

Dissecting Bonding Interactions in Cysteine Dimers

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Supplementary information

1 Electrostatic potential of the cysteine monomers

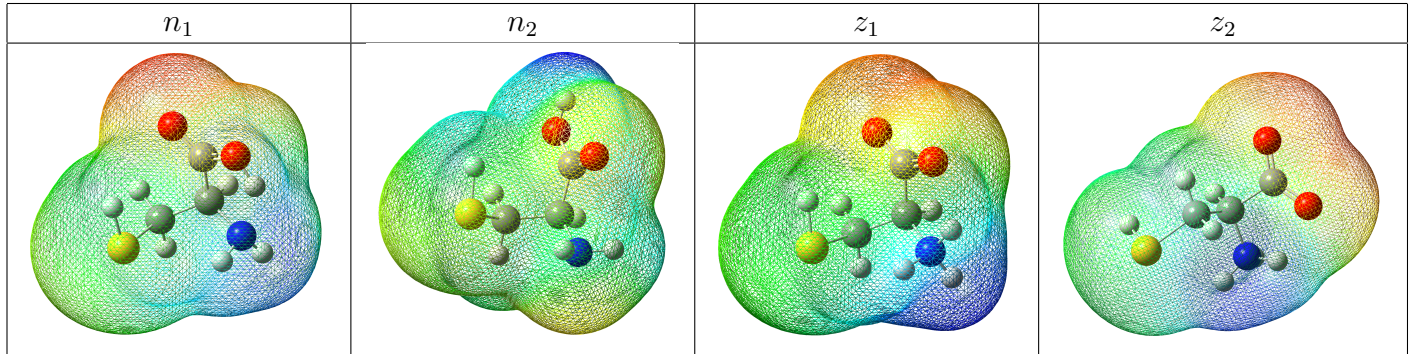


Figure S1: Electrostatic potential surfaces for the cysteine monomers.

2 Energetics for cysteine dimers

Table S1: Binding energies and energy differences in kcal mol⁻¹ for neutral dimers. $\Delta\Delta G$: Gibbs energies relative to the global minimum. We list electronic ($BE_{B3LYP-D3}$) and Gibbs (BE_{Gibbs}) binding energies corrected by the B3LYP-D3 vibrational ZPE (values within parentheses are calculated for the bare B3LYP functional with no dispersion corrections). Isomer populations $\% \chi_i(G)$ derived from Boltzmann distributions of the Gibbs energies are also reported.

Dimer	Composition	$BE_{B3LYP-D3}$	BE_{Gibbs}	$\Delta\Delta G$	$\% \chi_i(G)$
D_1^{nn}	$n_2 + n_2$	27.1	15.7 (-2.4)	≈ 0.0	35.7
D_2^{nn}	$n_2 + n_2$	27.0	15.6 (-1.4)	0.1	31.8
D_3^{nn}	$n_2 + n_2$	27.3	14.9 (-2.1)	0.7	10.4
D_4^{nn}	$n_2 + n_2$	26.8	14.2	1.5	3.1
D_5^{nn}	$n_2 + n_2$	26.3	13.9	1.8	1.7
D_6^{nn}	$n_1 + n_1$	20.3	9.3	1.9	1.3
D_7^{nn}	$n_2 + n_2$	26.3	13.7	2.0	1.3
D_8^{nn}	$n_1 + n_1$	19.0	9.2	2.0	1.2
D_9^{nn}	$n_1 + n_1$	20.3	9.1	2.1	1.0
D_{10}^{nn}	$n_1 + n_1$	20.4	9.0	2.2	0.9
D_{11}^{nn}	$n_1 + n_1$	20.7	9.0	2.2	0.8
D_{12}^{nn}	$n_1 + n_1$	20.6	8.9	2.3	0.7
D_{13}^{nn}	$n_1 + n_1$	20.5	8.8	2.4	0.6
D_{14}^{nn}	$n_1 + n_1$	20.5	8.8	2.4	0.6
D_{15}^{nn}	$n_1 + n_1$	20.5	8.8	2.5	0.6
D_{16}^{nn}	$n_1 + n_1$	20.5	8.7	2.6	0.5
D_{17}^{nn}	$n_1 + n_1$	20.2	8.7	2.6	0.5

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₁₈ ⁿⁿ	$n_1 + n_1$	20.4	8.6	2.7	0.4
D ₁₉ ⁿⁿ	$n_1 + n_1$	20.4	8.6	2.7	0.4
D ₂₀ ⁿⁿ	$n_1 + n_1$	19.9	8.5	2.7	0.4
D ₂₁ ⁿⁿ	$n_1 + n_1$	20.2	8.5	2.7	0.4
D ₂₂ ⁿⁿ	$n_1 + n_1$	20.7	8.4	2.8	0.3
D ₂₃ ⁿⁿ	$n_1 + n_1$	20.0	8.3	3.0	0.2
D ₂₄ ⁿⁿ	$n_1 + n_1$	19.2	8.2	3.0	0.2
D ₂₅ ⁿⁿ	$n_1 + n_1$	18.8	8.2	3.0	0.2
D ₂₆ ⁿⁿ	$n_1 + n_1$	20.3	8.2	3.0	0.2
D ₂₇ ⁿⁿ	$n_1 + n_1$	18.8	8.2	3.0	0.2
D ₂₈ ⁿⁿ	$n_1 + n_1$	19.8	8.1	3.1	0.2
D ₂₉ ⁿⁿ	$n_1 + n_1$	18.3	8.1	3.2	0.2
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D ₃₄ ⁿⁿ	$n_1 + n_1$	19.7	8.0	3.2	0.2
D ₃₅ ⁿⁿ	$n_1 + n_1$	19.4	8.0	3.2	0.2
D ₃₆ ⁿⁿ	$n_1 + n_1$	19.6	7.9	3.3	0.1
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D ₄₃ ⁿⁿ	$n_1 + n_1$	19.5	7.7	3.5	0.1
D ₄₄ ⁿⁿ	$n_1 + n_1$	19.5	7.7	3.5	0.1
D ₄₅ ⁿⁿ	$n_1 + n_1$	20.3	7.7	3.6	0.1
D ₄₆ ⁿⁿ	$n_1 + n_1$	17.9	7.7	3.6	0.1
D ₄₇ ⁿⁿ	$n_1 + n_1$	20.0	7.6	3.6	0.1
D ₄₈ ⁿⁿ	$n_1 + n_1$	20.0	7.6	3.6	0.1
D ₄₉ ⁿⁿ	$n_1 + n_1$	19.5	7.6	3.6	0.1
D ₅₀ ⁿⁿ	$n_1 + n_1$	19.6	7.6	3.7	0.1
D ₅₁ ⁿⁿ	$n_1 + n_1$	19.9	7.5	3.7	0.1
D ₅₂ ⁿⁿ	$n_1 + n_1$	19.2	7.5	3.7	0.1

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₅₃ ⁿⁿ	$n_1 + n_1$	18.3	7.5	3.7	0.1
D ₅₄ ⁿⁿ	$n_1 + n_1$	19.5	7.5	3.8	0.1
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D ₆₁ ⁿⁿ	$n_1 + n_1$	19.4	7.3	3.9	0.1
D ₆₂ ⁿⁿ	$n_1 + n_1$	19.2	7.2	4.0	≈ 0.0
D ₆₃ ⁿⁿ	$n_1 + n_1$	18.8	7.2	4.0	≈ 0.0
D ₆₄ ⁿⁿ	$n_1 + n_1$	17.9	7.2	4.0	≈ 0.0
D ₆₅ ⁿⁿ	$n_1 + n_1$	17.4	7.1	4.1	≈ 0.0
D ₆₆ ⁿⁿ	$n_1 + n_1$	17.3	7.1	4.1	≈ 0.0
D ₆₇ ⁿⁿ	$n_1 + n_1$	17.8	7.1	4.2	≈ 0.0
D ₆₈ ⁿⁿ	$n_2 + n_2$	24.1	11.5	4.2	≈ 0.0
D ₆₉ ⁿⁿ	$n_1 + n_1$	18.0	7.0	4.2	≈ 0.0
D ₇₀ ⁿⁿ	$n_1 + n_1$	18.0	7.0	4.2	≈ 0.0
D ₇₁ ⁿⁿ	$n_1 + n_1$	17.7	7.0	4.2	≈ 0.0
D ₇₂ ⁿⁿ	$n_1 + n_1$	17.3	7.0	4.3	≈ 0.0
D ₇₃ ⁿⁿ	$n_1 + n_1$	18.4	6.9	4.3	≈ 0.0
D ₇₄ ⁿⁿ	$n_1 + n_1$	18.0	6.9	4.3	≈ 0.0
D ₇₅ ⁿⁿ	$n_1 + n_1$	18.0	6.9	4.4	≈ 0.0
D ₇₆ ⁿⁿ	$n_1 + n_1$	17.4	6.9	4.4	≈ 0.0
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D ₈₀ ⁿⁿ	$n_1 + n_1$	18.2	6.8	4.4	≈ 0.0
D ₈₁ ⁿⁿ	$n_1 + n_1$	17.1	6.7	4.5	≈ 0.0
D ₈₂ ⁿⁿ	$n_1 + n_1$	18.9	6.7	4.6	≈ 0.0
D ₈₃ ⁿⁿ	$n_1 + n_1$	17.9	6.5	4.8	≈ 0.0
D ₈₄ ⁿⁿ	$n_1 + n_1$	16.6	6.4	4.8	≈ 0.0
D ₈₅ ⁿⁿ	$n_1 + n_1$	17.5	6.4	4.8	≈ 0.0
D ₈₆ ⁿⁿ	$n_1 + n_1$	17.7	6.3	4.9	≈ 0.0
D ₈₇ ⁿⁿ	$n_1 + n_1$	18.0	6.3	5.0	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₈₈ ⁿⁿ	$n_2 + n_2$	22.3	10.7	5.0	≈ 0.0
D ₈₉ ⁿⁿ	$n_1 + n_1$	17.0	6.2	5.0	≈ 0.0
D ₉₀ ⁿⁿ	$n_1 + n_1$	17.3	6.2	5.0	≈ 0.0
D ₉₁ ⁿⁿ	$n_2 + n_2$	21.4	10.6	5.1	≈ 0.0
D ₉₂ ⁿⁿ	$n_1 + n_1$	16.4	6.1	5.1	≈ 0.0
D ₉₃ ⁿⁿ	$n_1 + n_1$	17.1	6.0	5.2	≈ 0.0
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D ₁₅₅ ⁿⁿ	$n_2 + n_2$	18.0	7.2	8.5	≈ 0.0
D ₁₅₆ ⁿⁿ	$n_2 + n_2$	18.1	7.1	8.5	≈ 0.0
D ₁₅₇ ⁿⁿ	$n_2 + n_2$	18.7	7.0	8.6	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₁₅₈ ⁿⁿ	$n_2 + n_2$	17.4	7.0	8.7	≈ 0.0
D ₁₅₉ ⁿⁿ	$n_2 + n_2$	18.8	6.9	8.7	≈ 0.0
D ₁₆₀ ⁿⁿ	$n_2 + n_2$	17.0	6.8	8.8	≈ 0.0
D ₁₆₁ ⁿⁿ	$n_2 + n_2$	19.1	6.8	8.9	≈ 0.0
D ₁₆₂ ⁿⁿ	$n_2 + n_2$	17.9	6.7	8.9	≈ 0.0
D ₁₆₃ ⁿⁿ	$n_2 + n_2$	17.0	6.5	9.1	≈ 0.0
D ₁₆₄ ⁿⁿ	$n_2 + n_2$	18.1	6.4	9.2	≈ 0.0
D ₁₆₅ ⁿⁿ	$n_1 + n_2$	7.2	-2.3	15.7	≈ 0.0
D ₁₆₆ ⁿⁿ	$n_1 + n_2$	9.0	-2.3	15.7	≈ 0.0
D ₁₆₇ ⁿⁿ	$n_1 + n_2$	8.1	-2.6	16.0	≈ 0.0
D ₁₆₈ ⁿⁿ	$n_1 + n_2$	9.0	-2.6	16.0	≈ 0.0
D ₁₆₉ ⁿⁿ	$n_1 + n_2$	8.4	-2.8	16.2	≈ 0.0
D ₁₇₀ ⁿⁿ	$n_1 + n_2$	6.6	-3.6	17.0	≈ 0.0
D ₁₇₁ ⁿⁿ	$n_1 + n_2$	5.2	-3.8	17.2	≈ 0.0
D ₁₇₂ ⁿⁿ	$n_1 + n_2$	6.3	-4.4	17.8	≈ 0.0
D ₁₇₃ ⁿⁿ	$n_1 + n_2$	6.8	-4.5	17.9	≈ 0.0
D ₁₇₄ ⁿⁿ	$n_1 + n_2$	5.6	-4.6	18.0	≈ 0.0
D ₁₇₅ ⁿⁿ	$n_1 + n_2$	5.9	-4.6	18.0	≈ 0.0
D ₁₇₆ ⁿⁿ	$n_1 + n_2$	5.9	-4.8	18.2	≈ 0.0
D ₁₇₇ ⁿⁿ	$n_1 + n_2$	6.7	-4.8	18.2	≈ 0.0
D ₁₇₈ ⁿⁿ	$n_1 + n_2$	5.0	-5.0	18.5	≈ 0.0
D ₁₇₉ ⁿⁿ	$n_1 + n_2$	4.9	-5.1	18.5	≈ 0.0
D ₁₈₀ ⁿⁿ	$n_1 + n_2$	3.1	-5.2	18.6	≈ 0.0
D ₁₈₁ ⁿⁿ	$n_1 + n_2$	2.3	-5.3	18.8	≈ 0.0
D ₁₈₂ ⁿⁿ	$n_1 + n_2$	3.1	-5.4	18.9	≈ 0.0
D ₁₈₃ ⁿⁿ	$n_1 + n_2$	4.4	-5.5	18.9	≈ 0.0
D ₁₈₄ ⁿⁿ	$n_1 + n_2$	4.8	-5.5	18.9	≈ 0.0
D ₁₈₅ ⁿⁿ	$n_1 + n_2$	5.1	-5.5	18.9	≈ 0.0
D ₁₈₆ ⁿⁿ	$n_1 + n_2$	3.0	-5.5	19.0	≈ 0.0
D ₁₈₇ ⁿⁿ	$n_1 + n_2$	3.1	-5.5	19.0	≈ 0.0
D ₁₈₈ ⁿⁿ	$n_1 + n_2$	3.9	-5.6	19.0	≈ 0.0
D ₁₈₉ ⁿⁿ	$n_1 + n_2$	6.5	-5.6	19.0	≈ 0.0
D ₁₉₀ ⁿⁿ	$n_1 + n_2$	3.4	-5.6	19.0	≈ 0.0
D ₁₉₁ ⁿⁿ	$n_1 + n_2$	6.3	-5.6	19.1	≈ 0.0
D ₁₉₂ ⁿⁿ	$n_1 + n_2$	4.9	-5.6	19.1	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₁₉₃ ⁿⁿ	$n_1 + n_2$	3.6	-5.7	19.1	≈ 0.0
D ₁₉₄ ⁿⁿ	$n_1 + n_2$	4.8	-5.7	19.2	≈ 0.0
D ₁₉₅ ⁿⁿ	$n_1 + n_2$	5.7	-5.7	19.2	≈ 0.0
D ₁₉₆ ⁿⁿ	$n_1 + n_2$	5.4	-5.8	19.3	≈ 0.0
D ₁₉₇ ⁿⁿ	$n_1 + n_2$	5.3	-5.8	19.3	≈ 0.0
D ₁₉₈ ⁿⁿ	$n_1 + n_2$	4.1	-5.9	19.3	≈ 0.0
D ₁₉₉ ⁿⁿ	$n_1 + n_2$	3.3	-5.9	19.3	≈ 0.0
D ₂₀₀ ⁿⁿ	$n_1 + n_2$	3.6	-6.0	19.4	≈ 0.0
D ₂₀₁ ⁿⁿ	$n_1 + n_2$	5.0	-6.0	19.4	≈ 0.0
D ₂₀₂ ⁿⁿ	$n_1 + n_2$	3.1	-6.0	19.4	≈ 0.0
D ₂₀₃ ⁿⁿ	$n_1 + n_2$	3.7	-6.1	19.5	≈ 0.0
D ₂₀₄ ⁿⁿ	$n_1 + n_2$	5.4	-6.1	19.6	≈ 0.0
D ₂₀₅ ⁿⁿ	$n_1 + n_2$	3.3	-6.2	19.6	≈ 0.0
D ₂₀₆ ⁿⁿ	$n_1 + n_2$	3.3	-6.2	19.6	≈ 0.0
D ₂₀₇ ⁿⁿ	$n_1 + n_2$	3.2	-6.2	19.7	≈ 0.0
D ₂₀₈ ⁿⁿ	$n_1 + n_2$	3.4	-6.2	19.7	≈ 0.0
D ₂₀₉ ⁿⁿ	$n_1 + n_2$	2.9	-6.3	19.7	≈ 0.0
D ₂₁₀ ⁿⁿ	$n_1 + n_2$	3.2	-6.3	19.7	≈ 0.0
D ₂₁₁ ⁿⁿ	$n_1 + n_2$	4.1	-6.3	19.7	≈ 0.0
D ₂₁₂ ⁿⁿ	$n_1 + n_2$	3.3	-6.3	19.8	≈ 0.0
D ₂₁₃ ⁿⁿ	$n_1 + n_2$	4.6	-6.3	19.8	≈ 0.0
D ₂₁₄ ⁿⁿ	$n_1 + n_2$	5.4	-6.3	19.8	≈ 0.0
D ₂₁₅ ⁿⁿ	$n_1 + n_2$	3.2	-6.4	19.9	≈ 0.0
D ₂₁₆ ⁿⁿ	$n_1 + n_2$	2.8	-6.4	19.9	≈ 0.0
D ₂₁₇ ⁿⁿ	$n_1 + n_2$	3.0	-6.4	19.9	≈ 0.0
D ₂₁₈ ⁿⁿ	$n_1 + n_2$	2.8	-6.5	19.9	≈ 0.0
D ₂₁₉ ⁿⁿ	$n_1 + n_2$	3.2	-6.5	19.9	≈ 0.0
D ₂₂₀ ⁿⁿ	$n_1 + n_2$	3.0	-6.5	19.9	≈ 0.0
D ₂₂₁ ⁿⁿ	$n_1 + n_2$	3.6	-6.5	19.9	≈ 0.0
D ₂₂₂ ⁿⁿ	$n_1 + n_2$	3.6	-6.5	20.0	≈ 0.0
D ₂₂₃ ⁿⁿ	$n_1 + n_2$	3.2	-6.5	20.0	≈ 0.0
D ₂₂₄ ⁿⁿ	$n_1 + n_2$	3.2	-6.6	20.0	≈ 0.0
D ₂₂₅ ⁿⁿ	$n_1 + n_2$	3.7	-6.7	20.1	≈ 0.0
D ₂₂₆ ⁿⁿ	$n_1 + n_2$	3.4	-6.7	20.1	≈ 0.0
D ₂₂₇ ⁿⁿ	$n_1 + n_2$	2.8	-6.7	20.1	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{228}^{nn}	$n_1 + n_2$	4.0	-6.7	20.1	≈ 0.0
D_{229}^{nn}	$n_1 + n_2$	4.5	-6.7	20.1	≈ 0.0
D_{230}^{nn}	$n_1 + n_2$	4.5	-6.8	20.2	≈ 0.0
D_{231}^{nn}	$n_1 + n_2$	3.0	-6.8	20.2	≈ 0.0
D_{232}^{nn}	$n_1 + n_2$	2.7	-6.8	20.3	≈ 0.0
D_{233}^{nn}	$n_1 + n_2$	4.5	-6.8	20.3	≈ 0.0
D_{234}^{nn}	$n_1 + n_2$	4.2	-6.8	20.3	≈ 0.0
D_{235}^{nn}	$n_1 + n_2$	3.9	-6.9	20.4	≈ 0.0
D_{236}^{nn}	$n_1 + n_2$	4.2	-6.9	20.4	≈ 0.0
D_{237}^{nn}	$n_1 + n_2$	3.5	-6.9	20.4	≈ 0.0
D_{238}^{nn}	$n_1 + n_2$	2.8	-7.0	20.4	≈ 0.0
D_{239}^{nn}	$n_1 + n_2$	3.5	-7.0	20.5	≈ 0.0
D_{240}^{nn}	$n_1 + n_2$	3.0	-7.1	20.6	≈ 0.0
D_{241}^{nn}	$n_1 + n_2$	1.5	-7.5	20.9	≈ 0.0
D_{242}^{nn}	$n_1 + n_2$	2.4	-7.6	21.0	≈ 0.0
D_{243}^{nn}	$n_1 + n_2$	2.7	-7.9	21.3	≈ 0.0
D_{244}^{nn}	$n_1 + n_2$	2.5	-7.9	21.4	≈ 0.0

Table S2: Binding energies and energy differences in kcal mol⁻¹ for mixed dimers. $\Delta\Delta G$: Gibbs energies relative to the global minimum. We list electronic ($BE_{B3LYP-D3}$) and Gibbs (BE_{Gibbs}) binding energies corrected by the B3LYP-D3 vibrational ZPE (values within parentheses are calculated for the bare B3LYP functional with no dispersion corrections). Isomer populations $\% \chi_i(G)$ derived from Boltzmann distributions of the Gibbs energies are also reported.

Dimer	Composition	$BE_{B3LYP-D3}$	BE_{Gibbs}	$\Delta\Delta G$	$\% \chi_i(G)$
D_1^{nz}	$n_1 + z_1$	28.2	15.5 (-7.6)	≈ 0.0	44.9
D_2^{nz}	$n_2 + z_2$	29.7	17.9 (-0.5)	0.1	37.6
D_3^{nz}	$n_2 + z_2$	29.8	17.0 (-0.4)	1.1	7.4
D_4^{nz}	$n_2 + z_2$	29.8	17.0 (-2.5)	1.1	7.3
D_5^{nz}	$n_2 + z_2$	28.7	15.4	2.6	0.5
D_6^{nz}	$n_2 + z_2$	29.0	15.2	2.9	0.3
D_7^{nz}	$n_2 + z_2$	28.7	15.1	2.9	0.3
D_8^{nz}	$n_1 + z_1$	24.5	12.5	3.1	0.2
D_9^{nz}	$n_2 + z_2$	25.5	14.9	3.1	0.2
D_{10}^{nz}	$n_2 + z_2$	27.2	14.7	3.3	0.2
D_{11}^{nz}	$n_1 + z_1$	23.9	12.2	3.3	0.2
D_{12}^{nz}	$n_1 + z_1$	22.8	11.9	3.6	0.1
D_{13}^{nz}	$n_2 + z_2$	26.7	14.2	3.8	0.1
D_{14}^{nz}	$n_2 + z_2$	26.6	14.2	3.9	0.1
D_{15}^{nz}	$n_1 + z_1$	23.4	11.4	4.1	≈ 0.0
D_{16}^{nz}	$n_1 + z_1$	22.9	11.4	4.2	≈ 0.0
D_{17}^{nz}	$n_2 + z_2$	25.6	13.9	4.2	≈ 0.0
D_{18}^{nz}	$n_2 + z_2$	25.4	13.9	4.2	≈ 0.0
D_{19}^{nz}	$n_2 + z_2$	26.5	13.8	4.2	≈ 0.0
D_{20}^{nz}	$n_1 + z_1$	23.8	11.3	4.2	≈ 0.0
D_{21}^{nz}	$n_2 + z_2$	25.4	13.8	4.3	≈ 0.0
D_{22}^{nz}	$n_2 + z_2$	25.8	13.8	4.3	≈ 0.0
D_{23}^{nz}	$n_1 + z_1$	22.8	11.2	4.4	≈ 0.0
D_{24}^{nz}	$n_1 + z_1$	23.2	11.1	4.5	≈ 0.0
D_{25}^{nz}	$n_1 + z_1$	22.1	11.0	4.6	≈ 0.0
D_{26}^{nz}	$n_1 + z_1$	22.7	10.9	4.6	≈ 0.0
D_{27}^{nz}	$n_1 + z_1$	23.3	10.9	4.6	≈ 0.0
D_{28}^{nz}	$n_2 + z_2$	26.3	13.4	4.7	≈ 0.0
D_{29}^{nz}	$n_1 + z_1$	22.3	10.8	4.7	≈ 0.0
D_{30}^{nz}	$n_1 + z_1$	23.5	10.8	4.7	≈ 0.0
D_{31}^{nz}	$n_2 + z_2$	24.0	13.3	4.8	≈ 0.0
D_{32}^{nz}	$n_2 + z_2$	23.8	13.2	4.8	≈ 0.0
D_{33}^{nz}	$n_1 + z_1$	21.4	10.7	4.8	≈ 0.0
D_{34}^{nz}	$n_1 + z_1$	22.3	10.7	4.9	≈ 0.0
D_{35}^{nz}	$n_1 + z_1$	22.6	10.7	4.9	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₃₆ ^{nz}	$n_2 + z_2$	23.4	13.2	4.9	≈ 0.0
D ₃₇ ^{nz}	$n_2 + z_2$	24.4	13.1	5.0	≈ 0.0
D ₃₈ ^{nz}	$n_2 + z_2$	25.6	13.0	5.0	≈ 0.0
D ₃₉ ^{nz}	$n_1 + z_1$	21.9	10.5	5.0	≈ 0.0
D ₄₀ ^{nz}	$n_1 + z_1$	21.6	10.4	5.1	≈ 0.0
D ₄₁ ^{nz}	$n_1 + z_1$	22.1	10.4	5.1	≈ 0.0
D ₄₂ ^{nz}	$n_1 + z_1$	22.2	10.3	5.2	≈ 0.0
D ₄₃ ^{nz}	$n_1 + z_1$	21.3	10.3	5.2	≈ 0.0
D ₄₄ ^{nz}	$n_1 + z_1$	21.9	10.3	5.2	≈ 0.0
D ₄₅ ^{nz}	$n_1 + z_1$	21.6	10.1	5.4	≈ 0.0
D ₄₆ ^{nz}	$n_2 + z_2$	25.3	12.5	5.5	≈ 0.0
D ₄₇ ^{nz}	$n_1 + z_1$	22.5	9.9	5.6	≈ 0.0
D ₄₈ ^{nz}	$n_2 + z_2$	26.1	12.3	5.7	≈ 0.0
D ₄₉ ^{nz}	$n_2 + z_2$	24.3	12.3	5.7	≈ 0.0
D ₅₀ ^{nz}	$n_1 + z_1$	21.6	9.8	5.7	≈ 0.0
D ₅₁ ^{nz}	$n_1 + z_1$	21.0	9.8	5.7	≈ 0.0
D ₅₂ ^{nz}	$n_1 + z_1$	21.1	9.8	5.7	≈ 0.0
D ₅₃ ^{nz}	$n_1 + z_1$	22.5	9.6	5.9	≈ 0.0
D ₅₄ ^{nz}	$n_1 + z_1$	21.3	9.6	5.9	≈ 0.0
D ₅₅ ^{nz}	$n_1 + z_1$	21.9	9.6	5.9	≈ 0.0
D ₅₆ ^{nz}	$n_2 + z_2$	22.7	12.0	6.0	≈ 0.0
D ₅₇ ^{nz}	$n_1 + z_1$	20.4	9.5	6.0	≈ 0.0
D ₅₈ ^{nz}	$n_2 + z_2$	25.0	12.0	6.1	≈ 0.0
D ₅₉ ^{nz}	$n_1 + z_1$	21.5	9.5	6.1	≈ 0.0
D ₆₀ ^{nz}	$n_2 + z_2$	25.0	12.0	6.1	≈ 0.0
D ₆₁ ^{nz}	$n_1 + z_1$	21.4	9.4	6.1	≈ 0.0
D ₆₂ ^{nz}	$n_1 + z_1$	21.5	9.4	6.2	≈ 0.0
D ₆₃ ^{nz}	$n_2 + z_2$	24.0	11.8	6.2	≈ 0.0
D ₆₄ ^{nz}	$n_1 + z_1$	21.4	9.3	6.2	≈ 0.0
D ₆₅ ^{nz}	$n_1 + z_1$	21.1	9.3	6.3	≈ 0.0
D ₆₆ ^{nz}	$n_2 + z_2$	23.6	11.7	6.3	≈ 0.0
D ₆₇ ^{nz}	$n_1 + z_1$	19.0	9.1	6.5	≈ 0.0
D ₆₈ ^{nz}	$n_1 + z_1$	20.4	9.1	6.5	≈ 0.0
D ₆₉ ^{nz}	$n_2 + z_2$	24.3	11.5	6.5	≈ 0.0
D ₇₀ ^{nz}	$n_1 + z_1$	19.1	9.0	6.6	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₇₁ ^{n₁z₁}	$n_1 + z_1$	20.3	8.8	6.7	≈ 0.0
D ₇₂ ^{n₁z₁}	$n_1 + z_1$	21.3	8.8	6.8	≈ 0.0
D ₇₃ ^{n₂z₂}	$n_2 + z_2$	22.2	11.3	6.8	≈ 0.0
D ₇₄ ^{n₂z₂}	$n_2 + z_2$	25.2	11.2	6.8	≈ 0.0
D ₇₅ ^{n₁z₁}	$n_1 + z_1$	20.1	8.7	6.9	≈ 0.0
D ₇₆ ^{n₁z₁}	$n_1 + z_1$	20.1	8.7	6.9	≈ 0.0
D ₇₇ ^{n₁z₁}	$n_1 + z_1$	21.0	8.6	6.9	≈ 0.0
D ₇₈ ^{n₁z₁}	$n_1 + z_1$	19.2	8.6	6.9	≈ 0.0
D ₇₉ ^{n₁z₁}	$n_1 + z_1$	17.9	8.5	7.0	≈ 0.0
D ₈₀ ^{n₁z₁}	$n_1 + z_1$	20.1	8.5	7.0	≈ 0.0
D ₈₁ ^{n₁z₁}	$n_1 + z_1$	19.3	8.5	7.1	≈ 0.0
D ₈₂ ^{n₁z₁}	$n_1 + z_1$	19.1	8.4	7.1	≈ 0.0
D ₈₃ ^{n₁z₁}	$n_1 + z_1$	18.5	8.3	7.2	≈ 0.0
D ₈₄ ^{n₁z₁}	$n_1 + z_1$	18.6	8.3	7.2	≈ 0.0
D ₈₅ ^{n₁z₁}	$n_1 + z_1$	18.4	8.2	7.3	≈ 0.0
D ₈₆ ^{n₁z₁}	$n_1 + z_1$	19.4	8.2	7.3	≈ 0.0
D ₈₇ ^{n₁z₁}	$n_1 + z_1$	19.0	8.1	7.5	≈ 0.0
D ₈₈ ^{n₁z₁}	$n_1 + z_1$	19.7	8.0	7.6	≈ 0.0
D ₈₉ ^{n₂z₂}	$n_2 + z_2$	22.3	10.4	7.6	≈ 0.0
D ₉₀ ^{n₁z₁}	$n_1 + z_1$	19.3	7.9	7.7	≈ 0.0
D ₉₁ ^{n₂z₂}	$n_2 + z_2$	22.1	10.3	7.8	≈ 0.0
D ₉₂ ^{n₁z₁}	$n_1 + z_1$	19.4	7.7	7.8	≈ 0.0
D ₉₃ ^{n₁z₁}	$n_1 + z_1$	19.5	7.7	7.8	≈ 0.0
D ₉₄ ^{n₁z₁}	$n_1 + z_1$	20.4	7.7	7.9	≈ 0.0
D ₉₅ ^{n₁z₁}	$n_1 + z_1$	18.4	7.6	7.9	≈ 0.0
D ₉₆ ^{n₁z₁}	$n_1 + z_1$	19.4	7.6	8.0	≈ 0.0
D ₉₇ ^{n₂z₂}	$n_2 + z_2$	22.3	10.1	8.0	≈ 0.0
D ₉₈ ^{n₁z₁}	$n_1 + z_1$	18.8	7.5	8.0	≈ 0.0
D ₉₉ ^{n₁z₁}	$n_1 + z_1$	17.6	7.2	8.3	≈ 0.0
D ₁₀₀ ^{n₂z₂}	$n_2 + z_2$	22.4	9.7	8.4	≈ 0.0
D ₁₀₁ ^{n₁z₁}	$n_1 + z_1$	18.3	7.2	8.4	≈ 0.0
D ₁₀₂ ^{n₁z₁}	$n_1 + z_1$	18.1	7.0	8.5	≈ 0.0
D ₁₀₃ ^{n₁z₁}	$n_1 + z_1$	17.6	7.0	8.5	≈ 0.0
D ₁₀₄ ^{n₁z₁}	$n_1 + z_1$	18.6	6.9	8.6	≈ 0.0
D ₁₀₅ ^{n₁z₁}	$n_1 + z_1$	17.6	6.8	8.7	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{106}^{nz}	$n_1 + z_1$	18.7	6.8	8.8	≈ 0.0
D_{107}^{nz}	$n_2 + z_2$	21.2	9.2	8.8	≈ 0.0
D_{108}^{nz}	$n_2 + z_2$	22.1	9.2	8.8	≈ 0.0
D_{109}^{nz}	$n_2 + z_2$	20.2	9.2	8.9	≈ 0.0
D_{110}^{nz}	$n_1 + z_1$	17.2	6.4	9.1	≈ 0.0
D_{111}^{nz}	$n_2 + z_2$	19.9	8.9	9.2	≈ 0.0
D_{112}^{nz}	$n_2 + z_2$	20.0	8.8	9.2	≈ 0.0
D_{113}^{nz}	$n_2 + z_2$	20.2	8.8	9.2	≈ 0.0
D_{114}^{nz}	$n_2 + z_2$	20.3	8.8	9.2	≈ 0.0
D_{115}^{nz}	$n_2 + z_2$	20.7	8.8	9.3	≈ 0.0
D_{116}^{nz}	$n_2 + z_2$	20.6	8.8	9.3	≈ 0.0
D_{117}^{nz}	$n_1 + z_1$	16.9	6.3	9.3	≈ 0.0
D_{118}^{nz}	$n_2 + z_2$	19.8	8.6	9.5	≈ 0.0
D_{119}^{nz}	$n_2 + z_2$	21.0	8.4	9.6	≈ 0.0
D_{120}^{nz}	$n_2 + z_2$	20.4	8.3	9.7	≈ 0.0
D_{121}^{nz}	$n_2 + z_2$	20.0	8.1	9.9	≈ 0.0
D_{122}^{nz}	$n_2 + z_2$	19.6	8.0	10.0	≈ 0.0
D_{123}^{nz}	$n_2 + z_2$	20.1	8.0	10.1	≈ 0.0
D_{124}^{nz}	$n_2 + z_2$	19.2	7.9	10.1	≈ 0.0
D_{125}^{nz}	$n_2 + z_2$	20.5	7.9	10.1	≈ 0.0
D_{126}^{nz}	$n_2 + z_2$	18.7	7.9	10.2	≈ 0.0
D_{127}^{nz}	$n_2 + z_2$	18.9	7.9	10.2	≈ 0.0
D_{128}^{nz}	$n_1 + z_1$	16.9	5.3	10.2	≈ 0.0
D_{129}^{nz}	$n_1 + z_1$	15.5	5.3	10.2	≈ 0.0
D_{130}^{nz}	$n_2 + z_2$	18.4	7.7	10.3	≈ 0.0
D_{131}^{nz}	$n_2 + z_2$	18.3	7.6	10.4	≈ 0.0
D_{132}^{nz}	$n_2 + z_2$	18.8	7.6	10.4	≈ 0.0
D_{133}^{nz}	$n_2 + z_2$	17.4	7.6	10.4	≈ 0.0
D_{134}^{nz}	$n_2 + z_2$	18.9	7.5	10.5	≈ 0.0
D_{135}^{nz}	$n_2 + z_2$	18.7	7.4	10.7	≈ 0.0
D_{136}^{nz}	$n_2 + z_2$	18.4	7.3	10.8	≈ 0.0
D_{137}^{nz}	$n_2 + z_2$	18.3	7.2	10.9	≈ 0.0
D_{138}^{nz}	$n_2 + z_2$	18.8	7.1	10.9	≈ 0.0
D_{139}^{nz}	$n_2 + z_2$	18.7	7.1	11.0	≈ 0.0
D_{140}^{nz}	$n_2 + z_2$	18.3	7.0	11.0	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{141}^{nz}	$n_2 + z_2$	16.9	6.9	11.1	≈ 0.0
D_{142}^{nz}	$n_2 + z_2$	18.4	6.8	11.2	≈ 0.0
D_{143}^{nz}	$n_2 + z_2$	17.9	6.6	11.5	≈ 0.0
D_{144}^{nz}	$n_2 + z_2$	16.8	6.5	11.6	≈ 0.0
D_{145}^{nz}	$n_2 + z_2$	18.0	6.4	11.6	≈ 0.0
D_{146}^{nz}	$n_2 + z_2$	17.7	6.4	11.7	≈ 0.0
D_{147}^{nz}	$n_2 + z_2$	16.6	5.9	12.1	≈ 0.0
D_{148}^{nz}	$n_2 + z_2$	16.3	5.2	12.9	≈ 0.0
D_{149}^{nz}	$n_2 + z_1$	14.3	3.3	14.4	≈ 0.0
D_{150}^{nz}	$n_2 + z_1$	11.9	2.0	15.7	≈ 0.0
D_{151}^{nz}	$n_2 + z_1$	13.6	2.0	15.8	≈ 0.0
D_{152}^{nz}	$n_2 + z_1$	13.8	1.3	16.4	≈ 0.0
D_{153}^{nz}	$n_2 + z_1$	11.1	1.3	16.4	≈ 0.0
D_{154}^{nz}	$n_2 + z_1$	13.8	1.3	16.5	≈ 0.0
D_{155}^{nz}	$n_2 + z_1$	11.2	1.0	16.8	≈ 0.0
D_{156}^{nz}	$n_2 + z_1$	12.2	0.9	16.9	≈ 0.0
D_{157}^{nz}	$n_2 + z_1$	12.3	0.8	16.9	≈ 0.0
D_{158}^{nz}	$n_2 + z_1$	11.1	0.8	16.9	≈ 0.0
D_{159}^{nz}	$n_2 + z_1$	11.9	0.7	17.0	≈ 0.0
D_{160}^{nz}	$n_2 + z_1$	11.9	0.7	17.1	≈ 0.0
D_{161}^{nz}	$n_2 + z_1$	10.9	0.6	17.1	≈ 0.0
D_{162}^{nz}	$n_2 + z_1$	10.9	0.6	17.1	≈ 0.0
D_{163}^{nz}	$n_1 + z_2$	9.5	-1.5	17.4	≈ 0.0
D_{164}^{nz}	$n_1 + z_2$	7.6	-1.6	17.4	≈ 0.0
D_{165}^{nz}	$n_2 + z_1$	11.5	0.3	17.4	≈ 0.0
D_{166}^{nz}	$n_1 + z_2$	10.0	-1.7	17.5	≈ 0.0
D_{167}^{nz}	$n_1 + z_2$	9.5	-2.0	17.9	≈ 0.0
D_{168}^{nz}	$n_1 + z_2$	7.4	-2.0	17.9	≈ 0.0
D_{169}^{nz}	$n_2 + z_1$	11.2	-0.1	17.9	≈ 0.0
D_{170}^{nz}	$n_2 + z_1$	10.0	-0.2	17.9	≈ 0.0
D_{171}^{nz}	$n_1 + z_2$	8.0	-2.1	17.9	≈ 0.0
D_{172}^{nz}	$n_1 + z_2$	7.5	-2.4	18.3	≈ 0.0
D_{173}^{nz}	$n_1 + z_2$	8.3	-2.5	18.3	≈ 0.0
D_{174}^{nz}	$n_2 + z_1$	11.5	-0.6	18.4	≈ 0.0
D_{175}^{nz}	$n_1 + z_2$	7.3	-2.6	18.4	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta G$	% $\chi_i(G)$
D ₁₇₆ ^{n_z}	$n_1 + z_2$	8.2	-2.7	18.5	≈ 0.0
D ₁₇₇ ^{n_z}	$n_1 + z_2$	8.5	-2.8	18.6	≈ 0.0
D ₁₇₈ ^{n_z}	$n_1 + z_2$	8.3	-2.8	18.6	≈ 0.0
D ₁₇₉ ^{n_z}	$n_1 + z_2$	7.9	-2.8	18.6	≈ 0.0
D ₁₈₀ ^{n_z}	$n_2 + z_1$	9.9	-1.0	18.7	≈ 0.0
D ₁₈₁ ^{n_z}	$n_2 + z_1$	10.3	-1.1	18.8	≈ 0.0
D ₁₈₂ ^{n_z}	$n_1 + z_1$	8.0	-3.3	18.9	≈ 0.0
D ₁₈₃ ^{n_z}	$n_1 + z_2$	8.0	-3.1	19.0	≈ 0.0
D ₁₈₄ ^{n_z}	$n_2 + z_1$	10.3	-1.3	19.0	≈ 0.0
D ₁₈₅ ^{n_z}	$n_2 + z_1$	9.8	-1.3	19.1	≈ 0.0
D ₁₈₆ ^{n_z}	$n_1 + z_2$	8.2	-3.5	19.3	≈ 0.0
D ₁₈₇ ^{n_z}	$n_1 + z_2$	7.9	-3.9	19.8	≈ 0.0
D ₁₈₈ ^{n_z}	$n_2 + z_1$	9.0	-2.1	19.8	≈ 0.0
D ₁₈₉ ^{n_z}	$n_1 + z_2$	5.7	-4.1	20.0	≈ 0.0
D ₁₉₀ ^{n_z}	$n_2 + z_1$	9.1	-2.3	20.1	≈ 0.0
D ₁₉₁ ^{n_z}	$n_1 + z_2$	7.3	-4.3	20.1	≈ 0.0
D ₁₉₂ ^{n_z}	$n_1 + z_2$	7.1	-4.3	20.2	≈ 0.0
D ₁₉₃ ^{n_z}	$n_1 + z_2$	7.9	-4.6	20.4	≈ 0.0
D ₁₉₄ ^{n_z}	$n_1 + z_2$	7.0	-4.6	20.4	≈ 0.0
D ₁₉₅ ^{n_z}	$n_2 + z_1$	8.6	-2.7	20.5	≈ 0.0
D ₁₉₆ ^{n_z}	$n_1 + z_2$	5.7	-4.7	20.5	≈ 0.0
D ₁₉₇ ^{n_z}	$n_1 + z_2$	5.7	-4.7	20.5	≈ 0.0
D ₁₉₈ ^{n_z}	$n_1 + z_1$	5.9	-5.0	20.5	≈ 0.0
D ₁₉₉ ^{n_z}	$n_2 + z_1$	9.7	-2.9	20.7	≈ 0.0
D ₂₀₀ ^{n_z}	$n_1 + z_2$	5.1	-4.9	20.7	≈ 0.0
D ₂₀₁ ^{n_z}	$n_1 + z_2$	5.4	-5.0	20.8	≈ 0.0
D ₂₀₂ ^{n_z}	$n_1 + z_1$	5.9	-5.3	20.8	≈ 0.0
D ₂₀₃ ^{n_z}	$n_1 + z_2$	5.8	-5.0	20.9	≈ 0.0
D ₂₀₄ ^{n_z}	$n_1 + z_2$	6.1	-5.0	20.9	≈ 0.0
D ₂₀₅ ^{n_z}	$n_1 + z_2$	5.4	-5.1	20.9	≈ 0.0
D ₂₀₆ ^{n_z}	$n_1 + z_2$	6.3	-5.1	20.9	≈ 0.0
D ₂₀₇ ^{n_z}	$n_1 + z_2$	6.5	-5.2	21.0	≈ 0.0
D ₂₀₈ ^{n_z}	$n_1 + z_2$	6.6	-5.2	21.0	≈ 0.0
D ₂₀₉ ^{n_z}	$n_1 + z_2$	4.7	-5.2	21.0	≈ 0.0
D ₂₁₀ ^{n_z}	$n_1 + z_2$	5.4	-5.2	21.0	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{211}^{nz}	$n_2 + z_1$	7.4	-3.3	21.0	≈ 0.0
D_{212}^{nz}	$n_1 + z_2$	6.4	-5.2	21.1	≈ 0.0
D_{213}^{nz}	$n_1 + z_2$	6.4	-5.3	21.1	≈ 0.0
D_{214}^{nz}	$n_1 + z_2$	6.0	-5.4	21.2	≈ 0.0
D_{215}^{nz}	$n_1 + z_2$	5.8	-5.4	21.2	≈ 0.0
D_{216}^{nz}	$n_1 + z_2$	5.7	-5.4	21.3	≈ 0.0
D_{217}^{nz}	$n_1 + z_2$	6.4	-5.4	21.3	≈ 0.0
D_{218}^{nz}	$n_2 + z_1$	7.2	-3.6	21.3	≈ 0.0
D_{219}^{nz}	$n_1 + z_2$	5.7	-5.5	21.3	≈ 0.0
D_{220}^{nz}	$n_2 + z_1$	7.4	-3.6	21.3	≈ 0.0
D_{221}^{nz}	$n_1 + z_2$	4.8	-5.5	21.4	≈ 0.0
D_{222}^{nz}	$n_1 + z_2$	6.0	-5.5	21.4	≈ 0.0
D_{223}^{nz}	$n_1 + z_2$	5.8	-5.6	21.4	≈ 0.0
D_{224}^{nz}	$n_1 + z_2$	5.2	-5.6	21.4	≈ 0.0
D_{225}^{nz}	$n_1 + z_2$	5.5	-5.6	21.5	≈ 0.0
D_{226}^{nz}	$n_1 + z_2$	4.6	-5.6	21.5	≈ 0.0
D_{227}^{nz}	$n_1 + z_2$	6.1	-5.6	21.5	≈ 0.0
D_{228}^{nz}	$n_1 + z_2$	5.8	-5.7	21.6	≈ 0.0
D_{229}^{nz}	$n_2 + z_1$	6.7	-3.8	21.6	≈ 0.0
D_{230}^{nz}	$n_1 + z_2$	5.4	-5.8	21.6	≈ 0.0
D_{231}^{nz}	$n_1 + z_2$	5.7	-5.8	21.6	≈ 0.0
D_{232}^{nz}	$n_1 + z_2$	5.5	-5.9	21.7	≈ 0.0
D_{233}^{nz}	$n_1 + z_2$	4.5	-5.9	21.7	≈ 0.0
D_{234}^{nz}	$n_1 + z_2$	5.6	-5.9	21.7	≈ 0.0
D_{235}^{nz}	$n_1 + z_2$	4.8	-5.9	21.8	≈ 0.0
D_{236}^{nz}	$n_2 + z_1$	7.2	-4.0	21.8	≈ 0.0
D_{237}^{nz}	$n_1 + z_2$	4.4	-6.0	21.8	≈ 0.0
D_{238}^{nz}	$n_1 + z_2$	4.9	-6.0	21.9	≈ 0.0
D_{239}^{nz}	$n_1 + z_2$	3.4	-6.0	21.9	≈ 0.0
D_{240}^{nz}	$n_1 + z_2$	3.2	-6.1	21.9	≈ 0.0
D_{241}^{nz}	$n_1 + z_2$	4.7	-6.1	21.9	≈ 0.0
D_{242}^{nz}	$n_1 + z_2$	5.0	-6.1	21.9	≈ 0.0
D_{243}^{nz}	$n_1 + z_2$	5.5	-6.1	22.0	≈ 0.0
D_{244}^{nz}	$n_1 + z_2$	5.3	-6.2	22.0	≈ 0.0
D_{245}^{nz}	$n_1 + z_2$	5.3	-6.2	22.0	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{246}^{nz}	$n_2 + z_1$	7.0	-4.3	22.0	≈ 0.0
D_{247}^{nz}	$n_1 + z_2$	4.9	-6.3	22.1	≈ 0.0
D_{248}^{nz}	$n_1 + z_2$	2.9	-6.3	22.1	≈ 0.0
D_{249}^{nz}	$n_1 + z_2$	3.7	-6.3	22.1	≈ 0.0
D_{250}^{nz}	$n_1 + z_2$	4.8	-6.3	22.1	≈ 0.0
D_{251}^{nz}	$n_2 + z_1$	6.6	-4.4	22.2	≈ 0.0
D_{252}^{nz}	$n_1 + z_2$	4.2	-6.4	22.2	≈ 0.0
D_{253}^{nz}	$n_1 + z_2$	5.2	-6.4	22.2	≈ 0.0
D_{254}^{nz}	$n_1 + z_2$	4.6	-6.5	22.3	≈ 0.0
D_{255}^{nz}	$n_1 + z_2$	2.8	-6.5	22.4	≈ 0.0
D_{256}^{nz}	$n_1 + z_2$	5.0	-6.6	22.4	≈ 0.0
D_{257}^{nz}	$n_1 + z_2$	3.4	-6.6	22.4	≈ 0.0
D_{258}^{nz}	$n_2 + z_1$	6.1	-4.7	22.5	≈ 0.0
D_{259}^{nz}	$n_1 + z_2$	4.1	-6.7	22.6	≈ 0.0
D_{260}^{nz}	$n_1 + z_2$	2.5	-6.8	22.6	≈ 0.0
D_{261}^{nz}	$n_1 + z_2$	2.4	-6.8	22.7	≈ 0.0
D_{262}^{nz}	$n_1 + z_2$	2.9	-6.8	22.7	≈ 0.0
D_{263}^{nz}	$n_1 + z_2$	5.2	-6.9	22.7	≈ 0.0
D_{264}^{nz}	$n_1 + z_2$	2.7	-6.9	22.7	≈ 0.0
D_{265}^{nz}	$n_2 + z_1$	5.2	-5.0	22.7	≈ 0.0
D_{266}^{nz}	$n_1 + z_2$	4.5	-7.0	22.8	≈ 0.0
D_{267}^{nz}	$n_1 + z_2$	3.9	-7.0	22.8	≈ 0.0
D_{268}^{nz}	$n_1 + z_2$	4.2	-7.1	22.9	≈ 0.0
D_{269}^{nz}	$n_1 + z_2$	3.7	-7.1	22.9	≈ 0.0
D_{270}^{nz}	$n_2 + z_1$	5.7	-5.2	23.0	≈ 0.0
D_{271}^{nz}	$n_2 + z_1$	6.1	-5.2	23.0	≈ 0.0
D_{272}^{nz}	$n_1 + z_2$	3.1	-7.2	23.0	≈ 0.0
D_{273}^{nz}	$n_2 + z_1$	5.5	-5.3	23.1	≈ 0.0
D_{274}^{nz}	$n_2 + z_1$	5.0	-5.3	23.1	≈ 0.0
D_{275}^{nz}	$n_2 + z_1$	5.5	-5.4	23.1	≈ 0.0
D_{276}^{nz}	$n_1 + z_2$	3.3	-7.3	23.2	≈ 0.0
D_{277}^{nz}	$n_2 + z_1$	5.2	-5.4	23.2	≈ 0.0
D_{278}^{nz}	$n_2 + z_1$	5.5	-5.5	23.2	≈ 0.0
D_{279}^{nz}	$n_2 + z_1$	5.9	-5.5	23.2	≈ 0.0
D_{280}^{nz}	$n_1 + z_2$	4.4	-7.4	23.2	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{281}^{nz}	$n_1 + z_2$	3.1	-7.4	23.3	≈ 0.0
D_{282}^{nz}	$n_2 + z_1$	5.5	-5.5	23.3	≈ 0.0
D_{283}^{nz}	$n_2 + z_1$	4.6	-5.6	23.3	≈ 0.0
D_{284}^{nz}	$n_1 + z_2$	3.6	-7.5	23.3	≈ 0.0
D_{285}^{nz}	$n_1 + z_2$	2.3	-7.5	23.3	≈ 0.0
D_{286}^{nz}	$n_2 + z_1$	5.5	-5.6	23.4	≈ 0.0
D_{287}^{nz}	$n_2 + z_1$	5.9	-5.6	23.4	≈ 0.0
D_{288}^{nz}	$n_2 + z_1$	4.7	-5.6	23.4	≈ 0.0
D_{289}^{nz}	$n_2 + z_1$	5.1	-5.7	23.4	≈ 0.0
D_{290}^{nz}	$n_2 + z_1$	5.8	-5.7	23.4	≈ 0.0
D_{291}^{nz}	$n_2 + z_1$	3.5	-5.7	23.5	≈ 0.0
D_{292}^{nz}	$n_2 + z_1$	4.3	-5.7	23.5	≈ 0.0
D_{293}^{nz}	$n_2 + z_1$	4.4	-5.8	23.6	≈ 0.0
D_{294}^{nz}	$n_2 + z_1$	3.9	-5.9	23.7	≈ 0.0
D_{295}^{nz}	$n_2 + z_1$	4.0	-6.0	23.8	≈ 0.0
D_{296}^{nz}	$n_2 + z_1$	4.6	-6.0	23.8	≈ 0.0
D_{297}^{nz}	$n_2 + z_1$	4.8	-6.1	23.9	≈ 0.0
D_{298}^{nz}	$n_2 + z_1$	4.2	-6.1	23.9	≈ 0.0
D_{299}^{nz}	$n_1 + z_2$	1.3	-8.0	23.9	≈ 0.0
D_{300}^{nz}	$n_2 + z_1$	3.0	-6.2	23.9	≈ 0.0
D_{301}^{nz}	$n_2 + z_1$	5.5	-6.2	24.0	≈ 0.0
D_{302}^{nz}	$n_1 + z_2$	2.2	-8.1	24.0	≈ 0.0
D_{303}^{nz}	$n_2 + z_1$	3.9	-6.2	24.0	≈ 0.0
D_{304}^{nz}	$n_2 + z_1$	4.2	-6.3	24.0	≈ 0.0
D_{305}^{nz}	$n_2 + z_1$	4.9	-6.3	24.1	≈ 0.0
D_{306}^{nz}	$n_2 + z_1$	2.9	-6.3	24.1	≈ 0.0
D_{307}^{nz}	$n_2 + z_1$	4.9	-6.5	24.2	≈ 0.0
D_{308}^{nz}	$n_1 + z_2$	2.4	-8.4	24.3	≈ 0.0
D_{309}^{nz}	$n_2 + z_1$	3.5	-6.5	24.3	≈ 0.0
D_{310}^{nz}	$n_1 + z_2$	2.0	-8.5	24.4	≈ 0.0
D_{311}^{nz}	$n_2 + z_1$	3.5	-6.7	24.5	≈ 0.0
D_{312}^{nz}	$n_2 + z_1$	3.1	-6.8	24.6	≈ 0.0
D_{313}^{nz}	$n_2 + z_1$	4.5	-6.8	24.6	≈ 0.0
D_{314}^{nz}	$n_2 + z_1$	4.8	-7.0	24.8	≈ 0.0
D_{315}^{nz}	$n_2 + z_1$	4.1	-7.1	24.8	≈ 0.0

Dimer	Composition	BE _{B3LYP-D3}	BE _{Gibbs}	$\Delta\Delta\mathbf{G}$	$\%\chi_i(G)$
D ₃₁₆ ^{nz}	$n_1 + z_2$	1.5	-9.7	25.5	≈ 0.0

Table S3: Binding energies and energy differences in kcal mol⁻¹ for zwitterionic dimers. $\Delta\Delta G$: Gibbs energies relative to the global minimum. We list electronic ($BE_{B3LYP-D3}$) and Gibbs (BE_{Gibbs}) binding energies corrected by the B3LYP-D3 vibrational ZPE (values within parentheses are calculated for the bare B3LYP functional with no dispersion corrections). Isomer populations $\% \chi_i(G)$ derived from Boltzmann distributions of the Gibbs energies are also reported.

Dimer	Composition	$BE_{B3LYP-D3}$	BE_{Gibbs}	$\Delta\Delta G$	$\% \chi_i(G)$
D ₁ ^{zz}	$z_2 + z_2$	35.2	21.8 (-0.2)	≈ 0.0	51.8
D ₂ ^{zz}	$z_1 + z_1$	31.1	20.5 (-0.9)	0.7	15.1
D ₃ ^{zz}	$z_2 + z_2$	33.6	20.6 (-1.2)	1.1	7.6
D ₄ ^{zz}	$z_1 + z_2$	32.5	20.2 (-0.5)	1.3	5.6
D ₅ ^{zz}	$z_1 + z_2$	32.6	20.0	1.5	4.0
D ₆ ^{zz}	$z_1 + z_2$	33.1	19.9	1.6	3.5
D ₇ ^{zz}	$z_2 + z_2$	32.7	20.0	1.8	2.4
D ₈ ^{zz}	$z_1 + z_2$	31.4	19.5	2.0	1.9
D ₉ ^{zz}	$z_1 + z_2$	32.0	19.5	2.0	1.8
D ₁₀ ^{zz}	$z_2 + z_2$	32.8	19.7	2.1	1.5
D ₁₁ ^{zz}	$z_2 + z_2$	32.1	19.6	2.2	1.4
D ₁₂ ^{zz}	$z_2 + z_2$	31.6	19.5	2.2	1.2
D ₁₃ ^{zz}	$z_1 + z_2$	31.5	19.2	2.3	1.0
D ₁₄ ^{zz}	$z_1 + z_2$	31.9	18.7	2.8	0.4
D ₁₅ ^{zz}	$z_1 + z_2$	29.5	17.9	3.6	0.1
D ₁₆ ^{zz}	$z_1 + z_2$	29.5	17.7	3.8	0.1
D ₁₇ ^{zz}	$z_2 + z_2$	30.1	17.9	3.8	0.1
D ₁₈ ^{zz}	$z_2 + z_2$	30.0	17.7	4.1	0.1
D ₁₉ ^{zz}	$z_1 + z_1$	29.2	17.1	4.1	≈ 0.0
D ₂₀ ^{zz}	$z_2 + z_2$	30.1	17.5	4.2	≈ 0.0
D ₂₁ ^{zz}	$z_2 + z_2$	30.1	17.5	4.2	≈ 0.0
D ₂₂ ^{zz}	$z_1 + z_1$	29.3	16.7	4.5	≈ 0.0
D ₂₃ ^{zz}	$z_1 + z_2$	29.2	17.0	4.5	≈ 0.0
D ₂₄ ^{zz}	$z_1 + z_2$	28.6	16.8	4.6	≈ 0.0
D ₂₅ ^{zz}	$z_1 + z_1$	27.8	16.5	4.7	≈ 0.0
D ₂₆ ^{zz}	$z_1 + z_2$	28.1	16.7	4.8	≈ 0.0
D ₂₇ ^{zz}	$z_1 + z_2$	28.9	16.6	4.8	≈ 0.0
D ₂₈ ^{zz}	$z_2 + z_2$	30.1	16.6	5.1	≈ 0.0
D ₂₉ ^{zz}	$z_1 + z_1$	28.1	16.0	5.2	≈ 0.0
D ₃₀ ^{zz}	$z_1 + z_2$	29.5	16.2	5.3	≈ 0.0
D ₃₁ ^{zz}	$z_1 + z_2$	28.9	16.2	5.3	≈ 0.0
D ₃₂ ^{zz}	$z_2 + z_2$	29.2	16.5	5.3	≈ 0.0
D ₃₃ ^{zz}	$z_1 + z_2$	28.0	16.2	5.3	≈ 0.0
D ₃₄ ^{zz}	$z_1 + z_2$	27.2	16.2	5.3	≈ 0.0
D ₃₅ ^{zz}	$z_1 + z_1$	28.1	15.8	5.4	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\% \chi_i(G)$
D_{36}^{zz}	$z_1 + z_2$	27.7	16.1	5.4	≈ 0.0
D_{37}^{zz}	$z_1 + z_1$	27.1	15.7	5.5	≈ 0.0
D_{38}^{zz}	$z_1 + z_1$	27.7	15.7	5.5	≈ 0.0
D_{39}^{zz}	$z_1 + z_1$	26.8	15.7	5.5	≈ 0.0
D_{40}^{zz}	$z_1 + z_1$	27.9	15.6	5.6	≈ 0.0
D_{41}^{zz}	$z_1 + z_2$	28.1	15.8	5.7	≈ 0.0
D_{42}^{zz}	$z_1 + z_2$	27.8	15.7	5.8	≈ 0.0
D_{43}^{zz}	$z_1 + z_2$	28.7	15.7	5.8	≈ 0.0
D_{44}^{zz}	$z_1 + z_1$	27.6	15.3	5.9	≈ 0.0
D_{45}^{zz}	$z_1 + z_1$	26.6	15.3	5.9	≈ 0.0
D_{46}^{zz}	$z_1 + z_2$	27.5	15.5	6.0	≈ 0.0
D_{47}^{zz}	$z_1 + z_2$	26.1	15.4	6.1	≈ 0.0
D_{48}^{zz}	$z_1 + z_1$	27.6	15.1	6.1	≈ 0.0
D_{49}^{zz}	$z_1 + z_1$	27.3	15.0	6.2	≈ 0.0
D_{50}^{zz}	$z_1 + z_2$	27.6	15.3	6.2	≈ 0.0
D_{51}^{zz}	$z_1 + z_2$	26.1	15.2	6.3	≈ 0.0
D_{52}^{zz}	$z_1 + z_1$	25.9	14.8	6.4	≈ 0.0
D_{53}^{zz}	$z_1 + z_1$	26.3	14.8	6.4	≈ 0.0
D_{54}^{zz}	$z_1 + z_2$	26.1	15.0	6.5	≈ 0.0
D_{55}^{zz}	$z_1 + z_1$	27.6	14.7	6.5	≈ 0.0
D_{56}^{zz}	$z_1 + z_1$	25.8	14.6	6.6	≈ 0.0
D_{57}^{zz}	$z_1 + z_2$	26.4	14.9	6.6	≈ 0.0
D_{58}^{zz}	$z_1 + z_2$	26.5	14.8	6.7	≈ 0.0
D_{59}^{zz}	$z_1 + z_1$	25.8	14.5	6.7	≈ 0.0
D_{60}^{zz}	$z_1 + z_2$	26.4	14.8	6.7	≈ 0.0
D_{61}^{zz}	$z_1 + z_2$	26.0	14.8	6.7	≈ 0.0
D_{62}^{zz}	$z_2 + z_2$	26.7	15.0	6.7	≈ 0.0
D_{63}^{zz}	$z_1 + z_1$	26.5	14.4	6.8	≈ 0.0
D_{64}^{zz}	$z_1 + z_2$	25.5	14.6	6.9	≈ 0.0
D_{65}^{zz}	$z_1 + z_2$	26.3	14.6	6.9	≈ 0.0
D_{66}^{zz}	$z_1 + z_2$	25.7	14.6	6.9	≈ 0.0
D_{67}^{zz}	$z_1 + z_2$	26.7	14.6	6.9	≈ 0.0
D_{68}^{zz}	$z_1 + z_1$	24.8	14.3	6.9	≈ 0.0
D_{69}^{zz}	$z_2 + z_2$	26.6	14.8	6.9	≈ 0.0
D_{70}^{zz}	$z_2 + z_2$	26.6	14.8	7.0	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{71}^{zz}	$z_1 + z_2$	26.0	14.5	7.0	≈ 0.0
D_{72}^{zz}	$z_1 + z_2$	26.4	14.5	7.0	≈ 0.0
D_{73}^{zz}	$z_1 + z_2$	25.6	14.4	7.1	≈ 0.0
D_{74}^{zz}	$z_1 + z_1$	27.1	14.1	7.1	≈ 0.0
D_{75}^{zz}	$z_1 + z_2$	25.6	14.4	7.1	≈ 0.0
D_{76}^{zz}	$z_2 + z_2$	27.1	14.6	7.2	≈ 0.0
D_{77}^{zz}	$z_1 + z_2$	25.8	14.2	7.3	≈ 0.0
D_{78}^{zz}	$z_1 + z_2$	25.7	14.2	7.3	≈ 0.0
D_{79}^{zz}	$z_1 + z_2$	25.7	14.2	7.3	≈ 0.0
D_{80}^{zz}	$z_2 + z_2$	25.2	14.5	7.3	≈ 0.0
D_{81}^{zz}	$z_1 + z_2$	25.9	14.2	7.3	≈ 0.0
D_{82}^{zz}	$z_2 + z_2$	26.0	14.4	7.3	≈ 0.0
D_{83}^{zz}	$z_1 + z_1$	25.4	13.9	7.3	≈ 0.0
D_{84}^{zz}	$z_1 + z_2$	25.7	14.1	7.3	≈ 0.0
D_{85}^{zz}	$z_1 + z_2$	25.9	14.1	7.3	≈ 0.0
D_{86}^{zz}	$z_2 + z_2$	27.2	14.4	7.4	≈ 0.0
D_{87}^{zz}	$z_1 + z_1$	26.8	13.7	7.5	≈ 0.0
D_{88}^{zz}	$z_2 + z_2$	26.9	14.3	7.5	≈ 0.0
D_{89}^{zz}	$z_2 + z_2$	26.4	14.3	7.5	≈ 0.0
D_{90}^{zz}	$z_2 + z_2$	26.1	14.2	7.5	≈ 0.0
D_{91}^{zz}	$z_1 + z_2$	26.3	13.9	7.6	≈ 0.0
D_{92}^{zz}	$z_1 + z_2$	25.4	13.9	7.6	≈ 0.0
D_{93}^{zz}	$z_1 + z_2$	26.0	13.9	7.6	≈ 0.0
D_{94}^{zz}	$z_1 + z_2$	25.1	13.8	7.7	≈ 0.0
D_{95}^{zz}	$z_2 + z_2$	26.3	14.1	7.7	≈ 0.0
D_{96}^{zz}	$z_2 + z_2$	25.1	14.0	7.7	≈ 0.0
D_{97}^{zz}	$z_2 + z_2$	26.2	14.0	7.8	≈ 0.0
D_{98}^{zz}	$z_2 + z_2$	26.5	13.8	7.9	≈ 0.0
D_{99}^{zz}	$z_2 + z_2$	26.4	13.8	8.0	≈ 0.0
D_{100}^{zz}	$z_1 + z_2$	24.7	13.5	8.0	≈ 0.0
D_{101}^{zz}	$z_1 + z_2$	25.3	13.5	8.0	≈ 0.0
D_{102}^{zz}	$z_2 + z_2$	24.8	13.8	8.0	≈ 0.0
D_{103}^{zz}	$z_1 + z_2$	25.9	13.5	8.0	≈ 0.0
D_{104}^{zz}	$z_2 + z_2$	25.8	13.8	8.0	≈ 0.0
D_{105}^{zz}	$z_2 + z_2$	26.2	13.7	8.0	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{106}^{zz}	$z_2 + z_2$	25.9	13.7	8.0	≈ 0.0
D_{107}^{zz}	$z_1 + z_1$	25.1	13.1	8.1	≈ 0.0
D_{108}^{zz}	$z_2 + z_2$	26.0	13.7	8.1	≈ 0.0
D_{109}^{zz}	$z_2 + z_2$	25.8	13.7	8.1	≈ 0.0
D_{110}^{zz}	$z_2 + z_2$	26.1	13.7	8.1	≈ 0.0
D_{111}^{zz}	$z_2 + z_2$	25.9	13.6	8.2	≈ 0.0
D_{112}^{zz}	$z_2 + z_2$	24.8	13.5	8.3	≈ 0.0
D_{113}^{zz}	$z_2 + z_2$	25.5	13.5	8.3	≈ 0.0
D_{114}^{zz}	$z_1 + z_1$	23.8	12.8	8.4	≈ 0.0
D_{115}^{zz}	$z_2 + z_2$	25.8	13.3	8.4	≈ 0.0
D_{116}^{zz}	$z_1 + z_1$	25.0	12.7	8.5	≈ 0.0
D_{117}^{zz}	$z_1 + z_2$	24.0	13.0	8.5	≈ 0.0
D_{118}^{zz}	$z_2 + z_2$	25.7	13.2	8.5	≈ 0.0
D_{119}^{zz}	$z_2 + z_2$	24.9	13.1	8.6	≈ 0.0
D_{120}^{zz}	$z_1 + z_2$	24.5	12.8	8.7	≈ 0.0
D_{121}^{zz}	$z_2 + z_2$	24.7	13.0	8.8	≈ 0.0
D_{122}^{zz}	$z_2 + z_2$	24.8	12.8	8.9	≈ 0.0
D_{123}^{zz}	$z_2 + z_2$	25.0	12.8	9.0	≈ 0.0
D_{124}^{zz}	$z_1 + z_2$	24.5	12.5	9.0	≈ 0.0
D_{125}^{zz}	$z_2 + z_2$	24.0	12.8	9.0	≈ 0.0
D_{126}^{zz}	$z_2 + z_2$	24.9	12.7	9.1	≈ 0.0
D_{127}^{zz}	$z_2 + z_2$	24.0	12.7	9.1	≈ 0.0
D_{128}^{zz}	$z_2 + z_2$	23.6	12.6	9.2	≈ 0.0
D_{129}^{zz}	$z_1 + z_1$	22.0	11.3	9.9	≈ 0.0
D_{130}^{zz}	$z_1 + z_1$	22.7	11.2	10.0	≈ 0.0
D_{131}^{zz}	$z_2 + z_2$	24.6	11.8	10.0	≈ 0.0
D_{132}^{zz}	$z_1 + z_1$	22.7	11.2	10.0	≈ 0.0
D_{133}^{zz}	$z_1 + z_1$	23.7	11.2	10.0	≈ 0.0
D_{134}^{zz}	$z_1 + z_1$	22.6	10.8	10.4	≈ 0.0
D_{135}^{zz}	$z_1 + z_2$	23.2	10.8	10.7	≈ 0.0
D_{136}^{zz}	$z_1 + z_1$	21.9	10.5	10.7	≈ 0.0
D_{137}^{zz}	$z_1 + z_2$	23.0	10.7	10.8	≈ 0.0
D_{138}^{zz}	$z_2 + z_2$	20.8	10.3	11.4	≈ 0.0
D_{139}^{zz}	$z_1 + z_1$	20.6	9.8	11.4	≈ 0.0
D_{140}^{zz}	$z_1 + z_1$	21.3	9.7	11.5	≈ 0.0

Dimer	Composition	$\text{BE}_{\text{B3LYP-D3}}$	BE_{Gibbs}	$\Delta\Delta\text{G}$	$\%\chi_i(G)$
D_{141}^{zz}	$z_1 + z_2$	21.7	9.9	11.6	≈ 0.0
D_{142}^{zz}	$z_1 + z_1$	21.1	9.3	11.9	≈ 0.0
D_{143}^{zz}	$z_1 + z_1$	21.7	9.1	12.1	≈ 0.0
D_{144}^{zz}	$z_2 + z_2$	22.2	9.4	12.4	≈ 0.0
D_{145}^{zz}	$z_2 + z_2$	21.7	9.4	12.4	≈ 0.0
D_{146}^{zz}	$z_1 + z_2$	21.6	8.9	12.6	≈ 0.0
D_{147}^{zz}	$z_1 + z_1$	19.2	8.6	12.6	≈ 0.0
D_{148}^{zz}	$z_1 + z_1$	19.9	8.4	12.8	≈ 0.0
D_{149}^{zz}	$z_1 + z_1$	20.2	8.3	12.9	≈ 0.0
D_{150}^{zz}	$z_2 + z_2$	21.1	8.8	12.9	≈ 0.0
D_{151}^{zz}	$z_1 + z_2$	19.8	8.5	13.0	≈ 0.0
D_{152}^{zz}	$z_2 + z_2$	20.4	8.7	13.1	≈ 0.0
D_{153}^{zz}	$z_1 + z_2$	20.6	8.3	13.2	≈ 0.0
D_{154}^{zz}	$z_1 + z_2$	19.7	8.3	13.2	≈ 0.0
D_{155}^{zz}	$z_2 + z_2$	20.3	8.5	13.2	≈ 0.0
D_{156}^{zz}	$z_2 + z_2$	20.0	8.2	13.5	≈ 0.0
D_{157}^{zz}	$z_1 + z_1$	18.0	7.6	13.6	≈ 0.0
D_{158}^{zz}	$z_2 + z_2$	20.0	8.0	13.8	≈ 0.0
D_{159}^{zz}	$z_2 + z_2$	19.9	8.0	13.8	≈ 0.0
D_{160}^{zz}	$z_1 + z_2$	19.0	7.6	13.9	≈ 0.0
D_{161}^{zz}	$z_2 + z_2$	18.8	7.6	14.2	≈ 0.0
D_{162}^{zz}	$z_1 + z_2$	19.2	7.2	14.3	≈ 0.0
D_{163}^{zz}	$z_2 + z_2$	20.1	7.5	14.3	≈ 0.0
D_{164}^{zz}	$z_2 + z_2$	20.2	7.4	14.3	≈ 0.0
D_{165}^{zz}	$z_1 + z_1$	18.3	6.9	14.3	≈ 0.0
D_{166}^{zz}	$z_1 + z_2$	18.5	7.1	14.4	≈ 0.0
D_{167}^{zz}	$z_1 + z_2$	18.1	7.1	14.4	≈ 0.0
D_{168}^{zz}	$z_1 + z_1$	17.8	6.8	14.4	≈ 0.0
D_{169}^{zz}	$z_1 + z_2$	17.6	7.0	14.5	≈ 0.0
D_{170}^{zz}	$z_2 + z_2$	18.4	7.2	14.6	≈ 0.0
D_{171}^{zz}	$z_1 + z_2$	17.7	6.7	14.8	≈ 0.0
D_{172}^{zz}	$z_2 + z_2$	18.2	6.9	14.9	≈ 0.0
D_{173}^{zz}	$z_1 + z_1$	17.3	6.3	14.9	≈ 0.0
D_{174}^{zz}	$z_1 + z_2$	16.7	6.4	15.1	≈ 0.0
D_{175}^{zz}	$z_1 + z_2$	18.0	6.3	15.2	≈ 0.0

Dimer	Composition	BE_{B3LYP-D3}	BE_{Gibbs}	$\Delta\Delta G$	$\% \chi_i(G)$
D ₁₇₆ ^{zz}	$z_2 + z_2$	18.0	6.6	15.2	≈ 0.0
D ₁₇₇ ^{zz}	$z_1 + z_1$	17.9	6.0	15.2	≈ 0.0
D ₁₇₈ ^{zz}	$z_2 + z_2$	17.9	6.5	15.3	≈ 0.0
D ₁₇₉ ^{zz}	$z_2 + z_2$	17.1	6.4	15.4	≈ 0.0
D ₁₈₀ ^{zz}	$z_2 + z_2$	17.1	5.9	15.9	≈ 0.0
D ₁₈₁ ^{zz}	$z_1 + z_2$	15.6	4.8	16.7	≈ 0.0
D ₁₈₂ ^{zz}	$z_1 + z_2$	16.6	4.7	16.8	≈ 0.0
D ₁₈₃ ^{zz}	$z_1 + z_2$	15.8	4.3	17.1	≈ 0.0
D ₁₈₄ ^{zz}	$z_1 + z_1$	12.6	1.7	19.5	≈ 0.0
D ₁₈₅ ^{zz}	$z_1 + z_1$	13.2	1.3	19.9	≈ 0.0
D ₁₈₆ ^{zz}	$z_1 + z_1$	4.1	-6.7	27.9	≈ 0.0

3 Laplacian of the electron density distributions

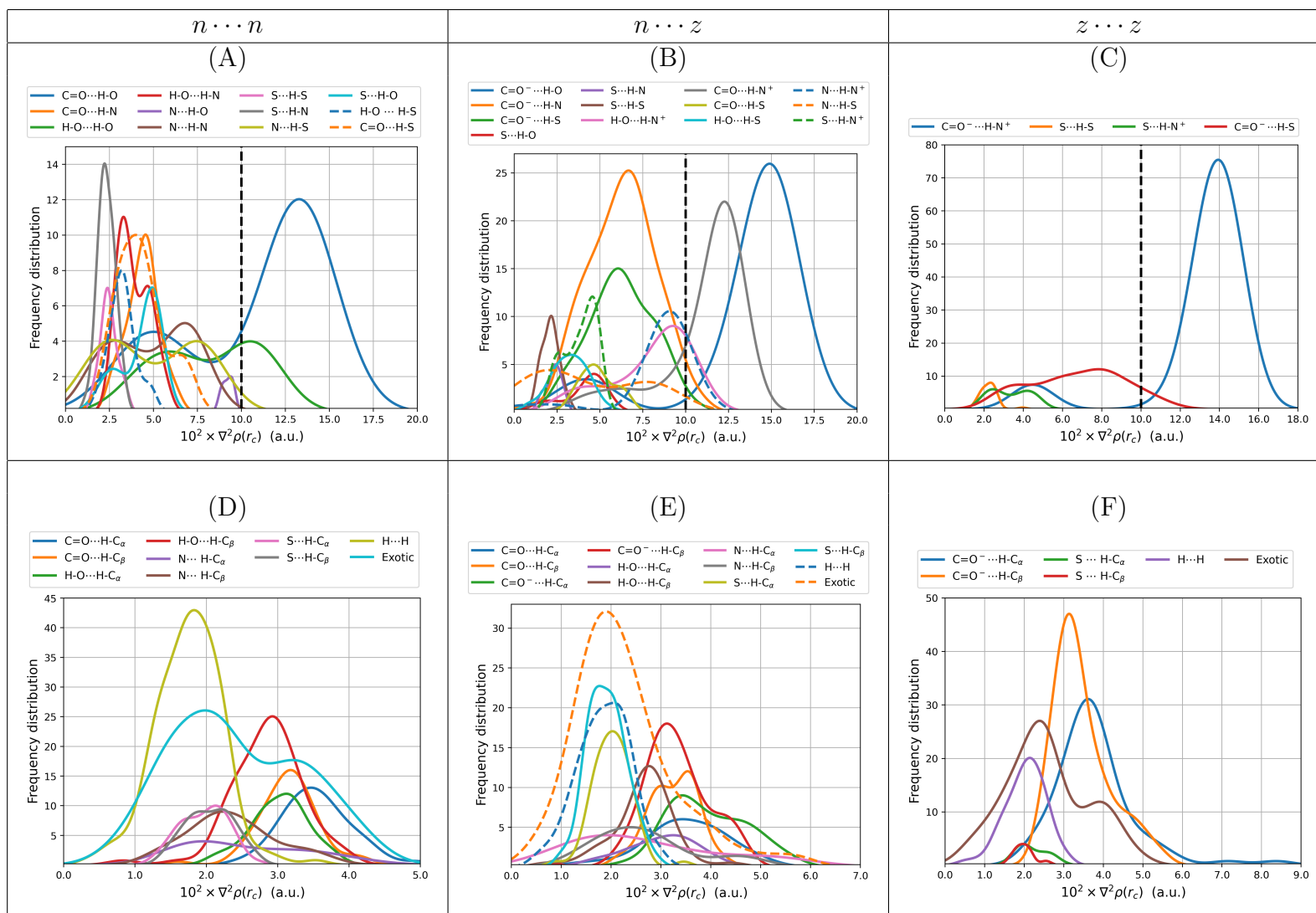


Figure S2: Laplacian of the electron densities at bond critical points for intermolecular contacts for all dimers of cysteine found in this work. The top row shows only primary hydrogen bonds including salt bridges. The bottom row shows secondary hydrogen bonds, dihydrogen bonds, and all exotic interactions. The left column is reserved for the $n \cdots n$ dimers, the middle column for $n \cdots z$ and the right column for $z \cdots z$. All values taken from the B3LYP-D3/6-311++G(d,p) potential energy surfaces with water represented as a continuum solvent. Dashed vertical lines mark the reference value for the gas phase water dimer.

4 NBO and NCI surfaces

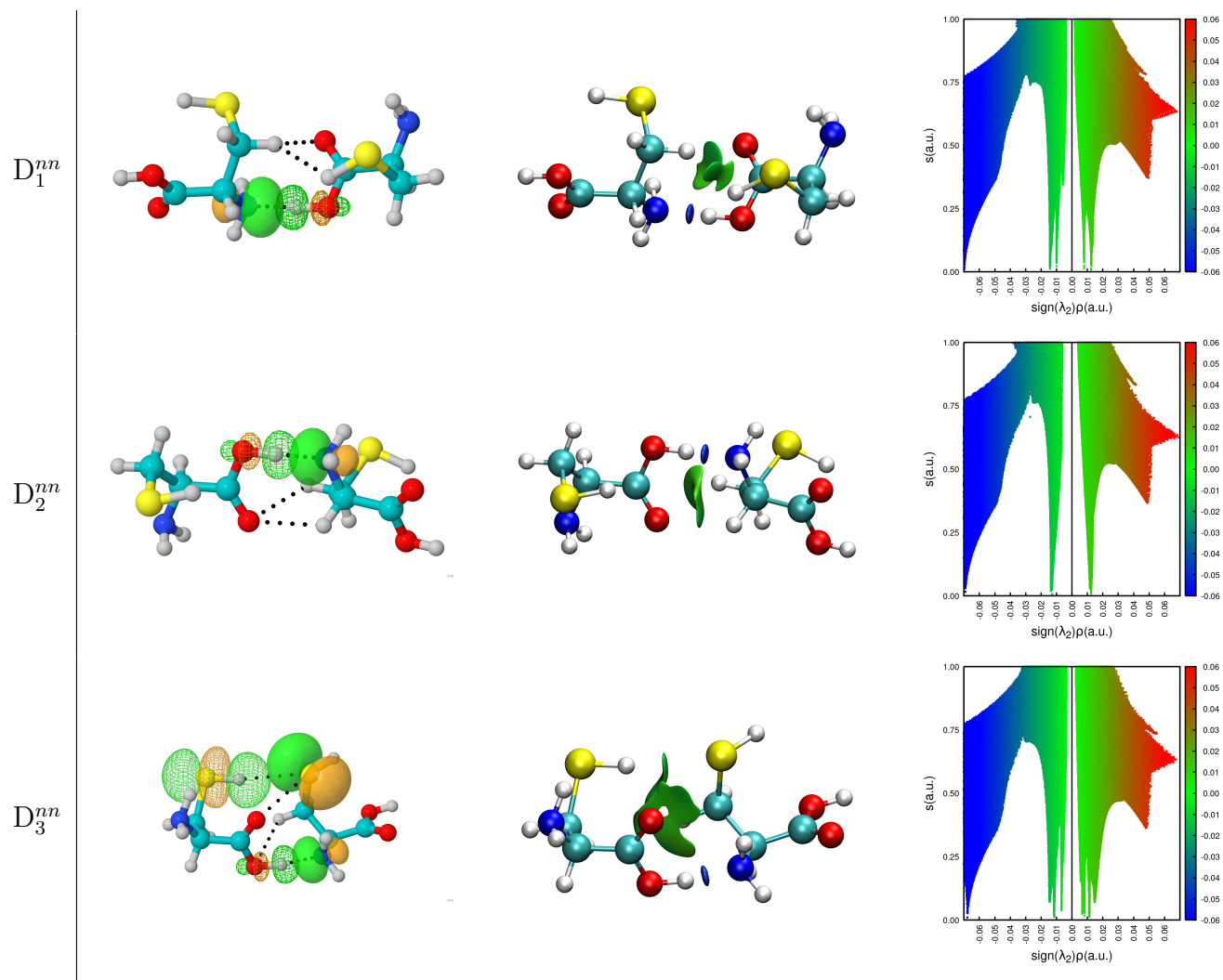


Figure S3: NBOs, NCI surfaces and thorough plots describing the intermolecular contacts for the $n \cdots n$ cysteine dimers with populations higher than 5%.

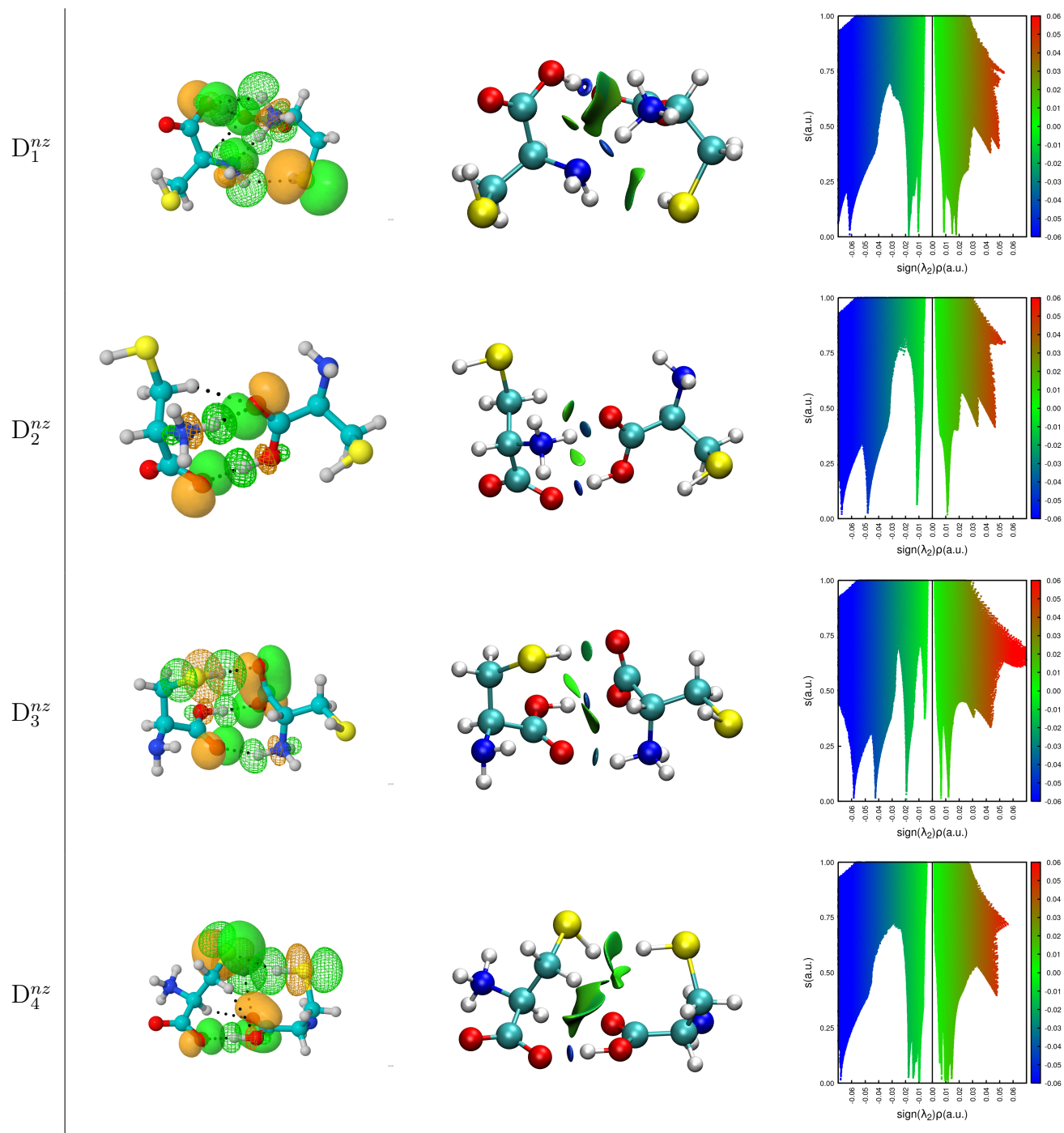


Figure S4: NBOs, NCI surfaces and thorough plots describing the intermolecular contacts for the $n \cdots z$ cysteine dimers with populations higher than 5%.

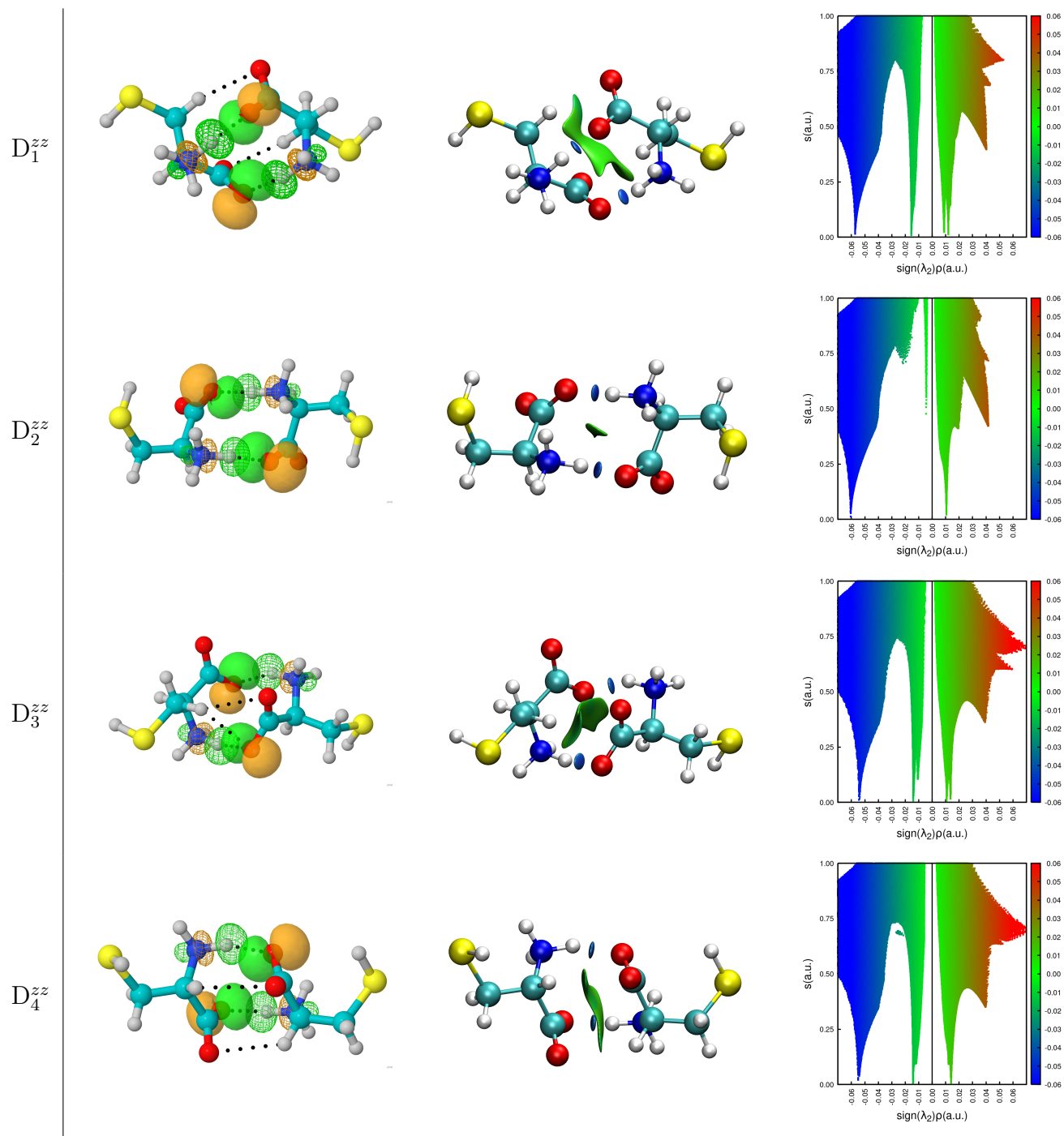


Figure S5: NBOs, NCI surfaces and thorough plots describing the intermolecular contacts for the $z \cdots z$ cysteine dimers with populations higher than 5%.

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28		
Dimer 1 of the n...n type		
C	-3.255452 0.495334 0.623992	
C	-3.518970 -1.002092 0.409208	
N	-3.875423 1.294425 -0.426063	
H	-3.452093 1.053962 -1.319783	
H	-3.659228 2.275665 -0.277475	
H	-3.721300 0.759962 1.581256	
C	-1.752201 0.763500 0.797845	
O	-1.161356 1.642731 0.196874	
O	-1.175646 -0.071587 1.649392	
H	-0.154551 0.087083 1.672313	
H	-3.243338 -1.571805 1.293514	
H	-4.579308 -1.151143 0.206303	
S	-2.625357 -1.722550 -1.043165	
H	-1.425145 -1.818590 -0.437937	
C	1.947061 -0.597683 0.454282	
C	1.327569 -0.181710 -0.888404	
N	1.448707 0.232773 1.552740	
H	1.652370 1.211816 1.357231	
H	1.937251 0.003891 2.414646	
H	1.638131 -1.632652 0.640791	
C	3.475136 -0.616124 0.391735	
O	4.199472 -0.086411 1.199612	
O	3.915727 -1.307850 -0.672455	
H	4.886417 -1.312505 -0.670289	
H	1.598230 -0.896296 -1.662193	
H	0.244914 -0.159626 -0.795791	
S	1.791759 1.514848 -1.441535	
H	3.037799 1.200684 -1.853457	
28		
Dimer 2 of the n...n type		
C	-3.021964 -1.109549 0.091679	
C	-3.962275 -0.232924 -0.749604	
N	-3.558203 -1.331534 1.427661	
H	-3.611574 -0.441071 1.916630	
H	-2.910336 -1.901266 1.963362	
H	-2.959649 -2.075836 -0.423166	
C	-1.596893 -0.534905 0.078314	
O	-0.967263 -0.296603 1.093835	
O	-1.141611 -0.333890 -1.147856	
H	-0.194052 0.077927 -1.131725	
H	-3.630875 -0.204363 -1.785379	
H	-4.968583 -0.649975 -0.709201	
S	-4.131883 1.503744 -0.137669	
H	-2.898360 1.915126 -0.496971	
C	1.905093 0.490935 0.199937	
C	2.090294 -1.011397 0.450777	
N	1.284641 0.736442 -1.103073	
H	1.877903 0.360031 -1.841014	
H	1.218402 1.736619 -1.274527	
H	1.214716 0.844551 0.971954	
C	3.206649 1.268518 0.376055	
O	3.642606 2.066715 -0.419218	
O	3.809493 0.964607 1.538622	
H	4.621504 1.489708 1.622797	
H	2.435821 -1.181390 1.468017	
H	1.127662 -1.504551 0.327358	
S	3.240872 -1.843439 -0.727140	
H	4.377306 -1.295452 -0.249307	
28		
Dimer 3 of the n...n type		
C	2.204763 0.494231 0.705661	
C	1.297969 -0.739079 0.576171	
N	1.617991 1.650872 0.027260	
H	1.547977 1.464150 -0.972074	
H	2.217966 2.464684 0.129912	
H	2.279861 0.725499 1.773817	
C	3.626991 0.197943 0.228171	

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O	4.233595 0.867244 -0.572585	
O	4.122828 -0.902124 0.819533	
H	5.027031 -1.055574 0.501551	
H	1.668533 -1.548244 1.200678	
H	0.298687 -0.478349 0.919961	
S	1.122899 -1.361960 -1.155085	
H	2.222640 -2.142486 -1.136202	
C	-3.084425 0.942048 0.267240	
C	-3.061442 -0.308069 1.169815	
N	-4.040025 0.799260 -0.820334	
H	-3.726368 0.069197 -1.454215	
H	-4.077261 1.656516 -1.363288	
H	-3.398719 1.772708 0.906436	
C	-1.648341 1.238464 -0.178684	
O	-1.219423 0.951955 -1.282063	
O	-0.918780 1.777160 0.789291	
H	0.066969 1.834539 0.496190	
H	-2.355198 -0.164666 1.987296	
H	-4.056263 -0.457126 1.590571	
S	-2.689048 -1.901127 0.310118	
H	-1.462076 -1.589476 -0.153307	
28		
Dimer 4 of the n...n type		
C	2.993992 0.744406 -0.564280	
C	2.899805 -0.779387 -0.786846	
N	4.128543 1.088348 0.281967	
H	3.964571 0.741171 1.223250	
H	4.211504 2.097814 0.355315	
H	3.144470 1.189487 -1.551895	
C	1.642551 1.240069 -0.041777	
O	1.393712 1.361675 1.144959	
O	0.769409 1.468083 -1.014371	
H	-0.153017 1.644701 -0.602456	
H	2.049891 -1.014593 -1.428288	
H	3.812553 -1.117427 -1.278545	
S	2.793127 -1.797776 0.748548	
H	1.588536 -1.347479 1.154372	
C	-2.597580 0.760608 -0.474081	
C	-1.950976 -0.317024 -1.366777	
N	-1.583587 1.572835 0.196086	
H	-1.224954 1.085512 1.015591	
H	-1.981491 2.446284 0.527541	
H	-3.182747 1.404802 -1.136384	
C	-3.575851 0.120265 0.509623	
O	-3.452100 0.136850 1.710946	
O	-4.581757 -0.494534 -0.134649	
H	-5.168101 -0.915048 0.514746	
H	-2.718564 -0.885760 -1.888256	
H	-1.316415 0.172968 -2.104552	
S	-0.828395 -1.474179 -0.475681	
H	-1.782384 -2.169639 0.177076	
28		
Dimer 5 of the n...n type		
C	3.282958 -0.585161 0.103305	
C	3.259882 0.728804 0.905649	
N	3.873176 -0.389681 -1.211041	
H	3.290521 0.246369 -1.750488	
H	3.880208 -1.266460 -1.722923	
H	3.903390 -1.289609 0.669379	
C	1.874639 -1.181832 0.064681	
O	1.312474 -1.485253 -0.978055	
O	1.325171 -1.293910 1.262277	
H	0.362150 -1.532959 1.179967	
H	3.018209 0.538542 1.948903	
H	4.245411 1.189307 0.846783	
S	2.075414 1.992398 0.254090	
H	0.961956 1.427796 0.764650	
C	-3.282901 -0.585239 -0.103308	
C	-3.259897 0.728727 -0.905647	

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N	-3.873139	-0.389809	1.211044	
H	-3.290564	0.246313	1.750491	
H	-3.880063	-1.266591	1.722924	
H	-3.903306	-1.289707	-0.669388	
C	-1.874569	-1.181878	-0.064696	
O	-1.312393	-1.485331	0.978023	
O	-1.325088	-1.293907	-1.262295	
H	-0.362041	-1.532904	-1.179952	
H	-3.018151	0.538477	-1.948885	
H	-4.245476	1.189130	-0.846843	
S	-2.075567	1.992442	-0.254060	
H	-0.962041	1.427969	-0.764623	
28				
Dimer 6 of the n...n type				
C	2.994012	-0.341362	-0.006800	
C	3.010077	1.117957	-0.477673	
N	2.619909	-1.343515	-1.006473	
H	1.972643	-0.961465	-1.689656	
H	3.428076	-1.698951	-1.502180	
H	4.002825	-0.576679	0.349721	
C	2.105455	-0.509246	1.239776	
O	2.081446	0.285049	2.151900	
O	1.387362	-1.632128	1.244796	
H	1.579359	-2.057696	0.369530	
H	3.323722	1.768831	0.336995	
H	3.714207	1.222313	-1.303220	
S	1.390706	1.716896	-1.129715	
H	0.725126	1.720989	0.045252	
C	-2.828832	-0.315440	0.623478	
C	-1.790954	-1.429580	0.432919	
N	-3.956846	-0.311237	-0.312375	
H	-3.693351	-0.727179	-1.202105	
H	-4.753386	-0.817794	0.053495	
H	-3.222156	-0.409178	1.641256	
C	-2.152322	1.067437	0.598086	
O	-1.108553	1.307224	1.165249	
O	-2.826295	1.988071	-0.085703	
H	-3.619214	1.499339	-0.432734	
H	-0.982728	-1.321973	1.153400	
H	-2.270099	-2.398152	0.577265	
S	-1.064280	-1.494600	-1.260907	
H	-0.365557	-0.340196	-1.183772	
28				
Dimer 7 of the n...n type				
C	3.280788	0.584037	-0.103978	
C	3.249814	-0.724104	-0.915948	
N	3.876265	0.377225	1.206121	
H	3.292690	-0.258590	1.744789	
H	3.891524	1.250884	1.723133	
H	3.900710	1.290456	-0.668009	
C	1.873984	1.183222	-0.055333	
O	1.311179	1.467832	0.992320	
O	1.325973	1.317946	-1.251272	
H	0.363073	1.556235	-1.165696	
H	3.000549	-0.525568	-1.955902	
H	4.235211	-1.186151	-0.867761	
S	2.069472	-1.991509	-0.264774	
H	0.951320	-1.420413	-0.757624	
C	-3.282174	0.582782	0.097786	
C	-3.264971	-0.733810	0.895514	
N	-3.862300	0.391475	-1.221848	
H	-3.276381	-0.244382	-1.758047	
H	-3.863175	1.269459	-1.731721	
H	-3.907451	1.285314	0.661059	
C	-1.874390	1.181848	0.071128	
O	-1.311509	1.503843	-0.965604	
O	-1.326582	1.275733	1.271132	
H	-0.363531	1.516128	1.193654	
H	-3.036584	-0.546872	1.942314	

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H	-4.248217	-1.197199	0.823139	
S	-2.067176	-1.990433	0.254184	
H	-0.965024	-1.425811	0.788577	
28				
Dimer 8 of the n...n type				
C	-1.897502	-0.563674	0.392203	
C	-3.102016	-0.972407	-0.460326	
N	-2.160512	-0.298830	1.808596	
H	-3.106138	0.045622	1.950301	
H	-2.028400	-1.127606	2.374278	
H	-1.159871	-1.366328	0.327804	
C	-1.175984	0.650561	-0.212629	
O	-1.012118	0.818092	-1.400327	
O	-0.715231	1.507727	0.700212	
H	-1.001641	1.109951	1.565684	
H	-2.782396	-1.185595	-1.479316	
H	-3.554876	-1.869922	-0.038727	
S	-4.453975	0.284996	-0.508374	
H	-3.771013	1.205875	-1.219045	
C	3.103995	-0.896558	0.092882	
C	3.492472	0.477100	0.652958	
N	3.360978	-1.119397	-1.332174	
H	3.233588	-0.259037	-1.859833	
H	4.302962	-1.453779	-1.494994	
H	3.664387	-1.649648	0.658704	
C	1.630280	-1.223715	0.387005	
O	1.056204	-0.904693	1.403641	
O	1.031952	-1.925830	-0.576808	
H	1.711831	-1.987776	-1.296308	
H	3.260630	0.524999	1.715991	
H	4.563791	0.628358	0.519994	
S	2.681140	1.892965	-0.207165	
H	1.435307	1.674896	0.262849	
28				
Dimer 9 of the n...n type				
C	2.996793	0.340783	0.003221	
C	3.014657	-1.118923	0.472765	
N	2.625876	1.342436	1.004490	
H	1.975351	0.961812	1.685420	
H	3.434955	1.692285	1.502714	
H	4.004483	0.576772	-0.356141	
C	2.104468	0.509876	-1.240378	
O	2.072909	-0.286326	-2.150584	
O	1.391838	1.636318	-1.245386	
H	1.587598	2.062106	-0.371155	
H	3.327798	-1.768847	-0.342863	
H	3.719925	-1.223406	1.297322	
S	1.396483	-1.719715	1.125939	
H	0.729548	-1.721161	-0.048189	
C	-2.827907	0.320879	-0.622935	
C	-1.782723	1.427680	-0.430352	
N	-3.959163	0.325816	0.308956	
H	-3.694421	0.737185	1.200462	
H	-4.749114	0.841507	-0.058481	
H	-3.217410	0.416293	-1.642059	
C	-2.162109	-1.067135	-0.594263	
O	-1.116439	-1.314639	-1.154498	
O	-2.848346	-1.983342	0.083405	
H	-3.639086	-1.488589	0.426647	
H	-0.973582	1.314485	-1.148886	
H	-2.254711	2.399520	-0.576275	
S	-1.059693	1.488234	1.265115	
H	-0.365728	0.330921	1.188660	
28				
Dimer 10 of the n...n type				
C	-1.231856	0.048852	0.038950	
C	-2.061890	-1.093056	-0.550333	
N	-1.044700	0.047584	1.490241	
H	-1.900746	-0.238816	1.959482	

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H	-0.304803	-0.588624	1.770313		
H	-0.244744	-0.005774	-0.427140		
C	-1.753015	1.426399	-0.397477		
O	-2.241638	1.648397	-1.481901		
O	-1.579231	2.380630	0.519836		
H	-1.218675	1.902998	1.308957		
H	-2.089305	-1.014147	-1.636261		
H	-1.595552	-2.039900	-0.279327		
S	-3.788710	-1.169343	0.092365		
H	-4.214091	-0.035186	-0.501069		
C	2.982851	-0.735401	-0.362236		
C	3.322439	0.638207	0.229930		
N	2.610754	-0.762207	-1.779196		
H	2.106882	0.081172	-2.042337		
H	3.422669	-0.843192	-2.379113		
H	3.862808	-1.375485	-0.232577		
C	1.875139	-1.431686	0.443588		
O	1.736041	-1.313750	1.642059		
O	1.059302	-2.183284	-0.294022		
H	1.362432	-2.035978	-1.227846		
H	3.646697	0.534286	1.263982		
H	4.131225	1.084935	-0.348150		
S	1.929124	1.849050	0.164009		
H	1.228383	1.324929	1.189496		
28					
Dimer 11 of the n...n type					
C	-2.719625	0.961317	-0.068753		
C	-3.312534	-0.370200	-0.553704		
N	-1.953357	1.735689	-1.039305		
H	-1.352480	1.139332	-1.602864		
H	-2.557114	2.264395	-1.656594		
H	-3.558447	1.580771	0.268679		
C	-1.870062	0.750338	1.194920		
O	-2.164889	-0.021468	2.079005		
O	-0.766468	1.499807	1.252588		
H	-0.721037	1.984970	0.391601		
H	-3.880818	-0.840631	0.247604		
H	-3.980725	-0.179173	-1.393648		
S	-2.060616	-1.565787	-1.188773		
H	-1.441644	-1.794190	-0.009750		
C	2.742453	-0.366590	-0.761711		
C	1.662067	-1.431204	-0.533399		
N	3.944526	-0.467233	0.070176		
H	3.734086	-0.910777	0.960706		
H	4.676026	-0.998577	-0.385428		
H	3.042265	-0.429344	-1.813208		
C	2.148283	1.047537	-0.616618		
O	1.068757	1.366412	-1.064028		
O	2.939734	1.901482	0.027423		
H	3.729918	1.355019	0.281703		
H	0.804909	-1.225861	-1.173176		
H	2.061064	-2.415350	-0.779074		
S	1.092072	-1.560802	1.215867		
H	0.594739	-0.311540	1.313347		
28					
Dimer 12 of the n...n type					
C	-3.055216	-0.591789	-0.352445		
C	-3.401708	0.902110	-0.351130		
N	-3.065273	-1.271141	0.945420		
H	-2.765837	-0.641350	1.686005		
H	-3.986639	-1.620207	1.179442		
H	-3.783698	-1.091251	-1.001351		
C	-1.703081	-0.856999	-1.037062		
O	-1.295623	-0.240133	-1.996215		
O	-1.017455	-1.861449	-0.492516		
H	-1.557263	-2.129384	0.296719		
H	-3.336511	1.299070	-1.363142		
H	-4.420822	1.034215	0.012403		
S	-2.349464	1.925226	0.767784		

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H	-1.198947	1.793249	0.072598		
C	1.643366	-0.187321	-0.559886		
C	3.108457	-0.162692	-1.009667		
N	0.953444	1.104812	-0.549875		
H	1.596605	1.864725	-0.344242		
H	0.513675	1.277729	-1.446139		
H	1.099770	-0.845401	-1.242399		
C	1.500219	-0.865216	0.811687		
O	2.128677	-1.847296	1.137170		
O	0.607082	-0.293911	1.622015		
H	0.271315	0.487655	1.123944		
H	3.510421	-1.174323	-1.034320		
H	3.169451	0.265172	-2.010479		
S	4.199028	0.890513	0.044045		
H	4.144602	0.106330	1.140273		
28					
Dimer 13 of the n...n type					
C	2.928047	0.602084	0.192906		
C	3.031131	-0.399173	-0.964194		
N	3.044244	0.053006	1.546764		
H	2.624646	-0.872473	1.597651		
H	4.011111	-0.022290	1.838759		
H	3.729375	1.338006	0.059580		
C	1.636895	1.433798	0.110462		
O	1.114858	1.778064	-0.925036		
O	1.139950	1.772078	1.302921		
H	1.721221	1.303634	1.955696		
H	2.923300	0.118876	-1.916011		
H	4.010599	-0.876562	-0.934281		
S	1.803452	-1.773557	-0.884430		
H	0.720428	-1.061529	-1.271778		
C	-1.801996	0.769156	0.270025		
C	-1.154202	-0.313454	1.137658		
N	-3.086564	1.293233	0.742963		
H	-3.642456	0.556729	1.171130		
H	-2.958305	2.029069	1.427098		
H	-1.095889	1.602821	0.211692		
C	-1.967035	0.317140	-1.188426		
O	-1.198081	-0.421493	-1.765615		
O	-3.035067	0.835953	-1.791325		
H	-3.505888	1.332108	-1.072828		
H	-0.163578	-0.563067	0.769845		
H	-1.052211	0.062549	2.155175		
S	-2.134376	-1.869350	1.264093		
H	-1.941643	-2.259146	-0.012574		
28					
Dimer 14 of the n...n type					
C	-2.492463	-0.737212	0.845934		
C	-3.090697	0.656887	0.630445		
N	-1.288801	-0.814151	1.678460		
H	-0.709049	0.019220	1.603278		
H	-1.517706	-0.946304	2.655859		
H	-3.267233	-1.354092	1.315165		
C	-2.209590	-1.437552	-0.496938		
O	-2.898832	-1.311993	-1.483033		
O	-1.128798	-2.220474	-0.468022		
H	-0.765553	-2.089379	0.447075		
H	-4.032986	0.582202	0.089934		
H	-3.279242	1.119925	1.599062		
S	-1.980255	1.821197	-0.274903		
H	-2.134622	1.250609	-1.486868		
C	1.307715	0.107590	-0.615140		
C	1.858549	-1.160455	0.046019		
N	1.891190	0.480181	-1.904519		
H	2.866762	0.198403	-1.958964		
H	1.393493	0.056178	-2.677814		
H	0.235277	-0.041311	-0.763448		
C	1.389090	1.309044	0.340154		
O	1.155639	1.230121	1.527781		

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O	1.713266	2.452097	-0.253817		
H	1.859396	2.201004	-1.203222		
H	1.350649	-1.337941	0.992438		
H	1.685927	-2.011513	-0.612442		
S	3.677054	-1.118812	0.348910		
H	3.643547	-0.175186	1.312128		
28					
Dimer 15 of the n...n type					
C	1.306489	0.107255	-0.614514		
C	1.858168	-1.159973	0.047466		
N	1.888804	0.478723	-1.904757		
H	2.864324	0.196931	-1.959859		
H	1.390361	0.054114	-2.677236		
H	0.234038	-0.042100	-0.761904		
C	1.388377	1.309735	0.339458		
O	1.156241	1.231883	1.527404		
O	1.711466	2.452249	-0.256153		
H	1.856763	2.200003	-1.205392		
H	1.350860	-1.336782	0.994336		
H	1.685530	-2.011705	-0.610119		
S	3.676823	-1.117451	0.349259		
H	3.643615	-0.172988	1.311655		
C	-2.492237	-0.737963	0.845166		
C	-3.091882	0.655366	0.628548		
N	-1.289656	-0.813455	1.679325		
H	-0.710201	0.020082	1.603695		
H	-1.519839	-0.944258	2.656603		
H	-3.266928	-1.355636	1.313515		
C	-2.206919	-1.438308	-0.497086		
O	-2.894291	-1.312850	-1.484478		
O	-1.126132	-2.221274	-0.466216		
H	-0.764320	-2.090048	0.449336		
H	-4.032786	0.579441	0.085808		
H	-3.283246	1.117984	1.596815		
S	-1.980823	1.821334	-0.273762		
H	-2.128458	1.249225	-1.485858		
28					
Dimer 16 of the n...n type					
C	-2.949066	-0.611656	0.168361		
C	-3.012957	0.375413	-1.004024		
N	-3.145884	-0.047276	1.506592		
H	-2.772235	0.897366	1.560007		
H	-4.125919	-0.014323	1.759661		
H	-3.726269	-1.366384	0.002552		
C	-1.636080	-1.412797	0.158209		
O	-1.079961	-1.788787	-0.848320		
O	-1.161204	-1.683402	1.376037		
H	-1.780589	-1.213522	1.992494		
H	-2.852059	-0.150762	-1.943785		
H	-3.999664	0.838059	-1.025463		
S	-1.808419	1.768280	-0.881550		
H	-0.704173	1.070901	-1.235607		
C	1.818046	-0.767765	0.292877		
C	1.199229	0.340767	1.148280		
N	3.112166	-1.287676	0.744025		
H	3.686515	-0.542767	1.131359		
H	2.998785	-1.999914	1.455234		
H	1.105817	-1.598112	0.275447		
C	1.946230	-0.356888	-1.181315		
O	1.173469	0.379731	-1.755951		
O	2.987103	-0.910045	-1.801223		
H	3.473373	-1.391406	-1.083120		
H	0.198903	0.582753	0.802741		
H	1.124846	-0.007295	2.178136		
S	2.189381	1.894677	1.206101		
H	1.965628	2.250340	-0.075452		
28					
Dimer 17 of the n...n type					
C	-3.085244	0.199527	0.026518		

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C	-3.002971	-1.331519	0.036782		
N	-2.895797	0.871934	-1.259273		
H	-2.127181	0.452763	-1.777172		
H	-3.730180	0.821195	-1.831454		
H	-4.083591	0.468533	0.392573		
C	-2.130897	0.830264	1.052917		
O	-1.777524	0.284057	2.074207		
O	-1.737129	2.063524	0.734997		
H	-2.073720	2.208969	-0.183085		
H	-3.203074	-1.706784	1.039648		
H	-3.755951	-1.732838	-0.641959		
S	-1.396487	-2.017718	-0.546318		
H	-0.647826	-1.607826	0.495986		
C	2.635765	0.518838	0.662534		
C	1.263184	1.132045	0.363810		
N	3.784560	1.123837	-0.017399		
H	3.519006	1.476209	-0.933698		
H	4.175455	1.890612	0.516258		
H	2.798766	0.599617	1.743040		
C	2.636916	-0.995664	0.389759		
O	1.703261	-1.723292	0.646733		
O	3.776303	-1.448647	-0.129772		
H	4.329797	-0.633674	-0.252164		
H	0.493818	0.616504	0.933796		
H	1.258334	2.180794	0.658486		
S	0.813534	1.121765	-1.423907		
H	0.532470	-0.195301	-1.503202		
28					
Dimer 18 of the n...n type					
C	1.828842	0.755758	-0.331300		
C	1.229542	-0.386360	-1.155385		
N	3.137205	1.253009	-0.766366		
H	3.724870	0.489243	-1.092110		
H	3.046927	1.924090	-1.519706		
H	1.120376	1.588446	-0.371287		
C	1.911834	0.414186	1.163622		
O	1.132692	-0.308995	1.746421		
O	2.920987	1.014868	1.792169		
H	3.428769	1.464895	1.069210		
H	0.214867	-0.603322	-0.835673		
H	1.193933	-0.084826	-2.202026		
S	2.208138	-1.948095	-1.111576		
H	1.947389	-2.240476	0.178924		
C	-2.943985	0.620462	-0.159764		
C	-2.981791	-0.346208	1.031082		
N	-3.189512	0.034625	-1.480664		
H	-2.840981	-0.920010	-1.523943		
H	-4.176053	0.022135	-1.708799		
H	-3.706479	1.387155	0.018219		
C	-1.621634	1.405084	-0.203622		
O	-1.042626	1.809770	0.778548		
O	-1.166837	1.626008	-1.438864		
H	-1.808889	1.148593	-2.026254		
H	-2.774835	0.192302	1.954742		
H	-3.975571	-0.789086	1.098005		
S	-1.810574	-1.765628	0.887280		
H	-0.679779	-1.083759	1.184645		
28					
Dimer 19 of the n...n type					
C	1.820497	0.765346	-0.302181		
C	1.205242	-0.350787	-1.150154		
N	3.118318	1.278535	-0.750427		
H	3.694632	0.528603	-1.124923		
H	3.010627	1.982475	-1.470726		
H	1.109604	1.597008	-0.297847		
C	1.938554	0.370743	1.177291		
O	1.163068	-0.360507	1.755089		
O	2.974112	0.932606	1.798342		
H	3.465498	1.405505	1.078149		

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H	0.201448	-0.586139	-0.810269
H	1.139724	-0.013467	-2.184215
S	2.191873	-1.907646	-1.184412
H	1.960329	-2.247916	0.099941
C	-2.948113	0.613918	-0.164687
C	-3.004370	-0.368426	1.012161
N	-3.158932	0.044459	-1.498674
H	-2.791705	-0.902789	-1.550390
H	-4.141094	0.016538	-1.743974
H	-3.721322	1.371767	0.005378
C	-1.632408	1.410714	-0.169391
O	-1.069417	1.793760	0.830643
O	-1.163454	1.668752	-1.392162
H	-1.789348	1.197272	-2.000885
H	-2.831560	0.160726	1.948143
H	-3.992764	-0.826773	1.045418
S	-1.807150	-1.767214	0.882908
H	-0.696227	-1.071933	1.220437
28			
Dimer 20 of the n...n type			
C	-1.525582	-0.265653	-0.043943
C	-2.600814	-1.016466	-0.836054
N	-1.234016	-0.769648	1.298366
H	-2.053791	-1.197835	1.719476
H	-0.480364	-1.447204	1.262787
H	-0.601527	-0.329799	-0.623473
C	-1.841753	1.237267	0.034468
O	-2.302305	1.874235	-0.886158
O	-1.545959	1.787051	1.212802
H	-1.246205	1.021607	1.769129
H	-2.699016	-0.588443	-1.832486
H	-2.312303	-2.063641	-0.929043
S	-4.257430	-1.029846	-0.022360
H	-4.505710	0.287068	-0.176253
C	2.923084	-0.200486	0.743582
C	1.890308	0.932241	0.761871
N	4.273266	0.150478	0.298698
H	4.245958	0.891869	-0.397020
H	4.854593	0.459292	1.068088
H	2.990312	-0.591584	1.764936
C	2.422320	-1.396222	-0.088394
O	1.266720	-1.764816	-0.106246
O	3.378919	-2.011767	-0.774023
H	4.193046	-1.469881	-0.598763
H	0.941387	0.559109	1.138069
H	2.235707	1.725269	1.425233
S	1.631337	1.754243	-0.867378
H	1.196279	0.666299	-1.534492
28			
Dimer 21 of the n...n type			
C	-3.113581	0.394002	-0.078962
C	-3.082963	-1.020355	0.513997
N	-3.294221	0.488463	-1.530052
H	-2.827790	-0.280621	-2.004839
H	-4.273121	0.473865	-1.789016
H	-3.941632	0.930421	0.398418
C	-1.861415	1.195114	0.311217
O	-1.297616	1.100187	1.376265
O	-1.440125	2.029473	-0.645330
H	-2.046168	1.853019	-1.411918
H	-2.965431	-0.972753	1.595431
H	-4.025140	-1.519286	0.286800
S	-1.756452	-2.103406	-0.181466
H	-0.748878	-1.673480	0.607850
C	1.317144	0.302509	-0.320599
C	2.193048	-0.654560	-1.138695
N	1.622166	1.725402	-0.486015
H	2.413311	1.886847	-1.098580
H	0.814342	2.234174	-0.825205

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H	0.288044	0.096537	-0.618286
C	1.407859	-0.058084	1.172930
O	1.135372	-1.160144	1.604846
O	1.843380	0.931320	1.938935
H	1.939354	1.690895	1.297783
H	1.895622	-1.682206	-0.934141
H	2.049562	-0.454378	-2.200961
S	4.008510	-0.479845	-0.854372
H	4.010743	-0.906511	0.425477
28			
Dimer 22 of the n...n type			
C	-1.643365	-0.178708	0.627496
C	-3.145851	-0.239540	0.919451
N	-1.015635	1.139423	0.737716
H	-1.681946	1.886832	0.567111
H	-0.592100	1.266916	1.648418
H	-1.143274	-0.850018	1.330373
C	-1.323549	-0.782459	-0.751295
O	-1.855211	-1.778516	-1.186624
O	-0.376544	-0.124938	-1.423986
H	-0.171138	0.662963	-0.858930
H	-3.498472	-1.266950	0.844441
H	-3.332450	0.124854	1.929740
S	-4.169178	0.828271	-0.185997
H	-3.954795	0.120331	-1.313911
C	2.923271	-0.683011	0.141587
C	3.436753	0.760341	0.160883
N	2.630242	-1.279536	-1.162008
H	2.091444	-0.639510	-1.740989
H	3.478300	-1.526691	-1.657944
H	3.698284	-1.300024	0.613816
C	1.696073	-0.883193	1.042988
O	1.417820	-0.189367	1.994125
O	0.955897	-1.940846	0.697747
H	1.335100	-2.247247	-0.162979
H	3.641721	1.068073	1.185613
H	4.364278	0.813385	-0.409785
S	2.311620	1.994538	-0.617167
H	1.368592	1.968925	0.345231
28			
Dimer 23 of the n...n type			
C	2.692755	-0.504102	-0.632530
C	1.362977	-1.221590	-0.373672
N	3.848442	-0.974450	0.136531
H	3.560881	-1.322748	1.047650
H	4.345805	-1.713771	-0.344349
H	2.921170	-0.619118	-1.697831
C	2.549791	1.016075	-0.435742
O	1.583340	1.650775	-0.797216
O	3.604794	1.585930	0.142763
H	4.214268	0.826731	0.339527
H	0.579165	-0.794032	-0.994552
H	1.464019	-2.276548	-0.627319
S	0.828769	-1.192612	1.390977
H	0.433961	0.097965	1.415874
C	-3.065626	-0.227143	-0.054585
C	-3.018923	1.302573	0.027154
N	-2.894559	-0.970162	1.194440
H	-2.151916	-0.564874	1.758605
H	-3.745420	-0.972860	1.744207
H	-4.048619	-0.494862	-0.461176
C	-2.074716	-0.779311	-1.091220
O	-1.696494	-0.165438	-2.063760
O	-1.681246	-2.029432	-0.845087
H	-2.033421	-2.234757	0.055122
H	-3.215525	1.733027	-0.954000
H	-3.789483	1.644819	0.718296
S	-1.434960	1.991145	0.668426
H	-0.673709	1.673106	-0.397334

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28		
Dimer 24 of the n...n type		
C	2.113182 -0.217223 0.794167	
C	1.962636 1.275719 0.483456	
N	3.382468 -0.641282 1.389431	
H	4.159036 -0.111158 1.001186	
H	3.383661 -0.511302 2.393956	
H	1.310010 -0.488835 1.488765	
C	1.838835 -1.078935 -0.447932	
O	1.045810 -0.779230 -1.312882	
O	2.532455 -2.216390 -0.477394	
H	3.134983 -2.159350 0.307090	
H	0.962762 1.483610 0.109781	
S	2.112740 1.847541 1.399265	
H	3.206182 1.920432 -0.717660	
H	2.719046 1.264630 -1.790630	
C	-1.878065 0.015845 -0.712786	
C	-2.971815 1.083151 -0.606303	
N	-2.258915 -1.249632 -1.343913	
H	-3.242502 -1.455190 -1.190188	
H	-2.084199 -1.238756 -2.340929	
H	-1.048387 0.442451 -1.283049	
C	-1.259299 -0.283367 0.660886	
O	-1.019240 0.568369 1.489087	
O	-0.959316 -1.566123 0.851937	
H	-1.265509 -2.009655 0.016824	
H	-2.565328 1.990351 -0.161660	
H	-3.346196 1.316930 -1.603059	
S	-4.449682 0.550256 0.363813	
H	-3.829488 0.504968 1.560664	
28		
Dimer 25 of the n...n type		
C	-1.557540 -0.327594 0.122470	
C	-1.587257 1.092230 -0.451704	
N	-1.614251 -1.426394 -0.844131	
H	-2.057225 -1.142712 -1.712691	
H	-0.699501 -1.816171 -1.041029	
H	-0.630896 -0.407996 0.696715	
C	-2.680108 -0.517182 1.159935	
O	-2.994176 0.326720 1.970334	
O	-3.266164 -1.711537 1.099099	
H	-2.829081 -2.148152 0.318308	
H	-1.511531 1.815605 0.356652	
H	-0.737477 1.240808 -1.115311	
S	-3.082022 1.460366 -1.469735	
H	-3.967553 1.430519 -0.452621	
C	2.854528 0.594612 -0.609847	
C	1.946099 -0.480625 -1.215584	
N	4.265647 0.245261 -0.440638	
H	4.372318 -0.738360 -0.205262	
H	4.800832 0.428676 -1.280602	
H	2.799149 1.469325 -1.267623	
C	2.299991 1.096738 0.736246	
O	1.116852 1.194000 0.976022	
C	3.242428 1.440881 1.610768	
H	4.094639 1.199118 1.165543	
H	0.939440 -0.087573 -1.337460	
H	2.325446 -0.766289 -2.196700	
S	1.875836 -2.050616 -0.250468	
H	1.394842 -1.514440 0.889830	
28		
Dimer 26 of the n...n type		
C	-2.927298 -0.017988 0.638196	
C	-2.272256 -1.379399 0.374802	
N	-3.952315 0.405390 -0.319650	
H	-3.764087 0.023153 -1.243206	
H	-4.878250 0.110198 -0.035294	
H	-3.385816 -0.066900 1.631908	
C	-1.874684 1.099372 0.768550	

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O	-0.823265 0.965617 1.356819	
O	-2.242057 2.249980 0.213938	
H	-3.124021 2.049662 -0.198389	
H	-1.522829 -1.588719 1.136284	
H	-3.035132 -2.157102 0.416231	
S	-1.508391 -1.536564 -1.295341	
H	-0.588182 -0.555989 -1.159385	
C	2.927370 -0.018212 -0.638046	
C	2.272106 -1.379584 -0.374778	
N	3.952283 0.405078 0.319925	
H	3.763357 0.023554 1.243635	
H	4.878075 0.108864 0.036158	
H	3.386075 -0.067143 -1.631672	
C	1.874947 1.099265 -0.768549	
O	0.823417 0.965631 -1.356615	
O	2.242572 2.250022 -0.214281	
H	3.124499 2.049838 0.198027	
H	1.522896 -1.588864 -1.136470	
H	3.034974 -2.157308 -0.416033	
S	1.508015 -1.536658 1.295165	
H	0.588226 -0.555704 1.159173	
28		
Dimer 27 of the n...n type		
C	3.137619 -0.489123 0.565300	
C	2.563499 0.865442 1.004198	
N	4.351287 -0.442108 -0.256631	
H	4.377725 0.405260 -0.818251	
H	5.191622 -0.477760 0.307052	
H	3.361840 -1.056219 1.475417	
C	2.078044 -1.339206 -0.157934	
O	0.932877 -1.442030 0.220404	
O	2.542574 -1.990361 -1.223301	
H	3.495363 -1.714699 -1.278866	
H	1.634483 0.721633 1.553489	
H	3.287431 1.365018 1.648100	
S	2.239376 2.033227 -0.387719	
H	1.042515 1.525200 -0.755578	
C	-2.124305 -0.826276 0.306304	
C	-3.270910 -0.906718 -0.706742	
N	-2.498881 -0.884589 1.721575	
H	-3.405643 -0.451725 1.878069	
H	-2.540133 -1.838713 2.058262	
H	-1.439190 -1.652961 0.100065	
C	-1.261893 0.421691 0.071368	
O	-0.988780 0.848426 -1.031013	
O	-0.818132 0.994083 1.186728	
H	-1.212498 0.446903 1.913930	
H	-2.875248 -0.898663 -1.721259	
H	-3.824339 -1.833044 -0.552087	
S	-4.516634 0.446058 -0.539190	
H	-3.705276 1.442289 -0.949944	
28		
Dimer 28 of the n...n type		
C	-3.132448 -0.428296 -0.266063	
C	-3.229167 0.898264 0.495595	
N	-3.120123 -1.649251 0.543528	
H	-2.612566 -1.503084 1.412984	
H	-4.057507 -1.956841 0.772761	
H	-3.996510 -0.481140 -0.938439	
C	-1.915757 -0.450182 -1.206165	
O	-1.503204 0.518716 -1.800510	
O	-1.357612 -1.658068 -1.330660	
H	-1.882751 -2.233052 -0.714505	
H	-3.270195 1.731670 -0.203994	
H	-4.139074 0.899398 1.095743	
S	-1.845736 1.188237 1.683488	
H	-0.917062 1.530105 0.763907	
C	2.077105 -0.880214 -0.277015	
C	1.726834 0.144956 -1.360755	

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N	1.047182	-1.169977	0.722822		
H	0.542394	-0.326867	0.983272		
H	0.368989	-1.827693	0.360294		
H	2.310346	-1.819837	-0.791647		
C	3.381942	-0.513389	0.450958		
O	4.317175	0.041570	-0.080391		
O	3.406072	-0.892113	1.730030		
H	2.502627	-1.264202	1.895567		
H	2.552093	0.235339	-2.065669		
H	0.833361	-0.178705	-1.891205		
S	1.308411	1.819876	-0.715705		
H	2.523141	2.092026	-0.195112		
28					
Dimer 29 of the n...n type					
C	3.100110	1.027208	-0.017870		
C	3.865272	-0.259013	-0.352273		
N	2.922043	1.338921	1.401846		
H	2.802476	0.487322	1.945438		
H	3.715944	1.843730	1.776872		
H	3.646470	1.858303	-0.478554		
C	1.724012	1.056398	-0.705455		
O	1.504620	0.581148	-1.796968		
O	0.784898	1.687716	0.000044		
H	1.228935	1.907372	0.859642		
H	3.934842	-0.379170	-1.432383		
H	4.872396	-0.195960	0.060216		
S	3.130350	-1.782718	0.381797		
H	1.975060	-1.752198	-0.313790		
C	-2.707200	0.537278	-0.597002		
C	-1.610843	-0.442298	-1.028133		
N	-2.285147	1.632846	0.281620		
H	-1.540031	1.314330	0.896677		
H	-1.902495	2.400507	-0.257436		
H	-3.129732	0.977202	-1.507735		
C	-3.889099	-0.196103	0.060682		
O	-4.289207	-1.282201	-0.294850		
O	-4.457988	0.489926	1.052664		
H	-3.893763	1.302283	1.140619		
H	-2.016560	-1.186953	-1.711190		
H	-0.810100	0.101552	-1.525692		
S	-0.801900	-1.310577	0.384482		
H	-1.829009	-2.141504	0.655791		
28					
Dimer 30 of the n...n type					
C	2.923512	-0.322064	0.702128		
C	2.350288	1.098524	0.780492		
N	4.079775	-0.504347	-0.179524		
H	4.033600	0.136578	-0.968250		
H	4.953266	-0.349114	0.308559		
H	3.218388	-0.612383	1.717228		
C	1.859760	-1.362034	0.315148		
O	0.708943	-1.345742	0.716107		
O	2.309171	-2.324367	-0.469394		
H	3.253644	-2.061109	-0.653663		
H	1.518836	1.136451	1.481967		
H	3.131357	1.766667	1.143938		
S	1.817340	1.789444	-0.843302		
H	0.738390	0.963794	-1.047850		
C	-2.049717	0.666992	-0.859753		
C	-3.378882	-0.121313	-0.820094		
N	-0.904335	-0.071782	-1.379440		
H	-0.861379	-1.014972	-1.001423		
H	-0.974880	-0.155378	-2.388309		
H	-2.215236	1.530820	-1.507907		
C	-1.808591	1.272743	0.529666		
O	-2.486493	2.198730	0.920778		
O	-0.893591	0.730718	1.333041		
H	-0.381011	-0.022145	0.957334		
H	-4.189598	0.520357	-0.475122		

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H	-3.610509	-0.467547	-1.828115		
S	-3.322581	-1.650347	0.210533		
H	-3.241549	-1.036474	1.408890		
28					
Dimer 31 of the n...n type					
C	-1.801341	-0.105094	-0.738074		
C	-2.454817	1.200429	-0.273037		
N	-2.591493	-0.945579	-1.640676		
H	-3.582841	-0.884290	-1.421874		
H	-2.463717	-0.676501	-2.608591		
H	-0.868130	0.148960	-1.248639		
C	-1.340297	-0.954314	0.457434		
O	-0.886657	-0.481839	1.477373		
O	-1.462157	-2.265840	0.269895		
H	-1.884513	-2.347830	-0.622867		
H	-1.766044	1.766164	0.352843		
H	-2.712876	1.804163	-1.143199		
S	-4.034605	0.960170	0.650202		
H	-3.478478	0.391169	1.739320		
C	2.195437	-0.106052	0.862547		
C	1.632406	1.276923	0.521295		
N	3.573870	-0.143905	1.357777		
H	4.145382	0.555471	0.889683		
H	3.616293	0.030603	2.354541		
H	1.540582	-0.533713	1.629058		
C	2.073169	-1.078955	-0.320581		
O	1.162354	-1.061139	-1.118892		
O	3.053704	-1.979727	-0.378329		
H	3.675211	-1.714630	0.346983		
H	0.577236	1.202142	0.277214		
H	1.735350	1.925827	1.391187		
S	2.517565	2.137217	-0.849209		
H	2.097237	1.311389	-1.829129		
28					
Dimer 32 of the n...n type					
C	-1.626377	-0.353966	-0.611017		
C	-2.091410	1.079447	-0.340009		
N	-2.385746	-1.110715	-1.609101		
H	-3.373643	-0.871407	-1.571901		
H	-2.051767	-0.927417	-2.547577		
H	-0.587551	-0.313829	-0.946059		
C	-1.544609	-1.177467	0.683280		
O	-1.224507	-0.712458	1.755281		
O	-1.833098	-2.467302	0.519578		
H	-2.103269	-2.539978	-0.431104		
H	-1.427169	1.568186	0.369224		
H	-2.072416	1.645043	-1.271437		
S	-3.825054	1.196177	0.282272		
H	-3.582758	0.630881	1.482665		
C	2.698467	0.054412	0.816629		
C	1.561165	1.081631	0.827648		
N	4.052437	0.575991	0.615025		
H	4.040564	1.379530	-0.008532		
H	4.478432	0.860606	1.488701		
H	2.674745	-0.462681	1.782576		
C	2.438073	-1.058276	-0.215043		
O	1.337451	-1.499230	-0.463685		
O	3.542676	-1.519198	-0.797716		
H	4.268309	-0.945179	-0.439258		
H	0.616638	0.588422	1.046512		
H	1.752371	1.819786	1.607020		
S	1.413396	2.060760	-0.728557		
H	1.095165	1.030929	-1.538330		
28					
Dimer 33 of the n...n type					
C	1.703060	0.526640	0.078905		
C	1.096564	-0.835401	-0.270503		
N	1.999299	1.420225	-1.042084		
H	2.346362	0.890528	-1.838414		

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H	1.156604	1.903617	-1.330986		
H	0.982289	1.038450	0.726581		
C	2.962268	0.376431	0.944309		
O	3.118520	-0.501466	1.763713		
O	3.870960	1.331775	0.736541		
H	3.500583	1.863260	-0.013949		
H	0.895781	-1.400038	0.638181		
H	0.160464	-0.683959	-0.805499		
S	2.142246	-1.865625	-1.386258		
H	3.123231	-2.099996	-0.490564		
C	-3.121046	0.748349	-0.180830		
C	-3.498216	-0.299610	0.872092		
N	-3.161777	0.314316	-1.579559		
H	-2.876728	-0.658238	-1.666991		
H	-4.089691	0.408193	-1.974456		
H	-3.814363	1.589938	-0.069412		
C	-1.735552	1.351922	0.102150		
O	-1.286520	1.532800	1.211159		
O	-1.060069	1.676032	-1.002587		
H	-1.633221	1.355011	-1.747604		
H	-3.503860	0.147751	1.864789		
H	-4.494999	-0.683265	0.654428		
S	-2.384265	-1.771748	0.887777		
H	-1.328402	-1.138182	1.433735		
28					
Dimer 34 of the n...n type					
C	2.921826	0.518305	0.680027		
C	3.152887	-0.997919	0.666631		
N	1.960441	1.018802	1.666779		
H	1.261866	0.311547	1.876257		
H	2.415304	1.273130	2.535079		
H	3.890019	0.992984	0.872825		
C	2.522294	1.022875	-0.718825		
O	2.999288	0.597693	-1.745580		
O	1.607669	1.994652	-0.702277		
H	1.357638	2.092375	0.252225		
H	3.890238	-1.255223	-0.091940		
H	3.523075	-1.316090	1.641249		
S	1.621630	-1.987631	0.378179		
H	1.396479	-1.560918	-0.881320		
C	-1.584547	-0.009333	0.580657		
C	-3.001897	-0.334168	1.066582		
N	-1.210665	1.403981	0.553726		
H	-2.001647	1.981993	0.281141		
H	-0.888385	1.720811	1.460220		
H	-0.886431	-0.534570	1.241629		
C	-1.313981	-0.637474	-0.795743		
O	-1.747090	-1.716856	-1.130900		
O	-0.517884	0.081441	-1.588244		
H	-0.323994	0.916889	-1.100182		
H	-3.152054	-1.412228	1.096166		
H	-3.138084	0.068414	2.070398		
S	-4.332423	0.429647	0.041273		
H	-4.135133	-0.340020	-1.048494		
28					
Dimer 35 of the n...n type					
C	-3.137046	-0.010089	-0.026388		
C	-2.709890	0.647826	-1.344085		
N	-3.247034	0.867420	1.141444		
H	-2.506954	1.565688	1.136306		
H	-4.136839	1.350913	1.162984		
H	-4.119773	-0.466706	-0.193691		
C	-2.225191	-1.191027	0.338870		
O	-1.667280	-1.893757	-0.475313		
O	-2.104689	-1.392941	1.651038		
H	-2.578979	-0.628281	2.065238		
H	-2.695855	-0.089426	-2.145445		
H	-3.426915	1.428103	-1.599833		
S	-1.066601	1.481454	-1.267174		

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H	-0.314726	0.363265	-1.340603		
C	2.197407	-0.421148	1.102535		
C	2.814581	-1.322090	0.025891		
N	0.751833	-0.562306	1.281209		
H	0.321605	-1.013937	0.481281		
H	0.504462	-1.096097	2.104369		
H	2.705481	-0.645153	2.046214		
C	2.529761	1.057425	0.816054		
O	3.635548	1.441394	0.502676		
O	1.493189	1.878971	0.951073		
H	0.727887	1.277086	1.158532		
H	3.888907	-1.156039	-0.032064		
H	2.630702	-2.366753	0.277128		
S	2.080293	-1.084331	-1.653478		
H	2.576454	0.152865	-1.861605		
28					
Dimer 36 of the n...n type					
C	-3.184756	0.421974	0.562816		
C	-2.794173	-1.050821	0.756892		
N	-3.987402	0.727923	-0.623756		
H	-3.845905	0.033531	-1.352670		
H	-4.976005	0.774915	-0.411860		
H	-3.737913	0.732389	1.454978		
C	-1.922953	1.302525	0.551246		
O	-1.006944	1.174142	1.333113		
O	-1.908522	2.219015	-0.415206		
H	-2.765465	2.072824	-0.900295		
H	-2.164737	-1.152700	1.639978		
H	-3.693116	-1.651780	0.893513		
S	-1.935086	-1.797196	-0.696456		
H	-0.855516	-0.992291	-0.674962		
C	1.801084	0.634589	0.231627		
C	1.510479	-0.703696	0.921137		
N	1.141284	0.882117	-1.050175		
H	1.035272	0.032517	-1.596970		
H	0.243872	1.336650	-0.942417		
H	1.478910	1.419207	0.923067		
C	3.316514	0.846590	0.058840		
O	4.143495	0.481752	0.864638		
O	3.643513	1.499458	-1.057012		
H	2.780095	1.618605	-1.530869		
H	2.073343	-0.767578	1.850957		
H	0.450096	-0.765681	1.157625		
S	1.893797	-2.181543	-0.113511		
H	3.231027	-2.002955	-0.132701		
28					
Dimer 37 of the n...n type					
C	3.091427	0.187923	-0.684764		
C	2.008282	-0.678518	-1.338916		
N	4.239124	-0.523991	-0.116958		
H	3.954322	-1.423295	0.263642		
H	4.959107	-0.687692	-0.810141		
H	3.465319	0.875897	-1.451431		
C	2.495724	1.109258	0.395397		
O	1.410944	1.638712	0.301550		
O	3.299228	1.300943	1.440472		
H	4.081338	0.718038	1.259605		
H	1.229642	-0.048289	-1.766026		
H	2.456096	-1.265368	-2.140921		
S	1.244902	-1.908362	-0.197162		
H	0.601126	-1.024385	0.594616		
C	-2.215213	-0.628032	-0.530652		
C	-1.526247	0.674063	-0.951720		
N	-3.578447	-0.835285	-1.026002		
H	-4.071672	0.050106	-1.111230		
H	-3.583843	-1.289452	-1.931095		
H	-1.589622	-1.453414	-0.888103		
C	-2.215612	-0.785679	0.999584		
O	-1.289062	-0.454589	1.708114		

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O -3.320055	-1.348877	1.483267	
H -3.900333	-1.470884	0.686901	
H -0.515127	0.723289	-0.557076	
H -1.485718	0.722919	-2.040116	
S -2.415900	2.198794	-0.415654	
H -2.128016	2.076965	0.896368	
28			
Dimer 38 of the n...n type			
C 1.296643	-0.239050	0.567975	
C 2.081852	1.077217	0.590852	
N 1.763596	-1.293692	1.468062	
H 2.771400	-1.244536	1.594611	
H 1.326175	-1.230210	2.379127	
H 0.266765	0.007441	0.832996	
C 1.208528	-0.800317	-0.862007	
O 1.019821	-0.102817	-1.836170	
O 1.346252	-2.118305	-0.940035	
H 1.470906	-2.407784	0.000327	
H 1.623151	1.798951	-0.081928	
H 2.069310	1.484957	1.601753	
S 3.864062	0.894793	0.149839	
H 3.663355	0.596521	-1.150287	
C -2.933915	-0.039884	0.496528	
C -2.980427	1.283055	-0.276720	
N -2.423627	0.026105	1.869811	
H -1.755267	0.785016	1.976534	
H -3.168280	0.168684	2.541088	
H -3.955667	-0.433584	0.531423	
C -2.141079	-1.108749	-0.279216	
O -2.174042	-1.228043	-1.481639	
O -1.419719	-1.914448	0.503812	
H -1.565392	-1.560910	1.419313	
H -3.376379	1.116064	-1.277095	
H -3.630544	1.983811	0.247081	
S -1.346971	2.132192	-0.408549	
H -0.763339	1.249118	-1.246603	
28			
Dimer 39 of the n...n type			
C 1.222008	0.509841	-0.138206	
C 1.852202	-0.479960	-1.118908	
N 1.511988	1.928758	-0.343602	
H 2.439605	2.064282	-0.736277	
H 0.830738	2.359599	-0.957478	
H 0.139987	0.391260	-0.224623	
C 1.531316	0.141419	1.321509	
O 1.619372	-0.997915	1.724084	
O 1.649854	1.198401	2.122525	
H 1.590433	1.976148	1.507070	
H 1.504101	-1.486788	-0.897404	
H 1.550226	-0.219238	-2.133631	
S 3.696789	-0.452550	-1.125806	
H 3.852321	-0.970755	0.109694	
C -2.610954	-0.547453	0.681947	
C -3.315354	0.583364	-0.076254	
N -1.676986	-0.136967	1.733173	
H -1.296672	0.787301	1.552306	
H -2.124587	-0.110310	2.640907	
H -3.392093	-1.163806	1.141119	
C -1.901747	-1.507688	-0.291729	
O -2.338061	-1.789771	-1.384923	
O -0.767399	-2.028627	0.175801	
H -0.602291	-1.595247	1.047923	
H -4.039036	0.172639	-0.777932	
H -3.837767	1.222775	0.635259	
S -2.171094	1.700440	-1.001884	
H -1.846055	0.809503	-1.960945	
28			
Dimer 40 of the n...n type			
C -3.099750	-0.507833	0.619164	

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C -1.773134	-1.251792	0.810424	
N -4.059322	-1.098809	-0.315862	
H -3.579162	-1.585815	-1.068662	
H -4.676788	-1.756180	0.144394	
H -3.577695	-0.444356	1.603096	
C -2.856619	0.959899	0.224455	
O -1.962811	1.637180	0.683739	
O -3.742297	1.437192	-0.645723	
H -4.320699	0.658526	-0.858238	
H -1.141622	-0.696585	1.502070	
H -1.968503	-2.241714	1.222659	
S -0.837810	-1.556940	-0.749736	
H -0.537205	-0.271310	-1.018970	
C 2.423612	0.867542	0.836832	
C 3.662985	-0.015946	0.643454	
N 1.300006	0.275184	1.559537	
H 1.166495	-0.689580	1.264437	
H 1.465345	0.276102	2.559116	
H 2.745412	1.755760	1.394136	
C 1.921569	1.429797	-0.502076	
O 2.634093	1.615295	-1.462547	
O 0.623359	1.741346	-0.523202	
H 0.231301	1.462689	0.336594	
H 4.444283	0.539952	0.127016	
H 4.037837	-0.323337	1.620095	
S 3.332651	-1.583882	-0.269030	
H 3.018036	-1.003730	-1.444863	
28			
Dimer 41 of the n...n type			
C -3.099513	0.508501	-0.618977	
C -1.772541	1.251828	-0.810368	
N -4.058598	1.099723	0.316375	
H -3.577970	1.585768	1.069507	
H -4.675322	1.758070	-0.143481	
H -3.577739	0.445491	-1.602804	
C -2.857063	-0.959460	-0.224694	
O -1.963431	-1.636975	-0.683911	
O -3.743223	-1.436703	0.645100	
H -4.321313	-0.657905	0.857795	
H -1.141519	0.696428	-1.502326	
H -1.967504	2.241919	-1.222395	
S -0.836668	1.556047	0.749582	
H -0.537769	0.270029	1.018827	
C 2.423966	-0.868072	-0.836325	
C 3.662998	0.015769	-0.642855	
N 1.300484	-0.276408	-1.559908	
H 1.166689	0.688524	-1.265458	
H 1.466276	-0.277912	-2.559416	
H 2.746154	-1.756549	-1.392989	
C 1.921328	-1.429804	0.502620	
O 2.633271	-1.614538	1.463631	
O 0.623178	-1.741866	0.522956	
H 0.231742	-1.463189	-0.337163	
H 4.444099	-0.539560	-0.125512	
H 4.038455	0.322568	-1.619449	
S 3.331831	1.584340	0.268331	
H 3.016500	1.004993	1.444361	
28			
Dimer 42 of the n...n type			
C -1.751732	-0.064256	0.814441	
C -1.842751	-1.349135	-0.016275	
N -2.777526	0.123259	1.842083	
H -3.673311	-0.247328	1.534186	
H -2.525709	-0.336663	2.708577	
H -0.775550	-0.049978	1.308928	
C -1.713836	1.182764	-0.082934	
O -1.176948	1.212815	-1.168961	
O -2.299276	2.250420	0.454956	
H -2.691112	1.916243	1.301975	

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H	-1.012413	-1.412119	-0.716898
H	-1.800421	-2.211455	0.649204
S	-3.419997	-1.520389	-0.956911
H	-3.177925	-0.513485	-1.821057
C	1.751813	-0.064290	-0.814586
C	1.842586	-1.349226	0.015987
N	2.777936	0.123271	-1.841926
H	3.673476	-0.247929	-1.534076
H	2.526033	-0.335932	-2.708769
H	0.775791	-0.049900	-1.309395
C	1.713919	1.182704	0.082907
O	1.176626	1.212798	1.168742
O	2.299922	2.250148	-0.454684
H	2.691955	1.915805	-1.301627
H	1.012087	-1.412341	0.716405
H	1.800457	-2.211508	-0.649554
S	3.419611	-1.520620	0.957045
H	3.177366	-0.513770	1.821206
28			
Dimer 43 of the n...n type			
C	-1.364356	0.287470	0.023859
C	-2.394386	0.660984	1.092251
N	-1.337406	1.109545	-1.184676
H	-2.264058	1.457244	-1.413881
H	-0.697221	1.888144	-1.085272
H	-0.376196	0.347251	0.493049
C	-1.479950	-1.189429	-0.387707
O	-1.804408	-2.081262	0.363037
O	-1.128599	-1.406534	-1.656557
H	-0.994906	-0.490663	-2.024329
H	-2.287240	0.010816	1.959281
H	-2.231927	1.692941	1.403639
S	-4.141143	0.590639	0.500994
H	-4.187522	-0.748882	0.350964
C	3.054282	0.645436	0.363605
C	3.296191	-0.858586	0.202288
N	2.604160	1.095751	1.684184
H	1.994238	0.406803	2.117803
H	3.383728	1.262272	2.309106
H	3.997341	1.157038	0.139552
C	2.070715	1.174463	-0.694019
O	1.985964	0.744602	-1.819835
O	1.313955	2.187082	-0.254279
H	1.549005	2.273715	0.706337
H	3.698801	-1.073923	-0.786129
H	4.015330	-1.187096	0.952465
S	1.783580	-1.883440	0.464819
H	1.224082	-1.621034	-0.732736
28			
Dimer 44 of the n...n type			
C	1.921135	0.659711	0.539234
C	1.341987	-0.665784	1.048228
N	1.261399	1.267699	-0.617234
H	0.910707	0.558368	-1.255339
H	0.475187	1.849491	-0.354382
H	1.873741	1.372087	1.370963
C	3.424410	0.523999	0.231682
O	4.184077	-0.164159	0.876354
O	3.824431	1.259558	-0.805257
H	2.985221	1.663409	-1.151870
H	1.901531	-1.006585	1.918084
H	0.302970	-0.518836	1.339221
S	1.317331	-2.014373	-0.210358
H	2.651996	-2.204305	-0.251573
C	-2.954856	-0.347972	-0.589807
C	-3.477190	0.329705	0.681032
N	-2.400987	-1.695756	-0.440852
H	-1.876207	-1.780048	0.426296
H	-3.129272	-2.399774	-0.434467

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H	-3.794652	-0.412414	-1.291874
C	-1.919822	0.523940	-1.318749
O	-1.885520	1.732629	-1.267728
O	-1.046547	-0.180439	-2.042445
H	-1.220363	-1.126177	-1.806135
H	-3.925179	1.292041	0.437840
H	-4.237273	-0.304666	1.137026
S	-2.193785	0.584024	1.981738
H	-1.543532	1.577082	1.343626
28			
Dimer 45 of the n...n type			
C	-2.361664	-1.125995	0.505985
C	-3.240706	-0.484633	-0.574661
N	-2.285592	-0.462464	1.807828
H	-2.182895	0.542415	1.686307
H	-3.116036	-0.635153	2.361619
H	-2.758009	-2.134844	0.676212
C	-0.929383	-1.381544	0.012282
O	-0.625157	-1.547128	-1.147232
O	-0.033289	-1.455421	1.000216
H	-0.534905	-1.182369	1.808461
H	-3.154019	-1.057865	-1.497162
H	-4.280929	-0.507112	-0.248046
S	-2.887728	1.289887	-0.918196
H	-1.580944	1.156483	-1.230926
C	2.361938	1.126040	0.505479
C	3.240506	0.484045	-0.575190
N	2.285863	0.462886	1.807546
H	2.183619	-0.542077	1.686432
H	3.115994	0.636256	2.361577
H	2.758695	2.134758	0.675410
C	0.929599	1.381914	0.011959
O	0.625249	1.547604	-1.147518
O	0.033736	1.456042	1.000067
H	0.535551	1.182735	1.808177
H	3.153600	1.056927	-1.497890
H	4.280866	0.506486	-0.249004
S	2.887173	-1.290529	-0.917911
H	1.580354	-1.157070	-1.230475
28			
Dimer 46 of the n...n type			
C	-1.589855	0.133377	0.321583
C	-2.542470	-0.833347	1.029295
N	-1.691426	1.545759	0.692680
H	-2.648398	1.794247	0.929252
H	-1.095811	1.776381	1.477992
H	-0.573819	-0.213394	0.532062
C	-1.698584	0.015407	-1.207228
O	-1.935013	-1.017352	-1.791927
O	-1.460179	1.163882	-1.844985
H	-1.375094	1.832542	-1.115361
H	-2.342814	-1.854931	0.709669
H	-2.389649	-0.765749	2.106542
S	-4.329464	-0.457895	0.757689
H	-4.344293	-0.777250	-0.552582
C	3.004364	-0.302262	0.907131
C	2.092551	0.911105	1.126175
N	4.335477	-0.028363	0.363010
H	4.304077	0.742907	-0.299491
H	4.996865	0.208278	1.092616
H	3.131117	-0.793626	1.878546
C	2.319997	-1.364797	0.028397
O	1.130494	-1.593967	0.056639
O	3.159605	-2.035973	-0.755663
H	4.038188	-1.600045	-0.609580
H	1.161629	0.598139	1.597530
H	2.589797	1.618585	1.789782
S	1.725003	1.860138	-0.409913
H	1.035963	0.886639	-1.035838

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28		
Dimer 47 of the n...n type		
C	2.909954	0.040607 -0.442694
C	2.538842	-1.445853 -0.511003
N	3.357262	0.546834 0.856763
H	2.854886	0.087272 1.612716
H	4.348953	0.396497 0.997217
H	3.716598	0.208537 -1.165552
C	1.759606	0.930100 -0.945052
O	1.003866	0.615054 -1.837237
O	1.681242	2.105778 -0.320678
H	2.374379	2.052234 0.387945
H	2.231359	-1.706767 -1.522729
H	3.408226	-2.045893 -0.241983
S	1.210707	-1.937517 0.669730
H	0.219713	-1.258477 0.060379
C	-2.433192	1.049298 0.271750
C	-3.293471	-0.040648 -0.379287
N	-1.599219	1.853767 -0.615208
H	-1.098333	1.283925 -1.293915
H	-2.140874	2.550934 -1.110944
H	-3.119788	1.732404 0.786765
C	-1.549710	0.483484 1.396026
O	-1.862747	-0.457386 2.090878
O	-0.400102	1.138861 1.561247
H	-0.365415	1.807109 0.831986
H	-3.956712	-0.493285 0.356469
H	-3.900497	0.410975 -1.163994
S	-2.324108	-1.380968 -1.197876
H	-2.034625	-2.054297 -0.067040
28		
Dimer 48 of the n...n type		
C	1.286127	0.192039 -0.018790
C	2.312354	0.937881 -0.876724
N	1.023640	0.738203 1.312231
H	1.891421	1.022463 1.760930
H	0.424004	1.554296 1.243401
H	0.338119	0.205227 -0.567055
C	1.622284	-1.300687 0.100631
O	2.186658	-1.935383 -0.758840
O	1.195220	-1.864071 1.237172
H	0.841136	-1.122217 1.781645
H	2.378431	0.484842 -1.864846
H	1.997021	1.975809 -0.986753
S	3.998180	1.004297 -0.130544
H	4.272018	-0.307213 -0.283982
C	-2.831597	-0.448243 0.451464
C	-3.266321	1.008590 0.255345
N	-1.947616	-0.726550 1.584718
H	-1.292682	0.034516 1.744068
H	-2.471328	-0.874196 2.438863
H	-3.743673	-1.040828 0.586606
C	-2.194660	-1.018456 -0.827797
O	-2.525798	-0.697376 -1.946012
O	-1.241220	-1.923403 -0.596397
H	-1.148720	-1.953144 0.389035
H	-3.994304	1.078183 -0.551394
H	-3.725550	1.372649 1.174322
S	-1.882171	2.176224 -0.105631
H	-1.642186	1.734830 -1.356840
28		
Dimer 49 of the n...n type		
C	-3.001218	0.538587 0.265779
C	-3.456784	-0.833681 -0.241363
N	-2.635595	1.528218 -0.750923
H	-2.179110	1.087109 -1.545480
H	-3.446412	2.028193 -1.095145
H	-3.823278	0.957906 0.857296
C	-1.836979	0.417536 1.263116

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O	-1.670184	-0.528301 2.001331
O	-1.015331	1.467269 1.254770
H	-1.340166	2.034392 0.509166
H	-3.775910	-1.457248 0.592288
H	-4.297743	-0.702164 -0.922216
S	-2.168830	-1.742255 -1.202356
H	-1.418817	-2.084953 -0.136713
C	1.739336	-0.705190 0.119920
C	1.099915	0.182447 -0.953542
N	1.448876	-0.359419 1.513799
H	1.314524	0.644174 1.608043
H	0.592834	-0.796551 1.836587
H	1.392640	-1.729871 -0.056784
C	3.266490	-0.778627 -0.062831
O	3.815097	-0.804512 -1.142216
O	3.935116	-0.835097 1.087851
H	3.225938	-0.742889 1.779925
H	1.351343	-0.188537 -1.945725
H	0.018682	0.156411 -0.846521
S	1.573140	1.960349 -0.839243
H	2.841391	1.801622 -1.269634
28		
Dimer 50 of the n...n type		
C	-3.112534	0.623264 -0.227493
C	-3.321404	-0.879207 -0.012441
N	-2.894628	1.057886 -1.610088
H	-2.341214	0.374026 -2.120904
H	-3.769715	1.187236 -2.103473
H	-4.004378	1.138397 0.147627
C	-1.962519	1.163140 0.639977
O	-1.680042	0.737274 1.735506
O	-1.300564	2.176102 0.070617
H	-1.698568	2.254662 -0.834836
H	-3.560731	-1.083703 1.029910
H	-4.150684	-1.216263 -0.634096
S	-1.861743	-1.902721 -0.494915
H	-1.157515	-1.665075 0.627549
C	1.443594	0.366552 -0.140958
C	2.560933	0.483773 -1.181103
N	1.437145	1.352917 0.936229
H	2.381199	1.631731 1.185848
H	0.890542	2.168259 0.689992
H	0.491258	0.452479 -0.676895
C	1.388219	-1.039086 0.477063
O	1.706515	-2.052542 -0.103361
O	0.887956	-1.050216 1.714044
H	0.768829	-0.090797 1.942443
H	2.434983	-0.272127 -1.954942
H	2.520755	1.470556 -1.642517
S	4.258627	0.336774 -0.471822
H	4.158828	-0.965403 -0.135634
28		
Dimer 51 of the n...n type		
C	-2.290704	0.139181 -1.098366
C	-2.718082	-1.243921 -0.592759
N	-0.923766	0.248766 -1.609741
H	-0.291859	-0.389807 -1.130143
H	-0.875022	0.041071 -2.599654
H	-2.980103	0.416709 -1.903861
C	-2.505460	1.216296 -0.019217
O	-3.444256	1.221752 0.745524
O	-1.567962	2.163005 -0.013336
H	-0.916945	1.876064 -0.706438
H	-3.777223	-1.243095 -0.340226
H	-2.544702	-1.980904 -1.376913
S	-1.768565	-1.840844 0.874425
H	-2.336834	-0.999031 1.761576
C	2.378103	0.227678 1.062806
C	2.907712	-1.093596 0.494594

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N	1.079820	0.177361	1.736475		
H	0.447149	-0.485400	1.290915		
H	1.173088	-0.089565	2.709054		
H	3.118017	0.587591	1.787288		
C	2.333431	1.328440	-0.011979		
O	3.133080	1.421338	-0.915524		
O	1.339289	2.200978	0.159989		
H	0.824872	1.845022	0.930597		
H	3.922212	-0.965575	0.120426		
H	2.918490	-1.843215	1.285782		
S	1.871618	-1.804225	-0.857643		
H	2.266419	-0.932700	-1.807742		
28					
Dimer 52 of the n...n type					
C	2.904685	-0.258336	0.369853		
C	2.723438	-1.227701	-0.804175		
N	2.376984	-0.692706	1.666994		
H	1.565509	-1.295876	1.550895		
H	3.070608	-1.196800	2.205606		
H	3.979947	-0.081028	0.482201		
C	2.327560	1.131655	0.036281		
O	2.403348	1.647546	-1.053502		
O	1.754436	1.734776	1.082077		
H	1.842556	1.076284	1.820204		
H	3.127532	-0.786376	-1.713972		
H	3.257758	-2.154431	-0.594028		
S	0.972624	-1.730954	-1.091128		
H	0.499481	-0.506262	-1.409029		
C	-2.255897	0.235337	1.071226		
C	-2.322038	1.582190	0.340815		
N	-0.934650	-0.145440	1.576373		
H	-0.212011	0.244851	0.980525		
H	-0.781529	0.196925	2.517148		
H	-2.949325	0.285221	1.917678		
C	-2.804903	-0.897567	0.185011		
O	-3.775880	-0.773303	-0.527577		
O	-2.129499	-2.041161	0.282435		
H	-1.365138	-1.836648	0.878625		
H	-3.346607	1.804504	0.047462		
H	-1.965175	2.369410	1.004941		
S	-1.240424	1.666276	-1.154821		
H	-1.991455	0.845765	-1.918172		
28					
Dimer 53 of the n...n type					
C	-1.645120	0.178342	0.606846		
C	-2.090339	-1.259033	0.321699		
N	-2.327921	0.872158	1.701355		
H	-3.293351	0.562864	1.782231		
H	-1.868258	0.712605	2.589441		
H	-0.578411	0.126580	0.837440		
C	-1.724233	1.043690	-0.660064		
O	-1.421234	0.642099	-1.762920		
O	-2.123730	2.293790	-0.437332		
H	-2.315788	2.318175	0.536193		
H	-1.476499	-1.684337	-0.468158		
H	-1.960105	-1.859180	1.222128		
S	-3.874410	-1.413631	-0.126946		
H	-3.778370	-0.795654	-1.321978		
C	3.041579	-0.380963	0.734279		
C	2.246955	0.892568	1.044548		
N	4.296365	-0.205280	0.000095		
H	4.224518	0.562827	-0.662787		
H	5.071239	-0.012996	0.623293		
H	3.274690	-0.860606	1.691646		
C	2.172960	-1.413519	-0.007729		
O	0.991025	-1.570993	0.205319		
O	2.845461	-2.143195	-0.894945		
S	3.759863	-1.759013	-0.888582		
H	1.373021	0.650757	1.648098		

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H	2.875875	1.578463	1.612251		
S	1.726125	1.836894	-0.450879		
H	0.942033	0.879048	-0.984615		
28					
Dimer 54 of the n...n type					
C	2.783799	0.480028	0.387381		
C	3.154035	-0.446680	-0.778140		
N	2.541913	-0.118608	1.697701		
H	1.914582	-0.914418	1.617725		
H	3.405946	-0.426215	2.127948		
H	3.626273	1.174760	0.501580		
C	1.611435	1.412504	0.044447		
O	1.310147	1.740460	-1.080440		
O	0.990788	1.906427	1.119051		
H	1.333965	1.374995	1.876687		
H	3.265507	0.145314	-1.686070		
H	4.106673	-0.930747	-0.559716		
S	1.985227	-1.833894	-1.096852		
H	0.871995	-1.083135	-1.184447		
C	-2.177895	-0.878847	-0.553355		
C	-1.814014	0.446546	-1.233187		
N	-3.606394	-1.123684	-0.336883		
H	-4.089613	-0.257889	-0.109702		
H	-4.045893	-1.524539	-1.156684		
H	-1.790948	-1.689474	-1.182307		
C	-1.442729	-1.049669	0.785610		
O	-0.313080	-0.663157	0.981710		
O	-2.148600	-1.695854	1.712329		
H	-3.033633	-1.843905	1.290933		
H	-0.744650	0.511618	-1.422944		
H	-2.341792	0.510449	-2.184854		
S	-2.307914	1.938073	-0.266916		
H	-1.265874	1.896074	0.588701		
28					
Dimer 55 of the n...n type					
C	2.917466	0.881493	-0.473552		
C	3.483211	-0.529570	-0.264515		
N	2.984799	1.795047	0.669655		
H	2.908488	1.280818	1.544229		
H	3.853519	2.315242	0.683877		
H	3.475645	1.331970	-1.302134		
C	1.468008	0.833741	-0.989513		
O	1.064069	0.016552	-1.786512		
O	0.695460	1.809995	-0.514304		
H	1.274810	2.287917	0.134261		
H	3.313633	-1.126602	-1.159500		
H	4.556272	-0.464782	-0.083064		
S	2.799094	-1.412725	1.202679		
H	1.501928	-1.412266	0.820586		
C	-2.029744	0.116817	-0.804493		
C	-2.439208	1.173152	0.223835		
N	-3.092218	-0.446722	-1.640842		
H	-3.947636	-0.571521	-1.104746		
H	-3.300325	0.154326	-2.429155		
H	-1.289626	0.576301	-1.465542		
C	-1.253796	-1.033983	-0.152391		
O	-0.555601	-0.906717	0.830407		
O	-1.387243	-2.199758	-0.783059		
H	-2.061970	-2.025417	-1.486228		
H	-1.554212	1.551732	0.730696		
H	-2.932894	2.000350	-0.286795		
S	-3.652475	0.570081	1.477694		
H	-2.800680	-0.264508	2.107375		
28					
Dimer 56 of the n...n type					
C	-2.848339	-0.500460	0.865123		
C	-3.651234	0.468947	-0.011764		
N	-2.051530	0.066181	1.952125		
H	-1.535367	0.884463	1.635360		

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H	-2.629840	0.330179	2.740594
H	-3.570987	-1.193254	1.313435
C	-1.940603	-1.414244	0.022839
O	-2.189213	-1.769989	-1.105212
O	-0.851328	-1.825829	0.679306
H	-0.874411	-1.327049	1.535906
H	-4.161942	-0.088621	-0.796240
H	-4.398920	0.972864	0.601398
S	-2.658796	1.823571	-0.768554
H	-1.766396	1.040007	-1.406205
C	2.098193	-0.843395	-0.144104
C	3.213473	-0.492003	0.845137
N	2.510054	-1.167472	-1.511944
H	3.312272	-0.608876	-1.792464
H	2.756549	-2.145233	-1.606191
H	1.558326	-1.706762	0.257066
C	1.028225	0.258284	-0.197198
O	0.687324	0.913997	0.761713
O	0.472367	0.404229	-1.400110
H	0.972237	-0.225257	-1.981393
H	2.795051	-0.322168	1.836135
H	3.921067	-1.319438	0.899071
S	4.210982	0.982053	0.354958
H	3.226223	1.886144	0.534016
28			
Dimer 57 of the n...n type			
C	-3.134731	0.159019	-0.569502
C	-3.419406	-0.955682	0.441938
N	-2.628415	-0.245366	-1.882396
H	-1.968098	-1.012945	-1.801953
H	-3.379113	-0.544326	-2.493332
H	-4.081725	0.687101	-0.735109
C	-2.206400	1.239998	0.005190
O	-2.128671	1.517153	1.178855
O	-1.508557	1.892902	-0.931358
H	-1.670827	1.382379	-1.763934
H	-3.888102	-0.541988	1.333651
H	-4.101605	-1.677905	-0.006638
S	-1.937541	-1.925185	0.961716
H	-1.412597	-0.958890	1.741562
C	1.545718	-0.248678	0.435341
C	2.731444	-1.221478	0.480492
N	0.674673	-0.334227	-0.732064
H	1.224453	-0.436196	-1.581446
H	0.061860	-1.138440	-0.650947
H	0.930052	-0.455487	1.319282
C	2.007610	1.203044	0.635627
O	2.987144	1.506286	1.280763
O	1.227880	2.125515	0.072672
H	0.507491	1.663175	-0.412366
H	3.273140	-1.117330	1.419452
H	2.356533	-2.242231	0.401456
S	3.916115	-1.019654	-0.919599
H	4.399766	0.175469	-0.524304
28			
Dimer 58 of the n...n type			
C	1.221681	0.034866	-0.539585
C	1.350166	-0.853293	0.700567
N	1.472290	-0.596408	-1.835122
H	2.181178	-1.321126	-1.759632
H	0.626345	-1.009362	-2.210237
H	0.197622	0.415806	-0.555203
C	2.093136	1.296953	-0.419514
O	2.299258	1.876810	0.622388
O	2.582489	1.718976	-1.586393
H	2.301354	1.022618	-2.234671
H	1.069417	-0.291065	1.587781
H	0.681147	-1.707489	0.605438
S	3.032286	-1.572847	0.931073

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H	3.645647	-0.409214	1.228811
C	-2.819515	0.726652	0.296402
C	-3.333714	-0.521547	-0.425970
N	-2.242544	1.778817	-0.545191
H	-1.782506	1.387604	-1.362970
H	-2.950024	2.426768	-0.870078
H	-3.668344	1.160686	0.837130
C	-1.812352	0.367223	1.403719
O	-1.846920	-0.660172	2.041240
O	-0.892195	1.309110	1.618277
H	-1.051828	1.987258	0.915373
H	-3.827235	-1.189274	0.278201
H	-4.052089	-0.224465	-1.189785
S	-2.022501	-1.475963	-1.310110
H	-1.472923	-2.007561	-0.201188
28			
Dimer 59 of the n...n type			
C	2.522749	-1.265346	0.130265
C	3.255247	-0.175063	0.922946
N	2.871112	-1.396081	-1.286400
H	3.141674	-0.496089	-1.675825
H	3.635093	-2.045436	-1.427743
H	2.733054	-2.220958	0.623487
C	0.996881	-1.108117	0.253646
O	0.439700	-0.771161	1.275311
O	0.332879	-1.407784	-0.859787
H	1.045015	-1.603702	-1.524123
H	2.880361	-0.151868	1.945197
H	4.322174	-0.397530	0.943654
S	3.123429	1.509608	0.183250
H	1.777813	1.602665	0.226632
C	-2.563242	0.916828	-0.704100
C	-3.495741	0.181470	0.268614
N	-2.106161	0.187171	-1.886362
H	-1.882482	-0.776619	-1.650884
H	-2.807947	0.186378	-2.616652
H	-3.108259	1.802293	-1.052380
C	-1.341846	1.515806	0.018072
O	-1.372300	1.967013	1.138934
O	-0.244574	1.560547	-0.741366
H	-0.490433	1.075547	-1.569776
H	-3.675815	0.811945	1.138667
H	-4.448724	-0.014548	-0.223697
S	-2.892770	-1.472483	0.818098
H	-1.656649	-1.086102	1.209827
28			
Dimer 60 of the n...n type			
C	2.810986	0.234531	0.465050
C	3.076782	-0.776451	-0.658048
N	2.372868	-0.296388	1.752530
H	1.627213	-0.976492	1.631794
H	3.138445	-0.729208	2.254822
H	3.756062	0.766062	0.635130
C	1.843151	1.343383	0.025232
O	1.746326	1.736465	-1.116887
O	1.138340	1.878782	1.020965
H	1.321697	1.303323	1.802570
H	3.484940	-0.268561	-1.530901
H	3.808303	-1.505640	-0.308824
S	1.610686	-1.763210	-1.186245
H	1.023541	-0.778349	-1.892106
C	-2.008488	-0.774558	-0.561451
C	-1.545780	0.569386	-1.132032
N	-3.443110	-1.059229	-0.657615
H	-3.989483	-0.214786	-0.506002
H	-3.689117	-1.434099	-1.565944
H	-1.474459	-1.563567	-1.103730
C	-1.568195	-0.960986	0.898387
O	-0.534756	-0.525256	1.349990

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O -2.419498	-1.683377	1.628653	
H -3.188641	-1.845568	1.025855	
H -0.462787	0.643559	-1.118879	
H -1.886444	0.650918	-2.164333	
S -2.219047	2.037958	-0.243978	
H -1.337839	1.981017	0.775122	
28			
Dimer 61 of the n...n type			
C -2.619067	-0.930070	-0.466048	
C -2.436396	0.303486	-1.361942	
N -3.650095	-0.839724	0.570134	
H -3.793406	0.125340	0.857202	
H -4.536482	-1.213542	0.254640	
H -2.859383	-1.772302	-1.123433	
C -1.283745	-1.328757	0.188237	
O -0.224549	-1.322298	-0.400090	
O -1.392623	-1.700250	1.460140	
H -2.357978	-1.582164	1.665709	
H -1.602333	0.139039	-2.043405	
H -3.339733	0.462085	-1.950975	
S -2.188089	1.883500	-0.439186	
H -1.093136	1.509786	0.268396	
C 2.518008	0.745282	-0.531086	
C 2.396905	1.364469	0.866855	
N 1.444529	0.988499	-1.491667	
H 0.542051	0.775987	-1.080131	
H 1.435995	1.952275	-1.803755	
H 3.437001	1.159608	-0.965857	
C 2.801671	-0.764950	-0.479414	
O 3.319113	-1.324548	0.460338	
O 2.496281	-1.405692	-1.609130	
H 1.986964	-0.755216	-2.145915	
H 3.275593	1.099697	1.454252	
H 2.354763	2.450288	0.773965	
S 0.884926	0.911347	1.815787	
H 0.989622	-0.424313	1.674743	
28			
Dimer 62 of the n...n type			
C -2.669327	0.075374	0.729207	
C -3.034721	0.783545	-0.579680	
N -1.828536	0.824953	1.664936	
H -1.152779	1.401379	1.169030	
H -2.380148	1.425345	2.265719	
H -3.607520	-0.169794	1.240450	
C -2.014597	-1.292488	0.463742	
O -2.304256	-2.011888	-0.464352	
O -1.107921	-1.632731	1.382494	
H -1.042938	-0.833547	1.968007	
H -3.708367	0.162177	-1.167881	
H -3.534371	1.725221	-0.351934	
S -1.574995	1.228733	-1.616256	
H -1.252341	-0.038591	-1.942044	
C 2.669284	-0.074161	0.729375	
C 3.034796	-0.784380	-0.578354	
N 1.828522	-0.822326	1.666282	
H 1.152695	-1.399438	1.171270	
H 2.380172	-1.421895	2.267855	
H 3.607428	0.171895	1.240289	
C 2.014463	1.293223	0.461760	
O 2.303977	2.011129	-0.467534	
O 1.107865	1.634926	1.380052	
H 1.042953	0.836698	1.966851	
H 3.708459	-0.163919	-1.167499	
H 3.534509	-1.725649	-0.349069	
S 1.575203	-1.231351	-1.614320	
H 1.252305	0.035435	-1.941938	
28			
Dimer 63 of the n...n type			
C 2.658320	0.907971	0.296038	

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C 3.479933	-0.290912	0.784468	
N 1.454024	1.221670	1.066146	
H 1.029026	0.369366	1.419803	
H 1.660053	1.817986	1.858516	
H 3.314477	1.785313	0.321910	
C 2.281132	0.755770	-1.188394	
O 2.984376	0.210231	-2.006844	
O 1.104491	1.300777	-1.511164	
H 0.722072	1.642089	-0.665954	
H 4.381351	-0.402084	0.184224	
H 3.766122	-0.129799	1.823741	
S 2.557167	-1.890564	0.764617	
H 2.537239	-2.026286	-0.577237	
C -2.035835	-0.806580	0.575523	
C -2.005079	0.519645	1.345563	
N -0.882769	-1.120678	-0.266535	
H -0.537162	-0.296689	-0.750036	
H -0.117518	-1.529632	0.258043	
H -2.131447	-1.606642	1.318776	
C -3.314661	-0.922899	-0.275282	
O -4.383005	-0.455856	0.048896	
O -3.148023	-1.618007	-1.401086	
H -2.179414	-1.824358	-1.425550	
H -2.912098	0.622467	1.939342	
H -1.151036	0.534842	2.020946	
S -1.819691	2.012145	0.280801	
H -3.025637	1.916061	-0.316387	
28			
Dimer 64 of the n...n type			
C 1.596213	-0.229425	-0.044418	
C 2.498483	-0.604055	1.133730	
N 1.647323	-1.105512	-1.216553	
H 2.596012	-1.432238	-1.383158	
H 1.045965	-1.913174	-1.100853	
H 0.566413	-0.215173	0.321550	
C 1.821468	1.221592	-0.495842	
O 2.146867	2.118304	0.248535	
O 1.596445	1.416647	-1.797265	
H 1.424425	0.510632	-2.157240	
H 2.333772	0.079563	1.965314	
H 2.261630	-1.617091	1.459774	
S 4.297486	-0.623365	0.720846	
H 4.413899	0.707818	0.539063	
C -2.993770	-0.100586	0.962784	
C -2.086226	-1.325203	0.799947	
N -4.358504	-0.222888	0.447147	
H -4.377825	-0.786726	-0.399223	
H -4.977849	-0.649939	1.125220	
H -3.057596	0.114846	2.035390	
C -2.347348	1.159551	0.358649	
O -1.154650	1.370571	0.365838	
O -3.223715	2.018384	-0.157334	
H -4.098483	1.558936	-0.078179	
H -1.128336	-1.150300	1.287611	
H -2.557740	-2.187602	1.271431	
S -1.806305	-1.823455	-0.954000	
H -1.177417	-0.694130	-1.337688	
28			
Dimer 65 of the n...n type			
C 3.208344	-0.304694	-0.844609	
C 1.723644	-0.660597	-0.711639	
N 4.166132	-1.351461	-0.477253	
H 3.808724	-1.916564	0.289134	
H 4.366267	-1.966468	-1.256566	
H 3.386783	-0.036844	-1.892108	
C 3.546493	0.975443	-0.057782	
O 2.797351	1.920915	0.040637	
O 4.762080	0.962811	0.490434	
H 5.114925	0.058870	0.286029	

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H	1.102631	0.164264	-1.054001		
H	1.505993	-1.539818	-1.317825		
S	1.218255	-1.102838	1.006181		
H	1.284821	0.149850	1.499688		
C	-2.340788	-0.463305	0.571778		
C	-3.698902	-0.982590	0.087672		
N	-2.360058	0.418687	1.741388		
H	-3.228457	0.944927	1.791732		
H	-2.248770	-0.098938	2.604333		
H	-1.720088	-1.331577	0.810072		
C	-1.580531	0.236384	-0.567821		
O	-1.538873	-0.184164	-1.702592		
O	-0.938660	1.341343	-0.191715		
H	-1.155003	1.430605	0.773388		
H	-3.560835	-1.649598	-0.761999		
H	-4.183453	-1.534422	0.893335		
S	-4.887170	0.350215	-0.381044		
H	-4.218162	0.766012	-1.476056		
28					
Dimer 66 of the n...n type					
C	-2.312119	-0.731052	0.196646		
C	-3.377704	-0.687360	-0.902951		
N	-2.782559	-1.010396	1.554967		
H	-3.709692	-0.621112	1.706984		
H	-2.821786	-2.005213	1.740046		
H	-1.587131	-1.505070	-0.074797		
C	-1.477513	0.560052	0.214413		
O	-1.149212	1.158169	-0.785847		
O	-1.112465	0.950511	1.435602		
H	-1.548112	0.296365	2.041078		
H	-2.908717	-0.518186	-1.871080		
H	-3.907709	-1.639503	-0.930217		
S	-4.678491	0.595287	-0.634905		
H	-3.876175	1.660334	-0.837818		
C	3.171253	-0.043905	-0.969486		
C	1.751662	-0.620213	-1.004404		
N	4.262905	-1.008030	-0.805466		
H	3.979195	-1.777761	-0.204200		
H	4.557479	-1.394159	-1.694189		
H	3.330798	0.487020	-1.914961		
C	3.305631	1.046492	0.109209		
O	2.424483	1.827618	0.387509		
O	4.502448	1.075158	0.697582		
H	4.988232	0.304222	0.307314		
H	1.023384	0.168879	-1.181607		
H	1.681479	-1.353944	-1.807595		
S	1.280136	-1.519673	0.537216		
H	1.120730	-0.418447	1.298239		
28					
Dimer 67 of the n...n type					
C	2.001090	-0.769141	-0.406507		
C	3.103360	-0.817907	0.655666		
N	2.432565	-0.741044	-1.805654		
H	3.280676	-0.189176	-1.910742		
H	2.617201	-1.672697	-2.157673		
H	1.373190	-1.656514	-0.269915		
C	1.036641	0.402854	-0.162326		
O	0.749796	0.820828	0.935960		
O	0.502498	0.895281	-1.281627		
H	0.973007	0.415430	-2.010250		
H	2.662447	-0.884254	1.649289		
H	3.727197	-1.695986	0.488169		
S	4.252836	0.624990	0.603634		
H	3.350631	1.540077	1.012700		
C	-3.123006	-0.004971	-0.438505		
C	-3.071252	-1.326881	0.336713		
N	-2.446732	0.034418	-1.733854		
H	-1.554867	-0.451692	-1.693406		
H	-3.010144	-0.392176	-2.459592		

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H	-4.182320	0.218474	-0.613169		
C	-2.639903	1.177286	0.421631		
O	-2.804445	1.241641	1.619634		
O	-2.073973	2.159430	-0.275688		
H	-1.976843	1.804737	-1.192502		
H	-3.626656	-1.233226	1.268844		
H	-3.525372	-2.115031	-0.264503		
S	-1.367644	-1.922508	0.709530		
H	-1.004651	-0.886177	1.492424		
28					
Dimer 68 of the n...n type					
C	2.756740	0.607552	-0.748556		
C	2.567870	1.523758	0.478407		
N	1.727886	0.823064	-1.746281		
H	0.800530	0.662833	-1.367043		
H	1.847460	0.200312	-2.537952		
H	3.727942	0.869466	-1.179147		
C	2.884473	-0.832881	-0.250164		
O	1.999388	-1.668490	-0.286187		
O	4.082079	-1.075757	0.282314		
H	4.105740	-1.980858	0.635105		
H	3.373704	1.361762	1.193238		
H	2.598995	2.560536	0.143328		
S	0.940928	1.357146	1.331624		
H	0.980365	0.031732	1.579723		
C	-2.856641	-1.063527	-0.237066		
C	-3.014282	0.185470	-1.119654		
N	-3.769166	-1.039103	0.895256		
H	-3.554439	-0.238640	1.484672		
H	-3.624199	-1.862275	1.471623		
H	-3.113494	-1.919238	-0.873522		
C	-1.387731	-1.277700	0.151433		
O	-0.998884	-1.426072	1.290515		
O	-0.588849	-1.294238	-0.918954		
H	0.352104	-1.455672	-0.654034		
H	-2.392093	0.101075	-2.008388		
H	-4.057115	0.269871	-1.425421		
S	-2.634420	1.780704	-0.269934		
H	-1.313116	1.566206	-0.079957		
28					
Dimer 69 of the n...n type					
C	-2.187292	0.620953	0.655598		
C	-3.116577	-0.542366	1.013347		
N	-2.792532	1.951335	0.568584		
H	-3.729540	1.897192	0.176330		
H	-2.856478	2.391897	1.478326		
H	-1.400148	0.665620	1.417043		
C	-1.415955	0.345892	-0.643043		
O	-1.060955	-0.753422	-1.000830		
O	-1.108350	1.451699	-1.326985		
H	-1.585515	2.177977	-0.849106		
H	-2.545172	-1.465897	1.095354		
H	-3.596669	-0.339460	1.970643		
S	-4.492782	-0.791090	-0.190300		
H	-3.718463	-1.227927	-1.204406		
C	1.889036	0.187149	-0.434346		
C	3.303935	0.555797	-0.896488		
N	1.301867	1.044982	0.598486		
H	2.017079	1.382294	1.238363		
H	0.844421	1.848841	0.185575		
H	1.237289	0.222912	-1.311454		
C	1.828300	-1.277447	0.031724		
O	2.395668	-2.180984	-0.540633		
O	1.093742	-1.475698	1.126084		
H	0.764083	-0.576383	1.370038		
H	3.623049	-0.111331	-1.695733		
S	3.304164	1.579478	-1.271488		
H	4.564584	0.523698	0.451701		
H	4.558189	-0.813800	0.626778		

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28		
Dimer 70 of the n...n type		
C	1.970457 -0.354905 0.803018	
C	2.592857 1.038164 0.652406	
N	2.771507 -1.361818 1.499682	
H	3.760882 -1.238907 1.297967	
H	2.644075 -1.313602 2.503208	
H	1.032302 -0.233986 1.357142	
C	1.538744 -0.926294 -0.558410	
O	1.089236 -0.246006 -1.456032	
O	1.651590 -2.247025 -0.649125	
H	2.080670 -2.517763 0.204114	
H	1.893738 1.716081 0.165573	
H	2.830247 1.432538 1.640345	
S	4.181701 1.045181 -0.283524	
H	3.643175 0.740193 -1.481951	
C	-1.802863 -0.391640 -0.167188	
C	-1.356569 0.987664 0.330906	
N	-1.951802 -0.543199 -1.614851	
H	-2.361007 0.298054 -2.015418	
H	-1.043037 -0.677484 -2.046251	
H	-1.055147 -1.121346 0.164342	
C	-3.096258 -0.854576 0.522583	
O	-3.380194 -0.586939 1.668162	
O	-3.872588 -1.614508 -0.251397	
H	-3.418427 -1.619202 -1.131762	
H	-1.197512 0.972097 1.408345	
H	-0.424404 1.248138 -0.167697	
S	-2.531321 2.346466 -0.081436	
H	-3.512137 1.949310 0.754842	
28		
Dimer 71 of the n...n type		
C	3.277871 -0.078002 -0.459018	
C	3.035813 1.433691 -0.389451	
N	2.629597 -0.805014 -1.550978	
H	1.689822 -0.454422 -1.716184	
H	3.152471 -0.722954 -2.414739	
H	4.359706 -0.223647 -0.563471	
C	2.938043 -0.772269 0.872065	
O	3.047796 -0.240993 1.954136	
O	2.551020 -2.040010 0.733303	
H	2.461748 -2.172594 -0.242649	
H	3.615920 1.869386 0.422661	
H	3.347572 1.891320 -1.328441	
S	1.265214 1.902777 -0.175354	
H	1.145379 1.423833 1.079132	
C	-2.689714 0.686356 -0.483453	
C	-1.634786 -0.153747 -1.211845	
N	-2.203740 1.565672 0.582833	
H	-1.450272 1.120843 1.100759	
H	-1.862371 2.446204 0.216986	
H	-3.184099 1.313479 -1.233835	
C	-3.815959 -0.199435 0.078731	
O	-4.225708 -1.194665 -0.474551	
O	-4.328467 0.244272 1.227520	
H	-3.776504 1.032914 1.459834	
H	-2.101118 -0.740776 -2.001309	
H	-0.889867 0.508220 -1.651101	
S	-0.691636 -1.283628 -0.099457	
H	-1.691356 -2.171192 0.080931	
28		
Dimer 72 of the n...n type		
C	2.357116 -0.214442 -0.721596	
C	3.694630 -0.896328 -0.414264	
N	2.418099 1.004825 -1.530960	
H	3.283787 1.511787 -1.365347	
H	2.351929 0.801815 -2.520684	
H	1.728146 -0.939984 -1.245708	
C	1.579592 0.083786 0.571302	

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O	1.524173 -0.677147 1.511304	
O	0.939466 1.252546 0.560801	
H	1.172956 1.650943 -0.317451	
H	3.525776 -1.810960 0.152030	
H	4.194596 -1.147953 -1.349664	
S	4.884907 0.170288 0.510289	
H	4.191908 0.193770 1.667340	
C	-3.215511 -0.467491 0.767057	
C	-1.731757 -0.793089 0.567383	
N	-4.176966 -1.420670 0.205611	
H	-3.824932 -1.820928 -0.660628	
H	-4.369930 -2.179561 0.847982	
H	-3.392803 -0.406978 1.846904	
C	-3.551392 0.941306 0.244394	
O	-2.797086 1.884469 0.323442	
O	-4.771167 1.040584 -0.285703	
H	-5.128769 0.116253 -0.257327	
H	-1.109577 -0.051526 1.063126	
H	-1.514555 -1.773402 0.991079	
S	-1.225905 -0.894509 -1.203363	
H	-1.299653 0.429101 -1.449435	
28		
Dimer 73 of the n...n type		
C	-2.944950 -0.733070 -0.438123	
C	-3.474791 0.328388 0.531100	
N	-2.375814 -1.944189 0.159378	
H	-1.886336 -1.730752 1.024686	
H	-3.092129 -2.629147 0.368493	
H	-3.784353 -1.038989 -1.073393	
C	-1.919383 -0.144076 -1.422021	
O	-1.936025 1.000055 -1.814593	
O	-1.000599 -1.025218 -1.823832	
H	-1.194251 -1.842360 -1.297787	
H	-3.948001 1.139403 -0.020195	
H	-4.214716 -0.125666 1.189913	
S	-2.190572 1.051171 1.642732	
H	-1.593985 1.802339 0.696561	
C	1.404371 -0.360356 0.355202	
C	1.313663 0.743452 -0.702943	
N	1.304625 0.056854 1.755214	
H	1.739986 0.965913 1.892044	
H	0.335618 0.125485 2.046774	
H	0.589713 -1.062820 0.155635	
C	2.678005 -1.204148 0.174964	
O	3.158586 -1.474220 -0.902778	
O	3.194871 -1.643294 1.323014	
H	2.626000 -1.227725 2.021740	
H	1.350096 0.307511 -1.698558	
H	0.366990 1.271176 -0.601430	
S	2.620285 2.034654 -0.545503	
H	3.652111 1.244048 -0.905846	
28		
Dimer 74 of the n...n type		
C	-2.122182 0.093390 0.860262	
C	-3.062986 -1.066037 0.513068	
N	-2.691063 1.195843 1.636564	
H	-3.663941 1.352032 1.384266	
H	-2.646705 1.015199 2.632076	
H	-1.286890 -0.325417 1.433983	
C	-1.460146 0.670896 -0.400198	
O	-1.121845 -0.002878 -1.349284	
O	-1.226931 1.979290 -0.336288	
H	-1.640363 2.261995 0.521140	
H	-2.518685 -1.844079 -0.020236	
H	-3.467831 -1.487660 1.433031	
S	-4.526478 -0.559310 -0.489095	
H	-3.840931 -0.289143 -1.618760	
C	1.865937 0.375775 -0.196461	
C	1.504769 -0.963620 0.456923	

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N	1.905565	0.397015	-1.659415		
H	2.309376	-0.467088	-2.013989		
H	0.963673	0.471174	-2.030622		
H	1.119567	1.112344	0.120721		
C	3.188861	0.935191	0.349732		
O	3.563205	0.786939	1.491346		
C	3.882669	1.637667	-0.547409		
H	3.365737	1.545676	-1.387862		
H	1.412236	-0.847868	1.535963		
H	0.554179	-1.307650	0.050735		
S	2.705002	-2.316692	0.097217		
H	3.720373	-1.805214	0.822683		
28					
Dimer 75 of the n...n type					
C	-3.158494	0.674716	-0.374578		
C	-3.536053	-0.145117	0.864723		
N	-3.404580	0.040564	-1.672270		
H	-3.243673	-0.962627	-1.624917		
H	-4.353493	0.194074	-1.991195		
H	-3.734360	1.606341	-0.340270		
C	-1.688264	1.122864	-0.320595		
O	-1.108363	1.425008	0.697804		
O	-1.093332	1.151924	-1.515198		
H	-1.781725	0.809355	-2.142859		
H	-3.381990	0.440945	1.769245		
H	-4.588094	-0.422796	0.801941		
S	-2.600844	-1.730094	1.018894		
H	-1.472670	-1.178594	1.503067		
C	1.912488	-0.207489	-0.796862		
C	2.010683	1.254909	-0.347665		
N	0.833606	-0.992661	-0.186372		
H	0.572410	-0.585455	0.707192		
H	0.010189	-1.005463	-0.774282		
H	1.771873	-0.207206	-1.882819		
C	3.247211	-0.941997	-0.567065		
O	4.330557	-0.452090	-0.798810		
O	3.101269	-2.180658	-0.100067		
H	2.117112	-2.272533	0.021687		
H	2.833986	1.747997	-0.861883		
H	1.078741	1.763450	-0.578733		
S	2.231927	1.456674	1.472827		
H	3.504706	1.011126	1.519207		
28					
Dimer 76 of the n...n type					
C	-3.049040	-0.299067	-0.759167		
C	-2.159612	0.948406	-0.776916		
N	-4.451641	-0.099237	-0.385120		
H	-4.538118	0.637591	0.310644		
H	-5.020385	0.152591	-1.184397		
H	-3.026188	-0.728011	-1.767330		
C	-2.450614	-1.398922	0.136550		
O	-1.261839	-1.603001	0.245568		
O	-3.364897	-2.132282	0.769593		
H	-4.228955	-1.705928	0.533546		
H	-1.159581	0.698910	-1.125372		
H	-2.587098	1.685598	-1.456991		
S	-2.031070	1.802559	0.851261		
H	-1.370193	0.813565	1.484933		
C	2.689969	-0.112640	0.860669		
C	1.389629	0.564483	0.416080		
N	3.812739	0.774309	1.178731		
H	3.808115	1.592013	0.573790		
H	3.777232	1.092869	2.139440		
H	2.459836	-0.699673	1.757222		
C	3.159686	-1.155041	-0.170544		
O	2.407054	-1.848533	-0.816647		
O	4.486245	-1.246579	-0.273539		
H	4.829430	-0.533706	0.324288		
H	0.607485	-0.177847	0.267580		

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H	1.069710	1.266576	1.185312		
S	1.561001	1.572945	-1.119060		
H	1.759509	0.531728	-1.952992		
28					
Dimer 77 of the n...n type					
C	-2.838337	0.271316	-0.166823		
C	-2.779033	-1.204518	-0.573859		
N	-2.402513	1.251592	-1.163431		
H	-1.591951	0.908584	-1.674421		
H	-3.135439	1.455332	-1.832285		
H	-3.881910	0.496153	0.084266		
C	-2.073169	0.533787	1.142373		
O	-1.925910	-0.284342	2.019834		
O	-1.604798	1.782486	1.240939		
H	-1.812069	2.194976	0.364830		
H	-3.171125	-1.828315	0.228293		
H	-3.388391	-1.355503	-1.465025		
S	-1.090268	-1.793891	-1.017447		
H	-0.571702	-1.682045	0.220946		
C	2.838417	-0.271226	-0.166770		
C	2.778936	1.204628	-0.573772		
N	2.402820	-1.251563	-1.163405		
H	1.592162	-0.908735	-1.674372		
H	3.135782	-1.455127	-1.832275		
H	3.882010	-0.495888	0.084390		
C	2.073188	-0.533781	1.142367		
O	1.925668	0.284372	2.019775		
O	1.604982	-1.782518	1.240922		
H	1.812612	-2.195031	0.364931		
H	3.170883	1.828434	0.228440		
H	3.388353	1.355739	-1.464880		
S	1.090134	1.793808	-1.017464		
H	0.571249	1.681334	0.220748		
28					
Dimer 78 of the n...n type					
C	2.171064	0.521655	-0.706738		
C	1.686493	-0.924983	-0.832772		
N	3.591824	0.756215	-0.984288		
H	4.159637	-0.005130	-0.619946		
H	3.768004	0.830097	-1.979165		
H	1.581327	1.112327	-1.415208		
C	1.835565	1.143625	0.659391		
O	0.866969	0.853951	1.324843		
O	2.708283	2.077172	1.045483		
H	3.424433	2.044457	0.361452		
H	0.602749	-0.956092	-0.785936		
H	1.995951	-1.314146	-1.803214		
S	2.399029	-2.084050	0.410653		
H	1.772832	-1.550916	1.479337		
C	-2.171190	0.521623	0.706816		
C	-1.686471	-0.925016	0.832755		
N	-3.592002	0.755881	0.984204		
H	-4.159646	-0.005735	0.620181		
H	-3.768301	0.830318	1.979010		
H	-1.581628	1.112346	1.415408		
C	-1.835587	1.143756	-0.659241		
O	-0.866552	0.854645	-1.324303		
O	-2.708724	2.076740	-1.045689		
H	-3.424985	2.043700	-0.361751		
H	-0.602727	-0.956031	0.785996		
H	-1.996005	-1.314275	1.803131		
S	-2.398814	-2.084022	-0.410850		
H	-1.772880	-1.550478	-1.479484		
28					
Dimer 79 of the n...n type					
C	3.100540	-0.016920	0.702061		
C	3.161253	-1.262806	-0.187517		
N	2.384122	-0.156418	1.973037		
H	1.623782	-0.826633	1.892240		

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H	2.997341	-0.470687	2.715366		
H	4.133248	0.272619	0.927644		
C	2.530788	1.192737	-0.062714		
O	2.709895	1.384589	-1.243583		
O	1.841181	2.035456	0.706781		
H	1.806809	1.593248	1.592448		
H	3.754899	-1.061318	-1.077609		
H	3.622910	-2.079776	0.367007		
S	1.503494	-1.888092	-0.703591		
H	1.219255	-0.877065	-1.549425		
C	-2.135744	-0.440138	0.693921		
C	-1.088454	0.640906	0.408507		
N	-1.972403	-1.714823	-0.009522		
H	-1.641329	-1.556336	-0.958602		
H	-1.293332	-2.305995	0.454682		
H	-2.101213	-0.646146	1.770051		
C	-3.563299	0.079752	0.450509		
O	-3.907013	1.221535	0.657499		
O	-4.407564	-0.855475	0.012811		
H	-3.844500	-1.661051	-0.111626		
H	-1.280979	1.526434	1.011570		
H	-0.105966	0.252164	0.661147		
S	-0.971338	1.127769	-1.364064		
H	-2.209960	1.654376	-1.453704		
28					
Dimer 80 of the n...n type					
C	3.026002	0.979580	0.086458		
C	3.567433	-0.374627	-0.386600		
N	2.806258	1.129387	1.527398		
H	2.493387	0.254025	1.940190		
H	3.650339	1.418630	2.006644		
H	3.746195	1.745223	-0.224094		
C	1.728493	1.355174	-0.649996		
O	1.495174	1.061467	-1.800272		
O	0.872507	2.055927	0.096555		
H	1.293667	2.086693	0.993958		
H	3.731418	-0.358752	-1.462914		
H	4.517160	-0.572896	0.110135		
S	2.479495	-1.806373	0.030836		
H	1.526583	-1.545796	-0.884402		
C	-1.996504	0.545996	0.499802		
C	-0.911376	-0.452316	0.092913		
N	-2.572964	0.377157	1.836132		
H	-2.628830	-0.607644	2.084562		
H	-2.021048	0.849147	2.542123		
H	-1.538141	1.539202	0.446938		
C	-3.133918	0.584854	-0.533431		
O	-2.963892	0.453568	-1.724953		
O	-4.336719	0.806399	-0.000757		
H	-4.174447	0.819544	0.977037		
H	-0.522402	-0.193147	-0.889183		
H	-0.095566	-0.406463	0.812157		
S	-1.452074	-2.213551	0.079892		
H	-2.267461	-2.105654	-0.988960		
28					
Dimer 81 of the n...n type					
C	-2.110414	0.487177	0.632420		
C	-2.706474	-0.913977	0.794624		
N	-2.855398	1.597728	1.229279		
H	-3.857874	1.445650	1.147390		
H	-2.632578	1.710638	2.210864		
H	-1.116026	0.462368	1.090455		
C	-1.837007	0.811849	-0.844760		
O	-1.507449	-0.013551	-1.666602		
O	-1.954409	2.107222	-1.139264		
H	-2.289105	2.521506	-0.303647		
H	-2.035344	-1.652062	0.360390		
H	-2.828517	-1.131903	1.855900		
S	-4.384575	-1.103062	0.050812		

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H	-3.981610	-1.012424	-1.232968		
C	2.986331	0.385546	-0.677745		
C	1.485753	0.245962	-0.400658		
N	3.572496	-0.598911	-1.590975		
H	3.119318	-1.503512	-1.485869		
H	3.482683	-0.311624	-2.558007		
H	3.146634	1.381122	-1.106807		
C	3.797723	0.395869	0.630827		
O	3.410172	0.910817	1.655557		
O	4.987487	-0.196672	0.529632		
H	5.004054	-0.560875	-0.392522		
H	1.147223	1.060065	0.239693		
H	0.937143	0.286425	-1.340041		
S	1.012698	-1.363369	0.365937		
H	1.652480	-1.161282	1.536211		
28					
Dimer 82 of the n...n type					
C	2.198120	-1.261467	-0.446371		
C	3.401281	-0.312859	-0.450587		
N	1.233377	-1.102449	-1.537324		
H	1.137052	-0.120534	-1.785398		
H	1.525707	-1.605510	-2.366633		
H	2.593088	-2.283160	-0.497411		
C	1.446460	-1.226249	0.896285		
O	1.974634	-0.994539	1.959152		
O	0.151606	-1.530564	0.791992		
H	-0.023918	-1.598110	-0.178404		
H	4.058315	-0.540181	0.387509		
H	3.957620	-0.442293	-1.379046		
S	2.951382	1.474778	-0.391505		
H	2.423161	1.450105	0.848648		
C	-2.197997	1.261129	-0.447251		
C	-3.401116	0.312518	-0.451332		
N	-1.232802	1.101385	-1.537733		
H	-1.136595	0.119353	-1.785368		
H	-1.524596	1.604203	-2.367375		
H	-2.592957	2.282779	-0.499143		
C	-1.446758	1.226851	0.895695		
O	-1.975232	0.995743	1.958547		
O	-0.151958	1.531380	0.791552		
H	0.023694	1.598001	-0.178908		
H	-4.058477	0.540343	0.386373		
H	-3.957111	0.441333	-1.380079		
S	-2.951211	-1.475092	-0.390851		
H	-2.424089	-1.449555	0.849755		
28					
Dimer 83 of the n...n type					
C	-2.661274	0.135776	-0.949903		
C	-1.238423	0.607210	-0.631196		
N	-3.683939	1.181850	-1.046800		
H	-3.507642	1.927979	-0.378675		
H	-3.716155	1.589572	-1.973370		
H	-2.624267	-0.386116	-1.912874		
C	-3.139555	-0.934266	0.048686		
O	-2.421547	-1.789647	0.513063		
O	-4.440832	-0.857765	0.335156		
H	-4.755159	-0.054319	-0.152599		
H	-0.549169	-0.234233	-0.635966		
H	-0.921008	1.326579	-1.386173		
S	-1.094233	1.466974	0.997296		
H	-0.914267	0.347608	1.725135		
C	3.202238	-0.868443	0.105606		
C	3.489779	0.553498	0.603432		
N	3.469287	-1.123458	-1.312788		
H	3.303817	-0.287856	-1.868547		
H	4.423875	-1.423790	-1.467680		
H	3.819320	-1.553795	0.697032		
C	1.754502	-1.283941	0.421653		
O	1.185278	-1.005214	1.452526		

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O	1.179377	-2.002834	-0.543425		
H	1.864207	-2.040088	-1.261219		
H	3.263826	0.630983	1.665910		
H	4.545237	0.779528	0.451209		
S	2.559881	1.864956	-0.304300		
H	1.357751	1.643009	0.278768		
28					
Dimer 84 of the n...n type					
C	2.528236	0.262541	0.839039		
C	1.921754	-1.144596	0.781085		
N	1.763928	1.339392	0.209520		
H	1.319050	1.021886	-0.647494		
H	1.041555	1.708939	0.815299		
H	2.655899	0.517786	1.897302		
C	3.958432	0.273860	0.266806		
O	4.731438	-0.651589	0.369627		
O	4.285786	1.418356	-0.334347		
H	3.454068	1.956460	-0.315461		
H	2.576010	-1.854159	1.285157		
H	0.957460	-1.148806	1.289004		
S	1.595094	-1.746742	-0.932494		
H	2.889517	-1.908310	-1.274471		
C	-2.720304	-0.636635	-0.475525		
C	-1.419151	0.167193	-0.559468		
N	-3.727907	-0.365424	-1.502272		
H	-3.720101	0.616223	-1.768232		
H	-3.571958	-0.919302	-2.335659		
H	-2.449971	-1.696792	-0.539092		
C	-3.367235	-0.487724	0.913683		
O	-2.732890	-0.393958	1.940319		
O	-4.699771	-0.498022	0.889695		
H	-4.930550	-0.533884	-0.073393		
H	-0.749526	-0.137992	0.240578		
H	-0.932076	-0.022810	-1.515372		
S	-1.648432	1.993759	-0.464714		
H	-2.025010	2.024573	0.830349		
28					
Dimer 85 of the n...n type					
C	1.969319	-0.101051	0.776267		
C	1.904667	1.300973	0.159389		
N	3.001962	-0.330509	1.786916		
H	3.845691	0.194312	1.569542		
H	2.688424	-0.058380	2.710759		
H	0.998051	-0.302152	1.241160		
C	2.088365	-1.178217	-0.316208		
O	1.549363	-1.094097	-1.397536		
O	2.812115	-2.235181	0.045873		
H	3.158389	-2.002891	0.944937		
H	1.093191	1.352140	-0.563942		
H	1.725825	2.035261	0.944995		
S	3.465260	1.826242	-0.670638		
H	3.380845	0.955247	-1.697111		
C	-2.374163	0.768743	-0.529481		
C	-1.695174	-0.507644	-1.039959		
N	-1.671259	1.523863	0.510264		
H	-1.174449	0.904873	1.144919		
H	-1.016544	2.191643	0.124418		
H	-2.506600	1.430926	-1.392438		
C	-3.808793	0.481068	-0.045331		
O	-4.539724	-0.334361	-0.560603		
O	-4.190094	1.236636	0.984808		
H	-3.382411	1.760914	1.219682		
H	-2.310908	-0.971183	-1.809110		
H	-0.719460	-0.268977	-1.461613		
S	-1.342018	-1.748588	0.277887		
H	-2.625448	-1.984882	0.619160		
28					
Dimer 86 of the n...n type					
C	2.673546	0.757507	0.447680		

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C	2.295248	-0.276991	1.514784		
N	1.573585	1.430808	-0.243385		
H	0.806583	0.792228	-0.425087		
H	1.219218	2.222530	0.279074		
H	3.273328	1.527811	0.945835		
C	3.623340	0.151272	-0.601833		
O	4.455624	-0.688391	-0.344561		
O	3.468124	0.654952	-1.826662		
H	2.698498	1.271922	-1.752429		
H	3.192661	-0.654503	2.002143		
H	1.663513	0.193436	2.268575		
S	1.325771	-1.712334	0.876368		
H	2.313465	-2.235497	0.122470		
C	-2.053577	-0.666097	0.021800		
C	-1.711032	0.443314	1.024113		
N	-1.346478	-0.660659	-1.258345		
H	-1.227168	0.284262	-1.614529		
H	-0.439720	-1.107074	-1.183761		
H	-1.831761	-1.619503	0.514817		
C	-3.568787	-0.715942	-0.250567		
O	-4.410406	-0.433588	0.571509		
O	-3.879562	-1.133926	-1.478572		
H	-3.008752	-1.232781	-1.938409		
H	-2.338530	0.350033	1.908853		
H	-0.671736	0.351832	1.333184		
S	-1.866834	2.149118	0.346280		
H	-3.205021	2.124969	0.179438		
28					
Dimer 87 of the n...n type					
C	-2.535191	-0.759502	0.858359		
C	-3.519630	0.415283	0.835321		
N	-1.286254	-0.567801	1.600504		
H	-0.923038	0.368523	1.433831		
H	-1.431135	-0.677107	2.597530		
H	-3.061104	-1.606977	1.314861		
C	-2.201292	-1.258259	-0.557238		
O	-2.923894	-1.121680	-1.515740		
O	-1.038924	-1.918453	-0.630734		
H	-0.626749	-1.805539	0.256451		
H	-4.410640	0.138620	0.273219		
H	-3.812396	0.655452	1.857777		
S	-2.832776	1.979810	0.146805		
H	-2.619556	1.511541	-1.099280		
C	2.722696	-0.810824	-0.111770		
C	1.839723	-0.512407	-1.329064		
N	2.040498	-1.253057	1.106244		
H	1.137976	-0.800434	1.225030		
H	1.903596	-2.256049	1.123476		
H	3.424486	-1.599321	-0.406671		
C	3.621771	0.391627	0.230998		
O	4.107156	1.124812	-0.600853		
O	3.844066	0.541337	1.537041		
H	3.289452	-0.160793	1.963859		
H	2.460461	-0.259583	-2.187239		
H	1.243043	-1.391499	-1.569444		
S	0.615017	0.838447	-1.054638		
H	1.511789	1.843400	-0.985349		
28					
Dimer 88 of the n...n type					
C	3.139650	0.045431	-0.755270		
C	3.179622	1.227052	0.236259		
N	2.256319	0.306643	-1.873802		
H	1.283675	0.348581	-1.579279		
H	2.322887	-0.439609	-2.558372		
H	4.162381	-0.066925	-1.129026		
C	2.823961	-1.237731	0.014182		
O	1.748085	-1.805387	0.017330		
O	3.871078	-1.669610	0.722447		
H	3.616823	-2.456965	1.231753		

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H	3.901977	1.032331	1.028241		
H	3.491773	2.116490	-0.311013		
S	1.559506	1.685766	0.990718		
H	1.397611	0.580495	1.745293		
C	-2.359576	0.907220	0.336324		
C	-3.372258	-0.003240	1.044870		
N	-3.015992	1.823030	-0.584359		
H	-3.484268	1.290166	-1.313358		
H	-2.319438	2.391623	-1.056249		
H	-1.868032	1.496997	1.120845		
C	-1.228522	0.094823	-0.301999		
O	-0.822194	0.272885	-1.431089		
O	-0.723909	-0.810539	0.537670		
H	0.096235	-1.208071	0.163750		
H	-2.891724	-0.562681	1.844446		
H	-4.163118	0.613887	1.470660		
S	-4.230667	-1.194319	-0.077837		
H	-3.172242	-2.007313	-0.273743		
28					
Dimer 89 of the n...n type					
C	-2.665482	0.022507	0.849421		
C	-1.614620	0.750579	0.004159		
N	-2.387749	-1.375322	1.183566		
H	-1.943748	-1.855051	0.404485		
H	-1.780888	-1.454239	1.990646		
H	-2.763415	0.577045	1.789762		
C	-4.060283	0.113749	0.204628		
O	-4.445323	1.070474	-0.428390		
O	-4.827529	-0.953583	0.429678		
H	-4.242320	-1.585985	0.917039		
H	-1.900750	1.790467	-0.143909		
H	-0.661258	0.723876	0.529987		
S	-1.303815	-0.025845	-1.638826		
H	-2.506774	0.268365	-2.172396		
C	2.456735	-0.377587	-0.684449		
C	2.112613	1.115275	-0.608851		
N	1.535851	-1.310500	-0.032862		
H	1.132778	-0.912579	0.810659		
H	0.788756	-1.608389	-0.647001		
H	2.506275	-0.642993	-1.746403		
C	3.881109	-0.638993	-0.155618		
O	4.803773	0.129659	-0.305755		
O	4.016333	-1.810649	0.465135		
H	3.100072	-2.188852	0.480933		
H	2.877977	1.695239	-1.121924		
H	1.156412	1.298211	-1.097380		
S	1.925568	1.757414	1.109822		
H	3.213674	1.590133	1.473554		
28					
Dimer 90 of the n...n type					
C	2.916450	-0.063243	0.957015		
C	3.194033	-1.259249	0.040953		
N	1.878481	-0.244543	1.976068		
H	1.150267	-0.872579	1.647290		
H	2.258526	-0.633544	2.830601		
H	3.854090	0.172863	1.473188		
C	2.604913	1.209970	0.148434		
O	3.088712	1.455730	-0.932773		
O	1.767372	2.044003	0.766534		
H	1.482080	1.554447	1.578732		
H	4.012675	-1.029379	-0.638912		
H	3.472258	-2.120684	0.648146		
S	1.734526	-1.805655	-0.948621		
H	1.699370	-0.736602	-1.770277		
C	-1.904719	-0.522201	0.467363		
C	-1.034543	0.660163	0.030210		
N	-1.889343	-1.699007	-0.404959		
H	-1.842085	-1.415220	-1.381214		
H	-1.078251	-2.276876	-0.218165		

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H	-1.554406	-0.836129	1.457913		
C	-3.362934	-0.091743	0.699777		
O	-3.681397	0.989197	1.141171		
O	-4.255752	-1.034322	0.394702		
H	-3.717003	-1.775034	0.016938		
H	-1.066027	1.455062	0.772753		
H	-0.010083	0.317081	-0.075282		
S	-1.469360	1.349001	-1.620455		
H	-2.658725	1.868856	-1.253831		
28					
Dimer 91 of the n...n type					
C	-2.202537	-0.516114	-0.618800		
C	-3.706907	-0.420709	-0.930728		
N	-1.916978	-1.609313	0.289185		
H	-2.253835	-1.395736	1.223165		
H	-0.917418	-1.760979	0.346065		
H	-1.689853	-0.710580	-1.566187		
C	-1.677557	0.841165	-0.147094		
O	-1.090149	1.039402	0.899286		
O	-1.957584	1.820509	-1.011679		
H	-1.601951	2.659458	-0.675322		
H	-3.895364	0.311791	-1.713204		
H	-4.048238	-1.397977	-1.270267		
S	-4.760903	-0.016705	0.531770		
H	-4.424839	1.287229	0.614493		
C	3.084286	-1.150903	0.238057		
C	3.984630	-0.022874	0.768532		
N	3.550111	-1.642752	-1.048869		
H	3.485414	-0.897938	-1.738478		
H	2.939241	-2.384263	-1.377507		
H	3.146432	-1.966115	0.968708		
C	1.619228	-0.701301	0.234468		
O	0.898747	-0.734274	-0.741977		
O	1.221734	-0.266136	1.434345		
H	0.308230	0.100551	1.364191		
H	3.720685	0.225833	1.794226		
H	5.021272	-0.357923	0.739569		
S	3.941387	1.522228	-0.245279		
H	2.701700	1.911123	0.118074		
28					
Dimer 92 of the n...n type					
C	2.764253	0.271164	0.940336		
C	1.451737	0.417180	0.163517		
N	3.585502	1.476980	1.068176		
H	3.512692	2.054966	0.234393		
H	3.309894	2.036418	1.866143		
H	2.507775	-0.071859	1.949150		
C	3.629124	-0.862234	0.358305		
O	3.172773	-1.886001	-0.098468		
O	4.939223	-0.625923	0.425335		
H	5.006795	0.293365	0.790133		
H	0.910109	-0.526782	0.165088		
H	0.838021	1.182351	0.636381		
S	1.667015	0.972843	-1.580698		
H	2.266035	-0.154470	-2.016078		
C	-2.101164	0.260783	0.562202		
C	-3.468109	0.305880	1.256941		
N	-1.789678	1.365505	-0.343746		
H	-2.618486	1.649632	-0.860547		
H	-1.444611	2.175212	0.157517		
H	-1.339381	0.245606	1.349811		
C	-1.903452	-1.070548	-0.184266		
O	-2.334382	-2.129220	0.213422		
O	-1.181596	-0.969880	-1.300786		
H	-0.984711	-0.006656	-1.409831		
H	-3.570451	-0.534304	1.941970		
H	-3.552332	1.234009	1.822467		
S	-4.896591	0.305162	0.088939		
H	-4.741377	-0.968122	-0.327697		

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28		
Dimer 93 of the n...n type		
C -2.726720	-0.511310	0.688968
C -1.955138	0.772893	1.015515
N -2.027179	-1.506120	-0.125252
H -1.424452	-1.056751	-0.810043
H -1.455934	-2.124207	0.437900
H -2.994633	-0.982035	1.641607
C -4.078790	-0.188737	0.025181
O -4.754405	0.773656	0.312331
O -4.457040	-1.085761	-0.885407
H -3.695160	-1.717315	-0.942364
H -2.560552	1.424976	1.642973
H -1.042641	0.522326	1.554940
S -1.411349	1.712922	-0.474310
H -2.641740	2.115808	-0.851759
C 2.726591	0.511335	0.688856
C 1.954996	-0.772843	1.015416
N 2.027067	1.506053	-0.125540
H 1.424552	1.056497	-0.810398
H 1.455540	2.123994	0.437482
H 2.994306	0.982171	1.641497
C 4.078756	0.188846	0.025250
O 4.754359	-0.773552	0.312464
O 4.457099	1.085925	-0.885211
H 3.695122	1.717423	-0.942190
H 2.560268	-1.424805	1.643146
H 1.042440	-0.522089	1.554671
S 1.411556	-1.713099	-0.474374
H 2.642060	-2.115940	-0.851505
28		
Dimer 94 of the n...n type		
C -2.659150	-1.023362	0.562543
C -3.532048	0.232359	0.649624
N -1.539361	-1.110222	1.506038
H -1.167699	-0.184643	1.703017
H -1.826338	-1.519635	2.387197
H -3.312291	-1.885838	0.739017
C -2.124365	-1.246046	-0.863284
O -2.706862	-0.903579	-1.865836
O -0.957023	-1.894285	-0.899584
H -0.689675	-1.977548	0.048192
H -4.348531	0.169553	-0.067957
H -3.951242	0.310517	1.652755
S -2.613650	1.808428	0.373543
H -2.373399	1.607833	-0.938202
C 1.801445	-0.153493	0.692431
C 0.992221	0.677359	-0.309115
N 2.385208	0.573692	1.822510
H 2.663412	1.511623	1.544056
H 1.733561	0.653939	2.593759
H 1.132282	-0.918518	1.101272
C 2.909738	-0.952014	-0.015659
O 2.783532	-1.443224	-1.114543
O 4.023405	-1.081421	0.706214
H 3.852206	-0.545434	1.522328
H 0.575998	0.034477	-1.081006
H 0.172541	1.174424	0.208358
S 1.951475	2.032983	-1.108967
H 2.741566	1.233650	-1.855071
28		
Dimer 95 of the n...n type		
C 2.544624	0.503242	0.834202
C 1.971706	-0.872164	1.196956
N 1.661782	1.413696	0.105660
H 1.140464	0.910356	-0.608096
H 0.994741	1.865376	0.720417
H 2.829982	0.993401	1.772163
C 3.865655	0.369878	0.055377

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O 4.657920	-0.528751	0.223903
O 4.081381	1.360161	-0.812626
H 3.259804	1.909551	-0.782392
H 2.720249	-1.463834	1.721587
H 1.112285	-0.742954	1.855318
S 1.354347	-1.827223	-0.255390
H 2.560524	-2.021669	-0.826256
C -1.849642	-0.003886	0.468671
C -3.148104	-0.711009	0.874102
N -1.659960	1.356713	0.978953
H -2.549490	1.848410	1.029689
H -1.257078	1.350626	1.908675
H -1.023802	-0.621494	0.833503
C -1.676228	0.003725	-1.060336
O -1.987117	-0.920271	-1.773733
O -1.125321	1.125564	-1.534689
H -1.055997	1.720750	-0.746238
H -3.157393	-1.727249	0.483094
H -3.210424	-0.751254	1.961624
S -4.674541	0.164112	0.320599
H -4.516471	-0.085438	-0.995402
28		
Dimer 96 of the n...n type		
C -3.216806	0.391601	0.458738
C -2.940295	-1.083130	0.809593
N -4.144838	0.501004	-0.656351
H -3.710744	0.116559	-1.491822
H -4.332811	1.478252	-0.858098
H -3.674388	0.844342	1.344908
C -1.889999	1.117774	0.229158
O -1.518557	1.541218	-0.843572
O -1.168147	1.211945	1.355862
H -0.295803	1.610197	1.138559
H -2.330411	-1.147608	1.710010
H -3.894233	-1.576701	0.993961
S -2.105854	-2.042510	-0.531890
H -0.842305	-1.603693	-0.234863
C 1.912501	-0.789500	-0.399760
C 1.617942	0.543614	-1.108775
N 0.906251	-1.113661	0.597012
H 0.879047	-0.410903	1.329329
H 1.132271	-1.992639	1.052925
H 1.884024	-1.556966	-1.180656
C 3.340621	-0.784656	0.152629
O 3.623614	-0.821455	1.326639
O 4.248672	-0.708602	-0.836081
H 5.139586	-0.680068	-0.451506
H 2.325272	0.691588	-1.922409
H 0.604399	0.520418	-1.507106
S 1.639485	2.043546	-0.028535
H 2.819662	1.820170	0.586652
28		
Dimer 97 of the n...n type		
C 2.039467	-0.286786	0.624632
C 1.514795	0.596425	-0.512439
N 2.300174	0.382409	1.900435
H 2.638093	1.330032	1.751579
H 1.469080	0.429036	2.477436
H 1.289184	-1.065670	0.798630
C 3.299408	-1.056829	0.194187
O 3.471948	-1.487303	-0.923920
O 4.181545	-1.235828	1.177661
H 3.799649	-0.739419	1.945814
H 1.305975	-0.009351	-1.392970
H 0.594527	1.080926	-0.190117
S 2.646876	1.971936	-0.985224
H 3.605581	1.190018	-1.522334
C -2.804434	0.814388	-0.238718
C -2.033587	0.038783	-1.313896

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N	-2.045728	1.253840	0.933098	
H	-1.366986	0.552125	1.215832	
H	-1.564789	2.130099	0.771883	
H	-3.222031	1.706201	-0.719621	
C	-4.038141	0.024525	0.237612	
O	-4.690567	-0.697534	-0.481375	
O	-4.347724	0.229582	1.518519	
H	-3.624142	0.810171	1.863040	
H	-2.699667	-0.221982	-2.134655	
H	-1.228849	0.660377	-1.704979	
S	-1.222036	-1.496011	-0.691257	
H	-2.360877	-2.175452	-0.445928	
28				
Dimer 98 of the n...n type				
C	2.203107	0.287475	-1.091420	
C	3.049812	1.351623	-0.372002	
N	0.790077	0.616847	-1.050650	
H	0.460333	0.585369	-0.089295	
H	0.255175	-0.060439	-1.583300	
H	2.536110	0.276556	-2.135761	
C	2.519672	-1.109431	-0.546060	
O	1.693599	-1.900678	-0.133025	
O	3.826694	-1.378623	-0.569682	
H	3.982308	-2.272465	-0.222281	
H	4.111057	1.163556	-0.520911	
H	2.801478	2.326640	-0.790020	
S	2.712989	1.493408	1.437545	
H	3.336674	0.354758	1.804201	
C	-3.111727	-0.860134	0.411089	
C	-3.367849	-0.151774	-0.935021	
N	-3.831964	-0.212548	1.495186	
H	-3.449239	0.716691	1.648941	
H	-3.695856	-0.726584	2.360097	
H	-3.489777	-1.880895	0.294508	
C	-1.603098	-0.969995	0.640356	
O	-0.990370	-0.316637	1.459880	
O	-1.029545	-1.829623	-0.205286	
H	-0.046987	-1.832869	-0.087888	
H	-2.867499	-0.681860	-1.744309	
H	-4.441106	-0.154112	-1.125251	
S	-2.887389	1.631964	-0.993696	
H	-1.551573	1.467504	-1.078805	
28				
Dimer 99 of the n...n type				
C	2.043172	-0.039342	0.887842	
C	3.580748	0.025222	0.939549	
N	1.557148	-1.404079	0.960815	
H	1.807536	-1.912361	0.117687	
H	0.544792	-1.397689	1.031251	
H	1.674828	0.506288	1.761653	
C	1.541613	0.736849	-0.331601	
O	0.988583	0.247502	-1.290695	
O	1.798062	2.051842	-0.222185	
H	1.480162	2.505814	-1.019405	
H	3.918673	1.059413	0.983864	
H	3.917404	-0.495095	1.836007	
S	4.435185	-0.827516	-0.458163	
H	4.108061	0.061592	-1.418426	
C	-2.043726	-0.037851	-0.888131	
C	-3.581343	0.027219	-0.938738	
N	-1.558057	-1.402544	-0.963173	
H	-1.807883	-1.911929	-0.120556	
H	-0.545765	-1.396134	-1.034401	
H	-1.675816	0.508892	-1.761405	
C	-1.541359	0.736615	0.332122	
O	-0.989704	0.245647	1.291191	
O	-1.795492	2.052115	0.223536	
H	-1.477266	2.504928	1.021288	
H	-3.918925	1.061614	-0.981022	

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H	-3.918647	-0.491391	-1.835945	
S	-4.435175	-0.827859	0.457867	
H	-4.107166	0.059298	1.419630	
28				
Dimer 100 of the n...n type				
C	2.607758	-1.008033	0.628522	
C	2.716637	0.496683	0.953577	
N	3.773953	-1.491156	-0.098002	
H	3.810851	-1.060902	-1.017890	
H	3.706389	-2.494204	-0.240732	
H	2.555693	-1.527398	1.588709	
C	1.279001	-1.244208	-0.091457	
O	1.123104	-1.086400	-1.286805	
O	0.304425	-1.598082	0.746941	
H	-0.561425	-1.653559	0.268024	
H	1.801214	0.840347	1.437330	
H	3.552825	0.646737	1.637248	
S	3.092428	1.600592	-0.478201	
H	2.053436	1.231929	-1.253281	
C	-2.987533	0.315602	0.737195	
C	-2.499465	1.661140	0.161641	
N	-2.268746	-0.041323	1.943714	
H	-1.268818	-0.089572	1.775797	
H	-2.567042	-0.944391	2.296221	
H	-4.046150	0.451774	0.979519	
C	-2.939125	-0.732310	-0.376331	
O	-2.093518	-1.601253	-0.486260	
O	-3.926548	-0.572714	-1.258547	
H	-3.833234	-1.223034	-1.974448	
H	-3.074419	1.921591	-0.725972	
H	-2.650321	2.432775	0.916608	
S	-0.697074	1.735147	-0.225130	
H	-0.664446	0.757770	-1.155314	
28				
Dimer 101 of the n...n type				
C	3.057171	-0.899698	0.035075	
C	3.251018	0.395948	0.841032	
N	3.658927	-0.793219	-1.285209	
H	3.157484	-0.095589	-1.829875	
H	3.551540	-1.669602	-1.786506	
H	3.577739	-1.687184	0.593349	
C	1.584232	-1.318952	0.003174	
O	0.962244	-1.558037	-1.007617	
O	1.050610	-1.382473	1.232549	
H	0.101056	-1.616231	1.171895	
H	2.910241	0.268430	1.866092	
H	4.313649	0.636347	0.850989	
S	2.411252	1.882578	0.124043	
H	1.230466	1.740205	0.754790	
C	-2.063102	-0.383525	-0.856000	
C	-1.116833	0.760166	-0.453456	
N	-3.023980	0.044883	-1.855284	
H	-3.652827	0.737826	-1.458565	
H	-3.599010	-0.737496	-2.150735	
H	-1.418569	-1.159261	-1.280324	
C	-2.701483	-0.992837	0.392771	
O	-3.873661	-0.970510	0.666339	
O	-1.773626	-1.577829	1.199361	
H	-2.210322	-1.934779	1.990041	
H	-0.375300	0.401022	0.249342	
H	-0.598042	1.114629	-1.342779	
S	-1.921741	2.248323	0.275797	
H	-2.255457	1.689795	1.457663	
28				
Dimer 102 of the n...n type				
C	2.583299	0.027583	-0.808485	
C	2.978850	0.656193	0.535942	
N	2.070603	1.027902	-1.731858	
H	1.272860	1.497189	-1.310111	

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H	1.731542	0.582615	-2.578898		
H	3.501045	-0.402258	-1.231247		
C	1.641613	-1.169218	-0.616663		
O	0.692300	-1.412239	-1.329949		
O	1.994291	-1.933352	0.425538		
H	1.295707	-2.589301	0.585263		
H	3.496919	-0.069785	1.158189		
H	3.645190	1.497520	0.346634		
S	1.566148	1.360222	1.496775		
H	0.918567	0.196304	1.713969		
C	-2.583416	0.028112	0.808394		
C	-2.978665	0.656382	-0.536252		
N	-2.070646	1.028587	1.731566		
H	-1.272680	1.497499	1.309812		
H	-1.731868	0.583452	2.578803		
H	-3.501291	-0.401464	1.231145		
C	-1.641861	-1.168840	0.617016		
O	-0.692416	-1.411626	1.330154		
O	-1.994878	-1.933455	-0.424798		
H	-1.296372	-2.589531	-0.584328		
H	-3.496710	-0.069706	-1.158397		
H	-3.644937	1.497847	-0.347341		
S	-1.565673	1.359938	-1.497060		
H	-0.918578	0.195741	-1.714160		
28					
Dimer 103 of the n...n type					
C	3.106829	0.861876	-0.227892		
C	3.428445	-0.639677	-0.304517		
N	3.360646	1.391730	1.102911		
H	2.738644	0.939487	1.768899		
H	3.132041	2.380580	1.131454		
H	3.776700	1.361320	-0.938281		
C	1.682569	1.131145	-0.728464		
O	0.861579	1.787180	-0.128548		
O	1.444203	0.540818	-1.908663		
H	0.492807	0.591606	-2.098846		
H	3.406103	-0.982342	-1.336614		
H	4.425214	-0.806118	0.102998		
S	2.297487	-1.711430	0.691491		
H	1.212812	-1.559537	-0.098262		
C	-2.097251	-0.707563	0.986380		
C	-3.360965	0.172450	0.930291		
N	-0.984929	-0.001794	1.592284		
H	-0.657339	0.736019	0.974451		
H	-0.195861	-0.625312	1.726182		
H	-2.353125	-1.573075	1.607992		
C	-1.798086	-1.262960	-0.410062		
O	-0.781529	-1.059210	-1.036308		
O	-2.816863	-1.999484	-0.882670		
H	-2.594431	-2.318653	-1.772277		
H	-4.218078	-0.406707	0.591464		
H	-3.561478	0.548490	1.933178		
S	-3.199744	1.677373	-0.126875		
H	-3.226293	1.043545	-1.317471		
28					
Dimer 104 of the n...n type					
C	-1.654586	-0.585819	-0.260549		
C	-1.178318	0.401729	0.815176		
N	-1.173970	-0.207295	-1.580054		
H	-1.520311	0.717500	-1.821502		
H	-1.539369	-0.844350	-2.281211		
H	-1.207884	-1.549312	0.008128		
C	-3.171378	-0.772187	-0.194425		
O	-3.932554	-0.599728	-1.117438		
O	-3.570489	-1.160052	1.033026		
H	-4.534890	-1.268617	1.032817		
H	-1.464482	0.054311	1.805377		
H	-0.096472	0.463365	0.762890		
S	-1.760504	2.136785	0.586720		

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H	-3.050596	1.923888	0.919882		
C	2.701443	-0.937309	-0.608401		
C	3.304100	0.473344	-0.690072		
N	1.751254	-1.180616	-1.678148		
H	0.897498	-0.628246	-1.554247		
H	1.451536	-2.150409	-1.654232		
H	3.544843	-1.631423	-0.722787		
C	2.141049	-1.235481	0.788448		
O	1.081204	-1.775378	1.003730		
O	2.979239	-0.840173	1.767330		
H	2.592222	-1.072787	2.626644		
H	4.147724	0.574608	-0.010413		
H	3.652455	0.638227	-1.709242		
S	2.114223	1.845174	-0.348158		
H	2.114183	1.714266	0.994078		
28					
Dimer 105 of the n...n type					
C	-3.158745	-0.538295	-0.488303		
C	-3.125631	0.982707	-0.715347		
N	-3.978198	-0.884058	0.661824		
H	-3.556562	-0.501677	1.504779		
H	-3.994307	-1.891583	0.786066		
H	-3.609906	-0.975894	-1.386532		
C	-1.733562	-1.095591	-0.418495		
O	-1.294586	-1.743265	0.506079		
O	-1.010248	-0.765001	-1.498740		
H	-0.109471	-1.142897	-1.413186		
H	-2.635207	1.221024	-1.656941		
H	-4.149791	1.353657	-0.745398		
S	-2.299888	1.932421	0.638299		
H	-1.037898	1.606256	0.303763		
C	1.583185	-0.002806	0.814202		
C	1.601498	1.150620	-0.202789		
N	2.232309	0.382751	2.054839		
H	3.216445	0.572071	1.882075		
H	2.198606	-0.382248	2.721220		
H	0.532606	-0.230523	1.029110		
C	2.148960	-1.292320	0.209617		
O	2.958192	-2.011839	0.732470		
O	1.621395	-1.554033	-1.018332		
H	1.985275	-2.388454	-1.357565		
H	0.947426	0.946618	-1.048006		
H	1.252842	2.053076	0.299393		
S	3.279841	1.575928	-0.841510		
H	3.409656	0.503348	-1.649153		
28					
Dimer 106 of the n...n type					
C	1.848766	-0.172267	0.881311		
C	1.417445	1.067340	0.078347		
N	2.662889	0.201883	2.024091		
H	3.541056	0.603239	1.705186		
H	2.902132	-0.620343	2.568903		
H	0.927740	-0.647372	1.236744		
C	2.518403	-1.204698	-0.027952		
O	3.607498	-1.687259	0.138223		
O	1.726504	-1.536637	-1.085606		
H	2.174683	-2.200837	-1.634654		
H	0.670978	0.813480	-0.671581		
H	0.987291	1.784946	0.776839		
S	2.798089	1.969058	-0.748638		
H	3.003446	1.070924	-1.734275		
C	-3.146408	-0.756517	-0.385773		
C	-3.232392	0.721671	-0.807846		
N	-3.965354	-1.023445	0.784562		
H	-3.602033	-0.505067	1.580235		
H	-3.908286	-2.006006	1.033312		
H	-3.535914	-1.338089	-1.228842		
C	-1.680204	-1.170574	-0.227755		
O	-1.182966	-1.554396	0.808303		

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O	-1.001033 -1.040915 -1.375377	
H	-0.067465 -1.313850 -1.247669	
H	-2.690775 0.885359 -1.737698	
H	-4.280451 0.979544 -0.959110	
S	-2.625887 1.921251 0.459201	
H	-1.314054 1.643981 0.336694	
28		
Dimer 107 of the n...n type		
C	-3.154172 0.939437 0.744346	
C	-4.184497 -0.183516 0.944742	
N	-3.711749 2.040654 -0.025479	
H	-3.952043 1.712171 -0.957667	
H	-3.009257 2.762377 -0.154174	
H	-2.898890 1.307257 1.745641	
C	-1.847366 0.381473 0.164817	
O	-1.288193 0.833418 -0.810016	
O	-1.394444 -0.663883 0.868846	
H	-0.548726 -0.988131 0.475904	
H	-3.811745 -0.924034 1.649125	
H	-5.103510 0.249900 1.338940	
S	-4.678881 -1.044571 -0.613692	
H	-3.517859 -1.706417 -0.797269	
C	3.288392 0.855296 -0.399598	
C	1.851984 0.431455 -0.061068	
N	3.556466 0.739648 -1.823323	
H	3.523967 -0.237665 -2.102011	
H	4.497210 1.061689 -2.027846	
H	3.369738 1.910196 -0.112883	
C	4.295373 0.105071 0.480915	
O	5.223979 -0.546858 0.066822	
O	4.017772 0.257958 1.790244	
H	4.675880 -0.227002 2.313489	
H	1.620103 0.644661 0.980568	
H	1.151735 0.972086 -0.694801	
S	1.490958 -1.353368 -0.385247	
H	2.125959 -1.852545 0.695527	
28		
Dimer 108 of the n...n type		
C	1.467223 -0.458845 -0.190099	
C	1.779192 0.890722 -0.866091	
N	0.676675 -0.279815 1.017487	
H	1.253115 0.109942 1.758313	
H	0.308131 -1.161353 1.358741	
H	0.878341 -1.029328 -0.913214	
C	2.760052 -1.240731 0.046032	
O	3.201463 -1.531656 1.132390	
O	3.366064 -1.549375 -1.114988	
H	4.193532 -2.021002 -0.927468	
H	2.343344 0.730995 -1.783221	
H	0.842116 1.387281 -1.113610	
S	2.677264 2.094596 0.202424	
H	3.868120 1.460422 0.200815	
C	-3.133636 -0.308136 -0.608920	
C	-2.288165 0.900040 -1.062476	
N	-4.265400 0.108043 0.200329	
H	-3.931037 0.543438 1.055926	
H	-4.816587 -0.698331 0.476522	
H	-3.509381 -0.779705 -1.523172	
C	-2.242313 -1.354369 0.065182	
O	-2.260472 -1.641483 1.238302	
O	-1.412835 -1.940945 -0.825359	
H	-0.916070 -2.645655 -0.380096	
H	-1.453698 0.560110 -1.676526	
H	-2.919407 1.549071 -1.669008	
S	-1.647442 1.959827 0.305371	
H	-0.704478 1.061360 0.742035	
28		
Dimer 109 of the n...n type		
C	2.553747 -0.953890 0.391017	

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C	1.305152 -0.120225 0.710702	
N	3.507467 -0.928122 1.486722	
H	3.878040 0.012235 1.597855	
H	4.301866 -1.522801 1.272369	
H	2.204812 -1.984214 0.253951	
C	3.151253 -0.534085 -0.958442	
O	4.303139 -0.216340 -1.133370	
O	2.227559 -0.561413 -1.937916	
H	2.641411 -0.293802 -2.774106	
H	0.551520 -0.245472 -0.063261	
H	0.904497 -0.441570 1.671957	
S	1.624028 1.691960 0.897089	
H	1.694317 1.969789 -0.420971	
C	-3.356072 0.568218 -0.265015	
C	-3.502837 -0.529030 0.805288	
N	-3.797964 0.098820 -1.568178	
H	-3.178055 -0.640909 -1.888895	
H	-3.722331 0.846817 -2.250486	
H	-4.001842 1.395476 0.050100	
C	-1.923062 1.110772 -0.256458	
O	-1.166277 1.058003 -1.200755	
O	-1.592700 1.624023 0.936482	
H	-0.643001 1.888483 0.930119	
H	-3.293291 -0.128104 1.794961	
H	-4.526509 -0.902307 0.783334	
S	-2.439386 -2.015423 0.529197	
H	-1.275071 -1.457862 0.914621	
28		
Dimer 110 of the n...n type		
C	2.564202 0.982922 -0.326382	
C	1.310990 0.191182 -0.727062	
N	3.542218 1.013734 -1.400205	
H	3.902512 0.077222 -1.564447	
H	4.339199 1.581392 -1.129691	
H	2.226688 2.007142 -0.129410	
C	3.122764 0.462839 1.004265	
O	4.257113 0.085618 1.175977	
O	2.185327 0.473360 1.970622	
H	2.573163 0.138027 2.794771	
H	0.542177 0.277926 0.037406	
H	0.937115 0.581488 -1.673414	
S	1.609315 -1.609258 -1.026691	
H	1.665885 -1.970168 0.271784	
C	-3.341892 -0.578959 0.296869	
C	-3.542570 0.543195 -0.737001	
N	-3.722425 -0.142004 1.630885	
H	-3.096604 0.600525 1.933660	
H	-3.598019 -0.901567 2.293056	
H	-3.999726 -1.401733 -0.005684	
C	-1.909927 -1.118962 0.211586	
O	-1.131077 -1.137222 1.138873	
O	-1.608394 -1.543192 -1.023485	
H	-0.659097 -1.807278 -1.056976	
H	-3.406825 0.162467 -1.747102	
H	-4.555533 0.932535 -0.637513	
S	-2.430627 2.001317 -0.501088	
H	-1.313631 1.425153 -0.986266	
28		
Dimer 111 of the n...n type		
C	2.589181 -0.197113 -1.072720	
C	3.535232 -1.083397 -0.244185	
N	3.314614 0.840133 -1.783863	
H	3.756049 1.468097 -1.116967	
H	2.673538 1.405702 -2.331114	
H	2.109099 -0.857632 -1.804906	
C	1.452321 0.333634 -0.198101	
O	1.160291 1.507622 -0.090903	
O	0.801672 -0.653975 0.437176	
H	0.092394 -0.279137 0.990940	

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H	2.999715	-1.936742	0.166566		
H	4.329625	-1.444879	-0.896522		
S	4.395678	-0.199705	1.130817		
H	3.322893	-0.084569	1.940666		
C	-3.472283	0.296373	0.708662		
C	-2.968336	-1.152772	0.841046		
N	-4.661363	0.364341	-0.123645		
H	-4.427790	0.090745	-1.074742		
H	-4.997592	1.320747	-0.175853		
H	-3.730666	0.625099	1.721679		
C	-2.340295	1.214579	0.240482		
O	-2.352313	1.867120	-0.774488		
O	-1.297321	1.206509	1.100699		
H	-0.557479	1.733671	0.724507		
H	-2.167223	-1.219033	1.575315		
H	-3.797384	-1.771873	1.182874		
S	-2.410869	-1.928051	-0.741159		
H	-1.208434	-1.323441	-0.815395		
28					
Dimer 112 of the n...n type					
C	-3.154657	-0.521437	-0.226067		
C	-3.016322	0.840998	-0.940851		
N	-3.875814	-0.397735	1.028614		
H	-3.335418	0.161821	1.682649		
H	-4.000142	-1.310733	1.454577		
H	-3.729226	-1.161571	-0.902613		
C	-1.770726	-1.155300	-0.094007		
O	-1.122915	-1.189525	0.930779		
O	-1.328233	-1.632218	-1.266925		
H	-0.421405	-1.984550	-1.161957		
H	-2.466547	0.721616	-1.873996		
H	-4.016957	1.206946	-1.171452		
S	-2.253359	2.195480	0.054242		
H	-0.981830	1.739329	0.119780		
C	1.366585	0.187522	-0.148337		
C	2.504393	0.824963	-0.969671		
N	0.981457	1.014484	0.980998		
H	1.798466	1.249279	1.537738		
H	0.341281	0.504011	1.581428		
H	0.523562	0.112465	-0.838203		
C	1.761028	-1.233850	0.242914		
O	2.313687	-1.549887	1.264779		
O	1.445641	-2.124238	-0.736410		
H	1.757270	-3.007861	-0.479821		
H	2.728588	0.206688	-1.838599		
H	2.165749	1.801420	-1.317872		
S	4.061018	1.170897	-0.043800		
H	4.367319	-0.108577	0.252328		
28					
Dimer 113 of the n...n type					
C	-1.939045	0.775967	0.469174		
C	-3.209169	0.099477	1.011829		
N	-2.241372	1.789348	-0.526101		
H	-2.640734	1.350134	-1.351252		
H	-1.373092	2.228412	-0.817925		
H	-1.451614	1.260476	1.320283		
C	-0.953880	-0.285905	-0.018604		
O	-0.641582	-0.458211	-1.175717		
O	-0.463819	-1.012342	1.001380		
H	0.248146	-1.599065	0.665934		
H	-2.957373	-0.587869	1.818206		
H	-3.875645	0.869278	1.400741		
S	-4.210008	-0.800438	-0.253611		
H	-3.344616	-1.814259	-0.461330		
C	2.857879	0.700608	0.552028		
C	3.482560	-0.558926	-0.060296		
N	2.421744	0.482742	1.925334		
H	1.610822	-0.129618	1.940551		
H	2.112084	1.361627	2.328510		

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H	3.660370	1.449893	0.570132		
C	1.770013	1.333823	-0.327080		
O	0.835601	1.963567	0.115374		
O	1.968291	1.132017	-1.638284		
H	1.230369	1.524770	-2.132303		
H	3.955257	-0.326913	-1.012359		
H	4.241897	-0.933971	0.624871		
S	2.336280	-1.981614	-0.340116		
H	1.663096	-1.435196	-1.373397		
28					
Dimer 114 of the n...n type					
C	2.985029	-1.006295	0.317002		
C	3.063431	0.353391	1.038172		
N	4.009581	-1.120481	-0.707514		
H	3.825704	-0.449460	-1.448858		
H	3.974906	-2.040042	-1.136158		
H	3.165117	-1.769515	1.081542		
C	1.564430	-1.244468	-0.198163		
O	1.249791	-1.282037	-1.366588		
O	0.688593	-1.395705	0.808898		
H	-0.205160	-1.570243	0.451175		
H	2.326266	0.404595	1.838556		
H	4.058481	0.452822	1.471314		
S	2.855727	1.824650	-0.059307		
H	1.503543	1.806853	-0.098292		
C	-2.910788	0.139316	-0.874022		
C	-1.503340	0.750304	-0.926670		
N	-3.933227	1.171056	-0.832247		
H	-3.847019	1.705590	0.028568		
H	-4.856652	0.749833	-0.816337		
H	-3.030766	-0.434039	-1.801837		
C	-3.054029	-0.895438	0.246405		
O	-3.960284	-0.940676	1.036432		
O	-2.050882	-1.818759	0.235745		
H	-2.254050	-2.499155	0.900183		
H	-0.751979	-0.003655	-1.148898		
H	-1.485231	1.487708	-1.728690		
S	-1.015019	1.681843	0.590613		
H	-0.695102	0.617354	1.352926		
28					
Dimer 115 of the n...n type					
C	3.001558	-0.439677	-0.351139		
C	2.793322	0.934617	-1.008108		
N	2.391173	-1.504018	-1.128493		
H	1.378638	-1.400935	-1.132788		
H	2.577412	-2.401975	-0.692871		
H	4.085546	-0.603649	-0.321086		
C	2.550723	-0.413916	1.114722		
O	1.779724	-1.199447	1.613001		
O	3.119713	0.600132	1.794716		
H	2.814401	0.574669	2.715794		
H	3.383276	1.695425	-0.501067		
H	3.111711	0.874789	-2.048505		
S	1.034777	1.491961	-1.067352		
H	0.881174	1.708475	0.253791		
C	-2.567326	-0.241772	0.969118		
C	-1.331482	-1.065023	0.559055		
N	-3.795314	-0.994880	0.774454		
H	-3.944153	-1.155700	-0.218191		
H	-4.592411	-0.460383	1.105400		
H	-2.450401	-0.026635	2.035874		
C	-2.550123	1.106230	0.244488		
O	-3.262202	1.402103	-0.685533		
O	-1.619630	1.935800	0.760201		
H	-1.632459	2.771441	0.265943		
H	-0.414452	-0.513425	0.751137		
H	-1.312059	-1.976752	1.155409		
S	-1.321997	-1.637674	-1.193629		
H	-0.982578	-0.453097	-1.742748		

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28		
Dimer 116 of the n...n type		
C	2.018260 0.662891 -0.630055	
C	1.258469 -0.660646 -0.796661	
N	3.142474 0.754248 -1.547501	
H	3.817816 0.025099 -1.331496	
H	3.626712 1.637118 -1.418134	
H	1.300849 1.456148 -0.869565	
C	2.402199 0.894022 0.834084	
O	3.506880 1.185465 1.225120	
O	1.342039 0.744531 1.655917	
H	1.617566 0.918182 2.570151	
H	0.337972 -0.656616 -0.222131	
H	1.013018 -0.790232 -1.850464	
S	2.225958 -2.160698 -0.323968	
H	2.135758 -1.983903 1.010334	
C	-2.789051 0.306208 0.858574	
C	-3.023805 1.250193 -0.331135	
N	-1.809476 0.847030 1.784483	
H	-0.899486 0.914689 1.336556	
H	-1.685483 0.212508 2.567201	
H	-3.752388 0.219520 1.376292	
C	-2.460374 -1.113288 0.378609	
O	-1.518849 -1.768455 0.759490	
O	-3.356704 -1.558620 -0.521981	
H	-3.118659 -2.462097 -0.785326	
H	-3.860882 0.907520 -0.935777	
H	-3.249318 2.244575 0.053339	
S	-1.553953 1.475483 -1.425796	
H	-1.587677 0.252340 -1.992492	
28		
Dimer 117 of the n...n type		
C	2.551603 -0.954712 0.387990	
C	1.303236 -0.123653 0.715143	
N	3.510197 -0.929910 1.479512	
H	3.880150 0.010688 1.590691	
H	4.304322 -1.523211 1.260399	
H	2.203580 -1.985250 0.250245	
C	3.142524 -0.530915 -0.963065	
O	4.292789 -0.209546 -1.142002	
O	2.215077 -0.559301 -1.938955	
H	2.624830 -0.288822 -2.776239	
H	0.545877 -0.248808 -0.055140	
H	0.907735 -0.447590 1.677557	
S	1.620238 1.688646 0.903979	
H	1.678722 1.969953 -0.413909	
C	-3.352055 0.565672 -0.272860	
C	-3.507377 -0.532844 0.794596	
N	-3.780546 0.096225 -1.580683	
H	-3.154871 -0.640841 -1.896449	
H	-3.700226 0.845172 -2.261444	
H	-4.002505 1.391602 0.036252	
C	-1.920489 1.111629 -0.251636	
O	-1.159832 1.071593 -1.193404	
O	-1.596271 1.612939 0.948076	
H	-0.647512 1.880782 0.947240	
H	-3.314489 -0.131863 1.787596	
H	-4.528380 -0.912114 0.757614	
S	-2.429141 -2.011464 0.532705	
H	-1.281093 -1.455369 0.966111	
28		
Dimer 118 of the n...n type		
C	2.744672 0.849971 0.191546	
C	3.243949 -0.581681 0.442514	
N	2.207796 1.446001 1.402090	
H	1.366863 0.954506 1.692128	
H	1.957030 2.416051 1.244022	
H	3.621537 1.430323 -0.122337	
C	1.787381 0.912506 -1.005037	

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O	0.750308 1.539775 -1.028076	
O	2.232988 0.201780 -2.051486	
H	1.615550 0.299359 -2.794611	
H	3.746387 -0.974188 -0.438908	
H	3.951938 -0.559112 1.270383	
S	1.928860 -1.767279 0.961984	
H	1.288582 -1.841718 -0.225168	
C	-2.768328 -0.165061 0.855868	
C	-1.775183 -1.303634 0.550112	
N	-4.070826 -0.415360 0.262560	
H	-3.987619 -0.414581 -0.750749	
H	-4.712438 0.335431 0.498072	
H	-2.871878 -0.130734 1.945521	
C	-2.124820 1.153039 0.420583	
O	-2.513248 1.838291 -0.496189	
O	-1.021669 1.424038 1.140228	
H	-0.493219 2.083127 0.656438	
H	-0.853524 -1.155156 1.109490	
H	-2.223777 -2.252524 0.843426	
S	-1.356121 -1.503029 -1.238861	
H	-0.761088 -0.302247 -1.399563	
28		
Dimer 119 of the n...n type		
C	2.536627 -0.948308 -0.442973	
C	3.523451 0.167879 -0.831165	
N	1.375426 -0.967210 -1.312583	
H	0.810725 -0.127353 -1.174910	
H	0.773088 -1.744839 -1.060882	
H	3.084823 -1.890562 -0.560111	
C	2.203356 -0.847545 1.050697	
O	1.100048 -0.670984 1.513273	
O	3.308579 -0.971695 1.811140	
H	3.060325 -0.891587 2.746098	
H	4.448782 0.072505 -0.265793	
H	3.747722 0.074876 -1.893679	
S	2.873329 1.883519 -0.625512	
H	2.869721 1.895705 0.723468	
C	-2.189483 0.887057 -0.596573	
C	-2.471427 -0.402033 -1.390670	
N	-0.778664 1.023638 -0.292987	
H	-0.499752 0.378409 0.442521	
H	-0.564654 1.957162 0.039668	
H	-2.494590 1.715409 -1.245592	
C	-3.095028 0.957836 0.637141	
O	-2.706761 1.035623 1.778418	
O	-4.398420 0.905546 0.297664	
H	-4.937914 0.941281 1.103778	
H	-3.507663 -0.429259 -1.722939	
H	-1.819003 -0.416716 -2.263639	
S	-2.093098 -1.965587 -0.486613	
H	-3.105185 -1.894185 0.402318	
28		
Dimer 120 of the n...n type		
C	2.582471 0.920275 -0.576499	
C	1.940445 -0.322669 -1.225220	
N	4.012468 0.754022 -0.388218	
H	4.191604 0.044649 0.316955	
H	4.423013 1.616844 -0.045463	
H	2.408840 1.747779 -1.270608	
C	1.803980 1.230144 0.703705	
O	2.178352 0.956292 1.819541	
O	0.614217 1.788830 0.424429	
H	0.056053 1.772395 1.219076	
H	0.875121 -0.152731 -1.379727	
H	2.410431 -0.500703 -2.191871	
S	2.174474 -1.902578 -0.290415	
H	1.685901 -1.464592 0.889861	
C	-2.890494 -0.796499 0.383430	
C	-3.205106 -0.062962 -0.934013	

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N	-3.370805	-0.057255	1.538004		
H	-2.876361	0.827855	1.610307		
H	-3.170410	-0.571082	2.390327		
H	-3.419859	-1.754143	0.333123		
C	-1.397871	-1.137552	0.436424		
O	-0.615460	-0.666258	1.233460		
O	-1.055485	-2.005915	-0.525100		
H	-0.090129	-2.194060	-0.482287		
H	-2.892880	-0.666940	-1.784376		
H	-4.281126	0.100437	-0.993592		
S	-2.463035	1.621425	-1.079801		
H	-1.168425	1.247362	-1.082380		
28					
Dimer 121 of the n...n type					
C	-1.463643	-0.027120	0.735862		
C	-1.283558	-0.870911	-0.541487		
N	-1.947189	-0.837500	1.836814		
H	-2.879887	-1.183495	1.628214		
H	-2.022987	-0.279710	2.681311		
H	-0.479555	0.369948	1.003160		
C	-2.328594	1.199638	0.438903		
O	-3.420611	1.417093	0.894635		
O	-1.710533	2.041030	-0.431928		
H	-2.278589	2.807105	-0.614014		
H	-0.815467	-0.288430	-1.330851		
H	-0.639776	-1.716751	-0.301198		
S	-2.835524	-1.623693	-1.192952		
H	-3.378945	-0.488690	-1.679687		
C	2.945937	0.404242	-0.712629		
C	2.459937	-1.059576	-0.791649		
N	4.130069	0.534653	0.118060		
H	3.900616	0.323078	1.085099		
H	4.469421	1.491247	0.098089		
H	3.194870	0.698256	-1.736267		
C	1.762379	1.263526	-0.268538		
O	1.578037	1.639089	0.869311		
O	0.903655	1.483145	-1.273214		
H	0.092454	1.919645	-0.939984		
H	1.584453	-1.128935	-1.437133		
H	3.256328	-1.667144	-1.221762		
S	2.096734	-1.866946	0.828851		
H	1.178411	-0.987621	1.273319		
28					
Dimer 122 of the n...n type					
C	3.200824	0.529294	0.319412		
C	3.144378	-0.278075	-0.993474		
N	3.615933	-0.300986	1.436866		
H	2.903740	-1.001303	1.626227		
H	3.703064	0.260341	2.278127		
H	3.953520	1.309528	0.163361		
C	1.879851	1.263808	0.553179		
O	1.097779	1.029021	1.444446		
O	1.681691	2.224045	-0.372488		
H	0.858081	2.696524	-0.173904		
H	2.831477	0.358292	-1.819998		
H	4.147372	-0.649951	-1.201745		
S	2.072130	-1.780581	-0.945075		
H	0.874807	-1.229539	-1.263634		
C	-1.398457	-0.558493	0.061112		
C	-1.426579	0.910595	-0.381988		
N	-1.284660	-1.442890	-1.086889		
H	-2.075845	-1.306540	-1.710790		
H	-1.312862	-2.413433	-0.789707		
H	-0.500806	-0.672179	0.680231		
C	-2.574494	-0.890287	0.980918		
O	-3.309365	-1.839832	0.847977		
O	-2.686805	0.004248	1.981741		
H	-3.428487	-0.250624	2.553614		
H	-1.311940	1.565848	0.477389		

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H	-0.596797	1.072185	-1.069444
S	-2.934655	1.398315	-1.327954
H	-3.783385	1.383338	-0.279453
28			
Dimer 123 of the n...n type			
C	-2.079933	-0.049001	-0.959535
C	-1.866077	-1.429807	-0.308464
N	-0.838583	0.703769	-1.051822
H	-0.584515	1.061861	-0.134925
H	-0.958040	1.509437	-1.657171
H	-2.455503	-0.240792	-1.969723
C	-3.185728	0.707997	-0.218277
O	-3.031170	1.749328	0.374616
O	-4.361089	0.055218	-0.285378
H	-5.029038	0.550457	0.215323
H	-2.803278	-1.983040	-0.281939
H	-1.150220	-1.995574	-0.901704
S	-1.146951	-1.378594	1.388024
H	-2.244358	-0.908529	2.016975
C	3.007391	0.248096	0.551262
C	3.178510	-0.590536	-0.725582
N	2.657905	-0.571898	1.699505
H	1.747171	-0.997457	1.545492
H	2.560354	0.013210	2.523480
H	3.984043	0.712755	0.739722
C	2.056800	1.432561	0.336352
O	1.185030	1.760930	1.108336
O	2.320416	2.098300	-0.802546
H	1.723735	2.860811	-0.870339
H	3.494585	0.045288	-1.550220
H	3.950371	-1.338908	-0.546317
S	1.688407	-1.553736	-1.235125
H	0.794866	-0.521402	-1.323580
28			
Dimer 124 of the n...n type			
C	1.680134	0.296467	0.065404
C	2.941664	1.077813	-0.343348
N	1.437283	0.346774	1.496209
H	2.223425	-0.067514	1.989745
H	0.621927	-0.233451	1.684751
H	0.848689	0.777451	-0.452762
C	1.766121	-1.126345	-0.484623
O	2.189266	-2.080712	0.125608
O	1.346108	-1.191209	-1.764486
H	1.462908	-2.098373	-2.089843
H	3.054804	1.066575	-1.427359
H	2.826538	2.111870	-0.016654
S	4.516532	0.513732	0.437576
H	4.528476	-0.727617	-0.089532
C	-2.201450	-0.233257	0.879473
C	-1.892729	1.253688	0.627592
N	-1.123115	-1.088464	0.412556
H	-1.052810	-1.034751	-0.600568
H	-1.317785	-2.058818	0.636549
H	-2.292937	-0.347214	1.965545
C	-3.569453	-0.603116	0.297172
O	-3.758527	-1.470435	-0.522047
O	-4.548606	0.167950	0.806830
H	-5.396265	-0.090740	0.410904
H	-2.657990	1.881393	1.079677
H	-0.930261	1.495009	1.078293
S	-1.720939	1.708874	-1.153698
H	-3.019010	1.560051	-1.489424
28			
Dimer 125 of the n...n type			
C	1.625261	-0.057294	-0.398809
C	2.378787	1.260170	-0.162224
N	0.698494	-0.338137	0.685279
H	1.201874	-0.435140	1.562792

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H	0.214286	-1.214001	0.520302		
H	1.046664	0.085354	-1.320043		
C	2.587363	-1.211671	-0.688588		
O	2.564747	-2.283031	-0.131394		
O	3.465755	-0.892779	-1.657596		
H	4.046486	-1.652673	-1.823105		
H	2.963100	1.528301	-1.039662		
H	1.650843	2.048635	0.026852		
S	3.485301	1.245527	1.314772		
H	4.435014	0.443436	0.790557		
C	-3.305864	-0.363935	-0.567824		
C	-2.127418	0.249162	-1.349032		
N	-4.420321	0.565384	-0.485939		
H	-4.149271	1.372427	0.069962		
H	-5.203832	0.133356	-0.006367		
H	-3.624314	-1.246622	-1.132458		
C	-2.833223	-0.877067	0.794920		
O	-3.137943	-0.400012	1.861441		
O	-2.024803	-1.952436	0.669096		
H	-1.779428	-2.263017	1.555720		
H	-1.324824	-0.480602	-1.453526		
H	-2.482714	0.517501	-2.343503		
S	-1.434550	1.795470	-0.614509		
H	-0.644609	1.146243	0.289843		
28					
Dimer 126 of the n...n type					
C	-3.120104	0.433001	-0.137634		
C	-3.213472	-1.100790	-0.170865		
N	-2.932959	0.988221	-1.467966		
H	-2.098325	0.590062	-1.890253		
H	-2.777925	1.989863	-1.410708		
H	-4.076758	0.793349	0.261021		
C	-2.066980	0.895686	0.875946		
O	-1.169186	1.668105	0.634463		
O	-2.269715	0.351753	2.088929		
H	-1.589436	0.675347	2.699998		
H	-3.460008	-1.482481	0.817951		
H	-4.002353	-1.388553	-0.865623		
S	-1.682770	-1.939409	-0.777856		
H	-0.847795	-1.496288	0.212393		
C	1.633355	-0.753227	-0.059156		
C	1.292924	0.386364	-1.031804		
N	0.788705	-0.703089	1.125957		
H	0.753753	0.247037	1.485795		
H	1.168580	-1.290158	1.861911		
H	1.429443	-1.690666	-0.594573		
C	3.128786	-0.797698	0.258812		
O	3.597708	-0.884126	1.368572		
O	3.871591	-0.753442	-0.863146		
H	4.810855	-0.807577	-0.624912		
H	1.724016	0.192085	-2.010976		
H	0.211162	0.450522	-1.125445		
S	1.836100	2.057612	-0.465852		
H	3.141047	1.891943	-0.765525		
28					
Dimer 127 of the n...n type					
C	2.316951	-0.121759	1.145082		
C	2.130199	-1.534462	0.568777		
N	1.137925	0.322562	1.872063		
H	0.288623	0.040774	1.392412		
H	1.115563	1.336358	1.919956		
H	3.164557	-0.181936	1.841265		
C	2.780150	0.856009	0.061399		
O	2.291719	1.939882	-0.151975		
O	3.837219	0.371149	-0.619676		
H	4.117173	1.026613	-1.278402		
H	3.091345	-1.981961	0.327289		
H	1.632218	-2.154271	1.314215		
S	1.066899	-1.613968	-0.941662		

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H	2.010773	-1.204537	-1.812814		
C	-3.091348	0.159596	0.077624		
C	-2.558734	1.066322	-1.050933		
N	-3.236988	0.891067	1.324442		
H	-2.324046	1.194294	1.653156		
H	-3.618771	0.285887	2.044452		
H	-4.078396	-0.187149	-0.245988		
C	-2.211982	-1.086779	0.189967		
O	-1.472422	-1.331647	1.116472		
O	-2.338404	-1.880163	-0.886901		
H	-1.717891	-2.622797	-0.808947		
H	-2.494992	0.508907	-1.984415		
H	-3.257614	1.892193	-1.183723		
S	-0.930305	1.861274	-0.701341		
H	-0.156920	0.767980	-0.880801		
28					
Dimer 128 of the n...n type					
C	-2.973996	0.398384	-0.532836		
C	-3.138523	-0.508194	0.696879		
N	-2.922149	-0.375922	-1.763113		
H	-2.113973	-0.993285	-1.742711		
H	-2.786471	0.242627	-2.556738		
H	-3.862389	1.041746	-0.562506		
C	-1.787059	1.356455	-0.366760		
O	-0.943297	1.550408	-1.210799		
O	-1.794154	1.969523	0.828338		
H	-0.985268	2.500572	0.907626		
H	-3.305573	0.087224	1.591786		
H	-3.999442	-1.157509	0.539266		
S	-1.716546	-1.650461	0.996636		
H	-0.835354	-0.704742	1.380387		
C	2.091123	0.638276	-0.722795		
C	1.338177	-0.666515	-1.021812		
N	3.414083	0.635135	-1.327062		
H	3.978006	-0.100024	-0.907482		
H	3.892004	1.508209	-1.126895		
H	1.492300	1.440086	-1.167623		
C	2.114788	0.929843	0.780147		
O	3.104844	1.179485	1.422939		
O	0.876881	0.884932	1.326871		
H	0.947806	1.070877	2.277372		
H	0.289707	-0.576145	-0.759575		
H	1.409780	-0.866808	-2.090557		
S	2.030486	-2.162223	-0.192596		
H	1.591045	-1.868640	1.048511		
28					
Dimer 129 of the n...n type					
C	2.217794	0.648093	0.968741		
C	3.444939	-0.238866	0.702437		
N	1.166111	-0.088478	1.646358		
H	0.938306	-0.925039	1.115967		
H	0.319066	0.468406	1.694870		
H	2.559521	1.461242	1.621032		
C	1.760977	1.337867	-0.321912		
O	0.634852	1.302491	-0.766684		
O	2.762335	2.013094	-0.907775		
H	2.429558	2.444999	-1.711208		
H	4.272896	0.356618	0.323945		
H	3.745985	-0.707443	1.639287		
S	3.129626	-1.639263	-0.460818		
H	2.987709	-0.891403	-1.574609		
C	-3.194956	-0.196049	0.532201		
C	-2.151485	-1.292489	0.811850		
N	-4.211297	-0.660065	-0.397194		
H	-3.781583	-0.861870	-1.296452		
H	-4.892853	0.073575	-0.564414		
H	-3.671078	0.030853	1.492754		
C	-2.492796	1.089947	0.085717		
O	-2.654202	1.629793	-0.982019		

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O	-1.649911	1.550918	1.031460	
H	-1.140204	2.286072	0.653516	
H	-1.492285	-0.990820	1.623277	
H	-2.674904	-2.199732	1.112824	
S	-1.135145	-1.782111	-0.650717	
H	-0.446953	-0.625055	-0.764418	
28				
Dimer 130 of the n...n type				
C	-1.810386	0.500769	-0.150214	
C	-1.663259	-0.840981	-0.895356	
N	-1.085371	0.496120	1.108656	
H	-1.576103	-0.074972	1.790709	
H	-1.030770	1.434191	1.491238	
H	-1.366800	1.253835	-0.807684	
C	-3.291881	0.848369	-0.002761	
O	-3.895488	0.873441	1.044330	
O	-3.861834	1.096143	-1.197331	
H	-4.806164	1.279721	-1.067773	
H	-2.203693	-0.809410	-1.840263	
H	-0.606675	-0.998921	-1.103339	
S	-2.196750	-2.321167	0.065111	
H	-3.511060	-2.022290	0.126748	
C	2.055613	0.102214	0.923132	
C	3.593519	0.153239	0.837970	
N	1.550193	-1.257634	0.861812	
H	1.735631	-1.654102	-0.055430	
H	0.541170	-1.216857	0.977146	
H	1.782495	0.531006	1.890120	
C	1.476730	1.025037	-0.147571	
O	1.125717	0.671614	-1.251006	
O	1.467660	2.311930	0.251173	
H	1.159660	2.867642	-0.482703	
H	3.942524	1.181122	0.937008	
H	4.004525	-0.435402	1.658586	
S	4.325881	-0.592390	-0.684194	
H	3.764970	0.255038	-1.570834	
28				
Dimer 131 of the n...n type				
C	2.604828	-0.758838	0.837741	
C	2.518548	0.782724	0.832543	
N	3.834012	-1.243900	0.230964	
H	3.848365	-1.015945	-0.759008	
H	3.885532	-2.255304	0.303183	
H	2.586399	-1.062208	1.887765	
C	1.324441	-1.281890	0.187490	
O	1.208657	-1.495064	-1.004425	
O	0.325280	-1.400691	1.062258	
H	-0.515632	-1.598237	0.586375	
H	1.564128	1.098854	1.250619	
H	3.329925	1.181274	1.442142	
S	2.743495	1.587883	-0.818505	
H	1.898234	0.801551	-1.513319	
C	-2.148831	1.030677	-0.774920	
C	-3.137556	-0.120815	-0.989144	
N	-0.952107	0.868249	-1.584052	
H	-0.515446	-0.032227	-1.407034	
H	-0.268279	1.576046	-1.333383	
H	-2.667667	1.940006	-1.107105	
C	-1.855934	1.284068	0.709019	
O	-0.766686	1.556847	1.153067	
O	-2.970143	1.211415	1.461812	
H	-2.745737	1.420480	2.382808	
H	-4.119201	0.132961	-0.596370	
H	-3.225524	-0.311062	-2.058156	
S	-2.642281	-1.737597	-0.232869	
H	-3.057698	-1.446823	1.017008	
28				
Dimer 132 of the n...n type				
C	3.098480	-0.270075	0.710734	

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C	2.037389	0.766933	1.131713	
N	4.333590	0.376162	0.301589	
H	4.173359	0.922095	-0.540728	
H	5.035147	-0.319905	0.069616	
H	3.293166	-0.885464	1.594343	
C	2.501940	-1.189307	-0.356887	
O	2.744472	-1.119006	-1.537009	
O	1.627580	-2.080474	0.163078	
H	1.198099	-2.543751	-0.575943	
H	1.162614	0.272323	1.546481	
H	2.470911	1.403570	1.902953	
S	1.510830	1.938861	-0.196065	
H	1.053915	1.015423	-1.066273	
C	-2.006870	0.889750	0.169403	
C	-3.341719	0.532596	0.844634	
N	-2.211153	1.603882	-1.077456	
H	-2.626814	0.983547	-1.767016	
H	-1.319641	1.905944	-1.456434	
H	-1.468433	1.546491	0.861695	
C	-1.130226	-0.357732	0.030646	
O	-0.675133	-0.773955	-1.010587	
O	-0.903585	-0.935703	1.223864	
H	-0.272447	-1.667057	1.110775	
H	-3.171015	0.119985	1.837063	
H	-3.937204	1.440483	0.936552	
S	-4.392197	-0.643175	-0.118151	
H	-3.647478	-1.744860	0.109217	
28				
Dimer 133 of the n...n type				
C	-2.005101	0.888846	0.168563	
C	-3.339176	0.533167	0.845687	
N	-2.210121	1.604189	-1.077516	
H	-2.628064	0.985090	-1.766811	
H	-1.318600	1.904695	-1.457713	
H	-1.464411	1.544345	0.860306	
C	-1.129811	-0.359444	0.027577	
O	-0.672913	-0.772684	-1.014001	
O	-0.906042	-0.941350	1.219478	
H	-0.274531	-1.672250	1.105486	
H	-3.167356	0.120420	1.837879	
H	-3.933705	1.441599	0.938523	
S	-4.391983	-0.641604	-0.115664	
H	-3.648058	-1.743976	0.110909	
C	3.095832	-0.270476	0.712652	
C	2.033692	0.766011	1.132190	
N	4.331936	0.376204	0.307133	
H	4.173926	0.922491	-0.535360	
H	5.034279	-0.319629	0.076870	
H	3.288489	-0.886805	1.596046	
C	2.501888	-1.188600	-0.357313	
O	2.745980	-1.116182	-1.536966	
O	1.627636	-2.081457	0.160043	
H	1.199923	-2.544217	-0.580307	
H	1.157641	0.270665	1.543367	
H	2.464881	1.401385	1.905766	
S	1.511081	1.939863	-0.195513	
H	1.056074	1.017646	-1.068015	
28				
Dimer 134 of the n...n type				
C	1.897362	-0.317438	0.032497	
C	2.003851	1.076999	-0.604653	
N	1.530880	-0.234319	1.435225	
H	2.293264	0.176262	1.967109	
H	1.377851	-1.164277	1.811477	
H	1.098908	-0.845419	-0.500729	
C	3.167525	-1.134368	-0.223649	
O	3.821295	-1.682343	0.631673	
O	3.475096	-1.175511	-1.535036	
H	4.279149	-1.705515	-1.656050	

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H	2.138168	0.998247	-1.681516		
H	1.083648	1.624520	-0.405011		
S	3.352521	2.130292	0.090483		
H	4.379840	1.467370	-0.479641		
C	-2.819181	0.885366	0.302766		
C	-1.479090	0.166438	0.087067		
N	-3.199392	0.888155	1.706000		
H	-3.343888	-0.068177	2.020537		
H	-4.088374	1.363805	1.825017		
H	-2.667366	1.921769	-0.021801		
C	-3.897758	0.314731	-0.625042		
O	-4.972645	-0.101186	-0.262737		
O	-3.503650	0.332235	-1.913673		
H	-4.213742	-0.029770	-2.467532		
H	-1.136901	0.295317	-0.938132		
H	-0.735487	0.578670	0.767463		
S	-1.500392	-1.636130	0.483492		
H	-2.216557	-2.032168	-0.589102		
28					
Dimer 135 of the n...n type					
C	1.557859	-0.116110	0.587192		
C	2.988225	0.066663	1.116795		
N	1.192942	-1.518378	0.497572		
H	1.829079	-1.992587	-0.138402		
H	0.263307	-1.621897	0.098698		
H	0.897466	0.379124	1.308814		
C	1.347930	0.662530	-0.715978		
O	0.871270	0.207685	-1.728167		
O	1.737399	1.947843	-0.594448		
H	1.565048	2.411017	-1.429741		
H	3.188450	1.114349	1.330848		
H	3.094901	-0.508937	2.035987		
S	4.304056	-0.569439	-0.013681		
H	4.197329	0.406985	-0.938355		
C	-2.947190	-0.577282	0.719010		
C	-3.136791	0.946051	0.712223		
N	-2.109052	-1.009649	1.825705		
H	-1.197932	-0.564186	1.766947		
H	-1.943530	-2.009653	1.771982		
H	-3.946890	-1.011011	0.851518		
C	-2.478908	-1.100185	-0.644904		
O	-1.614653	-1.932544	-0.797941		
O	-3.164128	-0.552552	-1.662604		
H	-2.854371	-0.938069	-2.498126		
H	-3.878330	1.236766	-0.028458		
H	-3.481338	1.259663	1.697405		
S	-1.586947	1.903445	0.413742		
H	-1.420019	1.537067	-0.873767		
28					
Dimer 136 of the n...n type					
C	-2.269539	-0.653985	-0.801116		
C	-1.776980	0.797401	-0.730508		
N	-3.526776	-0.755682	-1.525123		
H	-4.249638	-0.245698	-1.022921		
H	-3.832844	-1.723174	-1.556986		
H	-1.492992	-1.202919	-1.346986		
C	-2.316253	-1.292136	0.591614		
O	-3.249881	-1.916178	1.035702		
O	-1.171886	-1.086667	1.277922		
H	-1.233109	-1.524227	2.142005		
H	-0.762278	0.830458	-0.351397		
H	-1.791294	1.220292	-1.734562		
S	-2.820632	1.916923	0.300814		
H	-2.413723	1.439146	1.494927		
C	2.339917	-0.356292	-1.008883		
C	2.119117	1.163194	-0.910931		
N	1.091904	-1.089792	-0.894897		
H	0.706164	-0.987303	0.040126		
H	1.259447	-2.082815	-1.022184		

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H	2.763778	-0.538546	-2.003555		
C	3.412311	-0.811203	-0.012006		
O	3.269241	-1.690833	0.803407		
O	4.551295	-0.104238	-0.150394		
H	5.203376	-0.423739	0.493687		
H	3.028654	1.698620	-1.175163		
H	1.329872	1.444664	-1.607898		
S	1.544667	1.756617	0.742312		
H	2.702511	1.538376	1.398907		
28					
Dimer 137 of the n...n type					
C	-1.962439	0.262344	0.824682		
C	-1.669604	-0.939205	-0.089492		
N	-2.807228	-0.116815	1.943532		
H	-3.722785	-0.398659	1.602773		
H	-2.959525	0.681161	2.552043		
H	-0.991292	0.587975	1.212445		
C	-2.509810	1.434250	0.006625		
O	-3.557793	1.997827	0.204925		
O	-1.660443	1.773703	-0.989081		
H	-2.022154	2.526326	-1.483745		
H	-0.947330	-0.672391	-0.858233		
H	-1.253686	-1.739979	0.519736		
S	-3.153538	-1.663385	-0.912765		
H	-3.356331	-0.657315	-1.788386		
C	1.936209	0.066035	-0.801094		
C	3.460889	0.020445	-1.025769		
N	1.468249	1.421958	-0.588776		
H	1.738978	1.743761	0.335665		
H	0.456907	1.475755	-0.647978		
H	1.481327	-0.325754	-1.717220		
C	1.561670	-0.904862	0.323181		
O	1.091307	-0.580796	1.388599		
O	1.838116	-2.178683	-0.009645		
H	1.615094	-2.758994	0.736031		
H	3.781933	-0.987910	-1.282236		
H	3.704761	0.690523	-1.849669		
S	4.464588	0.626653	0.400120		
H	4.279165	-0.443251	1.200612		
28					
Dimer 138 of the n...n type					
C	2.215954	-0.649002	0.556333		
C	1.606237	0.758675	0.647477		
N	3.307086	-0.821438	1.500608		
H	4.059578	-0.176596	1.272252		
H	3.696710	-1.755229	1.417687		
H	1.418344	-1.353704	0.820111		
C	2.596062	-0.982022	-0.890661		
O	3.682963	-1.364173	-1.252061		
O	1.554853	-0.802317	-1.728800		
H	1.824499	-1.037263	-2.630960		
H	0.711550	0.843786	0.035657		
H	1.340156	0.955433	1.685492		
S	2.757240	2.119197	0.163333		
H	2.707766	1.896573	-1.166370		
C	-2.300143	0.211302	-0.852902		
C	-1.564655	-0.990733	-0.235441		
N	-1.551687	1.443994	-0.669193		
H	-1.559909	1.704039	0.313872		
H	-2.002171	2.204486	-1.168071		
H	-2.376491	0.004696	-1.926380		
C	-3.739334	0.285682	-0.331688		
O	-4.222092	1.239877	0.230430		
O	-4.412005	-0.857173	-0.568801		
H	-5.313792	-0.773264	-0.219699		
H	-2.082566	-1.918794	-0.468850		
H	-0.562839	-1.034583	-0.658665		
S	-1.336127	-0.884560	1.594946		
H	-2.600889	-1.204794	1.936703		

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28		
Dimer 139 of the n...n type		
C	-3.237903	0.123475
C	-2.216674	-0.985168
N	-4.471552	-0.427177
H	-4.289022	-0.871960
H	-5.140117	0.316017
H	-3.455297	0.619643
C	-2.595243	1.186105
O	-2.913338	1.415550
O	-1.610104	1.844331
H	-1.226550	2.504340
H	-1.330637	-0.561250
H	-2.675158	-1.686938
S	-1.709748	-2.012797
H	-1.023385	-1.048508
C	2.695554	0.311727
C	1.248067	0.136324
N	3.066616	1.715235
H	3.050070	2.117951
H	4.021238	1.807770
H	2.735557	-0.110972
C	3.654169	-0.538873
O	4.644185	-0.121216
O	3.258534	-1.825590
H	3.892100	-2.330966
H	0.934257	-0.901624
H	0.595402	0.763382
S	0.948743	0.687013
H	1.600130	-0.326892
28		
Dimer 140 of the n...n type		
C	-2.132777	0.115773
C	-3.654035	-0.034710
N	-1.752445	1.503135
H	-2.140617	1.843285
H	-0.744540	1.591910
H	-1.682243	-0.243508
C	-1.611441	-0.825993
O	-0.890379	-0.489712
O	-2.034302	-2.088898
H	-1.674280	-2.652050
H	-3.910658	-1.048079
H	-3.987702	0.659941
S	-4.625835	0.400992
H	-4.302910	-0.698308
C	1.855318	-0.387516
C	3.042882	-0.208541
N	1.923802	-1.647501
H	2.758007	-1.663060
H	1.129054	-1.717671
H	0.958548	-0.384632
C	1.755314	0.834460
O	2.035836	0.851987
O	1.350056	1.926838
H	1.332996	2.690324
H	2.917659	0.700413
H	3.068995	-1.063040
S	4.705824	-0.186671
H	4.577112	1.003343
28		
Dimer 141 of the n...n type		
C	-1.641878	-0.341392
C	-2.979570	0.234363
N	-1.671475	-1.790654
H	-2.327196	-2.087352
H	-0.760306	-2.150416
H	-0.885711	-0.046668
C	-1.212594	0.332351

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O	-0.917705	-0.246871
O	-1.163435	1.678492
H	-0.777129	2.051662
H	-2.895724	1.304578
H	-3.244290	-0.259919
S	-4.401060	-0.073384
H	-4.051514	0.829721
C	3.093733	0.403993
C	2.531376	-0.999804
N	4.233073	0.347029
H	3.941715	0.007278
H	4.617072	1.276044
H	3.418620	0.817137
C	1.944612	1.285692
O	1.769232	1.613989
O	1.105215	1.607035
H	0.344584	2.093014
H	1.697919	-0.921937
H	3.317772	-1.598029
S	2.010724	-1.979248
H	1.157856	-1.080012
28		
Dimer 142 of the n...n type		
C	-2.914843	-0.526383
C	-1.518699	-0.700233
N	-3.834231	-1.554260
H	-3.977566	-1.458427
H	-4.744418	-1.427445
H	-2.785863	-0.629197
C	-3.425164	0.901397
O	-4.467120	1.186268
O	-2.561663	1.817170
H	-2.917564	2.705364
H	-0.811008	-0.001208
H	-1.181633	-1.719812
S	-1.459027	-0.487032
H	-1.602184	0.854266
C	2.379668	0.887093
C	2.074115	-0.403185
N	1.237368	1.315620
H	1.035365	0.627071
H	1.451833	2.180897
H	2.595720	1.656692
C	3.667470	0.735891
O	3.768422	0.977830
O	4.691754	0.300197
H	5.487384	0.228449
H	2.872471	-0.623496
H	1.146553	-0.266731
S	1.801877	-1.887444
H	3.096928	-2.083534
28		
Dimer 143 of the n...n type		
C	1.895990	0.317060
C	2.003612	-1.077114
N	1.533031	0.233069
H	2.297720	-0.175386
H	1.378146	1.162623
H	1.095410	0.843814
C	3.164119	1.136263
O	3.819099	1.685205
O	3.468367	1.178002
H	4.271319	1.709219
H	2.135661	-0.998012
H	1.084802	-1.626333
S	3.355512	-2.128084
H	4.380535	-1.463511
C	-2.818003	-0.890397
C	-1.478263	-0.166905

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N	-3.202309	-0.913968	-1.692045	
H	-3.348499	0.037485	-2.020231	
H	-4.091273	-1.391981	-1.801441	
H	-2.664046	-1.921868	0.048887	
C	-3.894684	-0.307865	0.632514	
O	-4.971048	0.101613	0.267283	
O	-3.497082	-0.306719	1.920161	
H	-4.206139	0.062186	2.470786	
H	-1.133456	-0.280884	0.937758	
H	-0.735965	-0.587929	-0.764690	
S	-1.502304	1.629727	-0.510688	
H	-2.221899	2.039529	0.554393	
28				
Dimer 144 of the n...n type				
C	1.979053	-0.484059	0.597717	
C	1.579665	0.993617	0.459128	
N	2.963120	-0.674087	1.649200	
H	3.823382	-0.190818	1.403305	
H	3.200475	-1.657699	1.731187	
H	1.066371	-1.019938	0.877065	
C	2.404022	-1.057858	-0.757675	
O	3.451115	-1.616323	-0.979022	
O	1.449881	-0.866861	-1.692766	
H	1.740443	-1.252975	-2.534443	
H	0.764608	1.105739	-0.250001	
H	1.243694	1.354894	1.429267	
S	2.956564	2.113234	-0.047745	
H	3.035861	1.696940	-1.328643	
C	-1.784811	-0.563037	-0.517423	
C	-2.128617	0.912121	-0.784331	
N	-2.594582	-1.453318	-1.331351	
H	-3.572060	-1.368456	-1.064361	
H	-2.332631	-2.418600	-1.158032	
H	-0.736860	-0.693848	-0.806778	
C	-1.850893	-0.867923	0.982363	
O	-2.504022	-1.750608	1.484049	
O	-1.070030	-0.025161	1.690017	
H	-1.123197	-0.253064	2.631988	
H	-1.438452	1.571548	-0.262668	
H	-2.053071	1.098293	-1.855293	
S	-3.852417	1.388917	-0.323940	
H	-3.670750	1.359860	1.012538	
28				
Dimer 145 of the n...n type				
C	-2.056704	-0.439331	-0.653350	
C	-3.507010	-0.041188	-0.980831	
N	-1.988352	-1.741240	-0.015260	
H	-2.439929	-1.700174	0.894517	
H	-1.017477	-1.984872	0.150548	
H	-1.524629	-0.485959	-1.607983	
C	-1.381377	0.672592	0.150900	
O	-0.979383	0.564444	1.285265	
O	-1.292084	1.815080	-0.558573	
H	-0.904926	2.507879	0.000507	
H	-3.527600	0.880394	-1.559946	
H	-3.959159	-0.838890	-1.569993	
S	-4.606480	0.152452	0.490828	
H	-4.067212	1.301996	0.946282	
C	2.109191	-0.355447	0.880181	
C	2.127801	1.089122	0.347755	
N	3.210621	-0.602435	1.793998	
H	4.093315	-0.550978	1.292404	
H	3.147388	-1.541924	2.172941	
H	1.164465	-0.463904	1.420799	
C	2.046219	-1.333205	-0.294315	
O	2.889463	-2.150708	-0.571498	
O	0.913120	-1.162195	-1.012402	
H	0.917262	-1.774196	-1.766027	
H	1.257346	1.277028	-0.274872	

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H	2.107914	1.772226	1.196214	
S	3.641380	1.541559	-0.608395	
H	3.361314	0.814695	-1.709876	
28				
Dimer 146 of the n...n type				
C	-2.926445	-0.619245	0.459010	
C	-3.403915	0.825211	0.235421	
N	-2.180624	-0.748094	1.697974	
H	-1.327355	-0.197852	1.650896	
H	-1.876904	-1.708738	1.822326	
H	-3.830602	-1.236232	0.522944	
C	-2.165561	-1.122584	-0.772322	
O	-1.036469	-1.553184	-0.757600	
O	-2.906331	-1.021537	-1.892149	
H	-2.388647	-1.348099	-2.645592	
H	-4.081684	0.879182	-0.614086	
H	-3.929384	1.160318	1.129422	
S	-2.042305	2.047847	-0.013083	
H	-1.693479	1.655050	-1.255455	
C	1.487578	0.399794	-0.278090	
C	2.697811	0.202687	-1.197275	
N	1.433284	1.755230	0.249490	
H	2.228280	1.916176	0.862512	
H	0.596103	1.869527	0.812157	
H	0.593978	0.233753	-0.890644	
C	1.385478	-0.676596	0.809013	
O	0.929116	-0.479716	1.912827	
O	1.837517	-1.875928	0.404980	
H	1.686498	-2.522079	1.113119	
H	2.649465	-0.760149	-1.701342	
H	2.697270	0.993226	-1.947199	
S	4.331331	0.341387	-0.343100	
H	4.243105	-0.824451	0.328610	
28				
Dimer 147 of the n...n type				
C	-3.009376	0.333267	-0.715351	
C	-3.412864	-1.093335	-0.313997	
N	-2.105634	0.330884	-1.853877	
H	-1.301012	-0.255497	-1.652503	
H	-1.732356	1.262208	-2.008557	
H	-3.935865	0.847714	-1.001803	
C	-2.478526	1.124275	0.487221	
O	-1.471313	1.792058	0.480671	
O	-3.283290	1.007623	1.560051	
H	-2.924186	1.544087	2.285021	
H	-4.210093	-1.073526	0.425553	
H	-3.767662	-1.618666	-1.200603	
S	-2.020357	-2.119553	0.337206	
H	-1.898159	-1.479799	1.518439	
C	2.204475	-0.274702	0.869705	
C	1.120079	-0.169952	-0.213554	
N	2.167496	0.867641	1.767917	
H	2.351237	1.718544	1.242101	
H	2.908941	0.793325	2.457501	
H	1.974972	-1.180554	1.443934	
C	3.580294	-0.520897	0.242016	
O	4.565187	0.148196	0.447614	
O	3.566796	-1.590499	-0.577574	
H	4.454825	-1.717053	-0.948272	
H	1.050352	-1.097495	-0.777391	
H	0.167178	0.017976	0.272002	
S	1.332249	1.236230	-1.388821	
H	2.395007	0.731260	-2.050185	
28				
Dimer 148 of the n...n type				
C	2.825864	0.732205	-0.722135	
C	2.113797	-0.533574	-1.241783	
N	4.234029	0.485769	-0.459131	
H	4.329447	-0.181709	0.301355	

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H	4.691087	1.340782	-0.157866		
H	2.737105	1.480096	-1.515755		
C	2.050990	1.259227	0.486130		
O	2.364523	1.072711	1.638730		
O	0.933721	1.916301	0.118770		
H	0.404681	2.100630	0.913053		
H	1.077386	-0.314891	-1.498115		
H	2.634417	-0.876436	-2.136506		
S	2.157910	-1.986048	-0.099827		
H	1.530214	-1.409626	0.945564		
C	-2.279248	-0.477593	-0.945832		
C	-1.681129	-1.328282	0.186123		
N	-1.259796	0.308600	-1.618085		
H	-0.855559	0.984959	-0.976262		
H	-1.672966	0.843961	-2.374912		
H	-2.707401	-1.184250	-1.667081		
C	-3.459603	0.355494	-0.433582		
O	-3.578695	1.548528	-0.579752		
O	-4.365538	-0.409632	0.206809		
H	-5.099262	0.150491	0.506856		
H	-2.404552	-2.059428	0.540563		
H	-0.805820	-1.852434	-0.196903		
S	-1.073569	-0.362524	1.640245		
H	-2.283976	-0.073708	2.159856		
28					
Dimer 149 of the n...n type					
C	-1.665153	-0.156310	-0.364993		
C	-2.871695	-0.775472	-1.083643		
N	-1.083311	-1.081293	0.593193		
H	-1.780890	-1.335512	1.287878		
H	-0.330368	-0.623060	1.094757		
H	-0.916883	0.061506	-1.136212		
C	-2.002903	1.214802	0.233070		
O	-1.679395	1.584053	1.338829		
O	-2.680078	1.988894	-0.634013		
H	-2.838715	2.856256	-0.227719		
H	-3.193220	-0.145406	-1.909958		
H	-2.580666	-1.749688	-1.475939		
S	-4.322828	-1.101686	0.012831		
H	-4.688022	0.187639	0.167118		
C	2.749456	0.219533	-1.010142		
C	2.183176	-1.183989	-0.738766		
N	4.186117	0.178942	-1.229018		
H	4.649121	-0.147533	-0.384317		
H	4.538864	1.114894	-1.403189		
H	2.265142	0.575946	-1.927602		
C	2.325172	1.206976	0.083954		
O	3.070987	1.945664	0.679612		
O	0.996329	1.156663	0.300928		
H	0.735979	1.792014	0.988044		
H	1.095975	-1.182180	-0.751089		
H	2.540770	-1.856430	-1.518240		
S	2.746859	-1.938509	0.848407		
H	2.027724	-1.144303	1.667707		
28					
Dimer 150 of the n...n type					
C	3.142154	-0.669183	-0.626780		
C	1.634916	-0.566740	-0.351590		
N	3.737496	-1.796914	0.070785		
H	3.663095	-1.654291	1.074895		
H	4.729997	-1.849849	-0.136129		
C	3.246807	-0.830949	-1.706451		
C	3.839351	0.667298	-0.341888		
O	4.818481	0.800288	0.352806		
O	3.227708	1.691131	-0.968780		
H	3.704191	2.513758	-0.772709		
H	1.174382	0.182095	-0.991792		
H	1.173341	-1.533353	-0.549328		
S	1.205428	-0.177591	1.401442		

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H	1.587786	1.115681	1.370345		
C	-2.317792	-0.236479	0.745491		
C	-3.765098	-0.727677	0.562174		
N	-2.261019	1.007012	1.491912		
H	-2.694136	1.750496	0.950553		
H	-1.289555	1.271644	1.626014		
H	-1.796307	-1.012025	1.314093		
C	-1.623279	-0.166313	-0.615333		
O	-1.268453	0.849919	-1.164509		
O	-1.465846	-1.392033	-1.153029		
H	-1.062479	-1.304142	-2.031422		
H	-3.775547	-1.707898	0.088179		
H	-4.230375	-0.805621	1.544689		
S	-4.857888	0.413474	-0.394234		
H	-4.283795	0.219759	-1.599501		
28					
Dimer 151 of the n...n type					
C	-1.698213	-0.412827	0.128994		
C	-1.730808	1.043669	-0.357855		
N	-1.397302	-1.325662	-0.962398		
H	-2.157106	-1.319113	-1.637838		
H	-1.329384	-2.275894	-0.612416		
H	-0.886727	-0.491093	0.863049		
C	-2.974235	-0.769105	0.894170		
O	-3.652523	-1.748183	0.691393		
O	-3.253020	0.142297	1.847708		
H	-4.056345	-0.128775	2.320198		
H	-1.780509	1.731703	0.483497		
H	-0.822478	1.246225	-0.923872		
S	-3.111919	1.425636	-1.523611		
H	-4.099800	1.393960	-0.605683		
C	1.698185	-0.412494	-0.130233		
C	1.730792	1.042371	0.361452		
N	1.397617	-1.328996	0.958119		
H	2.157606	-1.324786	1.633362		
H	1.329484	-2.278032	0.604960		
H	0.886591	-0.488411	-0.864418		
C	2.974192	-0.765944	-0.896790		
O	3.653000	-1.745287	-0.697065		
O	3.252288	0.148406	-1.847710		
H	4.055694	-0.120830	-2.321109		
H	1.780407	1.733175	-0.477646		
H	0.822521	1.243158	0.928209		
S	3.111953	1.420490	1.528376		
H	4.099860	1.391424	0.610383		
28					
Dimer 152 of the n...n type					
C	-1.831964	-0.413006	-0.320700		
C	-3.140080	-0.904218	-0.961087		
N	-1.428040	-1.254146	0.789489		
H	-2.125122	-1.199622	1.527226		
H	-0.542524	-0.938402	1.189603		
H	-1.067083	-0.474748	-1.106203		
C	-1.913862	1.079035	0.030398		
O	-1.545111	1.561052	1.075457		
O	-2.417068	1.809225	-0.983649		
H	-2.417804	2.745811	-0.728359		
H	-3.346199	-0.368500	-1.885284		
H	-3.039634	-1.966428	-1.182207		
S	-4.615648	-0.771369	0.142533		
H	-4.741985	0.569597	0.067108		
C	1.874991	-0.667262	0.053185		
C	1.669281	0.781302	-0.414911		
N	1.554869	-0.810440	1.465246		
H	2.122153	-0.168657	2.013246		
H	1.789284	-1.745318	1.785281		
H	1.177179	-1.288357	-0.523310		
C	3.268455	-1.184762	-0.316151		
O	4.014676	-1.754575	0.443132		

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O	3.559980	-0.941566	-1.607911		
H	4.438153	-1.302610	-1.809716		
H	1.702354	0.844831	-1.500067		
H	0.697683	1.124456	-0.065505		
S	2.869963	1.989429	0.296379		
H	3.935969	1.591480	-0.428189		
28					
Dimer 153 of the n...n type					
C	1.827879	-0.878587	-0.279310		
C	1.499710	-0.045424	0.969937		
N	2.668560	-2.017986	0.046836		
H	3.569589	-1.692075	0.387330		
H	2.857786	-2.562392	-0.788772		
H	0.869694	-1.250163	-0.656035		
C	2.397499	0.015347	-1.384428		
C	3.453405	-0.157515	-1.944686		
O	1.562745	1.036123	-1.667902		
H	1.944688	1.576080	-2.378016		
H	0.787717	0.740187	0.734652		
H	1.060929	-0.700294	1.720893		
S	2.965400	0.728002	1.783762		
H	3.179813	1.678949	0.851065		
C	-2.756558	-0.299444	-0.861891		
C	-1.754067	0.863713	-0.859299		
N	-4.125383	0.176837	-0.975516		
H	-4.353138	0.751480	-0.167888		
H	-4.769721	-0.607552	-0.957783		
H	-2.522174	-0.905097	-1.746167		
C	-2.532366	-1.231785	0.335476		
O	-3.401911	-1.627490	1.073503		
O	-1.234860	-1.575524	0.467042		
H	-1.141741	-2.188168	1.214164		
H	-0.735067	0.503263	-0.963693		
H	-1.973201	1.512571	-1.707135		
S	-1.857435	1.961394	0.621711		
H	-1.432473	1.053225	1.524004		
28					
Dimer 154 of the n...n type					
C	-2.162599	0.957337	0.257136		
C	-1.639563	-0.142463	1.192780		
N	-3.538026	1.313361	0.558300		
H	-4.142065	0.510400	0.402444		
H	-3.857222	2.041130	-0.073318		
H	-1.528211	1.834555	0.436203		
C	-1.928399	0.591104	-1.214582		
O	-2.741969	0.698821	-2.097440		
O	-0.668018	0.143262	-1.411244		
H	-0.503898	-0.025362	-2.353097		
H	-0.577069	-0.305101	1.041250		
H	-1.804645	0.166903	2.224375		
S	-2.507618	-1.762484	1.028504		
H	-2.101068	-2.038028	-0.227828		
C	3.016320	-0.540016	0.413486		
C	2.292282	0.385054	1.409915		
N	4.171616	0.110008	-0.179114		
H	3.873094	0.914103	-0.724460		
H	4.636928	-0.521022	-0.823846		
H	3.355939	-1.405915	0.992265		
C	2.010395	-1.078556	-0.609366		
O	2.041290	-0.860461	-1.797280		
O	1.053786	-1.815102	-0.012579		
H	0.397681	-2.073294	-0.678683		
H	1.500079	-0.159337	1.921285		
H	3.011953	0.729348	2.152381		
S	1.600489	1.929162	0.668550		
H	0.806110	1.334271	-0.244014		
28					
Dimer 155 of the n...n type					
C	3.033553	-0.359326	0.628178		

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C	2.325801	0.971278	0.954080		
N	4.166354	-0.154118	-0.258103		
H	3.836809	0.152097	-1.169714		
H	4.660923	-1.028263	-0.405985		
H	3.398224	-0.753066	1.582194		
C	2.013724	-1.370549	0.101946		
O	1.926966	-1.738316	-1.045891		
O	1.183043	-1.793119	1.077386		
H	0.576759	-2.455568	0.709425		
H	1.496389	0.803967	1.638735		
H	3.049518	1.635204	1.426272		
S	1.700366	1.900836	-0.513462		
H	0.558819	1.208698	-0.669390		
C	-2.305976	-0.864367	0.444722		
C	-1.492919	-0.810166	-0.858040		
N	-3.660629	-1.331163	0.205297		
H	-4.144292	-0.675644	-0.403425		
H	-4.181789	-1.349526	1.076306		
H	-1.800455	-1.582969	1.101484		
C	-2.239404	0.475278	1.188974		
O	-3.194045	1.077009	1.616512		
O	-0.968903	0.907802	1.313801		
H	-0.961919	1.759357	1.779734		
H	-0.440343	-0.645957	-0.649629		
H	-1.590345	-1.766120	-1.371928		
S	-2.066415	0.453799	-2.072743		
H	-1.726744	1.540698	-1.348766		
28					
Dimer 156 of the n...n type					
C	2.523813	-0.658150	0.734316		
C	1.630844	0.568049	0.977225		
N	3.886070	-0.415720	1.183144		
H	4.289650	0.344414	0.640801		
H	4.463265	-1.230621	0.999593		
H	2.097141	-1.474145	1.330787		
C	2.441343	-1.132979	-0.722053		
O	3.395202	-1.387947	-1.417633		
O	1.166125	-1.247899	-1.142608		
H	1.160943	-1.562517	-2.060820		
H	0.585119	0.304097	0.858467		
H	1.785406	0.910206	2.000306		
S	2.019504	2.020523	-0.091458		
H	1.480612	1.527136	-1.224904		
C	-2.511950	-0.659206	-0.731651		
C	-1.618940	0.566796	-0.973841		
N	-3.868506	-0.424755	-1.201951		
H	-4.281380	0.339710	-0.672800		
H	-4.446144	-1.239273	-1.018053		
H	-2.075003	-1.479796	-1.314397		
C	-2.449458	-1.121919	0.729680		
O	-3.412228	-1.389951	1.407869		
O	-1.181089	-1.210785	1.176415		
H	-1.188425	-1.519958	2.096455		
H	-0.574358	0.305087	-0.842457		
H	-1.763431	0.901612	-2.000792		
S	-2.019896	2.025369	0.081652		
H	-1.488065	1.540224	1.221965		
28					
Dimer 157 of the n...n type					
C	-3.249519	-0.279809	-0.229150		
C	-2.579371	0.764718	-1.148398		
N	-4.156708	0.336564	0.722133		
H	-3.637541	0.909625	1.381065		
H	-4.635347	-0.376097	1.263847		
H	-3.820965	-0.940407	-0.887329		
C	-2.140691	-1.122081	0.405037		
O	-1.702720	-0.950188	1.521171		
O	-1.652886	-2.025818	-0.458012		
H	-0.853895	-2.448780	-0.087256		

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H	-1.918266	0.264268	-1.855694	
H	-3.356717	1.283332	-1.709645	
S	-1.659002	2.116334	-0.284667	
H	-0.961286	1.345989	0.570774	
C	2.069447	0.738917	-0.527809	
C	1.021093	-0.367057	-0.349511	
N	2.733805	0.641645	-1.815019	
H	3.291555	-0.207619	-1.851326	
H	3.380840	1.414688	-1.933731	
H	1.514768	1.683763	-0.488267	
C	3.026499	0.755991	0.668901	
O	4.225431	0.628176	0.599158	
O	2.359758	0.926361	1.827356	
H	2.992908	0.927508	2.563010	
H	0.480854	-0.233350	0.583409	
H	0.318846	-0.319773	-1.179942	
S	1.675394	-2.093670	-0.367430	
H	2.180895	-2.085544	0.883024	
28				
Dimer 158 of the n...n type				
C	3.208423	0.076297	0.930534	
C	1.705224	0.395278	0.895881	
N	4.003796	1.275606	1.134753	
H	3.881409	1.903289	0.344015	
H	4.990784	1.039260	1.160169	
H	3.361777	-0.596123	1.782930	
C	3.614022	-0.726341	-0.311510	
O	4.497523	-0.417675	-1.075499	
O	2.858428	-1.831906	-0.455412	
H	3.142427	-2.310283	-1.250712	
H	1.121217	-0.522824	0.883021	
H	1.447555	0.970039	1.785176	
S	1.181662	1.439045	-0.533796	
H	1.256130	0.468107	-1.466839	
C	-3.263606	-0.052664	0.905400	
C	-1.781331	-0.464096	0.961097	
N	-4.141115	-1.205177	1.020082	
H	-4.032268	-1.798702	0.201747	
H	-5.111120	-0.905861	1.029878	
H	-3.432168	0.605569	1.764748	
C	-3.520113	0.797032	-0.343408	
O	-4.251137	0.486973	-1.254331	
O	-2.811854	1.941507	-0.312698	
H	-2.974485	2.439366	-1.129749	
H	-1.143446	0.418056	0.963740	
H	-1.611099	-1.031006	1.876015	
S	-1.239783	-1.573033	-0.411323	
H	-1.124934	-0.612308	-1.350522	
28				
Dimer 159 of the n...n type				
C	1.549512	0.292667	-0.660348	
C	2.040112	-1.111622	-0.290994	
N	2.205690	0.794258	-1.857566	
H	3.205126	0.876979	-1.687543	
H	1.873553	1.730903	-2.066127	
H	0.479961	0.205742	-0.872763	
C	1.609838	1.266515	0.523074	
O	1.923216	2.429425	0.435858	
O	1.237023	0.683539	1.679290	
H	1.229325	1.349881	2.384830	
H	1.424237	-1.545970	0.492372	
H	1.970209	-1.747241	-1.172975	
S	3.809896	-1.178509	0.232668	
H	3.632927	-0.572124	1.424405	
C	-2.772650	0.039657	0.823458	
C	-1.645718	-1.005456	0.891895	
N	-4.079058	-0.586204	0.722645	
H	-4.146336	-1.101938	-0.150822	
H	-4.806023	0.121794	0.696402	

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H	-2.722340	0.601866	1.762997	
C	-2.488842	1.058876	-0.285803	
O	-3.210650	1.276809	-1.228477	
O	-1.314513	1.694262	-0.086726	
H	-1.175962	2.338291	-0.800014	
H	-0.694002	-0.520892	1.092783	
H	-1.861224	-1.693099	1.709754	
S	-1.495568	-2.089293	-0.594752	
H	-1.159236	-1.131844	-1.482763	
28				
Dimer 160 of the n...n type				
C	-2.724898	-0.786633	0.510735	
C	-1.359446	-0.225873	0.085227	
N	-3.140163	-1.880742	-0.351564	
H	-3.258328	-1.537919	-1.301765	
H	-4.048140	-2.228817	-0.059728	
H	-2.595707	-1.172429	1.529264	
C	-3.765015	0.334265	0.625429	
O	-4.853447	0.322183	0.101731	
O	-3.320821	1.348345	1.393670	
H	-4.009817	2.029726	1.449275	
H	-0.991580	0.483796	0.823861	
H	-0.652721	-1.048242	-0.004914	
S	-1.346956	0.583787	-1.573242	
H	-2.057191	1.674924	-1.219279	
C	2.196808	-0.273743	0.997562	
C	1.957124	1.094047	0.337384	
N	3.203873	-0.190726	2.042064	
H	4.096332	0.074535	1.632838	
H	3.344339	-1.102861	2.465205	
H	1.245563	-0.569889	1.454629	
C	2.498213	-1.339966	-0.062650	
O	3.468941	-2.058156	-0.065273	
O	1.536178	-1.385266	-1.005774	
H	1.753682	-2.074323	-1.653643	
H	1.114175	1.053790	-0.347633	
H	1.744244	1.823950	1.118189	
S	3.414579	1.762017	-0.579148	
H	3.323695	0.931745	-1.638522	
28				
Dimer 161 of the n...n type				
C	2.674516	-0.228275	1.019055	
C	1.926160	1.109877	0.856270	
N	4.114047	-0.026257	1.019542	
H	4.414143	0.291946	0.101664	
H	4.592391	-0.905049	1.191314	
H	2.375505	-0.632984	1.991448	
C	2.195536	-1.225643	-0.036669	
O	2.837652	-1.594739	-0.989526	
O	0.935666	-1.645910	0.212394	
H	0.654763	-2.241625	-0.502031	
H	0.849101	0.970665	0.921943	
H	2.246712	1.774173	1.658356	
S	2.282773	2.009460	-0.716158	
H	1.360621	1.371423	-1.464013	
C	-2.015738	-0.904746	0.406928	
C	-3.538831	-0.768504	0.209047	
N	-1.587035	-0.383568	1.692527	
H	-1.690311	0.626805	1.714987	
H	-0.605921	-0.597844	1.835645	
H	-1.797310	-1.974905	0.375247	
C	-1.310232	-0.261237	-0.786182	
O	-0.922073	0.883390	-0.820743	
O	-1.197980	-1.114213	-1.822985	
H	-0.790864	-0.651289	-2.573640	
H	-3.835855	-1.210618	-0.742119	
H	-4.037303	-1.307983	1.014773	
S	-4.200226	0.950211	0.316815	
H	-3.560089	1.444268	-0.762376	

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28		
Dimer 162 of the n...n type		
C 2.003201	-0.743709	0.418941
C 1.934480	0.707132	0.920608
N 3.107297	-1.466899	1.027951
H 3.988687	-1.048737	0.740502
H 3.123488	-2.424618	0.691569
H 1.062590	-1.211726	0.727348
C 2.011700	-0.787568	-1.112061
O 2.835793	-1.356944	-1.786298
O 0.967397	-0.108689	-1.629752
H 0.995172	-0.164147	-2.598310
H 1.019040	1.184806	0.584894
H 1.937962	0.696246	2.010094
S 3.376728	1.751981	0.432148
H 3.044529	1.877935	-0.869283
C -2.003302	-0.743382	-0.419525
C -1.934030	0.707930	-0.919733
N -3.107500	-1.465578	-1.029529
H -3.988760	-1.046558	-0.742910
H -3.124935	-2.423263	-0.693109
H -1.062731	-1.211439	-0.728109
C -2.012188	-0.788673	1.111439
O -2.837162	-1.357498	1.785045
O -0.966967	-0.111739	1.629803
H -0.994727	-0.168055	2.598310
H -1.018564	1.185000	-0.583267
H -1.937166	0.698143	-2.009233
S -3.376125	1.752723	-0.430702
H -3.044463	1.877070	0.871019
28		
Dimer 163 of the n...n type		
C 3.096585	-1.069813	-0.136602
C 1.633942	-0.602275	-0.199067
N 3.429471	-1.593695	1.177374
H 3.382638	-0.845183	1.864170
H 4.387672	-1.928958	1.186827
H 3.194453	-1.877494	-0.871385
C 4.036896	0.044248	-0.612143
O 4.971729	0.476130	0.019056
O 3.694147	0.492744	-1.835586
H 4.312798	1.191309	-2.102634
H 1.361478	-0.338587	-1.219284
H 0.990390	-1.414733	0.137989
S 1.245741	0.829466	0.903310
H 1.754930	1.789331	0.105256
C -1.923400	-0.278999	-0.209042
C -3.043922	-0.706730	-1.173075
N -1.685557	-1.282242	0.814441
H -2.545468	-1.447994	1.331588
H -1.018025	-0.929999	1.493528
H -1.023784	-0.172967	-0.821056
C -2.216150	1.113758	0.352183
O -2.452695	1.359451	1.511024
O -2.202137	2.046552	-0.619885
H -2.406056	2.912130	-0.231229
H -3.127618	0.005464	-1.992042
H -2.794632	-1.686012	-1.581984
S -4.703637	-0.923591	-0.392474
H -4.941901	0.381110	-0.146209
28		
Dimer 164 of the n...n type		
C -1.824793	0.510243	0.038392
C -3.170120	0.998411	0.587754
N -1.568785	1.044583	-1.292543
H -2.337947	0.794337	-1.909902
H -0.743986	0.609499	-1.693134
H -1.048937	0.874120	0.721594
C -1.678812	-1.011806	0.122342

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O -1.177651	-1.700094	-0.736888
O -2.145154	-1.504792	1.284018
H -1.982299	-2.461222	1.308216
H -3.272019	0.738490	1.638931
H -3.216632	2.082782	0.487752
S -4.644228	0.358406	-0.325883
H -4.545140	-0.914597	0.108731
C 1.724966	-0.332721	-0.134887
C 1.876210	1.161857	-0.463285
N 1.105606	-0.530533	1.163713
H 1.711801	-0.164688	1.893094
H 0.994580	-1.521979	1.349806
H 1.064554	-0.762551	-0.896737
C 3.060573	-1.066086	-0.296177
O 3.563031	-1.777303	0.541118
O 3.614266	-0.831008	-1.501882
H 4.448814	-1.322088	-1.568840
H 2.205715	1.296352	-1.491586
H 0.912989	1.655414	-0.339919
S 3.026616	2.073167	0.657200
H 4.168473	1.538788	0.176975
28		
Dimer 165 of the n...n type		
C -3.444051	0.564304	0.836848
C -4.010146	-0.861395	0.872978
N -4.257703	1.573073	0.155087
H -4.803063	1.156017	-0.595549
H -4.892650	2.040427	0.790756
H -3.301227	0.883280	1.875655
C -2.034721	0.595284	0.226841
O -1.196621	-0.265461	0.437205
O -1.792678	1.648398	-0.531660
H -2.659342	2.141301	-0.546038
H -3.332741	-1.522527	1.410549
H -4.969624	-0.851304	1.389847
S -4.360641	-1.576497	-0.789762
H -3.075782	-1.749916	-1.161178
C 3.479369	0.616734	-0.830907
C 4.040253	-0.813908	-0.852867
N 4.446680	1.553074	-0.278761
H 4.630967	1.316040	0.693057
H 4.056512	2.490328	-0.272133
H 3.295181	0.887429	-1.877933
C 2.104232	0.661204	-0.146426
O 1.824347	1.414447	0.762900
O 1.253070	-0.217212	-0.677299
H 0.364357	-0.163152	-0.232729
H 3.369628	-1.482570	-1.387637
H 5.005388	-0.803874	-1.359011
S 4.384061	-1.529507	0.814802
H 3.100283	-1.743159	1.169442
28		
Dimer 166 of the n...n type		
C 2.861957	-0.034961	-0.850278
C 1.538764	-0.800074	-0.957734
N 4.075693	-0.840466	-0.698293
H 3.890780	-1.678830	-0.152585
H 4.455765	-1.121182	-1.594343
H 2.964011	0.556770	-1.767722
C 2.844291	1.016299	0.272924
O 1.866998	1.672956	0.585576
O 4.013959	1.186610	0.863464
H 4.598669	0.494087	0.449960
H 0.714524	-0.115246	-1.148610
H 1.600754	-1.494947	-1.795411
S 1.143817	-1.853201	0.503287
H 0.874321	-0.850882	1.364524
C -3.051564	1.041895	0.223178
C -3.214900	-0.276415	1.002501

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N	-3.979952	1.110046	-0.893775	
H	-3.745022	0.394641	-1.576896	
H	-3.889855	2.002217	-1.369670	
H	-3.297811	1.842959	0.929206	
C	-1.584918	1.258651	-0.166415	
O	-1.179428	1.309614	-1.308837	
O	-0.796849	1.377385	0.906126	
H	0.145117	1.512930	0.639532	
H	-2.570185	-0.287349	1.879293	
H	-4.251440	-0.354606	1.329546	
S	-2.906524	-1.809130	0.019069	
H	-1.555719	-1.795234	0.084272	
28				
Dimer 167 of the n...n type				
C	-3.282856	0.325427	0.743611	
C	-2.467643	-0.953658	0.976496	
N	-4.607282	0.142712	0.144780	
H	-4.611473	-0.648042	-0.495173	
H	-5.322549	-0.008520	0.845791	
H	-3.415136	0.806279	1.719939	
C	-2.524259	1.371611	-0.091026	
O	-1.332789	1.604677	0.013627	
O	-3.291775	2.051293	-0.923434	
H	-4.191057	1.632756	-0.819536	
H	-1.516471	-0.727331	1.455345	
H	-3.030859	-1.606748	1.642991	
S	-2.160908	-1.948545	-0.545488	
H	-1.134785	-1.209253	-1.020255	
C	2.785928	-0.935364	0.528130	
C	3.765366	0.164984	0.970286	
N	3.407765	-1.848154	-0.417326	
H	3.634889	-1.349208	-1.273744	
H	2.752947	-2.578914	-0.677764	
H	2.529195	-1.495910	1.434856	
C	1.469909	-0.321862	0.032580	
O	1.010981	-0.503314	-1.076994	
O	0.881586	0.427374	0.966567	
H	0.047928	0.832500	0.613454	
H	3.329978	0.771206	1.761734	
H	4.672556	-0.307009	1.346932	
S	4.337977	1.279463	-0.386175	
H	3.195671	1.984529	-0.518714	
28				
Dimer 168 of the n...n type				
C	3.086602	0.731095	-0.289593	
C	3.486525	-0.742813	-0.124128	
N	3.094385	1.542386	0.930669	
H	2.977795	0.962126	1.757815	
H	3.948306	2.077758	1.028408	
H	3.773204	1.177649	-1.016359	
C	1.695322	0.843906	-0.930263	
O	1.342778	0.172146	-1.885031	
O	0.903626	1.732988	-0.355459	
H	1.461806	2.096484	0.391419	
H	3.419783	-1.254548	-1.082738	
H	4.515712	-0.797793	0.230271	
S	2.488392	-1.656965	1.128352	
H	1.308580	-1.620574	0.467713	
C	-3.099584	-0.759870	-0.392593	
C	-3.465447	0.713832	-0.137931	
N	-3.482697	-1.598572	0.732163	
H	-2.941951	-1.333523	1.551749	
H	-3.249671	-2.567798	0.539618	
H	-3.672559	-1.072270	-1.273248	
C	-1.618823	-0.866131	-0.777857	
O	-0.801921	-1.512315	-0.153093	
O	-1.330709	-0.144258	-1.860975	
H	-0.346778	-0.095049	-1.985982	
H	-3.321513	1.305069	-1.039548	

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H	-4.513168	0.767843	0.156872	
S	-2.532891	1.508687	1.245226	
H	-1.347147	1.611773	0.607589	
28				
Dimer 169 of the n...n type				
C	1.999992	0.200824	-0.835778	
C	1.448901	-1.105970	-0.246439	
N	3.148778	0.062080	-1.732976	
H	3.679467	-0.781119	-1.529980	
H	2.870969	0.042721	-2.706505	
H	1.174144	0.678472	-1.372967	
C	2.364961	1.207819	0.266952	
O	1.653822	1.447494	1.229996	
O	3.515196	1.824421	0.078342	
H	3.861173	1.426106	-0.769997	
H	0.611717	-0.901935	0.417720	
H	1.096497	-1.739755	-1.060181	
S	2.688105	-2.127470	0.656244	
H	2.828655	-1.311120	1.720949	
C	-3.112848	0.865925	0.325629	
C	-3.380662	-0.584350	0.766360	
N	-3.851668	1.193183	-0.882840	
H	-3.509756	0.628768	-1.656328	
H	-3.689704	2.161720	-1.140208	
H	-3.478163	1.501982	1.139933	
C	-1.604418	1.128390	0.230367	
O	-1.028965	1.435595	-0.793556	
O	-0.992583	0.969985	1.406729	
H	-0.019343	1.150421	1.318793	
H	-2.894847	-0.793934	1.717149	
H	-4.455829	-0.717441	0.884610	
S	-2.880562	-1.873886	-0.457360	
H	-1.550754	-1.805808	-0.249049	
28				
Dimer 170 of the n...n type				
C	-2.103496	0.180174	-0.677779	
C	-3.523406	-0.160423	-1.163717	
N	-1.215139	-0.956292	-0.468377	
H	-1.666158	-1.649496	0.123829	
H	-1.014720	-1.408772	-1.354403	
H	-1.652763	0.806263	-1.459931	
C	-2.150331	1.100213	0.555708	
O	-3.114415	1.809915	0.777206	
O	-1.094514	1.135812	1.352264	
H	-0.301754	0.549911	1.117374	
H	-4.092568	0.745155	-1.365804	
H	-3.451577	-0.738948	-2.085516	
S	-4.486587	-1.221950	-0.003330	
H	-4.683072	-0.273630	0.934451	
C	1.938945	-0.608663	0.109631	
C	1.933892	0.399599	-1.048736	
N	1.336961	-0.036355	1.308262	
H	1.911594	0.733569	1.646386	
H	1.321714	-0.727868	2.053132	
H	1.309099	-1.443122	-0.212435	
C	3.333452	-1.182356	0.357418	
O	3.908668	-1.173374	1.420137	
O	3.851554	-1.720629	-0.762243	
H	4.729965	-2.081774	-0.561634	
H	2.299105	-0.064930	-1.961928	
H	0.907867	0.725149	-1.212299	
S	2.888154	1.945709	-0.732712	
H	4.120763	1.411816	-0.857807	
28				
Dimer 171 of the n...n type				
C	-1.976817	-0.177480	-0.334488	
C	-2.969024	-1.343575	-0.248255	
N	-1.314976	0.210910	0.910668	
H	-1.914094	0.032766	1.712620	

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H	-0.432360	-0.298142	1.019727	
H	-1.199319	-0.477537	-1.047559	
C	-2.623117	1.068894	-0.970005	
O	-3.394926	1.031702	-1.903408	
O	-2.226895	2.209338	-0.407326	
H	-1.639355	1.907402	0.340435	
H	-3.382449	-1.562821	-1.231295	
H	-2.450830	-2.230068	0.117832	
S	-4.355601	-1.072578	0.937998	
H	-4.996411	-0.128424	0.218913	
C	2.074568	-0.468597	-0.397600	
C	2.101006	1.045338	-0.119463	
N	1.375146	-1.186762	0.658094	
H	1.910257	-1.136498	1.521575	
H	1.294268	-2.171235	0.423635	
H	1.519052	-0.599178	-1.333135	
C	3.485360	-1.001684	-0.668640	
O	4.029963	-1.874569	-0.035604	
O	4.057438	-0.374395	-1.713388	
H	4.947543	-0.736668	-1.850776	
H	2.546183	1.581121	-0.955049	
H	1.076706	1.391916	0.012478	
S	2.967835	1.526258	1.435851	
H	4.227388	1.325455	0.996199	
28				
Dimer 172 of the n...n type				
C	3.438653	-0.319661	-0.413920	
C	3.600578	0.891042	0.517910	
N	3.125749	-0.014754	-1.814028	
H	2.713225	0.910791	-1.902467	
H	3.944591	-0.062545	-2.407797	
H	4.373478	-0.887945	-0.373983	
C	2.367980	-1.282019	0.133052	
O	2.296504	-1.648705	1.279625	
O	1.507379	-1.698606	-0.811561	
H	1.818645	-1.227383	-1.639287	
H	3.741636	0.549830	1.542256	
H	4.476952	1.465678	0.217794	
S	2.199408	2.088320	0.452743	
H	1.225346	1.246333	0.863505	
C	-3.028005	-0.546470	0.879325	
C	-3.827650	-0.488975	-0.433292	
N	-3.407217	0.533405	1.775927	
H	-3.160016	1.426860	1.357867	
H	-2.881786	0.468629	2.642121	
H	-3.288512	-1.499936	1.354178	
C	-1.522114	-0.620746	0.594518	
O	-0.707033	0.162626	1.033134	
O	-1.212997	-1.655876	-0.193165	
H	-0.245980	-1.673524	-0.369496	
H	-3.632556	-1.369074	-1.042073	
H	-4.889864	-0.456181	-0.192185	
S	-3.522661	1.019913	-1.453267	
H	-2.300306	0.671661	-1.905180	
28				
Dimer 173 of the n...n type				
C	-2.150976	-0.280320	0.799376	
C	-3.599013	0.180188	1.036863	
N	-1.194991	0.774776	0.467803	
H	-1.567072	1.355235	-0.279922	
H	-1.054565	1.381813	1.268937	
H	-1.813066	-0.737392	1.738907	
C	-2.076444	-1.420822	-0.235304	
O	-3.073186	-1.925991	-0.720368	
O	-0.871702	-1.860688	-0.556863	
H	-0.086367	-1.452172	-0.037515	
H	-4.238610	-0.666571	1.282559	
H	-3.611941	0.877688	1.875615	
S	-4.358602	1.112835	-0.360980	

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H	-4.443697	0.065934	-1.205207	
C	2.318022	-0.658917	-0.381682	
C	1.852555	0.633909	-1.067572	
N	1.367140	-1.077792	0.647781	
H	1.200013	-0.308069	1.292833	
H	1.755534	-1.842158	1.194210	
H	2.347366	-1.435202	-1.155985	
C	3.748718	-0.549212	0.148351	
O	4.092776	-0.839456	1.269198	
O	4.592881	-0.108845	-0.800671	
H	5.491261	-0.074594	-0.434394	
H	2.463375	0.842241	-1.942577	
H	0.815982	0.509888	-1.374755	
S	1.851232	2.116810	0.029652	
H	3.171348	2.381045	-0.061107	
28				
Dimer 174 of the n...n type				
C	-2.151270	-0.613109	0.410311	
C	-2.075089	0.868420	0.801668	
N	-1.383535	-1.024381	-0.764626	
H	-1.389877	-0.287339	-1.466349	
H	-0.411948	-1.226141	-0.506728	
H	-1.776027	-1.185610	1.267774	
C	-3.608391	-1.083593	0.243338	
O	-4.531432	-0.697384	0.926382	
O	-3.757740	-1.996334	-0.716576	
H	-2.848239	-2.068413	-1.116615	
H	-2.696880	1.061621	1.674349	
H	-1.044475	1.123146	1.047591	
S	-2.549224	2.035377	-0.544367	
H	-3.868025	1.751932	-0.545166	
C	2.452440	-0.745259	-0.542127	
C	2.016531	0.688719	-0.897010	
N	1.459922	-1.411980	0.287551	
H	1.415159	-0.963177	1.199270	
H	1.727666	-2.377368	0.452518	
H	2.529625	-1.285446	-1.492164	
C	3.858527	-0.748426	0.066238	
O	4.133370	-1.142943	1.174448	
O	4.767761	-0.248115	-0.791203	
H	5.641482	-0.259742	-0.368282	
H	2.728179	1.145842	-1.581417	
H	1.044070	0.648313	-1.386327	
S	1.767597	1.806344	0.548478	
H	3.068472	1.987089	0.856380	
28				
Dimer 175 of the n...n type				
C	-3.243484	0.337840	0.450426	
C	-2.746523	-1.027542	0.956888	
N	-3.940161	0.326517	-0.839860	
H	-3.703421	-0.508320	-1.370946	
H	-4.946002	0.364539	-0.729769	
H	-3.917195	0.737756	1.215130	
C	-2.085697	1.353082	0.387339	
O	-1.304797	1.535607	1.295325	
O	-2.030491	2.038267	-0.753971	
H	-2.796261	1.682216	-1.282129	
H	-2.124971	-0.881282	1.839260	
H	-3.602856	-1.642682	1.233641	
S	-1.824745	-2.023365	-0.292238	
H	-0.806465	-1.131187	-0.529248	
C	1.516568	0.417207	0.191936	
C	1.925318	-0.898359	0.877457	
N	0.658963	0.169184	-0.956239	
H	1.196902	-0.228055	-1.721641	
H	0.246373	1.034326	-1.291048	
H	0.934777	0.980563	0.927969	
C	2.741140	1.272484	-0.136441	
O	3.053801	1.645601	-1.242668	

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O	3.447554	1.569729	0.971663		
H	4.215858	2.107198	0.720508		
H	2.499175	-0.700420	1.780480		
H	1.019958	-1.439828	1.150694		
S	2.870475	-2.068813	-0.191162		
H	4.048375	-1.411787	-0.164236		
28					
Dimer 176 of the n...n type					
C	2.687028	0.626573	-0.830792		
C	3.580337	-0.607366	-1.009600		
N	3.328300	1.823158	-0.278730		
H	4.082798	1.572432	0.356081		
H	3.706520	2.419036	-1.005302		
H	2.282687	0.880845	-1.817275		
C	1.446696	0.303586	0.018319		
O	0.819351	-0.726751	-0.047228		
O	1.098130	1.305711	0.837447		
H	1.803240	1.998036	0.695529		
H	3.005507	-1.429557	-1.432487		
H	4.394680	-0.365128	-1.692254		
S	4.399257	-1.176911	0.541008		
H	3.289669	-1.656408	1.139395		
C	-3.648950	0.476208	0.292443		
C	-3.496555	-0.973148	0.789468		
N	-4.432392	0.533846	-0.931323		
H	-3.936870	0.047098	-1.674125		
H	-4.532927	1.496599	-1.237490		
H	-4.188256	1.016147	1.079292		
C	-2.269101	1.135771	0.183124		
O	-1.796041	1.573230	-0.842284		
O	-1.632377	1.149774	1.362330		
H	-0.700105	1.422125	1.227114		
H	-3.028622	-0.991793	1.771368		
H	-4.486847	-1.422186	0.861846		
S	-2.546029	-2.080622	-0.342706		
H	-1.323723	-1.551195	-0.114060		
28					
Dimer 177 of the n...n type					
C	1.957395	-0.526062	0.471966		
C	3.439281	-0.510667	0.878941		
N	1.642695	-1.358971	-0.698533		
H	2.302963	-1.174165	-1.453738		
H	1.768859	-2.338698	-0.454739		
H	1.381986	-0.927679	1.311280		
C	1.432770	0.907670	0.317605		
O	1.657026	1.764478	1.136714		
O	0.685974	1.186547	-0.765428		
H	0.607390	0.401178	-1.330636		
H	3.574744	0.081009	1.782214		
H	3.764531	-1.531425	1.081032		
S	4.576165	0.111288	-0.432866		
H	4.244591	1.414448	-0.328328		
C	-3.205772	-0.960382	-0.124420		
C	-3.441751	0.326275	-0.938585		
N	-3.948596	-0.935921	1.125341		
H	-3.580437	-0.203368	1.726610		
H	-3.820673	-1.810046	1.625580		
H	-3.584211	-1.783794	-0.740033		
C	-1.701461	-1.201317	0.041942		
O	-1.116531	-1.159627	1.105122		
O	-1.097173	-1.435611	-1.126590		
H	-0.104999	-1.502681	-0.991815		
H	-2.953262	0.259733	-1.908934		
H	-4.513887	0.445649	-1.093258		
S	-2.906536	1.885272	-0.105552		
H	-1.577483	1.729708	-0.281443		
28					
Dimer 178 of the n...n type					
C	-2.175439	-0.729764	0.040700		

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C	-3.625802	-1.189335	-0.155404		
N	-1.750255	-0.478827	1.418711		
H	-2.525038	-0.140403	1.984039		
H	-1.376108	-1.312465	1.855604		
H	-1.528784	-1.511242	-0.375314		
C	-1.860324	0.512193	-0.811359		
O	-2.278212	0.698988	-1.928335		
O	-1.026747	1.372439	-0.205864		
H	-0.863430	0.983537	0.697524		
H	-3.828844	-1.358498	-1.211504		
H	-3.782438	-2.123988	0.383137		
S	-4.883335	-0.023367	0.522309		
H	-4.704363	0.950490	-0.393480		
C	3.642967	0.671124	0.067596		
C	3.724617	-0.518174	-0.906860		
N	4.295621	0.364108	1.329329		
H	3.791619	-0.381796	1.802094		
H	4.262748	1.169227	1.946828		
H	4.179823	1.497210	-0.412601		
C	2.188127	1.130443	0.212457		
O	1.567070	1.130591	1.252854		
O	1.666799	1.516872	-0.961619		
H	0.712187	1.699029	-0.836555		
H	3.348081	-0.237501	-1.888209		
H	4.768159	-0.817357	-1.001776		
S	2.842469	-2.040356	-0.344328		
H	1.586520	-1.603679	-0.572828		
28					
Dimer 179 of the n...n type					
C	-2.054628	0.376096	-0.051704		
C	-2.211336	-0.823704	-0.994968		
N	-1.551832	0.092602	1.291591		
H	-1.868412	-0.821226	1.607025		
H	-0.527086	0.113111	1.326719		
H	-1.356496	1.072254	-0.532773		
C	-3.366401	1.177485	0.064229		
O	-4.124518	1.376421	-0.859738		
O	-3.575420	1.664016	1.286222		
H	-2.812589	1.298635	1.815509		
H	-2.569836	-0.495966	-1.969376		
H	-1.244756	-1.310277	-1.126149		
S	-3.329728	-2.144302	-0.357544		
H	-4.480553	-1.454249	-0.493127		
C	2.090905	-0.503332	0.142310		
C	2.011932	0.534208	-0.990058		
N	1.514764	0.011814	1.375843		
H	1.999181	0.863328	1.651002		
H	1.657300	-0.652950	2.130938		
H	1.495791	-1.364334	-0.185864		
C	3.519721	-1.031854	0.311152		
O	4.143280	-1.024422	1.345639		
O	4.002072	-1.528746	-0.843164		
H	4.900895	-1.863065	-0.692448		
H	2.339321	0.098734	-1.931262		
H	0.977205	0.856177	-1.099698		
S	2.958141	2.087041	-0.680908		
H	4.190430	1.573561	-0.874732		
28					
Dimer 180 of the n...n type					
C	-2.071621	-0.263930	-0.142987		
C	-2.350480	1.003536	0.673393		
N	-2.134491	-0.127171	-1.598882		
H	-2.823952	0.569826	-1.869847		
H	-1.231004	0.148193	-1.970353		
H	-1.058150	-0.594029	0.112097		
C	-2.977282	-1.430865	0.291139		
O	-3.298739	-1.645407	1.438792		
O	-3.353673	-2.215642	-0.718562		
H	-2.976950	-1.772038	-1.523792		

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H	-2.252858	0.797000	1.737770	
H	-1.627723	1.772445	0.399853	
S	-4.001060	1.761236	0.354378	
H	-4.734432	0.797123	0.947438	
C	3.254223	0.637300	0.805335	
C	1.771710	0.491926	0.424497	
N	3.808029	1.883109	0.304095	
H	3.813053	1.874166	-0.712621	
H	4.774857	1.981660	0.596961	
H	3.285903	0.658972	1.901298	
C	4.053370	-0.607263	0.395334	
O	5.057295	-0.596481	-0.276442	
O	3.504640	-1.735051	0.887568	
H	4.045002	-2.493667	0.613967	
H	1.333932	-0.378253	0.908853	
H	1.241147	1.384336	0.754753	
S	1.455949	0.389071	-1.392101	
H	1.862487	-0.885782	-1.560409	
28				
Dimer 181 of the n...n type				
C	2.235566	-0.438625	0.308064	
C	1.857194	1.010126	-0.019236	
N	2.610872	-0.715631	1.696694	
H	3.086101	0.082784	2.110848	
H	1.801879	-0.932802	2.266600	
H	1.362970	-1.053697	0.061180	
C	3.342954	-0.959972	-0.623848	
O	3.425231	-0.674991	-1.797841	
O	4.195724	-1.794500	-0.027887	
H	3.907894	-1.803869	0.921321	
H	1.547687	1.093248	-1.059519	
H	1.025639	1.315322	0.615521	
S	3.190916	2.238282	0.318132	
H	4.009037	1.859992	-0.685141	
C	-3.268274	-0.040056	0.924426	
C	-1.769869	-0.083938	0.581173	
N	-3.759242	-1.352814	1.306419	
H	-3.700296	-1.986163	0.513100	
H	-4.740123	-1.301322	1.562276	
H	-3.364922	0.632039	1.785453	
C	-4.069501	0.617780	-0.206394	
O	-5.013638	0.117915	-0.770367	
O	-3.597477	1.845270	-0.500348	
H	-4.134413	2.226498	-1.213541	
H	-1.385386	0.919138	0.411404	
H	-1.236026	-0.528505	1.420818	
S	-1.345930	-1.136372	-0.875362	
H	-1.708385	-0.255544	-1.829995	
28				
Dimer 182 of the n...n type				
C	2.301462	0.152396	0.668343	
C	3.699910	0.779313	0.627073	
N	2.200212	-1.168359	1.295369	
H	3.059565	-1.698230	1.172072	
H	2.006801	-1.100695	2.287322	
H	1.649842	0.839633	1.218072	
C	1.671332	0.085977	-0.734947	
O	1.767422	0.967015	-1.559726	
O	0.971599	-1.027573	-0.955869	
H	1.090352	-1.558569	-0.124556	
H	3.659303	1.759347	0.154814	
H	4.071733	0.898157	1.644889	
S	4.966745	-0.250246	-0.232335	
H	4.481849	-0.088393	-1.480562	
C	-3.368191	0.415821	-0.752872	
C	-1.892807	0.824146	-0.610436	
N	-4.256885	1.472035	-0.298670	
H	-4.119977	1.631272	0.696311	
H	-5.225545	1.191872	-0.415010	

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H	-3.538410	0.254074	-1.824142	
C	-3.626203	-0.940581	-0.084460	
O	-4.466492	-1.150970	0.757983	
O	-2.799210	-1.893714	-0.557099	
H	-3.000443	-2.733065	-0.112959	
H	-1.238279	0.083760	-1.063648	
H	-1.746217	1.779784	-1.112921	
S	-1.341154	1.109124	1.128086	
H	-1.262894	-0.187236	1.492889	
28				
Dimer 183 of the n...n type				
C	1.758255	-0.018675	0.351351	
C	2.717728	-1.200891	0.530824	
N	0.947106	-0.017559	-0.867018	
H	1.460645	-0.417141	-1.648934	
H	0.099476	-0.556814	-0.725248	
H	1.063718	-0.038759	1.198401	
C	2.489241	1.329230	0.472086	
O	3.389913	1.541756	1.253076	
O	2.017002	2.270852	-0.347157	
H	1.327404	1.804340	-0.885504	
H	3.248144	-1.117273	1.477936	
H	2.145952	-2.129093	0.533148	
S	3.947059	-1.394487	-0.830779	
H	4.684462	-0.305320	-0.532082	
C	-2.836607	0.655331	0.765145	
C	-3.756041	0.514041	-0.463687	
N	-1.794263	1.638139	0.530942	
H	-1.175539	1.328333	-0.213156	
H	-1.223096	1.759572	1.360908	
H	-3.472832	1.006763	1.584157	
C	-2.320102	-0.725375	1.181280	
O	-1.177723	-1.107749	1.059437	
O	-3.302111	-1.491303	1.685663	
H	-2.941444	-2.365592	1.906001	
H	-4.591511	-0.148753	-0.245592	
H	-4.147294	1.500300	-0.712024	
S	-2.915623	-0.064002	-2.002107	
H	-2.782463	-1.359196	-1.649442	
28				
Dimer 184 of the n...n type				
C	2.633362	-0.731414	-0.632252	
C	2.201169	0.534237	-1.383274	
N	1.595326	-1.439904	0.119285	
H	0.814138	-0.845549	0.420081	
H	1.215533	-2.215992	-0.408686	
H	3.044416	-1.416182	-1.383044	
C	3.817810	-0.440161	0.311920	
O	4.755554	0.270332	0.019763	
O	3.723373	-1.067806	1.481209	
H	2.841387	-1.534792	1.418949	
H	3.021985	0.904547	-1.995182	
H	1.364111	0.296326	-2.039653	
S	1.608701	1.911760	-0.308130	
H	2.817042	2.261242	0.176838	
C	-1.814296	0.416599	0.004193	
C	-2.101713	-0.693041	-1.023078	
N	-0.992011	-0.075881	1.096426	
H	-1.521953	-0.734877	1.660725	
H	-0.720075	0.688218	1.706735	
H	-1.252092	1.191146	-0.529019	
C	-3.112960	1.086340	0.464822	
O	-3.496729	1.144183	1.608859	
O	-3.790579	1.614634	-0.572354	
H	-4.605122	2.025702	-0.240903	
H	-2.645487	-0.295533	-1.877420	
H	-1.152000	-1.096511	-1.372500	
S	-3.014463	-2.148110	-0.350589	
H	-4.226073	-1.561733	-0.261200	

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28		
Dimer 185 of the n...n type		
C	1.513086 0.122375 -0.672107	
C	1.993217 -1.215691 -0.100497	
N	2.224573 0.620364 -1.852653	
H	3.200744 0.334798 -1.837536	
H	1.808608 0.281154 -2.711709	
H	0.459120 -0.010259 -0.935100	
C	1.499574 1.222440 0.401099	
O	1.160638 1.035644 1.550440	
O	1.867491 2.419597 -0.049119	
H	2.110117 2.258563 -0.998553	
H	1.378447 -1.501608 0.749474	
H	1.896918 -1.986111 -0.865038	
S	3.770976 -1.236877 0.391851	
H	3.646057 -0.441742 1.474144	
C	-2.662759 -0.624992 0.897251	
C	-3.217583 0.737847 0.448232	
N	-1.653537 -0.473540 1.929365	
H	-0.845909 0.040807 1.584414	
H	-1.310795 -1.382703 2.222702	
H	-3.512428 -1.175560 1.319076	
C	-2.202683 -1.444204 -0.314599	
O	-1.087893 -1.882744 -0.475822	
O	-3.202333 -1.627093 -1.199251	
H	-2.869583 -2.150525 -1.946047	
H	-4.091918 0.609816 -0.186216	
H	-3.507919 1.299439 1.335613	
S	-2.002998 1.814380 -0.433954	
H	-2.086698 1.206229 -1.634827	
28		
Dimer 186 of the n...n type		
C	-2.555733 -0.801844 0.362681	
C	-1.907143 0.439957 0.986296	
N	-1.907493 -1.343648 -0.835845	
H	-1.472556 -0.603494 -1.380981	
H	-1.200462 -2.030862 -0.605102	
H	-2.552278 -1.584229 1.130329	
C	-4.048369 -0.570546 0.055705	
O	-4.793824 0.058852 0.772822	
O	-4.461290 -1.156454 -1.068516	
H	-3.637802 -1.557643 -1.451562	
H	-2.463815 0.748563 1.869703	
H	-0.877166 0.213415 1.270231	
S	-1.762653 1.874706 -0.162599	
H	-3.080741 2.140122 -0.272120	
C	1.962175 -0.580937 0.141292	
C	1.983460 0.612374 -0.829442	
N	1.477623 -0.188876 1.452725	
H	2.104468 0.500165 1.860207	
H	1.475345 -0.986142 2.081173	
H	1.261602 -1.307900 -0.286055	
C	3.322781 -1.288175 0.168433	
O	3.991113 -1.470770 1.158170	
O	3.691989 -1.698960 -1.060376	
H	4.553264 -2.142491 -0.999077	
H	2.247460 0.286452 -1.833174	
H	0.989323 1.056380 -0.858703	
S	3.101940 1.992978 -0.332991	
H	4.266934 1.386048 -0.640192	
28		
Dimer 187 of the n...n type		
C	2.932527 -0.443777 -0.833753	
C	1.525862 -0.833938 -0.364420	
N	4.004186 -1.403954 -0.555895	
H	3.826506 -1.905988 0.310810	
H	4.102867 -2.083563 -1.300537	
H	2.880468 -0.301846 -1.919392	
C	3.346604 0.935791 -0.284938	

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O	2.585076 1.869211 -0.164880	
O	4.641093 1.022205 0.021318	
H	4.992930 0.108001 -0.138979	
H	0.809991 -0.061274 -0.637260	
H	1.233793 -1.769020 -0.842920	
S	1.395618 -1.159544 1.446267	
H	1.565077 0.117298 1.846541	
C	-2.238703 0.108784 0.804146	
C	-2.339869 -1.130601 -0.098807	
N	-3.298576 0.127716 1.798026	
H	-4.200999 0.218658 1.338317	
H	-3.199513 0.937471 2.402023	
H	-1.276374 0.021357 1.323179	
C	-2.141237 1.396123 -0.022056	
O	-2.835681 2.373221 0.127062	
O	-1.158476 1.323128 -0.943017	
H	-1.109619 2.165149 -1.423467	
H	-1.473912 -1.207678 -0.751628	
H	-2.377491 -2.015836 0.535328	
S	-3.868847 -1.209928 -1.129407	
H	-3.508537 -0.273937 -2.031582	
28		
Dimer 188 of the n...n type		
C	-1.977283 -0.408690 -0.582791	
C	-2.512593 1.024091 -0.683433	
N	-2.796619 -1.455879 -1.198349	
H	-3.785540 -1.221854 -1.153425	
H	-2.549069 -1.603664 -2.169448	
H	-0.990961 -0.405562 -1.066925	
C	-1.683246 -0.798259 0.874121	
O	-1.197496 -0.043077 1.688679	
O	-1.964907 -2.069603 1.157925	
H	-2.367863 -2.421085 0.320722	
H	-1.823067 1.718055 -0.205618	
H	-2.608747 1.299705 -1.733825	
S	-4.195657 1.262393 0.034737	
H	-3.838252 1.109194 1.326225	
C	1.631250 0.483495 -0.077440	
C	1.942766 -0.925916 0.452720	
N	1.168007 0.436541 -1.455214	
H	1.902868 0.069825 -2.054744	
H	0.962370 1.373039 -1.789066	
H	0.818460 0.866228 0.550707	
C	2.813991 1.430895 0.144521	
O	3.357402 2.078395 -0.718984	
O	3.180076 1.472175 1.440558	
H	3.923810 2.088267 1.538362	
H	2.164257 -0.896705 1.517103	
H	1.069411 -1.558209 0.297729	
S	3.314575 -1.795560 -0.423926	
H	4.330023 -1.088003 0.112549	
28		
Dimer 189 of the n...n type		
C	2.635441 0.504290 0.971654	
C	3.403840 -0.657526 0.332151	
N	1.529252 0.164242 1.865241	
H	0.969341 -0.618652 1.531533	
H	1.852100 -0.047075 2.801628	
H	3.367605 1.070724 1.559848	
C	2.128695 1.512611 -0.076072	
O	2.720534 1.788231 -1.094610	
O	0.972373 2.086906 0.263718	
H	0.723482 1.641864 1.117759	
H	4.302486 -0.292592 -0.162252	
H	3.700819 -1.359922 1.110531	
S	2.466288 -1.661111 -0.903594	
H	2.551292 -0.772431 -1.914499	
C	-2.962675 -0.990103 -0.197773	
C	-3.188691 0.287523 -1.022657	

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N	-3.751824	-0.977257	1.023429	
H	-3.444761	-0.213469	1.620694	
H	-3.596056	-1.831701	1.548993	
H	-3.306678	-1.823396	-0.823125	
C	-1.467517	-1.243202	0.031425	
O	-0.968517	-1.464522	1.114825	
O	-0.768590	-1.204436	-1.107954	
H	0.182271	-1.382674	-0.921073	
H	-2.708548	0.209260	-1.995403	
H	-4.260281	0.418876	-1.169925	
S	-2.617436	1.841080	-0.204576	
H	-1.297658	1.681803	-0.434892	
28				
Dimer 190 of the n...n type				
C	1.600506	-0.049552	-0.272092	
C	1.924461	-0.337847	1.198824	
N	1.727482	-1.174967	-1.200536	
H	2.434814	-1.834325	-0.886570	
H	0.848399	-1.668355	-1.318304	
H	0.566558	0.309991	-0.304237	
C	2.427206	1.136475	-0.805324	
O	2.668248	2.132550	-0.160004	
O	2.829579	0.980506	-2.065500	
H	2.515823	0.068570	-2.307653	
H	1.778427	0.559202	1.797767	
H	1.259913	-1.116813	1.573320	
S	3.626161	-0.987609	1.485096	
H	4.280897	0.158723	1.208253	
C	-3.037698	-0.209022	0.925558	
C	-2.029770	-1.255558	0.428333	
N	-4.397063	-0.557906	0.552055	
H	-4.487804	-0.568918	-0.460467	
H	-5.047195	0.142297	0.894422	
H	-2.966650	-0.217406	2.020534	
C	-2.623728	1.211111	0.512185	
O	-3.356662	2.026467	0.007329	
O	-1.328430	1.459470	0.800232	
H	-1.119939	2.375462	0.554181	
H	-1.042599	-1.057300	0.838179	
H	-2.350889	-2.240150	0.766833	
S	-1.911894	-1.411585	-1.407293	
H	-1.478685	-0.159344	-1.663094	
28				
Dimer 191 of the n...n type				
C	2.348607	0.729064	0.928878	
C	3.060373	-0.626496	1.000434	
N	0.937090	0.733528	1.332911	
H	0.514610	-0.190391	1.281632	
H	0.827735	1.063800	2.284543	
H	2.898427	1.407119	1.590623	
C	2.492672	1.357005	-0.471445	
O	3.522365	1.335891	-1.107500	
O	1.386170	1.949141	-0.917163	
H	0.712971	1.778462	-0.212294	
H	4.125266	-0.503345	0.813493	
H	2.929657	-1.053871	1.994194	
S	2.433344	-1.909032	-0.174620	
H	2.971378	-1.372454	-1.288932	
C	-2.904362	-0.781069	-0.658767	
C	-2.862165	0.734191	-0.947012	
N	-3.984214	-1.117286	0.252771	
H	-3.805103	-0.708394	1.165828	
H	-4.035159	-2.122516	0.384710	
H	-3.091545	-1.268178	-1.620924	
C	-1.520369	-1.239742	-0.194197	
O	-1.237788	-1.521660	0.952380	
O	-0.633710	-1.248779	-1.196028	
H	0.256299	-1.492944	-0.850448	
H	-2.074971	0.963327	-1.663543	

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H	-3.820220	1.029300	-1.374638
S	-2.663576	1.815282	0.535627
H	-1.380600	1.501922	0.819017
28			
Dimer 192 of the n...n type			
C	2.994097	0.196009	0.622230
C	1.962890	1.330766	0.564055
N	4.117667	0.293367	-0.314224
H	3.845227	0.794031	-1.156813
H	4.912177	0.768778	0.096322
H	3.397282	0.180212	1.640927
C	2.323623	-1.181228	0.455082
O	1.278053	-1.487783	0.984771
O	3.019354	-2.028607	-0.299810
H	3.806398	-1.498813	-0.596688
H	1.152014	1.137079	1.264788
H	2.444706	2.270115	0.835507
S	1.247017	1.621246	-1.109264
H	0.486075	0.507788	-1.167728
C	-2.799387	-0.973858	0.186756
C	-3.186608	0.236273	1.056455
N	-1.844617	-1.835855	0.856893
H	-0.935776	-1.384762	0.929084
H	-1.698747	-2.682227	0.316106
H	-3.727977	-1.535784	0.030127
C	-2.357467	-0.521444	-1.210139
O	-1.283624	-0.762225	-1.713343
O	-3.317993	0.184790	-1.834599
H	-2.995072	0.448724	-2.711275
H	-3.960223	0.826808	0.569484
H	-3.574465	-0.134440	2.004943
S	-1.790784	1.345221	1.527831
H	-1.551899	1.867938	0.306681
28			
Dimer 193 of the n...n type			
C	2.868666	-0.436500	0.683029
C	1.875200	0.658773	1.086892
N	4.272978	-0.033451	0.568905
H	4.348318	0.931938	0.257036
H	4.762303	-0.120132	1.451602
H	2.803636	-1.224612	1.442039
C	2.444639	-1.129360	-0.626574
O	1.293857	-1.367712	-0.920271
O	3.468400	-1.473566	-1.405556
H	4.266075	-1.116263	-0.934213
H	0.869965	0.252249	1.173840
H	2.164098	1.066690	2.055935
S	1.845014	2.110500	-0.050301
H	1.340811	1.464334	-1.121130
C	-1.901300	-0.897098	-0.156816
C	-1.725263	0.413729	-0.940023
N	-2.758243	-1.829772	-0.869658
H	-3.702339	-1.456940	-0.927841
H	-2.823910	-2.705619	-0.361012
H	-0.897195	-1.328530	-0.083746
C	-2.347586	-0.619696	1.281356
O	-3.331246	-1.080465	1.810747
O	-1.490144	0.208546	1.913813
H	-1.799106	0.350657	2.822863
H	-1.007558	1.065273	-0.447524
H	-1.350830	0.172183	-1.934102
S	-3.281014	1.364851	-1.228915
H	-3.414488	1.852206	0.021920
28			
Dimer 194 of the n...n type			
C	2.790018	-0.141651	0.990273
C	2.952880	-1.494556	0.284684
N	1.569523	0.071046	1.769950
H	0.741880	-0.394806	1.382539

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H	1.682733	-0.235807	2.728571		
H	3.642854	-0.045363	1.673474		
C	2.961877	1.036609	0.012128		
O	3.735440	1.037852	-0.920352		
O	2.195485	2.083942	0.312970		
H	1.655751	1.761431	1.086298		
H	3.954882	-1.576729	-0.133945		
H	2.817703	-2.295013	1.012349		
S	1.732540	-1.840914	-1.052878		
H	2.200115	-0.927214	-1.926805		
C	-2.275125	-0.107580	0.917331		
C	-1.822256	1.298753	0.487156		
N	-1.177310	-1.056643	0.844072		
H	-0.891380	-1.194146	-0.122421		
H	-1.465049	-1.964581	1.195145		
H	-2.592565	-0.020184	1.962869		
C	-3.519243	-0.545476	0.136504		
O	-3.601493	-1.546815	-0.534336		
O	-4.532701	0.328874	0.289359		
H	-5.298946	0.015227	-0.217406		
H	-2.616878	2.024809	0.644870		
H	-0.964503	1.582698	1.095529		
S	-1.236552	1.421780	-1.258648		
H	-2.450650	1.367590	-1.844377		
28					
Dimer 195 of the n...n type					
C	3.078525	-0.197505	-0.695982		
C	3.227493	1.213940	-0.110627		
N	2.211812	-0.331652	-1.865706		
H	1.394126	0.269735	-1.796616		
H	2.702273	-0.117160	-2.725387		
H	4.082122	-0.533282	-0.981447		
C	2.621130	-1.202812	0.376427		
O	3.004297	-1.196574	1.521910		
O	1.746778	-2.111559	-0.080202		
H	1.594319	-1.854231	-1.029760		
H	3.933088	1.209258	0.718437		
H	3.606270	1.881506	-0.884555		
S	1.648466	1.978246	0.462600		
H	1.525891	1.255504	1.594343		
C	-1.985769	0.769567	0.488313		
C	-3.367740	0.261515	0.939926		
N	-2.101209	1.808205	-0.520849		
H	-2.511730	1.421782	-1.366703		
H	-1.176465	2.145293	-0.772729		
H	-1.516332	1.198836	1.379251		
C	-1.106141	-0.408726	0.062456		
O	-0.786170	-0.652177	-1.079706		
O	-0.727763	-1.158891	1.110508		
H	-0.101109	-1.839255	0.799067		
H	-3.264894	-0.456135	1.752307		
H	-3.946725	1.112703	1.298058		
S	-4.404687	-0.482729	-0.392342		
H	-3.697641	-1.620976	-0.545674		
28					
Dimer 196 of the n...n type					
C	3.242323	-0.365010	0.250995		
C	3.185225	1.147904	0.512725		
N	3.507045	-0.760348	-1.136692		
H	3.204163	-0.033339	-1.780809		
H	4.489898	-0.943553	-1.297832		
H	4.033572	-0.775941	0.887117		
C	1.955506	-1.064239	0.731383		
O	1.432627	-0.850825	1.802807		
O	1.475402	-1.953910	-0.136359		
H	2.112923	-1.910745	-0.899715		
H	2.906690	1.332347	1.549354		
H	4.171335	1.577950	0.336828		
S	2.035971	2.067438	-0.600116		

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H	0.858637	1.608810	-0.051416		
C	-1.829386	0.772338	-0.346072		
C	-1.550914	-0.547688	-1.082324		
N	-0.856920	1.006381	0.709865		
H	-0.720176	0.170560	1.273785		
H	-1.176488	1.739101	1.336196		
H	-1.727516	1.569468	-1.095103		
C	-3.280824	0.863479	0.133382		
O	-3.623368	1.169022	1.250885		
O	-4.148520	0.589808	-0.858925		
H	-5.053742	0.685774	-0.521793		
H	-2.134752	-0.603499	-1.997916		
H	-0.492539	-0.589729	-1.337264		
S	-1.863054	-2.068513	-0.084257		
H	-3.210264	-2.005708	-0.131473		
28					
Dimer 197 of the n...n type					
C	3.162145	-0.816855	-0.001015		
C	3.508463	0.421340	0.839411		
N	3.319298	-0.676058	-1.451499		
H	3.229431	0.296857	-1.734335		
H	4.215873	-1.021351	-1.771470		
H	3.810504	-1.630130	0.342426		
C	1.733933	-1.310648	0.298502		
O	1.271595	-1.401156	1.415286		
O	1.046871	-1.657696	-0.787536		
H	1.670411	-1.466534	-1.539685		
H	3.284628	0.231977	1.887933		
H	4.572997	0.635335	0.743540		
S	2.663604	1.970443	0.303375		
H	1.400613	1.604670	0.612955		
C	-1.993388	-0.765540	-0.236037		
C	-3.453778	-0.590321	-0.688857		
N	-1.904314	-1.355943	1.086713		
H	-2.311414	-0.725132	1.771881		
H	-0.926234	-1.478307	1.341560		
H	-1.526619	-1.447711	-0.952759		
C	-1.233961	0.556809	-0.374446		
O	-0.784768	1.201312	0.546718		
O	-1.121158	0.937327	-1.660471		
H	-0.642492	1.781051	-1.698744		
H	-3.497760	-0.237193	-1.717545		
H	-3.950080	-1.558819	-0.629875		
S	-4.473591	0.525936	0.370424		
H	-3.915755	1.690233	-0.020490		
28					
Dimer 198 of the n...n type					
C	3.222221	0.701253	-0.279415		
C	3.095602	-0.473254	-1.260119		
N	3.908280	0.416925	0.984233		
H	3.814010	-0.564303	1.235913		
H	4.894769	0.641351	0.938060		
H	3.767410	1.497948	-0.797099		
C	1.842374	1.313334	0.028504		
O	0.992969	1.510137	-0.813091		
O	1.668506	1.631995	1.309669		
H	2.512554	1.341811	1.748032		
H	2.531272	-0.164191	-2.138347		
H	4.089738	-0.788834	-1.577014		
S	2.322576	-1.981666	-0.535634		
H	1.096849	-1.464097	-0.307753		
C	-2.559942	0.341555	1.057217		
C	-3.603557	0.683316	-0.020377		
N	-1.511940	1.341545	1.117282		
H	-0.980555	1.359242	0.249296		
H	-0.838957	1.114105	1.842120		
H	-3.100658	0.338998	2.011927		
C	-2.046258	-1.092509	0.880113		
O	-0.884254	-1.408009	0.768472		

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O -3.052702	-1.987794	0.876881	
H -2.681275	-2.878616	0.771965	
H -4.451408	0.003645	0.032157	
H -3.957266	1.699298	0.153200	
S -2.955107	0.693237	-1.748710	
H -2.849161	-0.643596	-1.894565	
28			
Dimer 199 of the n...n type			
C -2.357097	0.362116	0.890611	
C -1.813548	-1.036639	0.576162	
N -3.728484	0.425136	1.403878	
H -4.296960	-0.321248	1.010506	
H -3.756709	0.346831	2.413381	
H -1.693543	0.803862	1.643153	
C -2.240409	1.302201	-0.324516	
O -1.301369	1.301097	-1.089554	
O -3.260971	2.149735	-0.445415	
H -3.881432	1.892270	0.285769	
H -0.786656	-0.981509	0.223194	
H -1.840018	-1.643593	1.481411	
S -2.804669	-1.972489	-0.665906	
H -2.437897	-1.241363	-1.738413	
C 2.248641	-0.310035	0.957744	
C 1.785814	1.050854	0.410040	
N 3.419966	-0.171055	1.806102	
H 4.201808	0.176972	1.256951	
H 3.702319	-1.076637	2.167590	
H 1.421493	-0.690375	1.569724	
C 2.424058	-1.326861	-0.177259	
O 3.434822	-1.947244	-0.406311	
H 1.294652	-1.460291	-0.900993	
H 1.438694	-2.119778	-1.598505	
H 0.840595	0.962108	-0.120519	
H 1.652890	1.731342	1.250953	
S 3.003658	1.888773	-0.695737	
H 2.789399	1.125831	-1.787278	
28			
Dimer 200 of the n...n type			
C 2.365389	-0.485047	0.631124	
C 1.729984	0.910244	0.664238	
N 3.684126	-0.614597	1.258108	
H 4.213321	0.249773	1.170149	
H 3.612794	-0.843953	2.242265	
H 1.677408	-1.164925	1.146852	
C 2.443962	-1.035306	-0.805686	
O 1.574051	-0.878688	-1.634420	
O 3.550301	-1.734418	-1.052208	
H 4.076387	-1.662874	-0.212641	
H 0.752012	0.905904	0.186700	
H 1.607096	1.223639	1.701226	
S 2.754833	2.226325	-0.122386	
H 2.566761	1.829173	-1.397577	
C -2.431230	0.399560	-0.761296	
C -1.682974	-0.919062	-0.494606	
N -1.658600	1.545469	-0.312230	
H -1.611830	1.553493	0.703276	
H -2.115259	2.409160	-0.587358	
H -2.549954	0.465214	-1.848714	
C -3.850010	0.344498	-0.183246	
O -4.286970	1.090478	0.661213	
O -4.570144	-0.654094	-0.731057	
H -5.455687	-0.658504	-0.333459	
H -2.230927	-1.763946	-0.907006	
H -0.704897	-0.865189	-0.972002	
S -1.319754	-1.254987	1.283467	
H -2.565800	-1.610018	1.658446	
28			
Dimer 201 of the n...n type			
C -2.788696	-0.851824	0.635566	

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C -3.036066	0.558753	1.184456	
N -1.572305	-1.532633	1.079968	
H -0.778083	-0.903489	1.247347	
H -1.731462	-2.072193	1.922072	
H -3.647775	-1.462926	0.937915	
C -2.828407	-0.875345	-0.905110	
O -3.590795	-0.214496	-1.575296	
O -1.948976	-1.723081	-1.438970	
H -1.464701	-2.085440	-0.644900	
H -4.021439	0.912891	0.885338	
H -2.996897	0.528639	2.273487	
S -1.781634	1.813956	0.681905	
H -2.202699	1.950762	-0.591516	
C 1.867031	-0.722457	0.244449	
C 1.310187	0.023872	-0.978690	
N 1.208779	-0.294397	1.469402	
H 1.299252	0.712729	1.577656	
H 1.658519	-0.715665	2.276430	
H 1.640679	-1.784254	0.083880	
C 3.395687	-0.637055	0.306770	
O 4.031347	-0.281663	1.270707	
O 3.962453	-1.030789	-0.849764	
H 4.927704	-0.978281	-0.761491	
H 1.691078	-0.411501	-1.899510	
H 0.224951	-0.060136	-0.977218	
S 1.647594	1.837654	-0.993138	
H 2.939530	1.756875	-1.373407	
28			
Dimer 202 of the n...n type			
C 2.034005	-0.345359	0.122323	
C 2.030781	0.927721	-0.733188	
N 2.050017	-0.154942	1.573315	
H 2.547058	0.695370	1.825930	
H 1.104531	-0.104257	1.939922	
H 1.125095	-0.905803	-0.127481	
C 3.187525	-1.287374	-0.272253	
O 3.556724	-1.461432	-1.412422	
O 3.729271	-1.926239	0.764048	
H 3.253883	-1.552590	1.553088	
H 1.991638	0.672294	-1.790717	
H 1.153725	1.526448	-0.487618	
S 3.468252	2.043234	-0.435054	
H 4.399438	1.256321	-1.011854	
C -3.255405	0.898276	-0.255513	
C -1.794388	0.765940	0.206385	
N -4.107695	1.379683	0.817305	
H -4.152850	0.687653	1.560669	
H -5.057338	1.506806	0.482283	
H -3.253550	1.643882	-1.059398	
C -3.742801	-0.405928	-0.900691	
O -4.717933	-1.029504	-0.555127	
O -2.946947	-0.781083	-1.921022	
H -3.291532	-1.603829	-2.304024	
H -1.149319	0.519617	-0.634279	
H -1.476316	1.718334	0.629444	
S -1.523998	-0.467626	1.553259	
H -1.626013	-1.576758	0.792242	
28			
Dimer 203 of the n...n type			
C -1.978796	0.126512	0.793688	
C -1.972607	-1.308050	0.251746	
N -3.082268	0.480498	1.689468	
H -3.934517	-0.009221	1.427062	
H -2.870676	0.253966	2.653831	
H -1.039247	0.272794	1.337369	
C -1.910641	1.161384	-0.343235	
O -1.269016	1.005567	-1.359155	
O -2.598344	2.274988	-0.095739	
H -3.050248	2.097566	0.769768	

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H	-1.105918	-1.469216	-0.386878	
H	-1.922275	-2.008392	1.085710	
S	-3.493247	-1.773450	-0.681120	
H	-3.260964	-0.992867	-1.756179	
C	1.894991	-0.001366	-0.808241	
C	1.985745	-1.274266	0.048836	
N	2.805102	-0.059436	-1.939690	
H	3.767266	-0.063299	-1.611098	
H	2.699748	0.768632	-2.517041	
H	0.868438	0.046220	-1.190086	
C	2.054686	1.257417	0.051233	
O	2.833855	2.154961	-0.163882	
O	1.194492	1.263971	1.092127	
H	1.316105	2.084940	1.595587	
H	1.221783	-1.278800	0.823235	
H	1.832921	-2.137955	-0.597752	
S	3.629020	-1.555908	0.841877	
H	3.517200	-0.607746	1.794938	
28				
Dimer 204 of the n...n type				
C	2.837746	-0.416745	0.735914	
C	1.848003	0.696154	1.096208	
N	4.223774	-0.011237	0.493756	
H	4.267957	0.911251	0.067917	
H	4.764304	0.010186	1.350200	
H	2.835880	-1.125697	1.571764	
C	2.344327	-1.242654	-0.467327	
O	1.179266	-1.506067	-0.670660	
O	3.323181	-1.672003	-1.259531	
H	4.145622	-1.267461	-0.879157	
H	0.860986	0.275786	1.282004	
H	2.184055	1.204391	1.999722	
S	1.707006	2.026628	-0.176762	
H	1.164138	1.261615	-1.147886	
C	-3.300388	0.498596	0.125477	
C	-2.967738	-0.589070	1.167116	
N	-4.124706	-0.030156	-0.947489	
H	-3.603031	-0.729270	-1.469251	
H	-4.365148	0.706071	-1.603692	
H	-3.870388	1.266262	0.659798	
C	-2.007268	1.171831	-0.344700	
O	-1.532956	1.063321	-1.453471	
O	-1.440097	1.886901	0.640819	
H	-0.566336	2.222564	0.342001	
H	-2.390173	-0.165294	1.986868	
H	-3.903356	-0.981123	1.565690	
S	-2.087847	-2.069456	0.505260	
H	-0.887761	-1.500183	0.260803	
28				
Dimer 205 of the n...n type				
C	2.381825	-0.133844	0.809958	
C	2.329193	1.222378	0.097596	
N	3.661985	-0.502536	1.419314	
H	4.441610	-0.137272	0.877321	
H	3.742228	-0.150970	2.365903	
H	1.621922	-0.104456	1.599037	
C	1.923838	-1.276703	-0.113553	
O	1.035682	-1.170469	-0.930227	
O	2.575046	-2.421988	0.089775	
H	3.261634	-2.196120	0.769830	
H	1.331399	1.402750	-0.295923	
H	2.568180	2.012413	0.809640	
S	3.555109	1.410828	-1.266764	
H	2.965915	0.553210	-2.124885	
C	-3.002862	0.803243	-0.598974	
C	-1.544140	0.909874	-0.122263	
N	-3.861891	1.730214	0.118173	
H	-3.897308	1.474178	1.101565	
H	-4.813436	1.670892	-0.230154	

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H	-2.997561	1.081761	-1.659219
C	-3.484540	-0.651819	-0.551718
O	-4.426059	-1.052593	0.091318
O	-2.726626	-1.449961	-1.328244
H	-3.061259	-2.359015	-1.266912
H	-0.884585	0.286376	-0.722007
H	-1.231527	1.950143	-0.211633
S	-1.280862	0.482997	1.654683
H	-1.320060	-0.857532	1.511072
28			
Dimer 206 of the n...n type			
C	-1.794111	0.229928	0.338877
C	-1.784696	-0.834947	-0.763422
N	-2.116155	-0.235537	1.690677
H	-2.791134	-0.996409	1.658909
H	-1.294096	-0.569513	2.179643
H	-0.790443	0.673149	0.349315
C	-2.717230	1.406016	-0.016625
O	-2.848704	1.846993	-1.136991
O	-3.340855	1.936234	1.037444
H	-3.077276	1.354527	1.796442
H	-1.534582	-0.381846	-1.721268
H	-1.032036	-1.586621	-0.525734
S	-3.366524	-1.767194	-0.936311
H	-4.098324	-0.747971	-1.431122
C	2.541741	0.964553	-0.036203
C	2.258871	0.314464	1.332217
N	1.333347	1.059873	-0.838303
H	1.104621	0.147612	-1.223403
H	1.482029	1.677124	-1.630128
H	2.900056	1.976856	0.177706
C	3.692768	0.239094	-0.741428
O	3.597825	-0.360654	-1.786297
O	4.839977	0.334356	-0.042955
H	5.536727	-0.152651	-0.511761
H	3.160659	0.285233	1.941039
H	1.510252	0.914641	1.848822
S	1.528978	-1.376688	1.250883
H	2.633941	-2.032441	0.841674
28			
Dimer 207 of the n...n type			
C	-2.253366	0.623432	0.452054
C	-2.443396	-0.767728	1.067733
N	-3.396793	1.535387	0.532249
H	-4.273981	1.024502	0.464303
H	-3.400664	2.056436	1.401032
H	-1.408785	1.096503	0.966433
C	-1.788197	0.536582	-1.012314
O	-1.028784	-0.310474	-1.427872
O	-2.268406	1.509323	-1.786061
H	-2.883869	2.013812	-1.193784
H	-1.530652	-1.352612	0.970232
H	-2.676945	-0.663761	2.127414
S	-3.847326	-1.726114	0.353180
H	-3.279070	-1.963791	-0.846633
C	2.884676	-0.736235	0.788354
C	1.483895	-0.104379	0.866026
N	3.786343	-0.144923	1.762278
H	3.949602	0.831801	1.531715
H	4.690809	-0.604582	1.730003
H	2.753638	-1.796502	1.033676
C	3.414038	-0.700546	-0.650057
O	4.424761	-0.141884	-1.006051
O	2.609081	-1.379006	-1.490359
H	2.973722	-1.325022	-2.388258
H	0.789874	-0.610346	0.198116
H	1.123629	-0.193251	1.890726
S	1.428675	1.702855	0.491655
H	1.465146	1.595283	-0.852050

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28		
Dimer 208 of the n...n type		
C -1.941631	-0.806398	-0.274097
C -1.666316	0.548004	-0.939698
N -3.045266	-1.592479	-0.830481
H -3.772776	-0.986470	-1.202261
H -2.733513	-2.206840	-1.573080
H -1.022009	-1.394419	-0.362544
C -2.152022	-0.652583	1.242737
O -1.507882	0.105509	1.934135
O -3.086674	-1.460559	1.740723
H -3.450121	-1.932001	0.945973
H -0.839986	1.052532	-0.443391
H -1.399591	0.389665	-1.984617
S -3.114717	1.688385	-0.973723
H -3.129899	1.962331	0.346914
C 2.828859	-0.665245	0.597908
C 1.844918	0.393047	1.125807
N 4.205833	-0.283559	0.858588
H 4.432260	0.564116	0.345056
H 4.841278	-1.002698	0.527853
H 2.610405	-1.585802	1.151433
C 2.542789	-0.984806	-0.874179
O 3.323042	-0.835478	-1.783709
O 1.293206	-1.464304	-1.047136
H 1.156639	-1.648046	-1.990758
H 0.816015	0.048241	1.055344
H 2.070035	0.575864	2.176459
S 1.982468	2.051363	0.328189
H 1.500145	1.706373	-0.883542
28		
Dimer 209 of the n...n type		
C -2.941695	0.712978	-0.449833
C -2.219524	-0.360047	-1.274317
N -2.105061	1.530598	0.432769
H -1.336919	0.980828	0.809502
H -1.710970	2.326075	-0.055484
H -3.435692	1.385364	-1.160632
C -4.095735	0.113265	0.375993
O -4.810374	-0.781630	-0.016265
O -4.263107	0.695500	1.563830
H -3.521895	1.351978	1.623971
H -2.930511	-0.897390	-1.899383
H -1.475256	0.117234	-1.911349
S -1.264441	-1.573117	-0.266834
H -2.326073	-2.203584	0.275983
C 3.095191	0.602283	0.874174
C 1.669386	0.844359	0.350167
N 3.998280	1.661653	0.459726
H 4.093544	1.656987	-0.552498
H 4.926271	1.503540	0.839373
H 3.023440	0.613188	1.968137
C 3.575233	-0.806447	0.502901
O 4.572597	-1.056872	-0.131382
O 2.742918	-1.753311	0.977885
H 3.079248	-2.626980	0.721404
H 0.981721	0.103835	0.753946
H 1.348966	1.837017	0.665637
S 1.512510	0.855249	-1.488055
H 1.629066	-0.475807	-1.674895
28		
Dimer 210 of the n...n type		
C -2.001375	-0.500579	-0.132975
C -3.431449	-0.829660	-0.579318
N -1.657491	-0.846621	1.249762
H -2.468408	-0.756880	1.858096
H -1.316044	-1.797753	1.322799
H -1.319952	-1.041749	-0.796285
C -1.665323	0.982272	-0.376103

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O -1.997972	1.592399	-1.366829
O -0.946722	1.539743	0.600053
H -0.853592	0.822204	1.277932
H -3.576465	-0.539151	-1.618421
H -3.599192	-1.903151	-0.491259
S -4.745821	-0.050328	0.453720
H -4.538617	1.217821	0.043835
C 2.123063	-0.665269	0.662068
C 2.381829	0.845838	0.796244
N 3.098349	-1.438025	1.411182
H 4.024475	-1.301896	1.014291
H 2.894659	-2.429757	1.338030
H 1.131914	-0.845400	1.095215
C 2.014004	-1.066482	-0.813666
O 2.700011	-1.893614	-1.364428
O 1.039341	-0.377092	-1.442800
H 1.006690	-0.652671	-2.373151
H 1.577957	1.417201	0.338538
H 2.425323	1.092857	1.856805
S 3.995267	1.417138	0.106176
H 3.652347	1.353684	-1.196847
28		
Dimer 211 of the n...n type		
C 1.893448	0.583389	0.255222
C 3.376221	0.843904	0.558289
N 1.183456	-0.276168	1.201697
H 1.739575	-1.102005	1.414654
H 1.042094	0.216850	2.077623
H 1.384709	1.555129	0.260330
C 1.703631	0.068711	-1.178768
O 2.420459	0.398817	-2.097914
O 0.668303	-0.748554	-1.371447
H 0.203534	-0.891622	-0.519599
H 3.797283	1.540785	-0.164273
H 3.465586	1.279239	1.553929
S 4.417343	-0.678035	0.599497
H 4.401050	-0.909136	-0.728829
C -3.040521	-0.170301	0.988309
C -3.173026	1.258859	0.425417
N -2.003810	-0.253357	2.001083
H -1.083811	-0.218094	1.565582
H -2.058795	-1.145879	2.481807
H -4.006217	-0.402554	1.449448
C -2.857584	-1.166968	-0.159645
O -1.840929	-1.784140	-0.386232
O -3.963755	-1.268603	-0.916360
H -3.792305	-1.884072	-1.647620
H -4.010838	1.323646	-0.266967
H -3.355730	1.936137	1.259237
S -1.662510	1.923487	-0.398359
H -1.746624	1.195293	-1.530324
28		
Dimer 212 of the n...n type		
C -2.151313	-0.588539	0.278172
C -1.917203	0.748609	0.993553
N -1.460568	-0.779901	-0.997772
H -1.382122	0.098399	-1.504740
H -0.532266	-1.168749	-0.873301
H -1.819669	-1.379410	0.961064
C -3.655317	-0.859279	0.075238
O -4.508943	-0.566291	0.882395
O -3.933925	-1.481443	-1.069999
H -3.056015	-1.549604	-1.529840
H -2.488983	0.784746	1.919097
H -0.860683	0.851296	1.238980
S -2.318947	2.233539	-0.022118
H -3.658488	2.075683	-0.008917
C 2.250148	-0.143725	0.921518
C 1.956631	0.995998	-0.071322

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N	3.279727	0.238062	1.870558		
H	4.162348	0.378395	1.386135		
H	3.432077	-0.503691	2.546374		
H	1.319711	-0.320597	1.473368		
C	2.545360	-1.450294	0.175452		
O	3.568772	-2.083687	0.254310		
O	1.503980	-1.827551	-0.600536		
H	1.729767	-2.653708	-1.058015		
H	1.115859	0.746394	-0.714121		
H	1.706490	1.890972	0.497890		
S	3.383816	1.489492	-1.130637		
H	3.351035	0.429403	-1.964423		
28					
Dimer 213 of the n...n type					
C	3.164855	0.407757	0.223228		
C	3.266530	-0.992172	-0.396770		
N	3.099337	0.466822	1.686290		
H	2.607077	-0.341415	2.060092		
H	4.021728	0.497301	2.104220		
H	4.050412	0.968811	-0.097251		
C	1.977775	1.199812	-0.354861		
O	1.622360	1.143097	-1.509443		
O	1.376269	1.987885	0.540642		
H	1.845825	1.791772	1.394177		
H	3.314364	-0.922498	-1.482068		
H	4.175941	-1.474989	-0.039349		
S	1.891154	-2.129229	0.071010		
H	0.953839	-1.603709	-0.744715		
C	-1.439054	0.237375	0.460393		
C	-2.395848	-0.864723	0.951149		
N	-1.689039	1.502663	1.124361		
H	-2.575678	1.889775	0.814045		
H	-0.962770	2.166339	0.873732		
H	-0.432762	-0.099717	0.728820		
C	-1.473665	0.321357	-1.069221		
O	-1.875358	1.262985	-1.708505		
O	-1.016536	-0.816042	-1.635765		
H	-1.050417	-0.723950	-2.601484		
H	-2.122530	-1.829014	0.526615		
H	-2.318202	-0.925437	2.036378		
S	-4.183499	-0.549618	0.621346		
H	-4.158846	-0.797951	-0.704414		
28					
Dimer 214 of the n...n type					
C	2.875508	-0.162881	-0.749221		
C	2.083359	-1.404728	-0.321045		
N	4.171616	0.034650	-0.094389		
H	4.155404	-0.322400	0.858019		
H	4.921032	-0.428007	-0.594816		
H	3.049835	-0.247186	-1.827917		
C	2.046155	1.125062	-0.591236		
O	0.859060	1.200651	-0.831671		
O	2.754828	2.172533	-0.182992		
H	3.666766	1.806860	-0.031433		
H	1.159944	-1.484060	-0.891044		
H	2.683127	-2.294130	-0.515166		
S	1.688611	-1.469931	1.479401		
H	0.765145	-0.486516	1.477975		
C	-2.987890	-0.142932	0.736445		
C	-2.199866	-1.334189	0.158959		
N	-4.301747	-0.037946	0.123800		
H	-4.201905	0.174715	-0.865478		
H	-4.821232	0.732148	0.533280		
H	-3.113691	-0.345570	1.805856		
C	-2.149952	1.134586	0.629195		
O	-2.435144	2.097246	-0.042584		
O	-1.023410	1.055975	1.364689		
H	-0.455174	1.810046	1.134115		
H	-1.289360	-1.508567	0.727760		

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H	-2.825610	-2.223763	0.225537		
S	-1.765154	-1.181369	-1.629170		
H	-0.805235	-0.240450	-1.484395		
28					
Dimer 215 of the n...n type					
C	1.997865	0.820989	-0.175788		
C	1.867792	-0.424305	-1.060705		
N	3.107168	1.726882	-0.485338		
H	3.909376	1.212105	-0.840779		
H	2.844470	2.419913	-1.175880		
H	1.061387	1.378924	-0.279361		
C	2.061637	0.447760	1.315495		
O	1.416503	-0.449924	1.811087		
O	2.870191	1.228660	2.030947		
H	3.281461	1.834596	1.360941		
H	0.998161	-1.008427	-0.767194		
H	1.740736	-0.115489	-2.098300		
S	3.356106	-1.513437	-1.059785		
H	3.213553	-1.970323	0.201213		
C	-2.613206	0.788628	0.510576		
C	-1.918106	-0.464380	1.067500		
N	-4.009704	0.839623	0.910284		
H	-4.511366	0.053270	0.505256		
H	-4.449881	1.679237	0.547183		
H	-2.093339	1.647965	0.951626		
C	-2.402347	0.913139	-1.003147		
O	-3.283073	1.035574	-1.820359		
O	-1.094145	0.879884	-1.330670		
H	-1.009636	0.972080	-2.293513		
H	-0.841656	-0.419231	0.924908		
H	-2.117638	-0.517424	2.137616		
S	-2.543792	-2.061645	0.385945		
H	-1.942515	-1.975972	-0.818525		
28					
Dimer 216 of the n...n type					
C	2.577640	-0.337075	-0.770676		
C	1.730707	0.931029	-0.604432		
N	2.017233	-1.577666	-0.229905		
H	1.488803	-1.402110	0.621103		
H	1.414504	-2.046906	-0.895083		
H	2.730968	-0.480408	-1.846534		
C	3.997746	-0.145295	-0.203550		
O	4.618479	0.891064	-0.279611		
O	4.504862	-1.243992	0.356500		
H	3.770707	-1.908558	0.309008		
H	2.249964	1.786964	-1.032039		
H	0.779258	0.810000	-1.121245		
S	1.277100	1.315702	1.141004		
H	2.510114	1.667664	1.558893		
C	-2.473847	0.488560	0.716368		
C	-1.747386	-0.863153	0.614679		
N	-3.639815	0.398391	1.576925		
H	-4.324637	-0.230680	1.165748		
H	-4.089862	1.304556	1.657379		
H	-1.758712	1.184988	1.170582		
C	-2.770576	1.056786	-0.676778		
O	-3.858914	1.398429	-1.072678		
O	-1.650899	1.144676	-1.424051		
H	-1.876355	1.518718	-2.290989		
H	-0.819401	-0.759364	0.059116		
H	-1.514719	-1.208291	1.621481		
S	-2.736122	-2.221649	-0.145948		
H	-2.652123	-1.793036	-1.422397		
28					
Dimer 217 of the n...n type					
C	2.071619	-0.390928	-0.064761		
C	2.156088	1.006504	-0.691069		
N	1.535509	-0.465363	1.295824		
H	1.743720	0.380315	1.820222		

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H	0.532270	-0.608292	1.286260		
H	1.423795	-0.993223	-0.711636		
C	3.435237	-1.107871	-0.104926		
O	4.207320	-1.037215	-1.035303		
O	3.678627	-1.847168	0.976547		
H	2.897189	-1.674985	1.566736		
H	2.556619	0.942527	-1.701291		
H	1.158833	1.442926	-0.741193		
S	3.158488	2.212607	0.278796		
H	4.361434	1.658777	0.022947		
C	-2.261086	0.650404	-0.460067		
C	-2.906160	0.757376	0.933741		
N	-3.032535	1.371211	-1.456410		
H	-3.944516	0.935929	-1.567810		
H	-2.574728	1.323175	-2.361008		
H	-1.276103	1.122716	-0.375639		
C	-1.996481	-0.815338	-0.822666		
O	-2.436494	-1.385722	-1.790234		
O	-1.195037	-1.416846	0.085462		
H	-1.067410	-2.344735	-0.171077		
H	-2.263734	0.316535	1.693090		
H	-3.048403	1.812569	1.165230		
S	-4.586969	0.007562	1.064497		
H	-4.194705	-1.283155	1.073292		
28					
Dimer 218 of the n...n type					
C	2.921883	0.604426	0.516841		
C	1.703368	-0.278551	0.808694		
N	2.735988	1.645906	-0.497940		
H	2.083733	1.338341	-1.215467		
H	2.376017	2.502250	-0.093725		
C	3.197587	1.095430	1.457236		
C	4.156720	-0.238126	0.145295		
O	4.431994	-1.295574	0.666578		
O	4.924546	0.321439	-0.790118		
H	4.436214	1.145891	-1.048318		
H	1.935597	-1.004143	1.585948		
H	0.878465	0.346707	1.147550		
S	1.055178	-1.173709	-0.668724		
H	2.005880	-2.130090	-0.697279		
C	-3.153998	-0.249528	0.964506		
C	-2.789587	1.246353	0.961578		
N	-2.048419	-1.071837	1.423962		
H	-1.313765	-1.101945	0.721227		
H	-2.356162	-2.030542	1.552732		
H	-3.982649	-0.354872	1.674244		
C	-3.715816	-0.670643	-0.399078		
O	-3.253850	-1.535631	-1.104834		
O	-4.805822	0.049654	-0.730000		
H	-5.126257	-0.244757	-1.597745		
H	-3.663395	1.854138	0.735049		
H	-2.424508	1.512042	1.953351		
S	-1.422016	1.716635	-0.183633		
H	-2.100694	1.563559	-1.339281		
28					
Dimer 219 of the n...n type					
C	-2.332902	-0.725290	0.312428		
C	-3.460046	-0.802553	-0.723190		
N	-2.736805	-0.740278	1.720655		
H	-3.635954	-0.281428	1.846375		
H	-2.808388	-1.684242	2.081198		
H	-1.672647	-1.583104	0.141948		
C	-1.421604	0.491337	0.070837		
O	-1.110260	0.893437	-1.027890		
O	-0.961213	1.046089	1.193104		
H	-1.413166	0.539823	1.918280		
H	-3.047018	-0.797033	-1.730462		
H	-4.017442	-1.728366	-0.580485		
S	-4.713131	0.543197	-0.578925		

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H	-3.918528	1.544291	-1.009695		
C	3.332492	-0.023452	-0.909332		
C	1.953362	-0.687513	-1.074518		
N	4.379075	-1.014631	-0.729272		
H	4.234405	-1.514469	0.144061		
H	5.285729	-0.563535	-0.660094		
H	3.521966	0.519933	-1.841779		
C	3.280418	1.037111	0.196471		
O	3.904013	0.996524	1.231103		
O	2.437072	2.038295	-0.120022		
H	2.414435	2.675028	0.612245		
H	1.187639	0.052928	-1.297027		
H	2.009380	-1.397032	-1.899848		
S	1.400340	-1.691385	0.372690		
H	1.101144	-0.660008	1.188813		
28					
Dimer 220 of the n...n type					
C	-2.820703	-0.660774	0.805038		
C	-2.368197	0.716084	1.306118		
N	-1.826219	-1.452407	0.077802		
H	-1.189550	-0.865612	-0.459135		
H	-1.269550	-2.022645	0.703093		
H	-3.129455	-1.235872	1.685859		
C	-4.097057	-0.558847	-0.052443		
O	-5.004936	0.208450	0.178788		
O	-4.128191	-1.423199	-1.066322		
H	-3.246802	-1.879889	-1.023384		
H	-3.161903	1.187000	1.883571		
H	-1.496907	0.594822	1.949983		
S	-1.832833	1.873444	-0.026006		
H	-3.059353	2.099542	-0.538624		
C	3.171233	0.761806	0.404497		
C	1.684422	0.443571	0.173055		
N	3.666466	1.711123	-0.576907		
H	3.636054	1.295881	-1.504403		
H	4.638933	1.934883	-0.391304		
H	3.231708	1.223237	1.397217		
C	3.997469	-0.527416	0.495442		
O	4.943104	-0.797896	-0.206161		
O	3.543728	-1.338730	1.470924		
H	4.093833	-2.138160	1.497553		
H	1.292139	-0.176944	0.976221		
H	1.130257	1.381116	0.150628		
S	1.308743	-0.364713	-1.442821		
H	1.801655	-1.583603	-1.140389		
28					
Dimer 221 of the n...n type					
C	-1.834786	-0.117466	-0.280579		
C	-3.081590	-0.598325	-1.033184		
N	-1.417525	-0.925667	0.867414		
H	-2.218489	-1.354464	1.324531		
H	-0.776336	-1.656352	0.581486		
H	-1.007548	-0.114502	-0.998727		
C	-1.976005	1.350744	0.163081		
O	-2.489663	2.212370	-0.514699		
O	-1.447261	1.601791	1.361347		
H	-1.143362	0.714592	1.685962		
H	-3.292078	0.060571	-1.873774		
H	-2.905890	-1.604382	-1.414453		
S	-4.592151	-0.736997	0.015961		
H	-4.785554	0.586445	0.190388		
C	2.250861	-0.310911	0.835635		
C	2.121656	1.039615	0.105253		
N	3.369354	-0.304661	1.760528		
H	4.242991	-0.221564	1.247589		
H	3.411823	-1.179938	2.272701		
H	1.323815	-0.437857	1.405635		
C	2.285170	-1.458923	-0.178701		
O	3.218832	-2.199101	-0.369055		

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O	1.120160	-1.547973	-0.859816		
H	1.184540	-2.267807	-1.508209		
H	1.237755	1.054126	-0.528611		
H	2.025998	1.825653	0.853611		
S	3.583703	1.522419	-0.910162		
H	3.366314	0.675926	-1.937759		
28					
Dimer 222 of the n...n type					
C	1.717491	0.177419	-0.170045		
C	2.842453	1.072571	-0.704793		
N	1.250492	0.462250	1.188009		
H	2.013406	0.794120	1.773148		
H	0.518198	1.163233	1.181620		
H	0.865048	0.299439	-0.847194		
C	2.085070	-1.314605	-0.274442		
O	2.687456	-1.794852	-1.208325		
O	1.651663	-2.048090	0.750861		
H	1.229804	-1.393021	1.363772		
H	3.098920	0.788818	-1.724018		
H	2.506177	2.109605	-0.705837		
S	4.371309	1.061606	0.326455		
H	4.759029	-0.192982	0.018770		
C	-3.101456	0.508551	0.763345		
C	-2.236818	-0.751114	0.950263		
N	-4.499324	0.163093	0.574377		
H	-4.610768	-0.364428	-0.287567		
H	-5.061537	1.002488	0.476385		
H	-3.006039	1.083102	1.692182		
C	-2.534392	1.409592	-0.340049		
O	-3.122731	1.740910	-1.340019		
O	-1.274939	1.817510	-0.061551		
H	-0.971908	2.402404	-0.775145		
H	-1.215276	-0.487435	1.213477		
H	-2.662310	-1.337597	1.764331		
S	-2.211717	-1.901138	-0.492044		
H	-1.440059	-1.150949	-1.304610		
28					
Dimer 223 of the n...n type					
C	-2.037310	-0.753976	-0.280215		
C	-2.079839	0.580444	-1.033400		
N	-3.140087	-1.684576	-0.535187		
H	-4.008077	-1.181178	-0.702884		
H	-2.955700	-2.273280	-1.338738		
H	-1.102312	-1.245940	-0.568000		
C	-1.908478	-0.541824	1.238308		
O	-1.260706	0.348955	1.742061		
O	-2.552278	-1.456537	1.963974		
H	-3.022670	-2.015819	1.293079		
H	-1.199638	1.173848	-0.795652		
H	-2.086133	0.386468	-2.106262		
S	-3.594749	1.582599	-0.714064		
H	-3.293757	1.918285	0.557040		
C	2.391659	-0.833866	0.379968		
C	2.008739	0.500744	1.039568		
N	3.708850	-1.277139	0.806155		
H	4.410660	-0.608747	0.497850		
H	3.941821	-2.161391	0.365197		
H	1.650647	-1.567340	0.721527		
C	2.230648	-0.764549	-1.143578		
O	3.084129	-1.056223	-1.946829		
O	0.999455	-0.342284	-1.497704		
H	0.939944	-0.322646	-2.466537		
H	0.963205	0.738190	0.862687		
H	2.161073	0.406604	2.114515		
S	3.052496	1.935808	0.530285		
H	2.498323	2.117322	-0.686061		
28					
Dimer 224 of the n...n type					
C	2.120167	-0.632514	0.409466		

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C	3.608441	-0.986796	0.532988		
N	1.482854	-0.940604	-0.870844		
H	2.125124	-0.771372	-1.641895		
H	1.191964	-1.910264	-0.917518		
H	1.591192	-1.192127	1.190316		
C	1.865404	0.844865	0.759749		
O	2.461227	1.438189	1.630425		
O	0.897601	1.421883	0.045350		
H	0.594925	0.749411	-0.612082		
H	3.975749	-0.742664	1.528196		
H	3.736773	-2.056448	0.366659		
S	4.683752	-0.168718	-0.722061		
H	4.609774	1.074879	-0.205457		
C	-2.366677	0.584453	0.625392		
C	-1.923527	-0.888192	0.667852		
N	-3.482924	0.827292	1.522313		
H	-4.297340	0.305589	1.208612		
H	-3.742478	1.808406	1.504547		
H	-1.506579	1.171357	0.968662		
C	-2.619333	1.037839	-0.817640		
O	-3.641998	1.533373	-1.225340		
O	-1.539586	0.824969	-1.599794		
H	-1.730928	1.134513	-2.499608		
H	-1.021112	-1.037114	0.079698		
H	-1.716337	-1.155780	1.703528		
S	-3.199181	-2.096323	0.104039		
H	-3.088178	-1.849773	-1.217556		
28					
Dimer 225 of the n...n type					
C	3.190443	0.514392	0.513701		
C	3.404738	-0.984778	0.273379		
N	2.504466	0.884311	1.754984		
H	1.823691	0.175371	2.017820		
H	3.153570	0.999639	2.524165		
H	4.180165	0.985536	0.521895		
C	2.459372	1.176105	-0.669954		
O	2.635568	0.876960	-1.828336		
O	1.621326	2.147615	-0.298394		
H	1.658333	2.134032	0.694989		
H	3.932366	-1.143914	-0.665487		
H	4.004639	-1.398032	1.084309		
S	1.849487	-1.975003	0.265421		
H	1.365014	-1.498398	-0.899737		
C	-1.651338	0.365564	0.449927		
C	-2.994444	0.185358	1.172602		
N	-1.509598	1.710643	-0.079345		
H	-2.196526	1.866555	-0.812088		
H	-0.592294	1.832140	-0.497320		
H	-0.869962	0.208586	1.205269		
C	-1.408157	-0.735496	-0.590709		
O	-0.948666	-0.553058	-1.693865		
O	-1.733227	-1.956833	-0.123945		
H	-1.540434	-2.617469	-0.808739		
H	-3.035580	-0.770514	1.689662		
H	-3.102812	0.985255	1.904354		
S	-4.474451	0.331367	0.078121		
H	-4.348515	-0.869657	-0.522596		
28					
Dimer 226 of the n...n type					
C	-1.944143	-0.175899	-0.489248		
C	-3.094670	-1.181079	-0.625586		
N	-1.063935	-0.349457	0.667127		
H	-1.586099	-0.688525	1.471610		
H	-0.315092	-1.004221	0.470827		
H	-1.330488	-0.265921	-1.393486		
C	-2.456518	1.276432	-0.516526		
O	-3.378217	1.652420	-1.205945		
O	-1.768681	2.104127	0.270082		
H	-1.107897	1.525392	0.729176		

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H	-3.670108	-0.978705	-1.527222
H	-2.684831	-2.189016	-0.692320
S	-4.237610	-1.218112	0.821214
H	-4.821281	-0.024318	0.590502
C	3.341887	-0.505851	0.732235
C	2.356157	0.594408	1.159501
N	4.675048	0.034307	0.528969
H	4.663083	0.700418	-0.239175
H	5.318705	-0.703702	0.262036
H	3.378643	-1.221365	1.562584
C	2.812422	-1.300404	-0.468567
O	3.400379	-1.459565	-1.510038
O	1.593715	-1.836502	-0.226770
H	1.323182	-2.352400	-1.004038
H	1.396736	0.175146	1.451686
H	2.781289	1.118006	2.015369
S	2.062557	1.906711	-0.102333
H	1.308818	1.168193	-0.941787
28			
Dimer 227 of the n...n type			
C	-2.380660	-0.796464	-0.308012
C	-1.626889	-0.405493	0.968604
N	-1.885781	-0.210151	-1.556789
H	-1.468968	0.703432	-1.394082
H	-1.197885	-0.802372	-2.005751
H	-2.319314	-1.886945	-0.397107
C	-3.888991	-0.503418	-0.183376
O	-4.527544	-0.685461	0.829120
O	-4.441983	-0.054803	-1.309717
H	-3.679721	0.025647	-1.940976
H	-2.063453	-0.904909	1.831736
H	-0.585206	-0.712389	0.881400
S	-1.579852	1.410640	1.288874
H	-2.875119	1.544241	1.639687
C	3.318060	0.069667	0.697291
C	2.223392	1.126802	0.477985
N	4.583063	0.489303	0.119820
H	4.490173	0.577082	-0.888852
H	5.296217	-0.213811	0.285094
H	3.443729	-0.018499	1.783248
C	2.850780	-1.313872	0.226169
O	3.444429	-2.019034	-0.553872
O	1.683129	-1.669741	0.801180
H	1.435914	-2.554867	0.487863
H	1.323731	0.868357	1.031202
H	2.589079	2.085849	0.843863
S	1.785880	1.430788	-1.287845
H	1.194995	0.241267	-1.520655
28			
Dimer 228 of the n...n type			
C	-2.598898	0.067408	0.977428
C	-2.909519	1.432288	0.351176
N	-1.240679	-0.094742	1.504052
H	-0.588792	0.557225	1.076072
H	-1.207301	0.044055	2.506569
H	-3.312156	-0.082765	1.795303
C	-2.901460	-1.072457	-0.015630
O	-3.890460	-1.104705	-0.714250
O	-1.986290	-2.039665	-0.026779
H	-1.286916	-1.736185	0.608144
H	-3.946984	1.470473	0.024131
H	-2.747981	2.215792	1.091711
S	-1.817229	1.872833	-1.070937
H	-2.339718	0.991058	-1.947819
C	2.575821	0.363413	-0.883113
C	1.451740	-0.682644	-0.945424
N	3.834444	-0.189621	-1.355164
H	4.133956	-0.939268	-0.736628
H	4.562696	0.516833	-1.323432

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H	2.277615	1.174144	-1.559535
C	2.673853	1.009618	0.504987
O	3.689349	1.119685	1.148037
O	1.480218	1.475201	0.933334
H	1.603119	1.900620	1.797679
H	0.481136	-0.220322	-0.781799
H	1.453791	-1.127478	-1.940057
S	1.654835	-2.099969	0.218050
H	1.267727	-1.449349	1.334340
28			
Dimer 229 of the n...n type			
C	2.117310	0.791577	-0.454287
C	1.827947	-0.557108	-1.126170
N	3.467663	1.329771	-0.635071
H	4.147618	0.580082	-0.737070
H	3.530107	1.930378	-1.448182
H	1.401640	1.513413	-0.865032
C	1.799339	0.752038	1.052958
O	0.826906	0.196019	1.521169
O	2.668501	1.419624	1.802433
H	3.350850	1.742573	1.154533
H	0.805682	-0.869530	-0.925614
H	1.956986	-0.455921	-2.203863
S	2.974549	-1.913321	-0.630766
H	2.527846	-2.050349	0.634378
C	-3.067177	-0.672992	-0.520465
C	-2.256712	0.275840	-1.425275
N	-4.377298	-0.123011	-0.217122
H	-4.274558	0.727521	0.330219
H	-4.907833	-0.772629	0.354750
H	-3.197427	-1.601734	-1.086865
C	-2.232210	-1.023110	0.715728
O	-2.514171	-0.721872	1.851708
O	-1.107225	-1.679034	0.378826
H	-0.507406	-1.683186	1.143862
H	-1.347783	-0.211310	-1.771529
H	-2.865543	0.536569	-2.290583
S	-1.812366	1.891550	-0.650249
H	-0.970740	1.399748	0.284565
28			
Dimer 230 of the n...n type			
C	2.121214	-0.791983	0.455799
C	1.827181	0.557085	1.125161
N	3.474771	-1.322791	0.634182
H	4.150571	-0.569578	0.737585
H	3.541367	-1.925393	1.445470
H	1.409855	-1.516080	0.869913
C	1.798881	-0.756210	-1.050654
O	0.819282	-0.210416	-1.515798
O	2.673377	-1.414120	-1.802622
H	3.359508	-1.731793	-1.156109
H	0.804181	0.865981	0.922899
H	1.955822	0.458539	2.203143
S	2.969505	1.916162	0.627808
H	2.523210	2.049372	-0.637926
C	-3.066715	0.670088	0.522354
C	-2.253528	-0.278756	1.424584
N	-4.376094	0.118076	0.219396
H	-4.272239	-0.731087	-0.329844
H	-4.908642	0.767890	-0.350376
H	-3.198325	1.597479	1.090671
C	-2.234585	1.025148	-0.714415
O	-2.518682	0.727766	-1.850845
O	-1.110196	1.682374	-0.377884
H	-0.515307	1.696340	-1.146489
H	-1.344419	0.209024	1.769513
H	-2.860290	-0.540652	2.290983
S	-1.809185	-1.893293	0.647269
H	-0.966061	-1.399998	-0.285490

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28		
Dimer 231 of the n...n type		
C 2.121594	-0.093703	0.285256
C 3.361691	-0.795482	0.851558
N 1.506369	-0.708256	-0.892386
H 2.201791	-1.177368	-1.467188
H 0.796919	-1.381297	-0.622638
H 1.370201	-0.081609	1.083377
C 2.399246	1.391986	-0.011999
O 3.080723	2.104200	0.691252
O 1.790003	1.839385	-1.110081
H 1.348336	1.034176	-1.488343
H 3.725469	-0.265566	1.730154
H 3.098366	-1.812647	1.142175
S 4.743994	-0.980107	-0.355322
H 5.076323	0.325808	-0.414462
C -3.188875	0.845104	0.201065
C -1.716710	0.407720	0.275040
N -3.759760	1.007441	1.526704
H -3.789430	0.109860	2.003198
H -4.719085	1.332099	1.460074
H -3.190563	1.820342	-0.300208
C -3.992819	-0.089231	-0.713005
O -4.998765	-0.676900	-0.393429
O -3.443473	-0.175695	-1.940257
H -3.984650	-0.767664	-2.487078
H -1.262891	0.402816	-0.713693
H -1.178772	1.115759	0.904956
S -1.439359	-1.237627	1.065600
H -1.925086	-1.991555	0.057651
28		
Dimer 232 of the n...n type		
C -1.958483	-0.491085	-0.243579
C -1.599594	0.998569	-0.196513
N -2.592136	-0.968861	-1.474967
H -3.168071	-0.241522	-1.892245
H -1.905048	-1.260295	-2.159965
H -1.023927	-1.045767	-0.113842
C -2.827490	-0.901996	0.958851
O -2.676047	-0.467473	2.078814
O -3.751942	-1.816280	0.663535
H -3.662494	-1.948145	-0.316011
H -1.138991	1.242248	0.759355
H -0.889837	1.217975	-0.993223
S -3.023946	2.133713	-0.479493
H -3.652949	1.893228	0.689160
C 2.205157	-0.714761	0.637827
C 2.194756	0.806874	0.873679
N 3.288054	-1.353226	1.364000
H 4.182464	-1.034149	1.000958
H 3.260714	-2.358824	1.228741
H 1.253593	-1.090408	1.031908
C 2.193159	-1.024863	-0.863536
O 3.048920	-1.635109	-1.457277
O 1.090667	-0.525069	-1.460995
H 1.124277	-0.729838	-2.409387
H 1.322800	1.263294	0.411361
H 2.155732	0.987657	1.947443
S 3.705459	1.692505	0.293591
H 3.428304	1.654677	-1.026047
28		
Dimer 233 of the n...n type		
C -2.735159	0.899121	-0.147108
C -3.256491	-0.370757	-0.831637
N -1.738380	1.680172	-0.884012
H -1.120896	1.068101	-1.413430
H -2.173500	2.328110	-1.530063
H -3.601545	1.546080	0.033726
C -2.183941	0.595961	1.258716

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O -2.647311	-0.235230	2.004524
O -1.144829	1.363982	1.601030
H -0.972942	1.916435	0.795419
H -3.975511	-0.873881	-0.187327
H -3.753658	-0.100047	-1.763269
S -1.942240	-1.565288	-1.322583
H -1.543202	-1.900170	-0.076996
C 2.898672	-0.284019	-0.697330
C 1.787111	-1.325047	-0.469728
N 4.086740	-0.595245	0.077128
H 3.878111	-0.536322	1.070168
H 4.819031	0.082292	-0.109829
H 3.150978	-0.339727	-1.762170
C 2.355159	1.130496	-0.467730
O 2.720019	1.886761	0.400861
O 1.396883	1.443431	-1.364284
H 1.071926	2.339216	-1.177747
H 0.928777	-1.113508	-1.104927
H 2.178640	-2.309055	-0.726933
S 1.211862	-1.493335	1.274138
H 0.571125	-0.310130	1.368533
28		
Dimer 234 of the n...n type		
C 2.911396	0.255981	-0.694796
C 2.064831	-0.992273	-0.971618
N 4.318485	0.029989	-0.354433
H 4.432216	-0.842868	0.155717
H 4.904091	-0.007819	-1.180153
H 2.876995	0.874996	-1.598771
C 2.274963	1.136287	0.397503
O 1.079733	1.293574	0.521170
O 3.161745	1.737195	1.186307
H 4.038940	1.384501	0.882260
H 1.054043	-0.707028	-1.256225
H 2.509286	-1.551855	-1.794958
S 1.996956	-2.187672	0.431327
H 1.346461	-1.385978	1.299317
C -1.660105	-0.138386	0.378618
C -2.822120	-1.136174	0.221242
N -1.713684	0.556570	1.651354
H -2.532024	1.158457	1.681513
H -0.897057	1.154376	1.736062
H -0.745746	-0.735786	0.349356
C -1.601009	0.792633	-0.834243
O -1.916442	1.958647	-0.839412
O -1.176183	0.137733	-1.935648
H -1.178061	0.752166	-2.687055
H -2.717464	-1.702977	-0.702532
H -2.791673	-1.830224	1.061147
S -4.512034	-0.398646	0.285206
H -4.490912	0.189607	-0.928239
28		
Dimer 235 of the n...n type		
C 2.726247	-0.499352	-0.877105
C 3.082936	0.967505	-0.607156
N 1.477612	-0.744380	-1.603735
H 0.777823	-0.031284	-1.410792
H 1.625790	-0.774272	-2.605323
H 3.548131	-0.924632	-1.464840
C 2.717115	-1.328199	0.421900
O 3.501765	-1.167612	1.329913
O 1.776376	-2.272517	0.443990
H 1.276592	-2.135554	-0.403516
H 4.060068	1.037282	-0.132422
H 3.117949	1.507448	-1.553458
S 1.855853	1.875881	0.428959
H 2.169172	1.279761	1.597149
C -1.615971	0.152171	0.772762
C -1.966509	-1.213872	0.164883

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N	-2.339866	0.384050	2.011284
H	-3.338281	0.429601	1.823727
H	-2.078769	1.281713	2.406677
H	-0.543844	0.125602	1.002854
C	-1.764428	1.285597	-0.249502
O	-2.316373	2.338905	-0.043638
O	-1.176215	0.981879	-1.427579
H	-1.257612	1.741024	-2.027279
H	-1.321506	-1.441450	-0.680751
H	-1.822876	-1.977972	0.928202
S	-3.724991	-1.387785	-0.368157
H	-3.631432	-0.632827	-1.482092
28			
Dimer 236 of the n...n type			
C	-2.500099	1.124055	-0.416553
C	-3.526143	-0.013785	-0.507462
N	-1.495981	1.185868	-1.476101
H	-1.220004	0.251877	-1.768280
H	-1.842661	1.678424	-2.290673
H	-3.065997	2.063254	-0.438438
C	-1.799537	1.145817	0.953974
O	-2.347329	0.843461	1.990942
O	-0.538788	1.576243	0.922039
H	-0.290877	1.678707	-0.029283
H	-4.232731	0.046985	0.318490
H	-4.076816	0.074433	-1.444177
S	-2.787997	-1.702808	-0.542719
H	-2.342919	-1.706199	0.730167
C	3.032332	0.028196	0.552796
C	2.714150	-1.477426	0.493537
N	2.446001	0.651764	1.725464
H	1.433748	0.687592	1.633071
H	2.760351	1.613796	1.802961
H	4.123581	0.102098	0.625113
C	2.658379	0.710967	-0.768744
O	1.855835	1.607744	-0.888962
O	3.340313	0.191633	-1.807217
H	3.069357	0.646609	-2.620937
H	3.225400	-1.946122	-0.345228
H	3.064002	-1.937333	1.417507
S	0.918550	-1.889757	0.414046
H	0.701842	-1.496102	-0.856752
28			
Dimer 237 of the n...n type			
C	-2.130588	-0.448750	0.429986
C	-1.643695	1.005897	0.393047
N	-1.722516	-1.305288	-0.685309
H	-1.638375	-0.768090	-1.544913
H	-0.836116	-1.765776	-0.501155
H	-1.742653	-0.892219	1.354533
C	-3.663036	-0.524395	0.579929
O	-4.311627	0.230672	1.269550
O	-4.215533	-1.528033	-0.100860
H	-3.453353	-1.937023	-0.590244
H	-2.026213	1.550161	1.254831
H	-0.555228	1.032255	0.423654
S	-2.095160	1.918206	-1.144196
H	-3.420072	1.996373	-0.903031
C	3.230822	0.205652	-0.704225
C	2.027473	-0.702878	-1.002782
N	4.472600	-0.546325	-0.679216
H	4.456940	-1.218067	0.083623
H	5.257067	0.073694	-0.504840
H	3.277165	0.926601	-1.529269
C	2.984291	1.044382	0.557334
O	3.714695	1.085588	1.518000
O	1.841530	1.755596	0.466723
H	1.735324	2.284045	1.274292
H	1.124752	-0.109824	-1.132861

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H	2.221579	-1.247230	-1.926481
S	1.715267	-2.017469	0.254988
H	1.362770	-1.205432	1.273827
28			
Dimer 238 of the n...n type			
C	2.956582	-0.829349	0.183608
C	1.551104	-0.354996	-0.203915
N	3.261443	-0.855280	1.616756
H	2.778856	-0.104203	2.104544
H	2.991080	-1.733829	2.042588
H	3.069651	-1.848634	-0.202909
C	4.047137	-0.019011	-0.543162
O	3.949453	0.365852	-1.686836
O	5.135602	0.197239	0.195580
H	4.914030	-0.191541	1.081033
H	1.429629	-0.387615	-1.285667
H	0.805997	-1.004853	0.254742
S	1.137217	1.340578	0.387814
H	1.913401	2.011139	-0.487516
C	-3.668164	-0.762121	-0.197376
C	-3.753888	0.680303	-0.730423
N	-4.203370	-0.862295	1.148591
H	-3.636311	-0.311157	1.787371
H	-4.163226	-1.822525	1.474913
H	-4.289074	-1.369399	-0.866059
C	-2.244281	-1.309594	-0.345499
O	-1.538720	-1.676607	0.564991
O	-1.860634	-1.342559	-1.636775
H	-0.964551	-1.710566	-1.693066
H	-3.411603	0.728403	-1.762303
H	-4.795707	0.997894	-0.692647
S	-2.842172	1.934987	0.268031
H	-1.585942	1.578064	-0.081047
28			
Dimer 239 of the n...n type			
C	-2.787558	-0.277740	0.863280
C	-1.444668	0.366063	0.499540
N	-2.907183	-1.715980	0.610178
H	-2.375725	-1.987424	-0.213638
H	-2.576425	-2.264925	1.394657
H	-2.943230	-0.111019	1.935294
C	-3.965721	0.447656	0.185104
O	-4.014411	1.646373	0.023806
O	-4.953902	-0.366724	-0.185387
H	-4.620724	-1.275193	0.032628
H	-1.445961	1.424755	0.752399
H	-0.648481	-0.128479	1.055047
S	-0.972048	0.173709	-1.272418
H	-1.872388	1.041673	-1.777031
C	3.313867	-0.495982	0.742196
C	2.608462	0.798553	1.187573
N	4.652214	-0.221644	0.248905
H	4.600434	0.335995	-0.599481
H	5.122212	-1.086706	0.001801
H	3.394304	-1.120745	1.638936
C	2.440843	-1.286369	-0.238786
O	2.724735	-1.528952	-1.387144
O	1.293872	-1.701193	0.340602
H	0.784847	-2.215313	-0.307128
H	1.639118	0.577257	1.630221
H	3.229374	1.280613	1.942180
S	2.394447	2.069387	-0.133996
H	1.345323	1.494232	-0.765292
28			
Dimer 240 of the n...n type			
C	1.988567	0.298764	-0.577298
C	1.554251	-0.755194	0.447895
N	2.333694	-0.197614	-1.912685
H	2.743973	-1.126965	-1.858303

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H	1.522340	-0.246216	-2.517150
H	1.153098	1.000725	-0.681060
C	3.149996	1.161033	-0.050815
O	3.252694	1.523903	1.099846
O	4.028179	1.508512	-0.992501
H	3.709151	1.041789	-1.808372
H	1.322519	-0.277881	1.398867
H	0.659954	-1.256900	0.078925
S	2.792392	-2.088923	0.736542
H	3.702813	-1.329725	1.380160
C	-2.690515	-0.892054	0.039225
C	-2.108042	-0.194625	1.282810
N	-1.662699	-1.148557	-0.955196
H	-1.368580	-0.271898	-1.377284
H	-2.034290	-1.720008	-1.707166
H	-3.085466	-1.852553	0.388267
C	-3.893507	-0.110372	-0.501846
O	-3.967205	0.373805	-1.606504
O	-4.876787	-0.018025	0.414176
H	-5.612292	0.491034	0.037027
H	-2.871454	-0.068627	2.047885
H	-1.311277	-0.818578	1.685799
S	-1.310404	1.436816	0.957538
H	-2.438797	2.143849	0.742315
28			
Dimer 241 of the n...n type			
C	2.026593	-0.465616	0.004977
C	2.091813	1.063234	-0.103519
N	1.920947	-1.017712	1.357681
H	2.402265	-0.425619	2.030205
H	0.957169	-1.116717	1.653203
H	1.150106	-0.795074	-0.564134
C	3.217165	-1.130640	-0.714092
O	3.681756	-0.728946	-1.757233
O	3.675018	-2.218195	-0.095049
H	3.134317	-2.273984	0.735544
H	2.148839	1.364831	-1.147967
H	1.192982	1.497034	0.333807
S	3.490121	1.827444	0.823086
H	4.474449	1.386679	0.013311
C	-2.384182	-0.757708	-0.367763
C	-1.674193	0.606842	-0.342410
N	-2.855586	-1.081225	-1.702725
H	-3.573497	-0.418750	-1.984750
H	-3.289265	-1.998882	-1.710625
H	-1.633219	-1.501089	-0.074822
C	-3.471760	-0.826997	0.711369
O	-4.634490	-1.085380	0.510482
O	-2.970873	-0.569830	1.935623
H	-3.687173	-0.628463	2.588097
H	-1.224905	0.787744	0.631559
H	-0.893543	0.602331	-1.102511
S	-2.742723	2.046705	-0.776642
H	-3.418331	2.110254	0.389333
28			
Dimer 242 of the n...n type			
C	1.855129	0.421952	-0.185972
C	2.047675	-1.077780	0.068452
N	1.882209	0.852287	-1.586881
H	2.509629	0.268850	-2.135292
H	0.963122	0.813027	-2.011024
O	0.880670	0.688929	0.235119
C	2.864147	1.264103	0.614688
O	3.217293	0.999906	1.742530
O	3.295390	2.345030	-0.036153
H	2.870810	2.277729	-0.930806
H	1.989646	-1.289729	1.134509
H	1.259621	-1.634563	-0.438543
S	3.624763	-1.761765	-0.599675

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H	4.445214	-1.154736	0.282073
C	-2.324823	-0.712550	-0.588409
C	-2.552721	0.775615	-0.904013
N	-3.386516	-1.538898	-1.135662
H	-4.268234	-1.312620	-0.682737
H	-3.204957	-2.518761	-0.942854
H	-1.385425	-0.989283	-1.081636
C	-2.082353	-0.926798	0.911410
O	-2.695179	-1.695436	1.612395
O	-1.077242	-0.151465	1.368090
H	-0.944924	-0.326890	2.313692
H	-1.699820	1.373911	-0.591396
H	-2.681425	0.884411	-1.980466
S	-4.083118	1.493493	-0.163526
H	-3.634513	1.566835	1.106551
28			
Dimer 243 of the n...n type			
C	2.505415	-0.743552	-0.572211
C	1.841498	0.573615	-0.993843
N	1.799241	-1.543333	0.431520
H	1.312788	-0.945405	1.095070
H	1.124556	-2.170550	0.010872
H	2.607498	-1.353984	-1.476856
C	3.954469	-0.519901	-0.095477
O	4.709201	0.287259	-0.589683
O	4.321172	-1.326845	0.900448
H	3.499931	-1.838461	1.119177
H	2.462527	1.086537	-1.726221
H	0.868546	0.369527	-1.439139
S	1.478747	1.723010	0.400371
H	2.759109	1.979123	0.739451
C	-2.050713	0.035485	0.794838
C	-2.119580	-1.284324	0.009596
N	-2.903799	-0.001885	1.969722
H	-3.876786	-0.085515	1.686601
H	-2.826760	0.867630	2.487604
H	-1.011494	0.144558	1.128319
C	-2.304641	1.240558	-0.119485
O	-3.106458	2.118172	0.092976
O	-1.499954	1.220384	-1.201382
H	-1.667659	2.013425	-1.735462
H	-1.390401	-1.294230	-0.797322
H	-1.898376	-2.104213	0.692416
S	-3.781117	-1.676910	-0.690626
H	-3.744006	-0.792567	-1.708501
28			
Dimer 244 of the n...n type			
C	2.165182	0.615271	0.446217
C	3.214565	-0.056460	1.340918
N	0.997973	-0.199396	0.097138
H	1.260382	-1.177562	-0.004140
H	0.277562	-0.134909	0.807944
H	1.807565	1.503213	0.980142
C	2.796708	1.173665	-0.842599
O	3.893785	1.682493	-0.887258
O	2.008941	1.079045	-1.914916
H	1.208043	0.595278	-1.594813
H	4.027771	0.635285	1.553076
H	2.750235	-0.348010	2.283068
S	3.914108	-1.613690	0.643769
H	4.634419	-1.036301	-0.339514
C	-3.591845	-0.282019	0.704338
C	-2.725874	-1.457775	0.222352
N	-4.812682	-0.177231	-0.076400
H	-4.585569	0.050612	-1.041028
H	-5.389974	0.581663	0.271576
H	-3.862743	-0.508237	1.742869
C	-2.791640	1.024392	0.771666
O	-3.105353	2.059975	0.237192

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O	-1.683923	0.901398	1.537988
H	-1.254568	1.770661	1.596102
H	-1.877594	-1.614502	0.885392
H	-3.339902	-2.357653	0.232391
S	-2.113984	-1.305625	-1.513402
H	-1.064824	-0.499851	-1.245493
28			
Dimer 1 of the n...z type			
C	1.600758	-0.103114	-0.595542
C	2.843504	0.616669	-1.136454
N	0.732437	0.720715	0.264632
H	1.302274	1.202128	0.959592
H	0.280869	1.443571	-0.289932
H	0.994117	-0.403352	-1.455308
C	1.944066	-1.399869	0.160065
O	3.061886	-1.674284	0.545581
O	0.921158	-2.217144	0.384860
H	0.080257	-1.944129	-0.116883
H	3.463641	-0.082609	-1.697294
H	2.521420	1.409413	-1.813439
S	3.885983	1.470770	0.123359
H	4.284607	0.351826	0.758311
C	-2.308106	-1.069979	-0.711329
C	-2.622546	-0.575278	0.729981
O	-1.169474	-1.587933	-0.915625
O	-3.219428	-0.919523	-1.535554
H	-3.282511	-1.317495	1.186822
C	-3.350444	0.766624	0.743444
N	-1.371385	-0.527814	1.558835
H	-1.535158	-0.080194	2.461109
H	-3.541709	1.096857	1.765994
H	-4.307138	0.632367	0.244275
S	-2.450882	2.152352	-0.074836
H	-1.026501	-1.469363	1.747224
H	-0.568505	-0.008381	1.052953
H	-2.540170	1.647609	-1.322750
28			
Dimer 2 of the n...z type			
C	-2.554882	-0.610801	-1.098294
C	-3.794634	0.187847	-0.664892
N	-2.721793	-2.033004	-0.843408
H	-2.811952	-2.188194	0.157745
H	-1.887267	-2.534866	-1.130692
H	-2.452135	-0.459157	-2.179609
C	-1.288460	-0.009154	-0.479904
O	-0.478432	-0.687557	0.142112
O	-1.169010	1.282681	-0.690701
H	-0.291986	1.643121	-0.323375
H	-3.721331	1.220265	-0.999975
H	-4.678145	-0.267989	-1.111094
S	-4.104449	0.176832	1.157167
H	-3.095453	1.007937	1.490157
C	2.201522	1.839990	-0.166989
C	2.690494	0.518770	0.488995
O	1.044817	2.237090	0.178464
O	2.988059	2.364721	-0.962155
H	3.660137	0.697385	0.953271
C	2.795662	-0.585403	-0.562972
N	1.736895	0.106222	1.573772
H	1.583028	0.870311	2.231290
H	3.461948	-0.243115	-1.351694
H	1.814905	-0.788273	-0.996869
S	3.379828	-2.204914	0.096704
H	0.817405	-0.137463	1.140902
H	2.086530	-0.711616	2.078333
H	4.620850	-1.794542	0.429722
28			
Dimer 3 of the n...z type			
C	3.168597	0.228119	0.624494

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C	3.273704	-0.710299	-0.596082
N	3.341721	-0.506192	1.867433
H	2.568405	-1.156689	1.982643
H	3.296578	0.130303	2.657286
H	3.977497	0.959515	0.525216
C	1.851902	0.998504	0.528939
O	0.932558	0.827201	1.316142
O	1.804321	1.803129	-0.518388
H	0.854282	2.068947	-0.716992
H	3.279227	-0.132478	-1.518353
H	4.207350	-1.267069	-0.520782
S	1.940712	-1.988388	-0.708522
H	0.982971	-1.199424	-1.247562
C	-0.990857	0.752557	-1.209172
C	-1.810088	0.118742	-0.054764
O	-0.731235	1.987319	-1.087164
O	-0.650870	-0.021364	-2.115833
H	-1.292050	-0.782564	0.272861
C	-3.228274	-0.213122	-0.506154
N	-1.806909	1.061593	1.111607
H	-0.819168	1.186083	1.404867
H	-3.166060	-0.863954	-1.376245
H	-3.761772	0.694659	-0.794969
S	-4.266689	-1.003990	0.795951
H	-2.159424	1.977764	0.826447
H	-2.371305	0.702522	1.885867
H	-3.552685	-2.144644	0.885942
28			
Dimer 4 of the n...z type			
C	2.707594	-1.177571	-0.466876
C	3.214615	-0.549798	0.843238
N	3.339979	-0.569390	-1.627457
H	3.060277	0.406339	-1.689640
H	3.001571	-1.013740	-2.475395
H	2.991739	-2.235068	-0.426764
C	1.173412	-1.153974	-0.502174
O	0.537144	-0.543748	-1.344676
O	0.636866	-1.850463	0.484353
H	-0.387103	-1.850388	0.470574
H	2.784477	-1.063662	1.700908
H	4.299880	-0.644317	0.882130
S	2.894143	1.262671	1.003518
H	1.559766	1.195888	1.174817
C	-2.815065	-1.170167	0.385433
C	-2.307539	0.112649	-0.322126
O	-4.034947	-1.261303	0.596317
O	-1.906716	-1.993847	0.690063
H	-1.705354	-0.168005	-1.183212
C	-1.474092	0.970300	0.627685
N	-3.489974	0.893779	-0.828027
H	-3.938009	0.414142	-1.610133
H	-0.691016	0.347159	1.052184
H	-2.083822	1.346735	1.451530
S	-0.728574	2.452674	-0.172924
H	-4.197184	0.970169	-0.090489
H	-3.205874	1.828875	-1.138965
H	0.059192	1.755891	-1.018185
28			
Dimer 5 of the n...z type			
C	-2.981810	-0.479014	0.232318
C	-3.117462	0.712202	-0.727258
N	-3.244647	-0.075642	1.607856
H	-2.526620	0.581162	1.905998
H	-3.153150	-0.878365	2.223153
H	-3.742474	-1.210609	-0.066374
C	-1.626530	-1.174335	0.048615
O	-0.922088	-1.493235	0.997280
O	-1.296738	-1.360643	-1.213249
H	-0.329555	-1.702320	-1.302096

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H	-3.142816	0.376499	-1.761022
H	-4.043435	1.240115	-0.502369
S	-1.760277	1.966950	-0.569984
H	-0.916462	1.368502	-1.432963
C	1.861150	-1.683766	-0.424930
C	1.602263	-0.225920	0.059876
O	2.771975	-2.283417	0.166695
O	1.140474	-2.098011	-1.377639
H	0.645955	0.145952	-0.291698
C	2.727576	0.695854	-0.397333
N	1.515484	-0.266424	1.557978
H	0.630495	-0.727644	1.812909
H	2.771727	0.683336	-1.485688
H	3.685315	0.344782	-0.010366
S	2.549327	2.433274	0.196204
H	2.298645	-0.815149	1.927311
H	1.538194	0.676732	1.958435
H	1.423416	2.720185	-0.488017
28			
Dimer 6 of the n...z type			
C	-2.671210	-1.152976	-0.641450
C	-3.456489	0.051104	-0.082534
N	-2.713385	-2.282084	0.273561
H	-2.229440	-2.036957	1.133666
H	-2.210205	-3.070249	-0.121977
H	-3.159401	-1.434933	-1.580067
C	-1.259882	-0.681298	-0.990999
O	-0.268872	-1.034555	-0.370544
O	-1.242126	0.187534	-1.987908
H	-0.355642	0.660970	-2.030696
H	-3.520424	0.838273	-0.831844
H	-4.463264	-0.279249	0.172307
S	-2.761950	0.767514	1.474715
H	-1.675391	1.358683	0.921311
C	0.987947	1.582094	-0.447403
C	2.103390	0.812110	0.321981
O	0.148486	2.159713	0.271928
O	1.015456	1.514725	-1.704363
H	2.810039	1.539649	0.725706
C	2.823050	-0.228306	-0.522748
N	1.430917	0.166449	1.506162
H	2.104552	-0.322428	2.101049
H	3.282561	0.274205	-1.369958
H	2.107554	-0.954117	-0.907102
S	4.093460	-1.197867	0.399623
H	0.936239	0.879886	2.046863
H	0.727599	-0.503865	1.160592
H	4.933957	-0.170474	0.638712
28			
Dimer 7 of the n...z type			
C	-2.741365	-0.827352	-0.549221
C	-2.567618	0.694218	-0.727508
N	-3.832617	-1.144360	0.359819
H	-3.586364	-0.865610	1.305538
H	-3.980040	-2.148723	0.384428
H	-2.982047	-1.223541	-1.539417
C	-1.380433	-1.404666	-0.143590
O	-1.067937	-1.601466	1.020049
O	-0.574140	-1.579162	-1.175024
H	0.370939	-1.863186	-0.878238
H	-1.753448	0.892836	-1.425236
H	-3.487765	1.112248	-1.135860
S	-2.278570	1.645780	0.835772
H	-1.398481	0.794618	1.402094
C	2.542283	-1.359951	0.061153
C	1.875365	0.016647	0.355318
O	3.724813	-1.495357	0.414559
O	1.813314	-2.187379	-0.552882
H	0.896514	-0.134827	0.804567

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C	1.766337	0.819200	-0.946040
N	2.727023	0.744140	1.356767
H	2.508193	0.461338	2.312695
H	1.091536	0.292143	-1.616685
H	2.742766	0.890958	-1.429312
S	1.209468	2.562256	-0.735305
H	3.707827	0.486799	1.181901
H	2.596007	1.760300	1.281434
H	-0.016656	2.295931	-0.225776
28			
Dimer 8 of the n...z type			
C	-3.070508	0.797186	0.082632
C	-3.311162	-0.462840	0.930530
N	-3.354679	0.672486	-1.349604
H	-3.323230	-0.301212	-1.641759
H	-4.257970	1.057433	-1.595198
H	-3.688770	1.596711	0.503232
C	-1.628035	1.295436	0.248118
O	-1.079719	1.418459	1.329103
O	-1.023281	1.601540	-0.886954
H	-1.709524	1.399084	-1.584335
H	-2.960374	-0.288275	1.946965
H	-4.380531	-0.672006	0.960601
S	-2.532665	-1.993775	0.257362
H	-1.225438	-1.609593	0.368385
C	1.133683	-0.590304	-0.559302
C	1.908255	0.743234	-0.355287
O	0.604770	-1.079442	0.472017
O	1.145335	-1.032187	-1.722940
H	1.471481	1.493830	-1.013104
C	3.393692	0.597153	-0.671052
N	1.695548	1.225711	1.051980
H	2.195279	2.095672	1.239900
H	3.919040	1.545311	-0.542214
H	3.487359	0.288112	-1.710299
S	4.285123	-0.606932	0.408248
H	0.677217	1.368062	1.229066
H	2.018856	0.510052	1.707853
H	3.629567	-1.705965	-0.018120
28			
Dimer 9 of the n...z type			
C	-2.070052	-0.289384	0.757014
C	-1.914694	0.994910	-0.083829
N	-1.120439	-1.326597	0.350643
H	-1.501089	-1.839806	-0.442241
H	-0.999192	-2.003345	1.098588
H	-1.866951	-0.009601	1.793615
C	-3.517737	-0.770945	0.684252
O	-3.884052	-1.750633	0.077921
O	-4.344133	0.060118	1.338745
H	-5.259138	-0.245409	1.228918
H	-2.677074	1.718925	0.200705
H	-0.934606	1.434013	0.097539
S	-1.952227	0.734138	-1.905981
H	-3.201269	0.229615	-1.988560
C	1.804750	1.663761	0.545382
C	2.155245	0.150110	0.374524
O	1.155498	2.181798	-0.398507
O	2.238018	2.189524	1.588227
H	1.918831	-0.380623	1.296458
C	3.642350	0.012441	0.052640
N	1.303415	-0.422866	-0.711357
H	0.371381	-0.756123	-0.313615
H	4.212889	0.472215	0.856972
H	3.881123	0.530342	-0.878956
S	4.207622	-1.725653	-0.202178
H	1.111951	0.330162	-1.383152
H	1.754834	-1.214350	-1.176091
H	3.899346	-2.167342	1.034385

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28		
Dimer 10 of the n...z type		
C	1.999786 0.200509 0.834391	
C	1.573528 -1.217931 0.408841	
N	0.916560 1.166744 0.652719	
H	0.821762 1.384218 -0.337196	
H	1.150095 2.044314 1.109790	
H	2.245896 0.147722 1.898517	
C	3.271920 0.606226 0.091603	
O	3.325383 1.466389 -0.755435	
O	4.320191 -0.142110 0.471520	
H	5.100985 0.113793 -0.045665	
H	2.399441 -1.911762 0.558515	
H	0.727192 -1.544266 1.012246	
S	0.958858 -1.353299 -1.322659	
H	2.101679 -0.985605 -1.939758	
C	-2.228887 -1.651996 0.173784	
C	-2.453834 -0.133606 0.480800	
O	-1.492380 -2.269447 0.984214	
O	-2.823919 -2.080224 -0.833403	
H	-3.485184 -0.018161 0.818260	
C	-2.207876 0.730863 -0.751294	
N	-1.563995 0.266117 1.621431	
H	-1.412819 -0.575230 2.189442	
H	-2.929421 0.452421 -1.515155	
H	-1.212194 0.545262 -1.153903	
S	-2.281949 2.547230 -0.441724	
H	-0.611863 0.599702 1.276178	
H	-1.968164 1.012215 2.184504	
H	-3.587936 2.601203 -0.108623	
28		
Dimer 11 of the n...z type		
C	-2.757754 -0.230289 0.737031	
C	-1.705047 -1.346623 0.691312	
N	-3.890536 -0.370868 -0.182456	
H	-3.641696 -0.948730 -0.981315	
H	-4.699269 -0.778132 0.270036	
H	-3.138982 -0.186829 1.762513	
C	-2.103528 1.145828 0.515725	
O	-1.087346 1.498979 1.076456	
O	-2.769903 1.932730 -0.319336	
H	-3.547141 1.377132 -0.601209	
H	-0.874557 -1.090959 1.348315	
H	-2.152310 -2.279368 1.035143	
S	-1.058768 -1.711561 -0.995737	
H	-0.473066 -0.510530 -1.229398	
C	1.890646 0.435855 -1.399627	
C	2.625459 0.969189 -0.126239	
O	0.818962 1.032215 -1.688369	
O	2.444483 -0.508740 -1.986603	
H	3.417748 1.639103 -0.467654	
C	3.239930 -0.127337 0.734643	
N	1.649538 1.805093 0.649261	
H	2.091121 2.525636 1.219305	
H	3.786247 0.293869 1.579754	
H	3.932045 -0.691678 0.114156	
S	1.999187 -1.277178 1.470100	
H	0.996398 2.219491 -0.030953	
H	1.059362 1.216856 1.250342	
H	1.496584 -1.726820 0.299261	
28		
Dimer 12 of the n...z type		
C	3.099587 -0.843913 0.121617	
C	3.301138 0.452375 0.921256	
N	3.510306 -0.807296 -1.285043	
H	3.457657 0.139790 -1.652461	
H	4.454400 -1.149499 -1.413105	
H	3.667702 -1.630357 0.629952	
C	1.640691 -1.324518 0.198113	

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O	0.989440 -1.338043 1.220887	
O	1.156193 -1.762720 -0.960175	
H	1.904425 -1.622866 -1.602595	
H	2.881055 0.336760 1.919616	
H	4.369139 0.651095 1.012226	
S	2.590966 1.957052 0.125589	
H	1.273324 1.664401 0.302126	
C	-1.213041 0.776273 -0.453155	
C	-1.798327 -0.617082 -0.063310	
O	-0.651048 1.403546 0.487656	
O	-1.345617 1.105062 -1.642635	
H	-1.129347 -1.365967 -0.485097	
C	-3.209762 -0.852866 -0.583703	
N	-1.708257 -0.738787 1.432712	
H	-1.318384 -1.630552 1.733070	
H	-3.563262 -1.850495 -0.319563	
H	-3.188006 -0.763246 -1.667491	
S	-4.463157 0.314924 0.102498	
H	-1.057824 0.023917 1.702586	
H	-2.611481 -0.568640 1.882057	
H	-3.912151 1.432257 -0.415172	
28		
Dimer 13 of the n...z type		
C	-1.685630 0.351205 0.414489	
C	-1.348187 0.090318 -1.063336	
N	-0.807518 -0.385921 1.324863	
H	-0.800283 -1.372016 1.067283	
H	-1.192793 -0.352975 2.266219	
H	-1.521806 1.422091 0.572510	
C	-3.163200 0.073954 0.691642	
O	-3.574604 -0.698125 1.525503	
O	-3.958703 0.806482 -0.106309	
H	-4.886465 0.608142 0.098547	
H	-2.027701 0.655178 -1.697854	
H	-0.339327 0.433630 -1.276834	
S	-1.373489 -1.683195 -1.565992	
H	-2.693825 -1.890888 -1.381990	
C	1.465535 1.873156 -0.583167	
C	2.312429 0.841991 0.234008	
O	0.632399 2.539993 0.074518	
O	1.716907 1.910341 -1.805652	
H	3.324127 1.241835 0.324041	
C	2.351607 -0.530990 -0.431422	
N	1.740573 0.730151 1.612848	
H	1.621616 1.660348 2.014583	
H	2.706603 -0.410392 -1.451385	
H	1.355041 -0.972611 -0.468549	
S	3.381945 -1.778570 0.456904	
H	0.767840 0.290480 1.545400	
H	2.330150 0.159462 2.220872	
H	4.566821 -1.160988 0.270837	
28		
Dimer 14 of the n...z type		
C	-3.047606 -0.948093 -0.331346	
C	-3.515801 0.403663 0.238662	
N	-3.165579 -2.008700 0.659683	
H	-2.533235 -1.811437 1.431627	
H	-2.850353 -2.887388 0.259811	
H	-3.709869 -1.176592 -1.173697	
C	-1.635460 -0.781483 -0.906106	
O	-0.659052 -1.348266 -0.454915	
O	-1.604682 0.084186 -1.913445	
H	-0.647286 0.361705 -2.098265	
H	-3.550980 1.150504 -0.552277	
H	-4.513982 0.283820 0.660021	
S	-2.470491 1.053984 1.618881	
H	-1.375331 1.342310 0.873683	
C	1.114971 1.194917 -0.909058	
C	2.480774 0.725205 -0.349139	

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O	0.377483	1.828325	-0.127753	
O	0.873775	0.818869	-2.084952	
H	3.275586	0.909465	-1.068784	
C	2.387204	-0.764437	-0.013145	
N	2.785982	1.523558	0.889325	
H	3.172429	2.440111	0.659930	
H	2.143306	-1.301955	-0.925837	
H	1.578355	-0.946817	0.695049	
S	3.906849	-1.458925	0.760860	
H	1.899944	1.685397	1.386166	
H	3.454942	1.031447	1.492072	
H	4.727247	-1.249065	-0.289094	
28				
Dimer 15 of the n...z type				
C	3.088838	0.481130	-0.535630	
C	3.533741	-0.912618	-0.076374	
N	3.089540	1.535807	0.480690	
H	2.846506	1.162577	1.395123	
H	3.991692	1.990157	0.551451	
H	3.754029	0.791460	-1.349277	
C	1.691910	0.437767	-1.165000	
O	1.263977	-0.494717	-1.819525	
O	0.955067	1.516849	-0.927811	
H	1.512991	2.069033	-0.314833	
H	3.572302	-1.596736	-0.922511	
H	4.529164	-0.840707	0.361196	
S	2.452972	-1.642763	1.231002	
H	1.458697	-2.012293	0.400331	
C	-3.426461	-0.764967	-0.126997	
C	-1.864084	-0.685739	-0.226337	
O	-4.036754	-0.615617	-1.214448	
O	-3.881748	-0.991606	1.010584	
H	-1.498936	-1.711637	-0.316834	
C	-1.198350	-0.028826	0.975975	
N	-1.516159	0.008080	-1.511071	
H	-0.598892	-0.283380	-1.884788	
H	-0.114005	-0.029246	0.885634	
H	-1.470362	-0.595470	1.863016	
S	-1.678866	1.734191	1.213395	
H	-2.289150	-0.189921	-2.161598	
H	-1.483045	1.021831	-1.363079	
H	-2.969789	1.474445	1.507782	
28				
Dimer 16 of the n...z type				
C	-2.024908	-0.578565	-0.684660	
C	-1.207675	0.680505	-0.977110	
N	-3.440979	-0.534284	-1.068866	
H	-3.826875	0.401548	-0.982978	
H	-3.582968	-0.846939	-2.021393	
H	-1.550950	-1.403614	-1.228753	
C	-1.939169	-1.005408	0.788778	
O	-0.919602	-0.979013	1.450632	
O	-3.078566	-1.460521	1.286532	
H	-3.727758	-1.358211	0.538770	
H	-0.176219	0.531242	-0.678491	
H	-1.233393	0.872346	-2.049635	
S	-1.803411	2.189361	-0.087748	
H	-0.665329	2.345794	0.627873	
C	2.109133	1.295718	0.070440	
C	2.688558	-0.014451	0.697514	
O	1.391486	1.972660	0.851728	
O	2.432074	1.534023	-1.107558	
H	3.624664	0.261550	1.190825	
C	2.983863	-1.141016	-0.282008	
N	1.751068	-0.451667	1.785876	
H	2.137139	-1.195734	2.367191	
H	3.375511	-2.015332	0.240880	
H	3.742594	-0.790531	-0.978131	
S	1.531507	-1.740419	-1.247969	

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H	1.541022	0.366459	2.365224	
H	0.831712	-0.759092	1.410748	
H	1.408635	-0.621673	-1.990354	
28				
Dimer 17 of the n...z type				
C	-3.782794	0.476517	0.377008	
C	-3.602234	-0.984675	0.824471	
N	-4.677320	0.571266	-0.769253	
H	-4.258058	0.080767	-1.555778	
H	-4.756190	1.541086	-1.060356	
H	-4.237107	1.007723	1.221419	
C	-2.402249	1.109416	0.149954	
O	-2.051326	1.578117	-0.916501	
O	-1.642734	1.048521	1.233911	
H	-0.662989	1.210318	0.996837	
H	-3.080523	-1.022163	1.778510	
H	-4.583204	-1.446731	0.936032	
S	-2.687221	-2.041944	-0.386462	
H	-1.468703	-1.468636	-0.219016	
C	1.199279	0.198321	0.016688	
C	2.671243	0.194464	-0.471836	
O	0.844226	1.246784	0.634773	
O	0.549931	-0.831374	-0.206764	
H	2.724429	-0.195880	-1.486029	
C	3.516255	-0.657583	0.476926	
N	3.184259	1.609724	-0.501237	
H	2.853009	2.111011	-1.326701	
H	3.106710	-1.665770	0.480968	
H	3.464651	-0.262063	1.493351	
S	5.309446	-0.703843	0.058254	
H	2.815102	2.105406	0.319272	
H	4.210393	1.630540	-0.500361	
H	5.170522	-1.315083	-1.135983	
28				
Dimer 18 of the n...z type				
C	3.788120	0.473776	-0.294904	
C	3.611969	-0.949970	-0.850089	
N	4.633776	0.477141	0.891864	
H	4.183017	-0.075270	1.617793	
H	4.695265	1.420614	1.262879	
H	4.283734	1.056054	-1.080644	
C	2.407235	1.112783	-0.082756	
O	2.031007	1.544185	0.990775	
O	1.680268	1.106186	-1.190211	
H	0.694191	1.269372	-0.977167	
H	3.127130	-0.914709	-1.823397	
H	4.591858	-1.415692	-0.956349	
S	2.641503	-2.077433	0.249544	
H	1.443960	-1.452976	0.115252	
C	-1.189645	0.274231	-0.036772	
C	-2.668999	0.275890	0.428466	
O	-0.820381	1.309245	-0.667609	
O	-0.543537	-0.747923	0.228549	
H	-2.716730	0.021767	1.486403	
C	-3.475541	-0.725752	-0.399056	
N	-3.241053	1.660573	0.276588	
H	-2.889036	2.290000	0.999158	
H	-3.023752	-1.707323	-0.272728	
H	-3.437981	-0.466172	-1.459030	
S	-5.266552	-0.790419	0.027708	
H	-2.944879	2.051699	-0.623894	
H	-4.265859	1.639917	0.331328	
H	-5.106889	-1.254926	1.283852	
28				
Dimer 19 of the n...z type				
C	-3.069538	0.521620	0.562367	
C	-3.252468	-0.284720	-0.737487	
N	-3.238583	1.948376	0.323945	
H	-2.485705	2.274754	-0.277098	

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H	-3.138981	2.456823	1.197378	
H	-3.851325	0.182665	1.250347	
C	-1.722101	0.145892	1.188021	
O	-0.779405	0.910463	1.249950	
O	-1.693479	-1.118404	1.598357	
H	-0.735301	-1.405591	1.740993	
H	-3.248246	-1.351548	-0.520470	
H	-4.209551	-0.016754	-1.184930	
S	-1.983799	0.054453	-2.040656	
H	-0.968616	-0.626260	-1.456136	
C	1.125550	-1.541221	0.407429	
C	2.430112	-0.750814	0.134258	
O	0.453000	-1.859760	-0.595610	
O	0.846440	-1.707649	1.620967	
H	3.226923	-1.069810	0.802582	
C	2.134693	0.740209	0.303604	
N	2.863949	-1.033588	-1.278605	
H	3.365142	-1.919937	-1.350967	
H	1.785475	0.907840	1.318665	
H	1.330328	1.046850	-0.366848	
S	3.559111	1.841632	-0.085486	
H	2.013834	-1.115355	-1.853161	
H	3.472352	-0.288283	-1.635301	
H	4.371170	1.400721	0.897369	
28				
Dimer 20 of the n...z type				
C	2.719706	-0.073181	0.700860	
C	1.940332	1.241646	0.859919	
N	3.753836	-0.098121	-0.337106	
H	3.583975	0.616715	-1.040082	
H	4.681071	0.038768	0.045010	
C	3.181061	-0.291870	1.669263	
C	1.755030	-1.248788	0.468148	
O	0.759866	-1.423057	1.146260	
O	2.123092	-2.071648	-0.497365	
H	2.966047	-1.666159	-0.844082	
H	1.120749	1.085976	1.560585	
H	2.603533	2.009928	1.257279	
S	1.283371	1.939282	-0.715192	
O	0.566904	0.853844	-1.115960	
C	-1.744126	-0.068422	-1.442654	
C	-2.617372	-0.796159	-0.377788	
O	-0.632658	-0.601564	-1.693172	
O	-2.236881	0.974875	-1.909539	
H	-3.476181	-1.242205	-0.884965	
C	-3.133896	0.144499	0.705197	
N	-1.822583	-1.932173	0.205786	
H	-2.352056	-2.456906	0.903179	
H	-3.732964	-0.394253	1.441610	
H	-3.766846	0.884877	0.220896	
S	-1.820142	1.005854	1.669232	
H	-1.542088	-2.569077	-0.541238	
H	-0.929661	-1.608697	0.628895	
H	-1.273760	1.667946	0.626240	
28				
Dimer 21 of the n...z type				
C	3.788481	0.473532	-0.292576	
C	3.611916	-0.948887	-0.851043	
N	4.633278	0.473823	0.894802	
H	4.181615	-0.079773	1.619268	
H	4.695168	1.416488	1.267817	
H	4.284994	1.057258	-1.076671	
C	2.407791	1.112840	-0.080050	
O	2.030998	1.542088	0.994148	
O	1.681650	1.108987	-1.188076	
H	0.695429	1.271929	-0.975546	
H	3.127945	-0.911185	-1.824687	
H	4.591606	-1.414985	-0.957459	
S	2.639874	-2.078204	0.245264	

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H	1.442967	-1.452225	0.112251	
C	-1.189520	0.276318	-0.037909	
C	-2.669074	0.278076	0.426714	
O	-0.819507	1.311540	-0.667907	
O	-0.543780	-0.746046	0.227571	
H	-2.716552	0.028077	1.485663	
C	-3.474571	-0.727955	-0.396481	
N	-3.242794	1.661538	0.269588	
H	-2.891401	2.294135	0.989695	
H	-3.021780	-1.708470	-0.265675	
H	-3.437259	-0.473222	-1.457635	
S	-5.265544	-0.792430	0.030575	
H	-2.947409	2.049834	-0.632335	
H	-4.267571	1.639754	0.324549	
H	-5.105456	-1.251098	1.288805	
28				
Dimer 22 of the n...z type				
C	3.571713	-0.803984	0.053594	
C	3.751494	0.695041	0.351560	
N	4.097853	-1.148316	-1.260934	
H	3.558734	-0.658483	-1.971046	
H	3.951556	-2.137615	-1.438133	
H	4.147905	-1.343831	0.813851	
C	2.099022	-1.186960	0.262570	
O	1.400801	-1.652989	-0.618466	
O	1.685168	-0.916816	1.490990	
H	0.662132	-0.914208	1.538303	
C	3.513651	0.900244	1.393302	
H	4.787569	0.974830	0.160319	
S	2.729544	1.809495	-0.713919	
H	1.524242	1.480114	-0.186252	
C	-1.200340	0.283589	0.897505	
C	-2.722912	0.380262	0.618094	
O	-0.477271	1.162338	0.391589	
O	-0.866131	-0.720498	1.579683	
H	-3.284843	0.236372	1.539082	
C	-3.114077	-0.670527	-0.422187	
N	-3.026633	1.763818	0.110128	
H	-3.060293	2.443374	0.871915	
H	-2.855820	-1.649860	-0.024759	
H	-2.554325	-0.518727	-1.347479	
S	-4.889628	-0.631805	-0.911457	
H	-2.264356	2.054679	-0.514475	
H	-3.924445	1.789105	-0.385655	
H	-5.388813	-0.968375	0.295502	
28				
Dimer 23 of the n...z type				
C	3.059060	-0.303045	-0.414064	
C	2.122119	-1.469089	-0.754385	
N	3.799263	-0.389568	0.845651	
H	3.268497	-0.905737	1.543238	
H	4.694239	-0.847740	0.725570	
H	3.785433	-0.231457	-1.231681	
C	2.334218	1.053448	-0.467226	
O	1.492042	1.332139	-1.301631	
O	2.758277	1.923226	0.430842	
H	3.414879	1.408423	0.974497	
H	1.576841	-1.238007	-1.669709	
H	2.716013	-2.365005	-0.934134	
S	0.945299	-1.938179	0.588178	
H	0.397051	-0.704191	0.798311	
C	-1.598838	1.331925	0.688235	
C	-2.090709	0.925992	-0.734676	
O	-0.455075	0.939696	1.029431	
O	-2.420089	2.006454	1.336782	
H	-2.240334	1.838710	-1.314138	
C	-3.404613	0.149499	-0.679007	
N	-1.034870	0.129097	-1.449063	
H	-1.265498	-0.008633	-2.434381	

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H	-3.761378 -0.100513 -1.679420	
H	-4.146178 0.777489 -0.190656	
S	-3.275364 -1.461794 0.213378	
H	-0.110092 0.596970 -1.388010	
H	-0.944254 -0.795969 -1.011762	
H	-2.976443 -0.939993 1.420849	
28		
Dimer 24 of the n...z type		
C	-1.385847 0.200382 0.710297	
C	-1.968762 -1.145644 0.265306	
N	-2.116433 0.901445 1.769656	
H	-3.096393 0.631947 1.784329	
H	-1.720271 0.722996 2.683879	
H	-0.364443 0.001595 1.045583	
C	-1.231704 1.149701 -0.485068	
O	-0.766534 0.802837 -1.557911	
O	-1.640325 2.383829 -0.259107	
H	-1.960308 2.357178 0.685709	
H	-1.328142 -1.596557 -0.486947	
H	-2.004104 -1.815943 1.123248	
S	-3.700586 -1.046920 -0.365141	
H	-3.412030 -0.380230 -1.501787	
C	2.007658 -1.461952 0.616263	
C	2.576491 -0.821470 -0.690583	
O	0.924299 -2.080714 0.488003	
O	2.704612 -1.287998 1.635778	
H	3.375154 -1.474834 -1.050894	
C	3.149124 0.577194 -0.497611	
N	1.505408 -0.850138 -1.747520	
H	1.879900 -0.701065 -2.685035	
H	3.416770 1.027302 -1.455026	
H	4.051351 0.490641 0.103263	
S	2.009728 1.771558 0.326912	
H	1.047081 -1.765055 -1.702977	
H	0.748836 -0.156820 -1.582442	
H	2.035107 1.156348 1.526859	
28		
Dimer 25 of the n...z type		
C	3.100572 -1.116221 0.040555	
C	4.079503 -0.155768 0.727347	
N	3.330151 -1.383359 -1.380662	
H	3.731177 -0.571755 -1.844358	
H	3.950499 -2.171113 -1.521681	
H	3.141615 -2.069112 0.580063	
C	1.651425 -0.642781 0.207915	
O	1.229799 -0.116350 1.222842	
O	0.879341 -0.868575 -0.841852	
H	1.497025 -1.253996 -1.522249	
H	3.842504 -0.073135 1.786915	
H	5.092614 -0.543751 0.622792	
S	4.111553 1.531955 -0.017225	
H	2.887160 1.901913 0.410487	
C	-3.119001 1.379756 -0.576402	
C	-1.953307 0.390367 -0.250725	
O	-3.155589 2.415693 0.133164	
O	-3.862992 1.043974 -1.519694	
H	-1.127822 0.625430 -0.925353	
C	-2.304469 -1.081166 -0.418749	
N	-1.459251 0.675888 1.136553	
H	-0.462790 0.404963 1.260085	
H	-1.443761 -1.710682 -0.193120	
H	-2.599772 -1.246689 -1.451944	
S	-3.662120 -1.643598 0.696873	
H	-1.602023 1.681197 1.297646	
H	-2.035466 0.175678 1.820309	
H	-4.607836 -0.845546 0.158956	
28		
Dimer 26 of the n...z type		
C	-3.091455 -0.502937 -0.058736	

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C	-3.089072 0.991930 -0.409567	
N	-3.330223 -0.840139 1.348318	
H	-2.967127 -0.115443 1.962630	
H	-4.316265 -0.960120 1.545018	
H	-3.871580 -0.981101 -0.661389	
C	-1.789803 -1.179904 -0.505627	
O	-1.195318 -0.932734 -1.526560	
O	-1.340295 -2.104226 0.358368	
H	-1.975962 -2.061189 1.123783	
H	-2.881076 1.125706 -1.470098	
H	-4.074225 1.403684 -0.191508	
S	-1.885484 1.995308 0.569307	
H	-0.788262 1.805881 -0.215583	
C	1.397078 0.492473 -1.121312	
C	1.300315 -0.190848 0.276234	
O	1.975542 -0.174424 -2.011005	
O	0.936245 1.652410 -1.175126	
H	0.304289 -0.050262 0.688592	
C	2.306941 0.415346 1.252096	
N	1.514192 -1.664924 0.072873	
H	2.162513 -2.080830 0.742312	
H	2.175610 -0.003793 2.251048	
H	2.114744 1.486411 1.299862	
S	4.076932 0.105740 0.832861	
H	0.618359 -2.163762 0.112062	
H	1.913290 -1.735303 -0.881765	
H	4.024561 0.568711 -0.433425	
28		
Dimer 27 of the n...z type		
C	3.128844 0.658325 0.142488	
C	3.315171 -0.842041 -0.115153	
N	2.980223 1.063916 1.543253	
H	2.502819 0.344120 2.080745	
H	3.875641 1.245378 1.979913	
H	3.998678 1.178931 -0.273256	
C	1.928793 1.202875 -0.643933	
O	1.603574 0.828122 -1.747760	
O	1.239980 2.144234 0.011394	
H	1.679909 2.197326 0.903188	
H	3.478208 -1.024504 -1.176135	
H	4.186490 -1.191112 0.438598	
S	1.894640 -1.874289 0.456235	
H	1.069572 -1.593617 -0.575918	
C	-1.508923 -1.283533 -0.333833	
C	-1.375270 0.184679 0.187217	
O	-1.021445 -1.483187 -1.475474	
O	-2.031920 -2.093097 0.453242	
H	-0.423468 0.236040 0.721639	
C	-2.492267 0.639397 1.114696	
N	-1.242880 1.096087 -0.998726	
H	-0.745499 1.958715 -0.766611	
H	-2.327864 1.662304 1.456740	
H	-2.508511 -0.021558 1.977831	
S	-4.155321 0.633511 0.315170	
H	-0.709212 0.588035 -1.717785	
H	-2.168373 1.318025 -1.378526	
H	-4.193968 -0.701065 0.120622	
28		
Dimer 28 of the n...z type		
C	-3.063991 -0.363657 -0.438314	
C	-3.019806 0.117149 1.023325	
N	-3.242949 -1.807791 -0.507451	
H	-2.414358 -2.259438 -0.126877	
H	-3.294049 -2.100185 -1.478698	
H	-3.930309 0.122658 -0.900442	
C	-1.818673 0.141641 -1.175730	
O	-0.979452 -0.598602 -1.647807	
O	-1.747627 1.470163 -1.194372	
H	-0.807514 1.758937 -1.410845	

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H	-3.039870	1.204303	1.065355
H	-3.890742	-0.275537	1.547548
S	-1.545285	-0.470353	1.978834
H	-0.686074	0.480946	1.543210
C	1.169494	1.665896	-0.211905
C	2.384369	0.707430	-0.129411
O	0.616980	1.949166	0.872428
O	0.815790	1.979333	-1.375389
H	3.158721	0.993451	-0.838015
C	1.885889	-0.713324	-0.401054
N	2.968154	0.794738	1.254861
H	3.550830	1.625427	1.367342
H	1.435727	-0.734587	-1.389611
H	1.107085	-0.987650	0.313828
S	3.181987	-2.012462	-0.246614
H	2.190279	0.876603	1.922350
H	3.536927	-0.032508	1.467750
H	3.950456	-1.587301	-1.270647
28			
Dimer 29 of the n...z type			
C	2.864108	-0.146259	0.769872
C	1.871827	1.016494	0.650367
N	4.251664	0.151293	0.406418
H	4.296033	0.883135	-0.298302
H	4.797956	0.444298	1.206934
H	2.843174	-0.486237	1.810995
C	2.404618	-1.369500	-0.043615
O	1.246898	-1.741060	-0.113861
O	3.383925	-2.004997	-0.660228
H	4.192796	-1.459382	-0.453280
H	0.885959	0.733909	1.009795
H	2.220862	1.843332	1.269352
S	1.728554	1.721264	-1.046601
H	1.304540	0.595730	-1.656381
C	-1.822808	1.249781	0.343545
C	-1.566198	-0.198234	-0.191398
O	-1.428787	1.453692	1.521926
O	-2.365133	2.033299	-0.454830
H	-0.676076	-0.153358	-0.819690
C	-2.710562	-0.770507	-1.014588
N	-1.206908	-1.061323	0.984662
H	-0.320109	-1.555094	0.807686
H	-2.471085	-1.772281	-1.374535
H	-2.869208	-0.118614	-1.870526
S	-4.289677	-0.938912	-0.076102
H	-1.088923	-0.385909	1.764066
H	-1.951924	-1.714593	1.232678
H	-4.440447	0.379520	0.167734
28			
Dimer 30 of the n...z type			
C	2.760537	0.205371	-0.295241
C	2.627617	-1.288635	-0.617808
N	2.903321	0.606154	1.102545
H	2.149490	0.208426	1.660388
H	3.794640	0.311240	1.482964
H	3.653641	0.557746	-0.828361
C	1.624596	1.037006	-0.896328
O	0.893807	0.674161	-1.793583
O	1.513521	2.256941	-0.361424
H	2.073903	2.230471	0.451604
H	2.493600	-1.414670	-1.692231
H	3.546214	-1.796870	-0.322244
S	1.281406	-2.168928	0.274307
H	0.284091	-1.369865	-0.144130
C	-1.243560	0.231825	1.472677
C	-2.236958	1.010586	0.544367
O	-0.089336	0.718240	1.543854
O	-1.718923	-0.766809	2.045526
H	-2.784869	1.710729	1.179929

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C	-3.235869	0.128852	-0.191902
N	-1.433894	1.848633	-0.411873
H	-1.976524	2.601062	-0.836247
H	-3.876657	0.719221	-0.848937
H	-3.861322	-0.365800	0.547325
S	-2.450711	-1.156227	-1.258918
H	-0.628006	2.240454	0.092769
H	-1.024579	1.274370	-1.162338
H	-1.991465	-1.897830	-0.230986
28			
Dimer 31 of the n...z type			
C	2.131084	0.100912	0.632298
C	2.448681	-1.403299	0.621628
N	0.981211	0.402861	-0.210808
H	1.196216	0.195702	-1.183407
H	0.738188	1.389908	-0.156893
H	1.879246	0.363460	1.666041
C	3.363118	0.931569	0.268287
O	3.401238	1.752087	-0.616379
O	4.407867	0.630590	1.059578
H	5.169647	1.175215	0.803929
H	3.227959	-1.631289	1.345701
H	1.548052	-1.954983	0.891579
S	2.946441	-2.060467	-1.029352
H	4.166883	-1.486680	-1.064257
C	-2.153699	1.792642	-0.316579
C	-2.423322	0.255430	-0.223158
O	-1.361251	2.269982	0.531254
O	-2.777132	2.370282	-1.230416
H	-2.200892	-0.193537	-1.191930
C	-3.878102	-0.009658	0.155070
N	-1.481496	-0.358141	0.763527
H	-0.480682	-0.221477	0.404981
H	-4.517959	0.486316	-0.571484
H	-4.098039	0.401552	1.142864
S	-4.324413	-1.798036	0.263345
H	-1.540807	0.138050	1.654405
H	-1.685481	-1.348843	0.911393
H	-4.145121	-2.079503	-1.043427
28			
Dimer 32 of the n...z type			
C	-3.662418	0.745009	0.594614
C	-4.213391	-0.640337	0.958968
N	-4.617495	1.499100	-0.208246
H	-4.776390	1.006285	-1.084150
H	-4.210725	2.393197	-0.466300
H	-3.514151	1.276447	1.543145
C	-2.261908	0.639485	-0.036196
O	-1.946437	1.244451	-1.044836
O	-1.460104	-0.160935	0.645213
H	-0.514215	-0.195133	0.242873
H	-3.575803	-1.123453	1.695766
H	-5.215058	-0.528195	1.374150
S	-4.407940	-1.779385	-0.484707
H	-3.090286	-1.984054	-0.688905
C	1.709465	0.540729	0.037379
C	3.171215	0.294018	-0.424641
O	1.482910	1.577134	0.684509
O	0.915249	-0.388228	-0.272818
H	3.190501	0.028271	-1.480065
C	3.796244	-0.817801	0.419659
N	3.943994	1.574760	-0.263126
H	3.770334	2.215339	-1.038320
H	3.204045	-1.719532	0.279246
H	3.772433	-0.553973	1.478933
S	5.567709	-1.154973	0.041013
H	3.618445	2.044953	0.590823
H	4.952909	1.393401	-0.214465
H	5.377989	-1.566812	-1.229264

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28		
Dimer 33 of the n...z type		
C	1.530220 0.249092 -0.083370	
C	2.629119 0.987680 -0.853412	
N	1.198752 0.772704 1.242118	
H	1.987612 1.254099 1.663512	
H	0.403699 1.401855 1.164887	
H	0.621978 0.310541 -0.688423	
C	1.842354 -1.252368 0.023642	
O	2.302281 -1.910156 -0.883362	
O	1.543261 -1.774913 1.213178	
H	1.243991 -0.990101 1.746711	
H	2.761075 0.540922 -1.837678	
H	2.342007 2.032177 -0.975997	
S	4.259230 1.023131 0.012711	
H	4.511850 -0.297569 -0.095267	
C	-2.430094 1.461714 -0.144966	
C	-2.878849 0.263249 0.758883	
O	-3.347533 2.004301 -0.804257	
O	-1.218120 1.751600 -0.090533	
H	-2.994774 0.653450 1.772038	
C	-1.902133 -0.904097 0.785727	
N	-4.245934 -0.156012 0.289784	
H	-4.860290 -0.473987 1.038697	
H	-2.251965 -1.695326 1.450483	
H	-0.951676 -0.537341 1.160096	
S	-1.659784 -1.716093 -0.851124	
H	-4.632712 0.679679 -0.184502	
H	-4.168482 -0.898738 -0.413712	
H	-1.246568 -0.612436 -1.506728	
28		
Dimer 34 of the n...z type		
C	2.056182 -0.331860 0.782479	
C	2.194792 1.170437 0.525095	
N	3.213604 -1.020681 1.357194	
H	4.082782 -0.639105 0.991688	
H	3.231515 -0.938410 2.366442	
H	1.207104 -0.464053 1.461950	
C	1.621730 -1.086157 -0.477516	
O	0.914253 -0.602358 -1.342281	
O	2.057132 -2.335542 -0.538236	
H	2.660658 -2.422055 0.245857	
H	1.247116 1.574507 0.176539	
H	2.456889 1.667579 1.459169	
S	3.536007 1.606745 -0.665312	
H	2.928221 1.098584 -1.756580	
C	-1.225421 0.125600 0.790471	
C	-1.819758 0.493641 -0.600776	
O	-1.131911 -1.098220 1.048056	
O	-0.916255 1.105625 1.497625	
H	-1.148737 1.199408 -1.089632	
C	-3.206916 1.117007 -0.477784	
N	-1.841841 -0.743143 -1.455148	
H	-0.863698 -1.001781 -1.657862	
H	-3.593058 1.413355 -1.454975	
H	-3.117222 2.008172 0.141224	
S	-4.491080 -0.003448 0.230470	
H	-2.261153 -1.509368 -0.920317	
H	-2.351441 -0.616731 -2.330360	
H	-3.909544 -0.164136 1.436879	
28		
Dimer 35 of the n...z type		
C	-3.089930 0.508328 0.068296	
C	-3.087461 -0.989325 0.406985	
N	-3.337530 0.857359 -1.334324	
H	-2.977823 0.138123 -1.956966	
H	-4.324799 0.978406 -1.524044	
H	-3.865294 0.982798 0.679999	
C	-1.784295 1.179731 0.511619	

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O	-1.182173 0.922470 1.525815	
O	-1.339494 2.110857 -0.346996	
H	-1.980186 2.075665 -1.108552	
H	-2.871053 -1.132077 1.464654	
H	-4.075142 -1.397476 0.193684	
S	-1.893716 -1.986927 -0.589931	
H	-0.791849 -1.814293 0.191555	
C	1.400837 -0.526095 1.114643	
C	1.300886 0.191649 -0.265322	
O	1.971500 0.122990 2.022527	
O	0.947142 -1.689807 1.138934	
H	0.303547 0.060349 -0.677260	
C	2.303782 -0.389064 -1.260487	
N	1.514294 1.660133 -0.024764	
H	0.623858 2.166306 -0.079579	
H	2.164591 0.051063 -2.249370	
H	2.115985 -1.459696 -1.330022	
S	4.074676 -0.080177 -0.844835	
H	1.887689 1.705940 0.942213	
H	2.187096 2.084183 -0.664226	
H	4.031956 -0.571495 0.411134	
28		
Dimer 36 of the n...z type		
C	-3.711539 -0.752091 -0.844645	
C	-4.171553 0.712347 -0.821082	
N	-4.710410 -1.630004 -0.248510	
H	-4.832445 -1.379218 0.729898	
H	-4.364656 -2.584912 -0.246558	
H	-3.600716 -1.022691 -1.902088	
C	-2.306576 -0.897186 -0.233492	
O	-2.035178 -1.730287 0.611435	
O	-1.447348 -0.026383 -0.738019	
H	-0.510802 -0.132599 -0.338357	
H	-3.504506 1.331471 -1.416664	
H	-5.179130 0.776592 -1.232098	
S	-4.289066 1.440902 0.874723	
H	-2.960877 1.499806 1.103489	
C	1.730210 0.697666 -0.036486	
C	3.185334 0.458147 0.451129	
O	0.929154 -0.257187 0.206802	
O	1.519538 1.753379 -0.641522	
H	3.570282 1.354944 0.932469	
C	4.059257 0.070582 -0.742993	
N	3.180869 -0.644518 1.477058	
H	2.896263 -0.299767 2.394778	
H	4.018856 0.880924 -1.468181	
H	3.676437 -0.834988 -1.218005	
S	5.810342 -0.305447 -0.310551	
H	2.483269 -1.342665 1.189162	
H	4.108341 -1.074018 1.568173	
H	6.125934 0.928541 0.133219	
28		
Dimer 37 of the n...z type		
C	1.740643 0.320332 0.169373	
C	2.243375 -0.804558 1.085285	
N	0.670235 -0.146280 -0.711138	
H	1.001613 -0.941687 -1.255157	
H	0.447019 0.577071 -1.389971	
H	1.326633 1.100018 0.819487	
C	2.881712 0.983897 -0.602960	
O	2.858935 1.218637 -1.787346	
O	3.910040 1.294511 0.204254	
H	4.602210 1.734775 -0.314786	
H	2.938086 -0.406999 1.821604	
H	1.398685 -1.245799 1.614380	
S	3.045096 -2.207899 0.194431	
H	4.166314 -1.543833 -0.154893	
C	-3.692445 -1.012017 -0.386260	
C	-2.794594 -0.061558 0.479509	

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O	-3.324425	-2.213363	-0.427312	
O	-4.682481	-0.472877	-0.916744	
H	-3.351083	0.166114	1.389869	
C	-2.453211	1.228555	-0.255629	
N	-1.562151	-0.819674	0.879155	
H	-1.290181	-0.641108	1.843344	
H	-3.379999	1.740341	-0.501593	
H	-1.932874	1.012954	-1.189909	
S	-1.334497	2.363146	0.675101	
H	-1.803645	-1.814468	0.746694	
H	-0.731894	-0.593726	0.251812	
H	-2.166481	2.590912	1.711761	
28				
Dimer 38 of the n...z type				
C	-2.552058	-0.596008	-0.815990	
C	-2.172690	0.887836	-0.638747	
N	-3.907099	-0.859138	-0.362300	
H	-3.968915	-0.716751	0.642067	
H	-4.149174	-1.830120	-0.533136	
H	-2.491536	-0.800090	-1.889377	
C	-1.474890	-1.450067	-0.138156	
O	-1.623510	-2.010218	0.926593	
O	-0.333467	-1.457447	-0.828950	
H	0.464737	-1.874985	-0.321809	
H	-1.180586	1.073595	-1.049331	
H	-2.887049	1.501868	-1.187226	
S	-2.259325	1.519911	1.094611	
H	-1.480218	0.581409	1.670259	
C	2.674985	-1.250533	0.479502	
C	2.510817	0.108005	-0.267011	
O	1.838846	-2.166258	0.200551	
O	3.589644	-1.288160	1.307569	
H	3.490136	0.571375	-0.367396	
C	1.566236	1.012352	0.525163	
N	1.984544	-0.086953	-1.669764	
H	2.585595	-0.711040	-2.209745	
H	1.973676	1.141582	1.526309	
H	0.585349	0.547366	0.618120	
S	1.254909	2.657366	-0.243112	
H	1.035068	-0.489423	-1.656698	
H	1.931071	0.813859	-2.155756	
H	2.533890	3.084708	-0.200489	
28				
Dimer 39 of the n...z type				
C	-1.767046	0.606682	-0.223245	
C	-1.480297	-0.733288	-0.909752	
N	-1.104138	0.859342	1.055328	
H	-0.983976	0.008153	1.596503	
H	-0.210394	1.331252	0.939213	
H	-1.435864	1.382567	-0.920729	
C	-3.280801	0.824327	-0.049639	
O	-4.113501	0.471726	-0.856478	
O	-3.598558	1.469076	1.073318	
H	-2.724325	1.573628	1.537860	
H	-2.057959	-0.805913	-1.829949	
H	-0.423189	-0.783941	-1.163424	
S	-1.835775	-2.210492	0.136462	
H	-3.171594	-2.031336	0.199372	
C	1.769561	1.346430	-0.552026	
C	3.106731	0.540824	-0.559613	
O	1.600196	2.111544	0.435844	
O	1.008624	1.126821	-1.507773	
H	3.727916	0.927720	-1.368084	
C	2.881857	-0.954693	-0.767849	
N	3.818150	0.825259	0.736960	
H	4.825734	0.943678	0.638793	
H	3.828088	-1.487616	-0.868078	
H	2.304643	-1.081223	-1.681189	
S	2.013936	-1.773748	0.640803	

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H	3.371614	1.682853	1.108021
H	3.631479	0.075710	1.413714
H	0.912145	-0.998438	0.619461
28			
Dimer 40 of the n...z type			
C	-2.144323	0.260793	0.782745
C	-1.986634	-1.221169	0.428010
N	-3.438687	0.667904	1.334807
H	-4.198898	0.155446	0.894140
H	-3.484706	0.503782	2.333181
H	-1.365387	0.503169	1.514005
C	-1.814109	1.170642	-0.407918
O	-0.985880	0.905736	-1.253977
O	-2.498806	2.311113	-0.418883
H	-3.137637	2.221545	0.334678
H	-0.965758	-1.436447	0.121807
H	-2.208770	-1.821557	1.310320
S	-3.149074	-1.809500	-0.878695
H	-2.583317	-1.121514	-1.891273
C	1.314695	-0.207954	0.941623
C	1.740445	-0.148785	-0.561036
O	0.928744	0.883853	1.435520
O	1.375677	-1.332401	1.468708
H	0.949538	-0.629195	-1.135314
C	3.065361	-0.841219	-0.849048
N	1.745181	1.301105	-0.961422
H	1.254040	1.474432	-1.836753
H	3.306782	-0.797543	-1.912030
H	2.970171	-1.883545	-0.553007
S	4.507426	-0.085806	0.019072
H	1.243227	1.767133	-0.179354
H	2.694223	1.680489	-1.002949
H	4.067012	-0.337070	1.269364
28			
Dimer 41 of the n...z type			
C	-1.240270	0.067063	0.011442
C	-2.064286	-1.071108	-0.590511
N	-1.012654	0.024139	1.456161
H	-1.846055	-0.303137	1.938841
H	-0.239313	-0.595664	1.691031
H	-0.264749	0.030598	-0.479676
C	-1.791143	1.448364	-0.367165
O	-2.314499	1.701050	-1.429389
O	-1.599573	2.374219	0.575935
H	-1.214834	1.866875	1.337412
H	-2.122332	-0.960663	-1.672577
H	-1.566074	-2.011583	-0.358123
S	-3.773250	-1.200677	0.091407
H	-4.233857	-0.053860	-0.449156
C	1.778729	-1.467411	0.441749
C	2.973964	-0.791039	-0.306401
O	1.000322	-2.132669	-0.283025
O	1.722166	-1.263016	1.671081
H	3.831524	-1.462723	-0.229166
C	3.359178	0.581942	0.229334
N	2.598900	-0.734458	-1.764125
H	3.397177	-0.772919	-2.397866
H	4.184547	1.007692	-0.342955
H	3.672618	0.468210	1.264147
S	1.989850	1.818240	0.148503
H	1.962353	-1.533811	-1.918759
H	2.065173	0.119434	-1.959431
H	1.237508	1.241417	1.107335
28			
Dimer 42 of the n...z type			
C	-2.724287	0.916160	-0.216008
C	-3.299829	-0.484926	-0.514284
N	-1.975807	1.547674	-1.289765
H	-1.234826	0.941358	-1.633131

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H -2.590313	1.754638	-2.069394	
H -3.585537	1.555647	0.010337	
C -1.946275	0.878060	1.107877	
O -2.439128	0.390883	2.104438	
O -0.723937	1.403377	1.154907	
H -0.329438	1.630866	0.271963	
H -3.889386	-0.841929	0.329205	
H -3.945148	-0.420424	-1.391169	
S -2.030033	-1.749881	-0.945033	
H -1.464871	-1.845513	0.277267	
C 2.135555	1.206496	-0.478725	
C 2.648345	-0.220816	-0.839872	
O 2.931683	1.944808	0.134443	
O 0.968835	1.452257	-0.870846	
H 2.880279	-0.224602	-1.906571	
C 1.637446	-1.323272	-0.544319	
N 3.943125	-0.444727	-0.104757	
H 4.583980	-1.072905	-0.589722	
H 2.004544	-2.293963	-0.880065	
H 0.719675	-1.089607	-1.079534	
S 1.261151	-1.530784	1.249730	
H 4.372051	0.481332	0.036251	
H 3.746981	-0.827584	0.828098	
H 0.662232	-0.333448	1.422937	
28			
Dimer 43 of the n...z type			
C -1.762194	-0.747807	-0.262426	
C -1.224166	0.416495	-1.096173	
N -2.998222	-1.373403	-0.742275	
H -3.619106	-0.681766	-1.155434	
H -2.806890	-2.082019	-1.440188	
H -0.975924	-1.508573	-0.241501	
C -1.946471	-0.361229	1.208951	
O -1.226920	0.412544	1.805193	
O -2.965696	-0.979882	1.804136	
H -3.400898	-1.489920	1.072711	
H -0.265139	0.749432	-0.711318	
H -1.073099	0.077911	-2.119902	
S -2.362176	1.866320	-1.193230	
H -2.233578	2.234489	0.098008	
C 1.612835	-1.410257	-0.349307	
C 2.947334	-0.595938	-0.278513	
O 1.121657	-1.519793	-1.502208	
O 1.197081	-1.871571	0.728151	
H 3.764174	-1.319817	-0.321729	
C 3.104834	0.264160	0.967874	
N 3.025691	0.222703	-1.538981	
H 3.975642	0.376781	-1.875650	
H 4.083888	0.744518	0.988885	
H 3.011655	-0.383068	1.836792	
S 1.870035	1.628863	1.088728	
H 2.458329	-0.298594	-2.230667	
H 2.572498	1.132114	-1.392119	
H 0.785351	0.854804	1.321627	
28			
Dimer 44 of the n...z type			
C -3.034135	-0.237847	0.718198	
C -2.092940	-1.400635	0.382069	
N -4.337594	-0.239492	0.054217	
H -4.276551	-0.657169	-0.871098	
H -5.033054	-0.745783	0.588291	
H -3.199268	-0.255949	1.801214	
C -2.360949	1.119344	0.457166	
O -1.181626	1.340754	0.669424	
O -3.175207	2.046539	-0.008688	
H -4.042756	1.571344	-0.127122	
H -1.184474	-1.332919	0.978597	
H -2.585265	-2.341299	0.627742	
S -1.661821	-1.535765	-1.405438	

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H -1.048861	-0.340474	-1.514429	
C 2.948735	-1.181585	0.396620	
C 1.618572	-0.386160	0.190756	
O 3.220946	-1.467392	1.586964	
O 3.567844	-1.463381	-0.649108	
H 0.843867	-1.125525	-0.022993	
C 1.649189	0.631510	-0.941118	
N 1.238949	0.276812	1.483321	
H 0.257016	0.599355	1.456704	
H 0.700539	1.166113	-1.008207	
H 1.832143	0.104426	-1.874159	
S 2.933964	1.936108	-0.714026	
H 1.417584	-0.376858	2.251084	
H 1.841175	1.092050	1.636261	
H 3.983489	1.091870	-0.795882	
28			
Dimer 45 of the n...z type			
C -2.036465	-0.858763	-0.032720	
C -3.157177	-0.333013	-0.934860	
N -2.444406	-1.454499	1.241415	
H -3.273639	-0.996126	1.610822	
H -2.642343	-2.442875	1.145792	
H -1.470693	-1.608139	-0.593763	
C -0.989100	0.226014	0.244967	
O -0.644122	1.049049	-0.581191	
O -0.470477	0.180352	1.464662	
H -0.957764	-0.563240	1.907839	
H -2.740390	0.043076	-1.868008	
H -3.849790	-1.143917	-1.160723	
S -4.182758	0.992717	-0.160221	
H -3.218635	1.935795	-0.154559	
C 1.931860	-1.455412	-0.114745	
C 2.737317	-0.404462	-0.954930	
O 0.869308	-1.853105	-0.654515	
O 2.447781	-1.801459	0.963272	
H 3.401509	-0.975499	-1.608956	
C 3.578474	0.569090	-0.142384	
N 1.764182	0.304087	-1.856313	
H 2.214423	0.796373	-2.627962	
H 4.178069	1.206522	-0.794490	
H 4.246947	-0.018958	0.482676	
S 2.601394	1.721398	0.912290	
H 1.111572	-0.403819	-2.212921	
H 1.182300	0.965881	-1.319118	
H 1.876968	0.771248	1.536456	
28			
Dimer 46 of the n...z type			
C 2.614365	-0.398568	0.778086	
C 2.735814	-1.165547	-0.548774	
N 2.015371	-1.223428	1.816771	
H 1.091912	-1.530813	1.521316	
H 1.879652	-0.678418	2.662567	
H 3.637204	-0.141924	1.082364	
C 1.898412	0.944103	0.579986	
O 1.040221	1.370675	1.325423	
O 2.312668	1.589681	-0.512571	
H 1.666649	2.283144	-0.737198	
H 3.324637	-0.596208	-1.264111	
H 3.234821	-2.115052	-0.356829	
S 1.122408	-1.610057	-1.340026	
H 0.745406	-0.349799	-1.678016	
C -1.137074	1.712697	-0.694569	
C -1.433736	0.418306	0.117615	
O -1.760076	2.734491	-0.334284	
O -0.316650	1.572128	-1.631566	
H -0.532568	-0.173219	0.214067	
C -2.511130	-0.417377	-0.556715	
N -1.824173	0.821184	1.509212	
H -0.978600	1.103767	2.014730	

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H -2.210103	-0.588690	-1.589402	
H -3.473512	0.097231	-0.559432	
S -2.789550	-2.039082	0.279416	
H -2.442264	1.639068	1.448416	
H -2.279720	0.058893	2.019086	
H -1.536837	-2.503537	0.080540	
28			
Dimer 47 of the n...z type			
C -2.242481	-1.166596	-0.232967	
C -3.267131	-0.109197	0.197829	
N -1.432285	-1.777582	0.809865	
H -0.983372	-1.091182	1.413910	
H -1.970566	-2.416151	1.381921	
H -2.808993	-1.971068	-0.719582	
C -1.313599	-0.646658	-1.340858	
O -1.635714	0.180176	-2.161330	
O -0.103086	-1.219498	-1.349698	
H -0.053139	-1.807706	-0.553740	
H -3.873659	0.203202	-0.651421	
H -3.923677	-0.543683	0.952005	
S -2.532091	1.389868	0.979258	
H -2.123187	1.959214	-0.171824	
C 1.814921	-0.894840	1.068185	
C 2.817452	-0.031517	0.227583	
O 1.767153	-2.099339	0.714214	
O 1.193830	-0.316426	1.979825	
H 3.818768	-0.268335	0.595479	
C 2.617585	1.474478	0.281501	
N 2.756254	-0.551754	-1.185505	
H 3.530485	-0.231770	-1.768329	
H 3.400931	1.991631	-0.275037	
H 2.673206	1.780996	1.323898	
S 1.022121	2.049184	-0.434580	
H 2.751218	-1.577117	-1.129982	
H 1.866291	-0.275471	-1.620521	
H 0.245040	1.421242	0.471252	
28			
Dimer 48 of the n...z type			
C 2.694552	-0.630902	-0.882602	
C 1.794402	-1.588744	-0.077304	
N 4.057026	-0.621975	-0.373628	
H 4.085505	-0.169367	0.535774	
H 4.648548	-0.066055	-0.983490	
H 2.701025	-1.017925	-1.905869	
C 2.011916	0.743793	-0.912548	
O 2.401929	1.687697	-0.252910	
O 0.910199	0.743541	-1.653276	
H 0.283656	1.492310	-1.364320	
H 0.822480	-1.676567	-0.559674	
H 2.261856	-2.572134	-0.049890	
S 1.543652	-1.120842	1.708521	
H 1.721455	0.211906	1.586390	
C -1.363982	1.766655	0.384217	
C -1.605585	0.237424	0.204505	
O -1.786586	2.270351	1.438739	
O -0.805690	2.338936	-0.592079	
H -0.747148	-0.230146	-0.266149	
C -2.850740	0.023948	-0.654783	
N -1.763992	-0.384514	1.559718	
H -0.836108	-0.646615	1.928737	
H -2.693929	0.517095	-1.612502	
H -3.727082	0.467527	-0.178356	
S -3.277247	-1.748585	-0.923626	
H -2.187003	0.316643	2.182487	
H -2.338794	-1.232253	1.522382	
H -2.150390	-2.075392	-1.589167	
28			
Dimer 49 of the n...z type			
C -1.971695	-0.782687	-0.704265	

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C -2.169229	-1.344195	0.718749	
N -0.700004	-0.081147	-0.840656	
H -0.772386	0.881275	-0.509916	
H -0.426291	-0.030398	-1.817149	
H -1.977716	-1.643997	-1.377015	
C -3.168828	0.093193	-1.072263	
O -3.134773	1.298237	-1.157689	
O -4.280237	-0.641616	-1.240522	
H -5.029837	-0.052151	-1.423055	
H -3.128373	-1.855838	0.786272	
H -1.377820	-2.066295	0.922064	
S -2.031340	-0.101806	2.075075	
H -2.960363	0.762665	1.617393	
C 2.004866	1.896383	0.071197	
C 2.451097	0.441521	0.439036	
O 0.842561	2.223280	0.411587	
O 2.875774	2.571097	-0.515146	
H 3.247507	0.511810	1.181631	
C 2.944129	-0.314865	-0.791068	
N 1.305828	-0.290500	1.068573	
H 0.894915	0.267370	1.818550	
H 3.747195	0.258195	-1.247582	
H 2.140917	-0.419478	-1.522833	
S 3.514166	-2.038335	-0.453162	
H 0.537010	-0.407848	0.341986	
H 1.590772	-1.203221	1.427006	
H 4.579832	-1.702394	0.302450	
28			
Dimer 50 of the n...z type			
C 2.064567	-0.779407	-0.413137	
C 1.720524	0.432845	-1.284544	
N 1.034981	-1.235959	0.523346	
H 0.619152	-0.436227	0.996025	
H 0.283201	-1.677122	-0.000342	
H 2.271076	-1.610328	-1.099185	
C 3.380844	-0.587757	0.354187	
O 4.315583	0.065206	-0.052072	
O 3.420319	-1.242885	1.517992	
H 2.517067	-1.637527	1.612628	
H 2.540671	0.647328	-1.968590	
H 0.813697	0.218826	-1.848114	
S 1.317172	1.959311	-0.336757	
H 2.529890	2.117246	0.233954	
C -1.802734	-0.375923	-1.294374	
C -3.086051	-0.448940	-0.402697	
O -1.197341	-1.471377	-1.444975	
O -1.534141	0.740229	-1.766972	
H -3.938500	-0.550053	-1.077857	
C -3.299062	0.760883	0.496401	
N -3.008587	-1.726189	0.390940	
H -3.918326	-2.136295	0.601619	
H -4.224943	0.667903	1.065409	
H -3.361675	1.644314	-0.134399	
S -1.959941	0.999640	1.742901	
H -2.432755	-2.369508	-0.177042	
H -2.507197	-1.563861	1.271542	
H -0.995705	1.337534	0.859253	
28			
Dimer 51 of the n...z type			
C -2.420711	-0.330523	0.835087	
C -1.300828	0.708275	0.695603	
N -2.086461	-1.646827	0.273026	
H -1.114807	-1.693680	-0.046744	
H -2.219685	-2.378735	0.960820	
H -2.657969	-0.401621	1.901670	
C -3.698399	0.191658	0.150717	
O -4.228391	1.244692	0.435968	
O -4.150289	-0.616961	-0.801875	
H -3.482290	-1.367143	-0.786196	

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H	-1.584043	1.627888	1.204683		
H	-0.399130	0.309590	1.157831		
S	-0.853985	1.125610	-1.049269		
H	-1.884012	1.970136	-1.264133		
C	1.571908	-1.308864	0.375216		
C	2.994915	-0.946453	-0.162618		
O	0.765446	-1.711870	-0.504669		
O	1.392960	-1.171995	1.597045		
H	3.611950	-1.841708	-0.062080		
C	3.666196	0.210817	0.565316		
N	2.854224	-0.677939	-1.636888		
H	3.685113	-0.912146	-2.179895		
H	4.675109	0.380997	0.187296		
H	3.723687	-0.043848	1.620903		
S	2.780568	1.815111	0.365027		
H	2.039073	-1.234973	-1.942750		
H	2.626509	0.311766	-1.789497		
H	1.645655	1.423114	0.976032		
28					
Dimer 52 of the n...z type					
C	2.642540	0.343757	0.763484		
C	1.460910	1.257557	0.422416		
N	3.933787	0.687183	0.160403		
H	3.806859	1.132190	-0.744937		
H	4.468295	1.314329	0.748816		
H	2.758340	0.363699	1.852629		
C	2.316216	-1.127624	0.442621		
O	1.234156	-1.632659	0.642053		
O	3.347130	-1.810718	-0.052400		
H	4.073258	-1.137532	-0.126322		
H	0.558044	0.919586	0.927672		
H	1.682168	2.273638	0.749862		
S	1.126012	1.399155	-1.388970		
H	0.762833	0.113200	-1.579021		
C	-2.196310	0.223876	1.437980		
C	-2.944002	0.482085	0.085396		
O	-1.522125	1.196808	1.859707		
O	-2.376656	-0.895513	1.950537		
H	-3.940011	0.850804	0.344022		
C	-3.095931	-0.739832	-0.807913		
N	-2.246392	1.618414	-0.611664		
H	-2.832064	2.090670	-1.300736		
H	-3.638494	-0.493026	-1.722015		
H	-3.666377	-1.482272	-0.254291		
S	-1.504365	-1.489091	-1.355375		
H	-1.950535	2.274163	0.123964		
H	-1.379930	1.308021	-1.076239		
H	-1.013222	-1.721767	-0.121818		
28					
Dimer 53 of the n...z type					
C	2.328416	-1.022648	-0.626855		
C	3.162895	-0.520360	0.561610		
N	2.225865	-0.173895	-1.811096		
H	1.977098	0.777799	-1.547180		
H	3.090451	-0.161580	-2.338337		
H	2.782266	-1.970915	-0.942624		
C	0.910061	-1.439610	-0.206252		
O	0.623018	-1.877406	0.883901		
O	0.015142	-1.340304	-1.196529		
H	0.513859	-0.882814	-1.922900		
H	3.022074	-1.198484	1.403120		
H	4.217505	-0.531306	0.283841		
S	2.835929	1.211531	1.096504		
H	1.476353	1.152012	1.180923		
C	-0.802504	1.389635	-0.043526		
C	-2.317621	1.185620	-0.378016		
O	-0.075226	1.591178	-1.044798		
O	-0.485246	1.348894	1.162603		
H	-2.727812	2.178130	-0.578777		

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C	-3.153377	0.514979	0.703062		
N	-2.367846	0.435175	-1.681954		
H	-3.263354	0.514728	-2.164898		
H	-4.214834	0.554230	0.454181		
H	-2.991357	1.063645	1.628451		
S	-2.775629	-1.267124	0.967421		
H	-1.609741	0.811645	-2.266243		
H	-2.166930	-0.558497	-1.510778		
H	-1.465244	-1.112647	1.248208		
28					
Dimer 54 of the n...z type					
C	2.663098	-1.218696	0.153297		
C	3.384186	-0.051341	0.839134		
N	2.961765	-1.433278	-1.263893		
H	3.174287	-0.552991	-1.727152		
H	3.745779	-2.060463	-1.394294		
H	2.922092	-2.131401	0.701479		
C	1.140191	-1.092180	0.311382		
O	0.612280	-0.677032	1.326979		
O	0.449701	-1.483158	-0.744809		
H	1.146412	-1.714492	-1.417575		
H	3.092064	0.000837	1.886858		
H	4.461031	-0.209124	0.780843		
S	3.078684	1.583908	0.041505		
H	1.757010	1.640478	0.311911		
C	-2.992204	-0.849132	-0.271549		
C	-2.906977	0.449649	0.602406		
O	-2.881011	-1.917626	0.375676		
O	-3.199897	-0.678176	-1.489431		
H	-3.908196	0.609583	1.012478		
C	-2.497628	1.715964	-0.134276		
N	-2.017013	0.152271	1.777001		
H	-2.022931	0.895002	2.476601		
H	-2.531858	2.582697	0.528394		
H	-3.214026	1.867520	-0.938945		
S	-0.796782	1.703215	-0.838643		
H	-2.344371	-0.721094	2.199472		
H	-1.033763	-0.035015	1.485961		
H	-0.933029	0.545771	-1.516018		
28					
Dimer 55 of the n...z type					
C	-2.490413	0.060604	0.919555		
C	-2.504836	1.525241	0.463526		
N	-1.292463	-0.382514	1.634395		
H	-0.461614	0.175674	1.414684		
H	-1.427269	-0.356300	2.637162		
H	-3.360603	-0.080176	1.570608		
C	-2.740935	-0.891472	-0.265916		
O	-3.548088	-0.675510	-1.143632		
O	-1.991807	-1.991613	-0.228479		
H	-1.417349	-1.860313	0.578096		
H	-3.493621	1.796008	0.096712		
H	-2.261115	2.163982	1.312391		
S	-1.270150	1.935524	-0.848711		
H	-1.951363	1.365146	-1.862912		
C	2.225167	1.013158	0.632736		
C	2.046556	0.363523	-0.780765		
O	3.355855	1.513846	0.839965		
O	1.230235	0.990744	1.385269		
H	1.643208	1.141135	-1.432568		
C	1.135255	-0.851183	-0.851095		
N	3.429634	0.045407	-1.285411		
H	3.514840	0.081016	-2.301141		
H	1.137873	-1.277174	-1.855980		
H	0.123965	-0.527553	-0.635539		
S	1.609438	-2.223488	0.278929		
H	4.050459	0.738781	-0.834606		
H	3.721651	-0.882440	-0.962261		
H	1.397815	-1.529569	1.415754		

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28		
Dimer 56 of the n...z type		
C	-2.701773	-0.585845
C	-3.255053	-1.439096
N	-3.762010	-0.148253
H	-4.414683	0.439490
H	-3.372553	0.438447
H	-2.017649	-1.234038
C	-1.824131	0.559376
O	-1.879483	1.697553
O	-0.979274	0.153264
H	-0.329203	0.884005
H	-2.444627	-1.902475
H	-3.890958	-2.220656
S	-4.329150	-0.509095
H	-3.336411	0.202399
C	1.997716	1.595772
C	2.466630	0.165773
O	0.980529	1.663260
O	2.676297	2.523270
H	2.259734	0.036598
C	3.957430	-0.028623
N	1.669161	-0.892908
H	0.681909	-0.888838
H	4.502013	0.754580
H	4.166003	0.064400
S	4.607186	-1.684993
H	1.678213	-0.721864
H	2.069832	-1.820334
H	4.420265	-1.541100
28		
Dimer 57 of the n...z type		
C	2.059782	0.615127
C	3.202902	-0.164846
N	2.433585	1.813570
H	3.367065	1.724017
H	2.406221	2.645649
H	1.364547	0.909665
C	1.223513	-0.294300
O	0.887239	-1.421391
O	0.851581	0.288502
H	1.248214	1.201597
H	2.803546	-1.012497
H	3.731760	0.490774
S	4.480990	-0.767023
H	3.701748	-1.687582
C	-3.280358	-0.951734
C	-2.980982	-0.237522
O	-2.524891	-1.913805
O	-4.224965	-0.465510
H	-3.834029	-0.393573
C	-2.768283	1.263405
N	-1.786448	-0.917682
H	-2.025349	-1.423914
H	-2.493218	1.732248
H	-3.705707	1.697486
S	-1.434605	1.718137
H	-1.470142	-1.601622
H	-1.003342	-0.288546
H	-2.041753	1.212174
28		
Dimer 58 of the n...z type		
C	-2.723676	-0.395155
C	-1.881898	-1.534216
N	-4.097645	-0.442481
H	-4.111806	-0.286427
H	-4.632130	0.316314
H	-2.718551	-0.552185
C	-2.019783	0.943732

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O	-2.482624	1.841214
O	-0.818689	0.983296
H	-0.277930	1.736252
H	-0.898614	-1.563272
H	-2.386168	-2.481158
S	-1.682776	-1.464384
H	-0.927081	-0.342450
C	1.224445	1.476483
C	2.402674	0.505714
O	1.044986	2.379515
O	0.533656	1.203524
H	2.941566	0.258772
C	1.821599	-0.753639
N	3.362598	1.179499
H	4.010585	1.792589
H	1.143909	-1.221798
H	1.252493	-0.485532
S	3.076982	-1.975722
H	2.806269	1.769707
H	3.909951	0.490639
H	3.566732	-2.266793
28		
Dimer 59 of the n...z type		
C	-2.919807	0.314933
C	-2.851079	-1.166267
N	-2.504956	1.272689
H	-1.880979	0.843110
H	-3.297567	1.655476
H	-3.958544	0.526500
C	-2.127471	0.577424
O	-2.212118	-0.123820
O	-1.371555	1.674540
H	-1.499188	2.031072
H	-3.154760	-1.785829
H	-3.531564	-1.347104
S	-1.191316	-1.720703
H	-0.533881	-1.617909
C	1.933234	-1.143914
C	2.738696	0.192650
O	2.390302	-2.031252
O	0.918762	-1.172518
H	3.214397	0.252521
C	1.862481	1.424684
N	3.833871	0.098947
H	4.723110	0.494935
H	2.430541	2.342674
H	1.041264	1.383534
S	1.171838	1.563282
H	3.919555	-0.912119
H	3.536703	0.558951
H	0.431056	0.431559
28		
Dimer 60 of the n...z type		
C	-2.722062	-0.393016
C	-1.879757	-1.532744
N	-4.096153	-0.441792
H	-4.110613	-0.289788
H	-4.630357	0.318721
H	-2.716543	-0.548156
C	-2.018653	0.945663
O	-2.480876	1.841108
O	-0.818695	0.987452
H	-0.277515	1.739496
H	-0.895982	-1.559279
H	-2.382705	-2.479727
S	-1.683311	-1.468826
H	-0.934931	-0.342389
C	1.223504	1.476246
C	2.401563	0.505116

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O	1.045795	2.380512	0.044690
O	0.531144	1.202187	-1.814069
H	2.939044	0.256908	-1.445012
C	1.820594	-0.752963	0.119909
N	3.363372	1.179280	0.407557
H	4.010659	1.791858	-0.090010
H	1.140572	-1.220616	-0.589265
H	1.253838	-0.483385	1.013158
S	3.075897	-1.976065	0.679081
H	2.808477	1.770070	1.042594
H	3.911434	0.490574	0.935822
H	3.562630	-2.268332	-0.544583
28			
Dimer 61 of the n...z type			
C	-2.523393	0.813787	-0.764203
C	-3.473143	0.045559	0.166072
N	-1.892057	0.092291	-1.865021
H	-1.412299	-0.746853	-1.536398
H	-2.561881	-0.157226	-2.582340
H	-3.120320	1.622847	-1.205272
C	-1.432810	1.574513	0.009620
O	-1.573834	2.032089	1.118877
O	-0.320221	1.774129	-0.707545
H	-0.456842	1.255255	-1.539453
H	-3.767273	0.701492	0.985616
H	-4.368151	-0.232276	-0.391716
S	-2.811026	-1.536371	0.846599
H	-1.533473	-1.112495	1.075343
C	0.919158	-1.107296	0.148053
C	2.469465	-1.243080	0.281075
O	0.439375	-1.480414	-0.950349
O	0.329354	-0.667088	1.153812
H	2.663642	-2.181006	0.805899
C	3.135903	-0.097297	1.032289
N	3.019504	-1.395883	-1.110463
H	3.857856	-1.973797	-1.162915
H	4.202815	-0.282656	1.163501
H	2.666916	-0.021853	2.010653
S	3.011229	1.522095	0.159134
H	2.249642	-1.800192	-1.669448
H	3.229877	-0.469065	-1.501069
H	1.661399	1.584802	0.142583
28			
Dimer 62 of the n...z type			
C	-2.917945	-0.034507	0.627465
C	-2.240407	-1.388704	0.381849
N	-3.912590	0.383111	-0.364691
H	-3.694579	-0.006270	-1.278758
H	-4.847025	0.089974	-0.107533
H	-3.410022	-0.091412	1.604565
C	-1.881071	1.091486	0.799769
O	-0.858048	0.967856	1.438206
O	-2.232980	2.237606	0.225929
H	-3.095021	2.028062	-0.222818
H	-1.499575	-1.579809	1.156590
H	-2.993106	-2.176429	0.421651
S	-1.454345	-1.550861	-1.277113
H	-0.546776	-0.544504	-1.161581
C	1.815900	1.151453	-0.814431
C	2.872194	0.003019	-0.681683
O	2.147695	2.244532	-0.297611
O	0.785781	0.861242	-1.454834
H	3.398793	-0.051869	-1.636425
C	2.286189	-1.364519	-0.354442
N	3.874255	0.441063	0.351876
H	4.830903	0.151808	0.151923
H	3.060098	-2.133366	-0.368791
H	1.541302	-1.607023	-1.108448
S	1.528726	-1.460381	1.322754

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H	3.790125	1.473115	0.382308
H	3.599339	0.080265	1.273738
H	0.604906	-0.488205	1.149620
28			
Dimer 63 of the n...z type			
C	-2.159150	-1.037239	-0.475822
C	-3.029502	-0.523196	0.684840
N	-1.073934	-1.863165	0.006832
H	-0.543060	-1.399480	0.737292
H	-0.419962	-2.119277	-0.724843
H	-2.816058	-1.647556	-1.108641
C	-1.731595	0.127982	-1.373416
O	-0.590945	0.381345	-1.704388
O	-2.775882	0.856288	-1.778889
H	-2.467103	1.574908	-2.354850
H	-3.935436	-0.052814	0.309610
H	-3.305205	-1.371365	1.310912
S	-2.162937	0.658615	1.810756
H	-2.182422	1.716341	0.973596
C	2.028325	-1.652306	0.418124
C	2.372746	-0.185458	-0.009809
O	1.997591	-2.489831	-0.517084
O	1.823690	-1.823460	1.635226
H	3.438805	-0.030870	0.166178
C	1.552821	0.854519	0.741403
N	2.155848	-0.074824	-1.493213
H	2.484361	-0.945697	-1.922966
H	1.742170	0.740213	1.805202
H	0.488312	0.698799	0.575043
S	1.862952	2.596957	0.224353
H	1.143077	0.005028	-1.687366
H	2.627500	0.734800	-1.897389
H	3.133884	2.673196	0.670311
28			
Dimer 64 of the n...z type			
C	-2.950196	0.583949	-0.137479
C	-2.968142	-0.464157	0.983135
N	-3.137489	0.079738	-1.501217
H	-2.763813	-0.861831	-1.593486
H	-4.114944	0.060578	-1.764892
H	-3.751176	1.301181	0.073710
C	-1.665633	1.428282	-0.093194
O	-1.141038	1.809089	0.928423
O	-1.177608	1.731053	-1.298370
H	-1.782657	1.262678	-1.931584
H	-2.786143	0.016660	1.943254
H	-3.949414	-0.938061	1.009451
S	-1.754578	-1.836233	0.754947
H	-0.629573	-1.161728	1.128155
C	1.940836	0.266843	1.292666
C	1.742295	0.785421	-0.168062
O	2.908877	0.775007	1.906734
O	1.113079	-0.575053	1.699800
H	1.049148	1.625104	-0.111795
C	1.208233	-0.236906	-1.158914
N	3.068360	1.341206	-0.615849
H	2.987547	2.096031	-1.296836
H	1.136266	0.193900	-2.158074
H	0.212245	-0.537878	-0.853164
S	2.263190	-1.739745	-1.318187
H	3.536407	1.666012	0.246405
H	3.647086	0.595052	-1.016214
H	2.084272	-2.150026	-0.045243
28			
Dimer 65 of the n...z type			
C	-2.186439	0.005620	-0.936027
C	-1.577472	-1.362126	-0.603976
N	-1.330265	1.180056	-0.808997
H	-0.762507	1.159939	0.037320

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H -0.686863	1.286995	-1.584691	
H -2.530111	-0.048656	-1.976362	
C -3.472978	0.254557	-0.127598	
O -4.233712	-0.619655	0.223184	
O -3.694067	1.544201	0.131435	
H -2.888330	2.004177	-0.222891	
H -2.319633	-2.145048	-0.754442	
H -0.734037	-1.553933	-1.264359	
S -0.897961	-1.510011	1.101064	
H -2.072112	-1.376864	1.751035	
C 1.760237	1.563757	0.100740	
C 2.899694	0.616223	0.606973	
O 0.949083	1.914388	0.996978	
O 1.776859	1.868261	-1.104836	
H 3.700437	1.256133	0.984934	
C 3.470410	-0.333045	-0.435133	
N 2.345403	-0.121013	1.796633	
H 3.056718	-0.421629	2.462797	
H 4.256958	-0.957120	-0.008466	
H 3.896144	0.263177	-1.238979	
S 2.226010	-1.494258	-1.143842	
H 1.674879	0.530339	2.236036	
H 1.809108	-0.939689	1.489186	
H 1.498589	-0.530291	-1.744090	
28			
Dimer 66 of the n...z type			
C -2.860907	-0.554102	-0.563513	
C -3.344662	-0.286537	0.875244	
N -1.895253	-1.630494	-0.606559	
H -1.104960	-1.489768	0.018381	
H -1.520528	-1.755046	-1.540633	
C -3.749671	-0.847659	-1.132648	
H -2.385077	0.762925	-1.176877	
O -1.221695	1.073822	-1.351053	
O -3.402978	1.569941	-1.485128	
H -3.059170	2.409913	-1.831718	
H -4.178838	0.412938	0.873238	
H -3.679374	-1.231725	1.302326	
S -2.050459	0.341216	2.037246	
H -2.040218	1.616857	1.598486	
C 1.686445	-1.777799	-0.224173	
C 2.042981	-0.264997	-0.379967	
O 0.829267	-2.044122	0.656315	
O 2.323847	-2.546918	-0.966695	
H 2.052220	0.004115	-1.435114	
C 3.410537	-0.003788	0.249436	
N 0.982442	0.553098	0.289843	
H 0.158487	0.676096	-0.327117	
H 4.143018	-0.635893	-0.248164	
H 3.397416	-0.262356	1.310494	
S 3.955142	1.757863	0.188080	
H 0.653451	0.043176	1.119887	
H 1.328309	1.480580	0.552506	
H 3.991181	1.859266	-1.156530	
28			
Dimer 67 of the n...z type			
C -2.624264	-0.514929	0.862606	
C -1.615825	-1.213683	-0.054985	
N -4.032763	-0.881719	0.681845	
H -4.229433	-1.085568	-0.295081	
H -4.280003	-1.696787	1.229730	
H -2.342867	-0.752324	1.894985	
C -2.498494	1.015935	0.772722	
O -1.444198	1.597414	0.647420	
O -3.662698	1.657959	0.872306	
H -4.338556	0.933154	0.922549	
H -0.597327	-0.934818	0.208342	
H -1.714501	-2.292773	0.066286	
S -1.897754	-0.890483	-1.849594	

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H -1.432888	0.375807	-1.839735	
C 2.634363	-1.080169	0.808630	
C 2.856771	0.470145	0.836286	
O 3.671951	-1.761489	0.612406	
O 1.465052	-1.458344	1.006365	
H 2.944342	0.763396	1.884635	
C 1.746639	1.278080	0.181517	
N 4.195566	0.732052	0.197802	
H 4.688967	1.535739	0.584866	
H 1.950864	2.348025	0.244080	
H 0.809176	1.073364	0.690621	
S 1.535177	0.915790	-1.613120	
H 4.731745	-0.142942	0.332908	
H 4.082530	0.866575	-0.813011	
H 1.129848	-0.360011	-1.450088	
28			
Dimer 68 of the n...z type			
C 2.304607	-0.178075	-0.838517	
C 1.295480	0.952434	-0.613971	
N 1.849604	-1.521606	-0.472563	
H 1.243607	-1.477145	0.347496	
H 1.236198	-1.880015	-1.198031	
H 2.549209	-0.182824	-1.907787	
C 3.644900	0.099980	-0.143204	
O 4.141027	1.200579	-0.042238	
O 4.236128	-1.001780	0.320782	
H 3.576902	-1.722746	0.130166	
H 1.659836	1.887711	-1.036118	
H 0.370704	0.666607	-1.112448	
S 0.855129	1.232561	1.156426	
H 2.007948	1.850553	1.485680	
C -1.485655	-1.366798	-0.190251	
C -2.962719	-0.953991	0.129545	
O -0.843142	-1.790631	0.804003	
O -1.123143	-1.259099	-1.376214	
H -3.570213	-1.854588	0.014223	
C -3.537203	0.148971	-0.747464	
N -3.001527	-0.593228	1.589808	
H -3.905044	-0.756553	2.033797	
H -4.587180	0.329546	-0.513528	
H -3.457873	-0.170002	-1.784146	
S -2.692135	1.774103	-0.542393	
H -2.259992	-1.164433	2.029403	
H -2.747512	0.394261	1.710146	
H -1.516081	1.375974	-1.061280	
28			
Dimer 69 of the n...z type			
C -2.930210	-0.506307	-0.535045	
C -2.412051	0.897679	-0.897339	
N -4.112836	-0.439941	0.306905	
H -3.874772	-0.018709	1.200862	
H -4.445476	-1.376984	0.511740	
H -3.198311	-0.984897	-1.483084	
C -1.780571	-1.334307	0.054623	
O -1.748498	-1.737547	1.196196	
O -0.802247	-1.534079	-0.835783	
H 0.020734	-1.979555	-0.427710	
H -1.592393	0.823710	-1.609873	
H -3.220917	1.464226	-1.358746	
S -1.884754	1.927066	0.543453	
H -1.026784	1.039216	1.081848	
C 2.461265	-1.619340	0.216745	
C 2.481744	-0.184756	-0.390680	
O 1.473628	-2.362651	-0.064299	
O 3.423848	-1.877766	0.948612	
H 3.484547	0.018289	-0.763716	
C 2.110986	0.836939	0.686528	
N 1.560763	-0.062119	-1.578516	
H 1.879778	-0.647563	-2.351720	

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H	2.844471	0.759758	1.486415		
H	1.132305	0.617662	1.112571		
S	2.012200	2.577686	0.090499		
H	0.598995	-0.356320	-1.355456		
H	1.531152	0.912883	-1.897983		
H	3.331223	2.723563	-0.153909		
28					
Dimer 70 of the n...z type					
C	-2.904236	-0.437791	-0.746480		
C	-1.475942	0.107140	-0.645476		
N	-3.842979	0.322699	-1.573634		
H	-3.664850	1.321449	-1.503008		
H	-3.780302	0.059760	-2.549669		
H	-2.832405	-1.449168	-1.162259		
C	-3.521464	-0.641035	0.649873		
O	-2.884024	-0.979693	1.621349		
O	-4.837319	-0.432422	0.689943		
H	-5.066923	-0.114926	-0.220196		
H	-0.857159	-0.569270	-0.057591		
H	-1.053707	0.192639	-1.647056		
S	-1.379325	1.805717	0.077245		
H	-1.783202	1.455393	1.316085		
C	1.852596	-1.231576	-0.326223		
C	2.019131	0.326064	-0.288186		
O	1.177031	-1.710191	0.622545		
O	2.378525	-1.808107	-1.292801		
H	1.274212	0.744672	-0.966984		
C	3.395288	0.820667	-0.709334		
N	1.642037	0.774147	1.095711		
H	1.033053	1.596261	1.092389		
H	3.443406	1.910216	-0.688834		
H	3.578939	0.479115	-1.725373		
S	4.758314	0.236429	0.386910		
H	1.132932	-0.043052	1.488419		
H	2.469486	0.941266	1.674796		
H	4.587770	-1.075402	0.121226		
28					
Dimer 71 of the n...z type					
C	2.840186	0.399966	-0.548965		
C	2.478063	1.736883	0.110182		
N	2.120055	-0.018509	-1.745622		
H	1.105016	-0.010719	-1.620395		
H	2.359700	0.557753	-2.543279		
H	3.899336	0.491377	-0.827361		
C	2.856244	-0.771094	0.448414		
O	3.008838	-0.650701	1.643013		
O	2.793942	-1.965521	-0.145103		
H	2.558425	-1.765385	-1.082885		
H	3.090167	1.864383	1.003094		
H	2.705291	2.547094	-0.583754		
S	0.704356	1.968600	0.556686		
H	0.471944	0.708996	0.982844		
C	-1.011525	-1.016429	-0.505858		
C	-2.492116	-1.302784	-0.097333		
O	-0.151197	-1.267923	0.375148		
O	-0.843604	-0.569334	-1.655498		
H	-2.764472	-2.276685	-0.508669		
C	-3.478888	-0.252368	-0.589074		
N	-2.512846	-1.437865	1.401624		
H	-3.202988	-2.104164	1.747294		
H	-4.498387	-0.496585	-0.287412		
H	-3.429445	-0.226202	-1.675052		
S	-3.141499	1.434480	0.079047		
H	-1.551170	-1.722843	1.658501		
H	-2.684019	-0.524415	1.837089		
H	-1.923308	1.564820	-0.489849		
28					
Dimer 72 of the n...z type					
C	2.571009	0.828010	-0.229060		

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C	3.049665	-0.164209	0.842524		
N	1.692380	1.905812	0.201624		
H	0.970264	1.607084	0.858729		
H	2.210653	2.672049	0.612101		
H	3.471176	1.279171	-0.663696		
C	1.921659	0.079091	-1.404262		
O	2.332634	-0.976131	-1.833968		
O	0.855729	0.683772	-1.931770		
H	0.674019	1.482849	-1.376129		
H	3.751071	-0.874555	0.406426		
H	3.555592	0.385870	1.636421		
S	1.696494	-1.094596	1.680321		
H	1.283731	-1.787170	0.598129		
C	-1.670286	1.289621	0.501907		
C	-2.728391	0.160581	0.701524		
O	-1.593638	1.755833	-0.664451		
O	-0.989568	1.556748	1.508110		
H	-3.302892	0.355142	1.605381		
C	-2.039954	-1.200893	0.826505		
N	-3.663536	0.214064	-0.481803		
H	-4.533018	0.700118	-0.263744		
H	-2.745522	-1.966457	1.151785		
H	-1.257944	-1.099800	1.578274		
S	-1.323515	-1.846774	-0.746854		
H	-3.137741	0.774815	-1.183042		
H	-3.884964	-0.703465	-0.872808		
H	-0.687461	-0.717829	-1.120228		
28					
Dimer 73 of the n...z type					
C	-2.598997	0.452281	0.825003		
C	-3.385784	0.048396	-0.438606		
N	-1.867848	1.686216	0.611597		
H	-1.197229	1.594117	-0.144190		
H	-1.349952	1.955743	1.441227		
H	-3.340782	0.612020	1.612771		
C	-1.733894	-0.728192	1.262879		
O	-0.554426	-0.858369	0.992362		
O	-2.425864	-1.636900	1.950438		
H	-1.852753	-2.393161	2.160745		
H	-4.012639	-0.819833	-0.240736		
H	-4.024698	0.885595	-0.718628		
S	-2.348969	-0.291977	-1.931027		
H	-1.979116	-1.543700	-1.591966		
C	2.960909	-1.344108	-0.110911		
C	2.353959	0.036987	-0.538703		
O	2.447927	-2.348154	-0.662520		
O	3.904832	-1.282308	0.700425		
H	3.022321	0.465140	-1.288198		
C	2.179693	0.997638	0.629345		
N	1.040997	-0.219124	-1.222040		
H	1.139293	-1.081418	-1.769354		
H	3.147046	1.143732	1.102227		
H	1.494294	0.579059	1.367865		
S	1.450203	2.628627	0.163133		
H	0.309125	-0.397859	-0.512610		
H	0.736827	0.553254	-1.815044		
H	2.441397	3.019110	-0.664367		
28					
Dimer 74 of the n...z type					
C	-2.923768	0.115952	0.121071		
C	-2.200930	0.589616	-1.159924		
N	-3.559071	1.212681	0.837249		
H	-2.858184	1.804407	1.273518		
H	-4.133332	0.845310	1.589826		
H	-3.697826	-0.578340	-0.214792		
C	-1.894983	-0.682616	0.924336		
O	-1.146585	-0.162171	1.732909		
O	-1.844308	-1.958657	0.563012		
H	-0.912842	-2.315953	0.692385		

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H	-1.704769	-0.255838	-1.635791
H	-2.933069	1.021584	-1.841396
S	-0.930259	1.929564	-0.907827
H	-0.611835	1.636353	0.369505
C	0.897080	-1.720528	-0.609151
C	2.073252	-0.707872	-0.503003
O	0.233454	-1.688997	-1.661392
O	0.722699	-2.450366	0.404705
H	3.008893	-1.237816	-0.690373
C	2.121125	-0.024995	0.861108
N	1.918820	0.299152	-1.610344
H	1.846029	-0.180867	-2.509053
H	2.274503	-0.792967	1.614640
H	1.171681	0.459840	1.084980
S	3.409369	1.283814	1.017777
H	1.036653	0.836206	-1.491394
H	2.700108	0.959523	-1.626752
H	4.477257	0.465871	0.916653
28			
Dimer 75 of the n...z type			
C	-2.496352	0.438707	-0.671660
C	-1.747839	-0.894599	-0.775984
N	-1.796533	1.531075	0.007422
H	-1.275663	1.174056	0.806921
H	-1.087256	1.920393	-0.606477
H	-2.711350	0.766150	-1.696221
C	-3.880650	0.262133	-0.028731
O	-4.573020	-0.721328	-0.170118
O	-4.270852	1.318565	0.686532
H	-3.488570	1.930147	0.661131
H	-2.330003	-1.614859	-1.348789
H	-0.800792	-0.721057	-1.284700
S	-1.323251	-1.640971	0.857916
H	-2.570040	-2.059513	1.154960
C	1.320135	0.670750	-0.206410
C	2.121030	-0.672113	-0.266860
O	0.933772	1.105636	-1.322330
O	1.116690	1.130573	0.930195
H	1.404665	-1.481450	-0.110718
C	3.233192	-0.788547	0.765087
N	2.637666	-0.818190	-1.672975
H	2.722944	-1.786645	-1.981475
H	3.743211	-1.749620	0.688595
H	2.785910	-0.704720	1.752663
S	4.543002	0.495973	0.575157
H	1.971011	-0.295660	-2.265678
H	3.550701	-0.358016	-1.761376
H	3.734720	1.543430	0.839374
28			
Dimer 76 of the n...z type			
C	1.697373	0.327328	-0.036228
C	2.147690	-0.681327	1.025761
N	1.111155	-0.220534	-1.257662
H	1.571591	-1.090396	-1.513964
H	0.109949	-0.405211	-1.180475
H	0.956687	0.975658	0.442918
C	2.840417	1.284036	-0.418188
O	3.669753	1.693071	0.364436
O	2.814890	1.650387	-1.699069
H	2.066120	1.116246	-2.080911
H	2.520893	-0.159856	1.905856
H	1.300163	-1.299106	1.320684
S	3.437030	-1.861388	0.434872
H	4.429745	-0.953490	0.336350
C	-2.874158	-0.776010	-0.964277
C	-3.132739	0.660966	-0.397863
O	-3.872077	-1.531063	-0.971933
O	-1.711764	-0.998937	-1.363126
H	-3.382370	1.299914	-1.247604

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C	-1.959120	1.267479	0.356833
N	-4.366146	0.582185	0.460882
H	-4.895247	1.453526	0.500395
H	-2.208595	2.255256	0.746645
H	-1.132132	1.377971	-0.340999
S	-1.430607	0.273753	1.818188
H	-4.937340	-0.180268	0.061802
H	-4.113649	0.306801	1.416364
H	-1.132172	-0.839798	1.117392
28			
Dimer 77 of the n...z type			
C	-2.792729	0.708930	-0.409772
C	-3.322147	-0.727764	-0.501394
N	-1.838999	1.127466	-1.429176
H	-1.162078	0.404184	-1.664032
H	-2.302592	1.422295	-2.279212
H	-3.665835	1.368449	-0.478958
C	-2.208361	1.000996	0.982744
O	-2.662991	0.542490	2.007364
O	-1.156127	1.819310	0.976971
H	-0.959511	2.009397	0.025384
H	-4.145207	-0.876349	0.195883
H	-3.683441	-0.910524	-1.513097
S	-2.073364	-2.049589	-0.171330
H	-2.036815	-1.876443	1.165960
C	1.301963	0.710855	-0.799566
C	1.482678	-0.078154	0.530779
O	0.991690	0.025412	-1.804201
O	1.474099	1.941115	-0.701409
H	0.714195	0.253924	1.230265
C	2.856727	0.132601	1.156918
N	1.227326	-1.534980	0.261774
H	1.316665	-2.107922	1.102443
H	2.955594	-0.422069	2.091597
H	2.968226	1.193735	1.369241
S	4.258058	-0.430321	0.095230
H	0.275928	-1.652731	-0.122624
H	1.886389	-1.874463	-0.444391
H	4.082919	0.488262	-0.877116
28			
Dimer 78 of the n...z type			
C	-2.052628	-0.461315	-0.560204
C	-3.330886	0.214986	-1.063850
N	-2.209861	-1.797788	0.021926
H	-3.118895	-1.900859	0.465491
H	-2.111291	-2.523600	-0.677014
H	-1.353277	-0.537826	-1.396141
C	-1.308871	0.431462	0.443608
O	-1.212772	1.634426	0.334347
O	-0.756020	-0.239560	1.454132
H	-1.023768	-1.181911	1.287432
H	-3.092757	1.180211	-1.508330
H	-3.800049	-0.414391	-1.820299
S	-4.616059	0.458410	0.240884
H	-3.930510	1.378806	0.949491
C	1.829453	-1.169835	-0.538363
C	2.280592	-0.398217	0.747059
O	2.402509	-2.273707	-0.716880
O	0.944585	-0.619757	-1.220051
H	1.617792	-0.711967	1.553881
C	2.234524	1.117231	0.636165
N	3.659455	-0.894890	1.094760
H	3.875338	-0.847749	2.090430
H	2.565807	1.587433	1.563309
H	1.207966	1.415135	0.443399
S	3.326095	1.791292	-0.690098
H	3.694675	-1.869616	0.753896
H	4.366305	-0.361708	0.576774
H	2.651951	1.215708	-1.707393

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28		
Dimer 79 of the n...z type		
C	-3.679766 -0.883103 0.107981	
C	-2.183138 -0.917091 0.434867	
N	-4.058827 -1.200025 -1.269753	
H	-3.375177 -0.840521 -1.931121	
H	-4.142898 -2.198790 -1.415080	
H	-4.169236 -1.609896 0.766184	
C	-4.304594 0.469141 0.499645	
O	-3.947165 1.119744 1.455522	
O	-5.300557 0.852014 -0.298742	
H	-5.328502 0.165357 -1.011970	
H	-2.024627 -0.727307 1.495189	
H	-1.777267 -1.896852 0.184180	
S	-1.185797 0.293823 -0.541552	
H	-1.655890 1.400734 0.069361	
C	3.636666 -1.311381 0.079947	
C	2.375383 -0.432499 -0.214216	
O	3.595850 -1.951283 1.159357	
O	4.520134 -1.294560 -0.798790	
H	1.692510 -1.038450 -0.815326	
C	2.657892 0.868074 -0.952984	
N	1.671233 -0.172971 1.085619	
H	0.673486 0.029965 0.926037	
H	1.735223 1.422343 -1.131958	
H	3.115444 0.626074 -1.909039	
S	3.764693 2.012654 -0.021424	
H	1.805301 -1.005150 1.674442	
H	2.105334 0.620626 1.568312	
H	4.836366 1.193038 -0.042870	
28		
Dimer 80 of the n...z type		
C	2.977636 -0.912979 0.266443	
C	3.369109 0.519244 0.651954	
N	3.141891 -1.266085 -1.147230	
H	3.016414 -0.451117 -1.742893	
H	4.054541 -1.662244 -1.335149	
C	3.585118 -1.598351 0.866732	
C	1.523639 -1.201558 0.677409	
O	1.026217 -0.842598 1.716399	
O	0.839557 -1.894086 -0.247132	
H	1.502588 -2.027878 -0.980670	
H	3.233218 0.670524 1.721636	
H	4.417751 0.682546 0.403776	
S	2.424236 1.816192 -0.261774	
H	1.252380 1.683257 0.399185	
C	-2.027684 1.543474 0.246398	
C	-2.262962 0.650832 -1.018792	
O	-0.857371 1.981212 0.379750	
O	-3.030667 1.746707 0.954218	
H	-2.601277 1.318442 -1.815020	
C	-3.292923 -0.454815 -0.831622	
N	-0.933272 0.103224 -1.460372	
H	-0.910773 -0.148873 -2.448875	
H	-3.406839 -1.045249 -1.742272	
H	-4.246869 0.012308 -0.598457	
S	-2.866648 -1.655632 0.500812	
H	-0.225267 0.825274 -1.269359	
H	-0.664813 -0.726425 -0.910747	
H	-2.930680 -0.756201 1.504105	
28		
Dimer 81 of the n...z type		
C	2.596276 -0.554154 0.663166	
C	1.705107 0.614742 1.095057	
N	4.043330 -0.339051 0.754108	
H	4.278375 0.625418 0.531992	
H	4.392573 -0.542357 1.682757	
H	2.342356 -1.408512 1.301211	
C	2.261575 -1.029347 -0.762003	

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O	1.143050 -1.024248 -1.227377	
O	3.316800 -1.473989 -1.441139	
H	4.087044 -1.302191 -0.839715	
H	0.654691 0.330141 1.109680	
H	1.982609 0.915797 2.105826	
S	1.910586 2.133695 0.067872	
H	1.432086 1.606914 -1.077702	
C	-2.158416 -0.502374 1.387443	
C	-1.743899 -0.824903 -0.083823	
O	-2.995260 -1.292144 1.893012	
O	-1.590212 0.481945 1.897941	
H	-0.806713 -1.380719 -0.048981	
C	-1.541275 0.398845 -0.963057	
N	-2.785118 -1.753413 -0.648759	
H	-2.419826 -2.409053 -1.338819	
H	-1.208632 0.113030 -1.960653	
H	-0.775467 1.019343 -0.510173	
S	-3.070103 1.406225 -1.186353	
H	-3.180623 -2.248078 0.168338	
H	-3.545859 -1.212481 -1.075068	
H	-3.184888 1.756414 0.111710	
28		
Dimer 82 of the n...z type		
C	3.094642 -0.414453 0.687453	
C	2.409218 0.910871 1.043042	
N	4.245108 -0.331105 -0.215403	
H	4.143778 0.448189 -0.861152	
H	5.113492 -0.212412 0.291658	
H	3.428000 -0.871456 1.625612	
C	2.080029 -1.419256 0.112173	
O	0.951292 -1.542599 0.533507	
O	2.562322 -2.165797 -0.878629	
H	3.482473 -1.820338 -1.019360	
H	1.577544 0.727712 1.722293	
H	3.125312 1.564210 1.541846	
S	1.815220 1.865853 -0.417977	
H	0.892041 0.979791 -0.849891	
C	-1.699083 1.138435 -0.656884	
C	-1.660386 0.215368 0.602707	
O	-2.177107 2.284063 -0.472170	
O	-1.218777 0.639008 -1.693879	
H	-0.638425 0.220130 0.982175	
C	-2.064058 -1.225264 0.326061	
N	-2.533125 0.853861 1.649799	
H	-2.200010 0.717847 2.603524	
H	-1.996060 -1.831413 1.230098	
H	-1.375257 -1.627598 -0.409814	
S	-3.800828 -1.399786 -0.272681	
H	-2.562004 1.857707 1.400293	
H	-3.492175 0.497006 1.576536	
H	-3.616865 -0.717335 -1.421993	
28		
Dimer 83 of the n...z type		
C	3.066077 -0.479212 -0.795801	
C	1.704201 0.216234 -0.730847	
N	3.168969 -1.779587 -0.128489	
H	2.610797 -1.798521 0.721539	
H	2.852105 -2.532177 -0.727712	
H	3.301565 -0.627736 -1.855824	
C	4.190663 0.436370 -0.279471	
O	4.202409 1.636678 -0.434870	
O	5.176200 -0.217135 0.336837	
H	4.873086 -1.159960 0.360907	
H	1.724636 1.146172 -1.296835	
H	0.927173 -0.432286 -1.132577	
S	1.149279 0.586985 0.990591	
H	1.980532 1.626689 1.206468	
C	-1.925941 -1.028909 0.216203	
C	-2.472319 0.307621 0.806806	

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O	-1.290403	-0.934953	-0.860470	
O	-2.222686	-2.042070	0.879548	
H	-2.131970	0.404469	1.838358	
C	-3.997858	0.353433	0.777938	
N	-1.879098	1.460673	0.045144	
H	-2.269578	2.362098	0.324374	
H	-4.373397	1.275534	1.225038	
H	-4.367039	-0.488765	1.360133	
S	-4.729633	0.302469	-0.915372	
H	-0.857506	1.469244	0.209819	
H	-2.028746	1.318300	-0.957774	
H	-4.298199	-0.935333	-1.233349	
28				
Dimer 84 of the n...z type				
C	2.625353	0.611240	0.616434	
C	2.077079	-0.614357	1.356446	
N	1.656405	1.448585	-0.086817	
H	0.900071	0.912991	-0.508606	
H	1.233322	2.137852	0.522141	
H	3.133422	1.235214	1.361137	
C	3.739505	0.211712	-0.369219	
O	4.533488	-0.679095	-0.163135	
O	3.767892	0.960386	-1.471128	
H	2.979013	1.557291	-1.377887	
H	2.878709	-1.118742	1.893970	
H	1.325427	-0.292442	2.078101	
S	1.233862	-1.837771	0.262117	
H	2.345288	-2.247417	-0.381874	
C	-1.788714	1.379062	0.064161	
C	-1.943535	-0.052694	0.677966	
O	-2.276968	2.308974	0.749626	
O	-1.173137	1.428469	-1.018295	
H	-1.016262	-0.273993	1.208386	
C	-2.214437	-1.143860	-0.348003	
N	-3.026570	0.020984	1.719504	
H	-2.898089	-0.629170	2.494868	
H	-2.284987	-2.123259	0.126800	
H	-1.386937	-1.155695	-1.051445	
S	-3.797118	-0.904235	-1.263282	
H	-3.025906	1.000962	2.048166	
H	-3.940340	-0.154170	1.285889	
H	-3.421198	0.239200	-1.873068	
28				
Dimer 85 of the n...z type				
C	2.970638	-0.735102	-0.361732	
C	1.614948	-0.025661	-0.430174	
N	3.197007	-1.601625	0.796784	
H	2.764967	-1.213326	1.631621	
H	2.818270	-2.529305	0.649262	
H	3.058406	-1.350978	-1.264032	
C	4.131894	0.270098	-0.468038	
O	4.090647	1.272195	-1.145501	
O	5.209012	-0.076476	0.237017	
H	4.936637	-0.896131	0.722037	
H	1.541526	0.551098	-1.351343	
H	0.813424	-0.764109	-0.417176	
S	1.297216	1.101805	0.998853	
H	2.136308	2.081339	0.606545	
C	-2.121855	-1.276406	-0.199844	
C	-2.177795	0.150359	0.445095	
O	-1.382836	-1.362658	-1.215527	
O	-2.784789	-2.156731	0.373922	
H	-1.460074	0.154873	1.267629	
C	-3.545678	0.545712	0.982127	
N	-1.664676	1.118733	-0.584688	
H	-1.041519	1.828392	-0.193285	
H	-3.517022	1.534147	1.442616	
H	-3.836238	-0.184475	1.733784	
S	-4.849947	0.634308	-0.319120	

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H	-1.151789	0.516416	-1.257808
H	-2.437862	1.563672	-1.088419
H	-4.796845	-0.673821	-0.645723
28			
Dimer 86 of the n...z type			
C	-1.494804	-0.460968	-0.182754
C	-1.446711	0.725425	0.784131
N	-1.175280	-0.181245	-1.585598
H	-1.497978	0.746780	-1.849760
H	-0.176544	-0.220251	-1.753286
H	-0.770347	-1.189533	0.195345
C	-2.851978	-1.178943	-0.120029
O	-3.498096	-1.314893	0.895521
O	-3.250810	-1.674927	-1.293278
H	-2.557342	-1.366593	-1.933215
H	-1.693084	0.390692	1.789721
H	-0.441276	1.141669	0.808578
S	-2.565226	2.117673	0.318599
H	-3.723197	1.464798	0.548001
C	1.844405	-0.155551	1.430100
C	3.052527	-0.611167	0.543393
O	1.022720	-1.065066	1.706792
O	1.840507	1.042551	1.765927
H	3.871480	-0.862113	1.220903
C	3.536293	0.427771	-0.457251
N	2.642295	-1.895609	-0.126548
H	3.415461	-2.538539	-0.296504
H	4.350642	0.036948	-1.068862
H	3.898691	1.289997	0.097290
S	2.234801	0.987311	-1.639099
H	1.938955	-2.312794	0.508540
H	2.172220	-1.705682	-1.016745
H	1.483014	1.611113	-0.709449
28			
Dimer 87 of the n...z type			
C	1.991216	-0.545396	0.502252
C	0.940642	0.506874	0.148648
N	2.619045	-0.426650	1.821637
H	2.727638	0.550449	2.082863
H	2.066728	-0.883587	2.537191
H	1.472245	-1.508984	0.448724
C	3.089807	-0.621193	-0.567102
O	2.890794	-0.460965	-1.750979
O	4.298171	-0.910902	-0.078375
H	4.166263	-0.932163	0.903832
H	0.504552	0.274398	-0.820065
H	0.150768	0.479114	0.896052
S	1.553942	2.244611	0.140887
H	2.324880	2.123767	-0.959118
C	-1.618431	-1.373502	-0.585805
C	-3.031839	-0.998088	-0.023892
O	-0.873801	-1.983497	0.223091
O	-1.397647	-1.037135	-1.762555
H	-3.719928	-1.785803	-0.338187
C	-3.565488	0.347949	-0.494356
N	-2.941314	-1.075877	1.477148
H	-3.800330	-1.388327	1.929038
H	-4.553255	0.545884	-0.075945
H	-3.643546	0.321121	-1.578524
S	-2.510449	1.779805	-0.001205
H	-2.159115	-1.730917	1.659220
H	-2.675475	-0.165438	1.866425
H	-1.477011	1.467669	-0.805841
28			
Dimer 88 of the n...z type			
C	2.846561	-0.077427	-0.853510
C	2.884425	1.362373	-0.325684
N	1.876665	-0.410408	-1.887634
H	0.923533	-0.222311	-1.579240

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H	2.067841	0.077941	-2.753885
H	3.845134	-0.263476	-1.271581
C	2.735347	-1.105751	0.283032
O	3.091493	-0.893614	1.420484
O	2.261958	-2.291667	-0.101128
H	1.937165	-2.162518	-1.021413
H	3.710894	1.473917	0.375412
H	3.042416	2.044963	-1.161169
S	1.352286	1.965714	0.498896
H	1.275217	0.998049	1.435743
C	-1.042387	-0.510892	0.622798
C	-1.931744	0.763568	0.522110
O	-0.578090	-0.937194	-0.463172
O	-0.929024	-0.978397	1.770458
H	-1.633741	1.472819	1.294430
C	-3.411838	0.430314	0.697527
N	-1.672628	1.424687	-0.803464
H	-2.261245	2.244162	-0.962126
H	-4.022890	1.334264	0.671969
H	-3.532303	-0.038297	1.672998
S	-4.116696	-0.663336	-0.610894
H	-0.681807	1.708252	-0.828910
H	-1.822202	0.744606	-1.555184
H	-3.317122	-1.724275	-0.377830
28			
Dimer 89 of the n...z type			
C	-2.271249	-0.799866	0.212814
C	-3.747742	-0.385273	0.068819
N	-1.776609	-0.548081	1.550938
H	-1.739274	0.449043	1.739689
H	-0.844119	-0.932246	1.662458
C	-2.228051	-1.877779	0.021348
H	-1.439796	-0.153022	-0.897675
O	-0.478256	0.569274	-0.719358
O	-1.892878	-0.462569	-2.114372
H	-1.339371	-0.032922	-2.787332
H	-4.141366	-0.690318	-0.898812
H	-4.319030	-0.878029	0.854752
S	-4.054180	1.420679	0.300545
H	-3.560961	1.822303	-0.889106
C	3.696556	1.064009	-0.138190
C	2.725122	0.036851	0.545521
O	3.414890	2.275328	0.053239
O	4.641484	0.563099	-0.772927
H	3.271654	-0.435206	1.361932
C	2.235248	-1.017039	-0.437491
N	1.595975	0.826330	1.155014
H	1.411125	0.575570	2.123815
H	3.104734	-1.509614	-0.865375
H	1.668004	-0.556144	-1.246876
S	1.098352	-2.277361	0.285705
H	1.927793	1.809622	1.091712
H	0.719781	0.744542	0.609798
H	1.956038	-2.764673	1.204889
28			
Dimer 90 of the n...z type			
C	-2.083033	-0.778681	0.406154
C	-3.158928	-0.894048	-0.677570
N	-2.557478	-0.683013	1.789232
H	-3.440316	-0.180598	1.839089
H	-2.690186	-1.598119	2.201834
H	-1.426115	-1.649771	0.329293
C	-1.132782	0.391497	0.126746
O	-0.771760	0.709626	-0.988329
O	-0.720526	1.032087	1.216091
H	-1.189269	0.572401	1.958959
H	-2.694599	-1.008288	-1.655957
H	-3.779622	-1.767861	-0.478465
S	-4.324757	0.537528	-0.732884

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H	-3.421680	1.440946	-1.165856
C	1.843222	-1.438109	-0.138775
C	3.034792	-0.617016	0.453429
O	2.006899	-1.867797	-1.309107
O	0.884494	-1.601281	0.636699
H	3.465760	-1.219420	1.254143
C	2.630940	0.746717	1.019921
N	4.076737	-0.489077	-0.625173
H	5.034235	-0.606991	-0.297111
H	3.430874	1.160583	1.634846
H	1.741763	0.608297	1.631895
S	2.288611	2.029278	-0.259525
H	3.819915	-1.207531	-1.326488
H	3.983507	0.427490	-1.083608
H	1.111135	1.521370	-0.694695
28			
Dimer 91 of the n...z type			
C	2.971120	0.265614	-0.186071
C	2.571287	-0.927903	-1.082678
N	3.585700	-0.190553	1.049163
H	2.891020	-0.655120	1.627929
H	3.933299	0.598905	1.584336
H	3.699997	0.849752	-0.754625
C	1.743661	1.145505	0.023123
O	1.047316	1.098260	1.022700
O	1.474569	1.923995	-1.021608
H	0.642774	2.425514	-0.857212
H	2.155099	-0.578102	-2.026802
H	3.472616	-1.503954	-1.290831
S	1.395193	-2.127930	-0.312981
H	0.245057	-1.505355	-0.622027
C	-2.553300	-1.494473	-0.099347
C	-2.310408	-0.055804	0.486830
O	-1.887555	-2.412052	0.447558
O	-3.360288	-1.553338	-1.041174
H	-3.253921	0.328839	0.868774
C	-1.763369	0.857998	-0.599445
N	-1.357771	-0.207643	1.647386
H	-1.759765	0.099806	2.531116
H	-2.456595	0.827710	-1.435820
H	-0.799750	0.494161	-0.957482
S	-1.548433	2.627810	-0.079960
H	-1.184018	-1.235299	1.677384
H	-0.458200	0.279168	1.511240
H	-2.417573	3.162722	-0.959039
28			
Dimer 92 of the n...z type			
C	3.092931	-0.072787	0.885543
C	2.240383	1.199443	0.961086
N	4.315302	0.003289	0.083049
H	4.193580	0.637191	-0.703027
H	5.104422	0.324852	0.630170
H	3.374595	-0.336033	1.911119
C	2.250767	-1.268258	0.403326
O	1.094470	-1.440325	0.718581
O	2.917573	-2.118325	-0.374491
H	3.809503	-1.699480	-0.489270
H	1.372604	1.024852	1.595849
H	2.830433	2.005937	1.396546
S	1.695732	1.832506	-0.683847
H	0.965345	0.758193	-1.064442
C	-1.492263	-0.654178	-0.986642
C	-1.621017	0.202289	0.318447
O	-0.919349	-0.058580	-1.937472
O	-1.933874	-1.814285	-0.935988
H	-0.671745	0.087134	0.843165
C	-2.762271	-0.189955	1.243567
N	-1.723024	1.646266	-0.100282
H	-1.344625	2.299596	0.585443

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H	-2.767695	0.423368	2.145950
H	-2.625508	-1.230782	1.527131
S	-4.430687	0.016878	0.481779
H	-1.202376	1.728067	-0.985453
H	-2.703878	1.886535	-0.284421
H	-4.232137	-0.897595	-0.490190
28			
Dimer 93 of the n...z type			
C	2.261813	0.753172	-0.455730
C	1.570997	-0.431670	-1.139402
N	3.710676	0.854197	-0.668088
H	4.130609	-0.061573	-0.802218
H	3.934929	1.426061	-1.472969
H	1.791850	1.666569	-0.837036
C	1.984670	0.775866	1.057962
O	0.891380	0.574968	1.542800
O	3.048370	1.072669	1.798766
H	3.780741	1.185027	1.135941
H	0.500316	-0.416411	-0.961774
H	1.758437	-0.377520	-2.211752
S	2.166170	-2.080961	-0.557913
H	1.196820	-2.232528	0.367777
C	-2.123151	-1.181661	0.538913
C	-3.010796	-0.379726	-0.474547
O	-2.506920	-1.137870	1.735232
O	-1.161916	-1.788446	0.035139
H	-3.587709	-1.111159	-1.042624
C	-2.211525	0.486713	-1.441759
N	-3.986483	0.430744	0.335655
H	-4.931720	0.447255	-0.044300
H	-2.859434	0.933005	-2.197175
H	-1.486924	-0.153348	-1.940891
S	-1.357583	1.907397	-0.632096
H	-3.961100	-0.011216	1.275663
H	-3.646060	1.394115	0.438230
H	-0.626847	1.187425	0.252194
28			
Dimer 94 of the n...z type			
C	2.783555	0.346324	0.234341
C	2.799536	-1.165533	0.475754
N	2.264120	1.185788	1.315222
H	1.465582	0.742083	1.763527
H	2.967386	1.361701	2.022672
H	3.819621	0.652637	0.046147
C	2.047036	0.708322	-1.067402
O	1.995772	-0.006430	-2.040239
O	1.495101	1.926251	-1.040571
H	1.649946	2.246056	-0.115945
H	3.230236	-1.674295	-0.385573
H	3.409677	-1.382844	1.352515
S	1.148058	-1.902463	0.829253
H	0.586647	-1.683726	-0.381238
C	-1.952009	-0.516471	-1.253343
C	-2.799270	-0.390805	0.060109
O	-1.367838	-1.621605	-1.395977
O	-1.975663	0.469085	-2.009846
H	-3.811538	-0.724425	-0.180129
C	-2.860461	1.009543	0.650557
N	-2.246586	-1.382188	1.048572
H	-2.918266	-1.666804	1.761951
H	-3.475432	1.031335	1.551421
H	-3.302176	1.669982	-0.091913
S	-1.209459	1.667171	1.139807
H	-1.934135	-2.193682	0.496243
H	-1.415196	-0.991332	1.510877
H	-0.701959	1.666091	-0.109089
28			
Dimer 95 of the n...z type			
C	3.379988	0.576547	0.396103

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C	2.115847	1.171067	1.030839
N	3.872378	1.239539	-0.814356
H	3.107211	1.656712	-1.338434
H	4.543358	1.966711	-0.599463
H	4.170785	0.612967	1.153209
C	3.195627	-0.925836	0.109503
O	2.646664	-1.687431	0.872764
O	3.727651	-1.322947	-1.046527
H	4.086161	-0.489915	-1.449565
H	1.822624	0.580089	1.897371
H	2.318514	2.192604	1.352641
S	0.684824	1.300579	-0.127875
H	0.448838	-0.026927	-0.266560
C	-1.999526	-1.494616	-0.414097
C	-2.782335	-0.819052	0.762792
O	-0.794836	-1.760030	-0.170390
O	-2.663089	-1.713613	-1.442951
H	-3.271889	-1.620210	1.321976
C	-3.834002	0.190282	0.324293
N	-1.776136	-0.205098	1.700420
H	-2.151414	-0.023098	2.631877
H	-4.345478	0.626614	1.183883
H	-4.565026	-0.334792	-0.286094
S	-3.155677	1.612426	-0.632490
H	-0.978972	-0.850910	1.756270
H	-1.404788	0.673519	1.310679
H	-2.704683	0.869275	-1.664144
28			
Dimer 96 of the n...z type			
C	1.930793	0.255998	-0.697018
C	3.416982	0.304723	-1.086701
N	1.405707	1.488148	-0.090405
H	2.082559	1.877172	0.565845
H	1.289732	2.193452	-0.813627
H	1.346488	0.057763	-1.596761
C	1.669439	-0.965375	0.189144
O	2.005403	-2.078408	-0.133702
O	1.066711	-0.748352	1.370423
H	0.911009	0.204467	1.471044
H	3.701812	-0.619956	-1.586177
H	3.581130	1.137566	-1.770943
S	4.557062	0.603557	0.334481
H	4.405460	-0.606364	0.911503
C	-1.621945	-0.938945	-0.257033
C	-2.025050	0.148743	0.786041
O	-0.929402	-0.541497	-1.222543
O	-2.053118	-2.081597	-0.004978
H	-1.541853	-0.088783	1.735011
C	-3.534004	0.208845	1.004688
N	-1.491533	1.482735	0.341618
H	-1.723281	2.228436	0.999865
H	-3.798984	0.978357	1.731663
H	-3.857322	-0.757223	1.385610
S	-4.492768	0.612858	-0.520419
H	-0.450907	1.453272	0.219393
H	-1.892027	1.717661	-0.570712
H	-4.198428	-0.527369	-1.178435
28			
Dimer 97 of the n...z type			
C	2.418952	0.053346	1.145738
C	3.296039	-0.515755	0.018814
N	1.469126	-0.932775	1.621665
H	0.937262	-1.360481	0.865881
H	0.804453	-0.517708	2.265530
H	3.098679	0.318317	1.964698
C	1.790234	1.374273	0.690243
O	0.600822	1.589697	0.618476
O	2.725383	2.279016	0.362472
H	2.291948	3.097113	0.069677

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H	4.155319	0.125367	-0.164277
H	3.647607	-1.503420	0.315473
S	2.408269	-0.757804	-1.588397
H	2.489684	0.523615	-2.002363
C	-1.649683	-1.918427	0.286386
C	-1.756921	-0.376439	0.047325
O	-0.603068	-2.446945	-0.166982
O	-2.574505	-2.435318	0.939945
H	-1.272737	0.110180	0.894436
C	-3.181229	0.132675	-0.108153
N	-0.922372	-0.002615	-1.146607
H	0.006583	-0.450980	-1.093590
H	-3.753271	-0.184144	0.759866
H	-3.654602	-0.293451	-0.995239
S	-3.303419	1.965204	-0.311920
H	-1.356899	-0.318720	-2.015400
H	-0.791463	1.010506	-1.196878
H	-2.800854	2.283491	0.898450
28			
Dimer 98 of the n...z type			
C	2.633944	0.555961	0.776957
C	1.155404	0.642711	0.385684
N	3.499364	1.632200	0.280793
H	3.202528	1.954910	-0.636216
H	3.507220	2.427722	0.907332
H	2.681164	0.566938	1.871695
C	3.247825	-0.800038	0.382930
O	2.673987	-1.857638	0.505707
O	4.500513	-0.713284	-0.069810
H	4.697685	0.258305	-0.064431
H	0.602696	-0.209285	0.777519
H	0.730409	1.559892	0.792780
S	0.873188	0.673899	-1.442519
H	0.466421	-0.607801	-1.542783
C	-2.002082	-1.300329	-0.647004
C	-3.076091	-0.815349	0.383617
O	-0.998688	-1.869443	-0.142946
O	-2.267411	-1.084204	-1.840713
H	-3.898109	-1.532776	0.352710
C	-3.617974	0.581119	0.101730
N	-2.457411	-0.909371	1.752445
H	-3.110641	-1.184615	2.484994
H	-4.431044	0.833144	0.784067
H	-3.995325	0.593225	-0.918224
S	-2.361418	1.915473	0.316610
H	-1.689307	-1.596577	1.651438
H	-2.032734	-0.008292	2.004271
H	-1.498383	1.473335	-0.629602
28			
Dimer 99 of the n...z type			
C	3.336962	-0.781115	0.441241
C	3.598938	0.680663	0.826512
N	3.779446	-1.193525	-0.893104
H	3.756382	-0.409409	-1.540507
H	4.720407	-1.567106	-0.879449
H	3.846055	-1.407588	1.181654
C	1.846379	-1.134128	0.608283
O	1.172311	-0.757315	1.540513
O	1.369319	-1.923468	-0.352873
H	2.136047	-2.041279	-0.972621
H	3.194639	0.877199	1.818408
H	4.673079	0.866237	0.839306
S	2.906836	1.903716	-0.368911
H	1.609169	1.548881	-0.233049
C	-3.627787	0.169563	0.862204
C	-2.994531	-0.790422	-0.202665
O	-4.751162	0.639366	0.548006
O	-2.960659	0.338177	1.898769
H	-3.238360	-1.811240	0.099409

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C	-1.487410	-0.662412	-0.352311
N	-3.713541	-0.538849	-1.502679
H	-3.804323	-1.365518	-2.092536
H	-1.095357	-1.351103	-1.100090
H	-1.014822	-0.891510	0.598054
S	-0.949017	1.017022	-0.886768
H	-4.639830	-0.167603	-1.226378
H	-3.235559	0.197868	-2.032405
H	-1.371167	1.650175	0.227210
28			
Dimer 100 of the n...z type			
C	-2.934226	-0.803534	-0.488932
C	-3.128323	-0.522520	1.008693
N	-2.380902	-2.127285	-0.710712
H	-1.531330	-2.258149	-0.170190
H	-2.137578	-2.260550	-1.686814
H	-3.931335	-0.758729	-0.944440
C	-2.139627	0.322572	-1.157808
O	-1.138915	0.154931	-1.825139
O	-2.677437	1.523847	-0.935148
H	-2.129320	2.204922	-1.358313
H	-3.699926	0.390638	1.157988
H	-3.670939	-1.356107	1.453078
S	-1.554108	-0.380046	1.972667
H	-1.235573	0.862082	1.551857
C	3.507443	-0.867620	-0.116615
C	2.242967	0.019764	-0.404193
O	3.292196	-2.106278	-0.087779
O	4.577152	-0.247441	0.019308
H	2.325232	0.366503	-1.435405
C	2.139580	1.207290	0.539835
N	1.037900	-0.877311	-0.343786
H	0.344273	-0.676180	-1.076407
H	3.069484	1.766690	0.473959
H	2.021256	0.872542	1.573109
S	0.711174	2.334154	0.224212
H	1.428338	-1.834011	-0.424780
H	0.539996	-0.816003	0.551934
H	0.944516	2.526603	-1.089967
28			
Dimer 101 of the n...z type			
C	1.702945	-0.211906	0.565177
C	1.419062	0.836274	-0.512955
N	2.212319	0.287556	1.845271
H	2.834084	1.079667	1.702262
H	1.462053	0.584988	2.457064
H	0.759922	-0.739787	0.741185
C	2.645103	-1.310663	0.050623
O	2.660775	-1.708610	-1.092575
O	3.438655	-1.821547	0.995645
H	3.254675	-1.268222	1.796643
H	0.948091	0.360558	-1.369896
H	0.740085	1.585228	-0.106344
S	2.907242	1.781382	-1.058211
H	3.513217	0.751452	-1.683336
C	-2.210483	-1.313954	-0.409537
C	-3.013069	-0.035158	-0.830705
O	-2.902224	-2.230350	0.098300
O	-0.988145	-1.276142	-0.642926
H	-3.232848	-0.129746	-1.895801
C	-2.272258	1.272034	-0.587893
N	-4.331251	-0.082873	-0.105804
H	-5.106714	0.323070	-0.629007
H	-2.863979	2.130549	-0.908735
H	-1.351713	1.245143	-1.165347
S	-1.878059	1.576011	1.188311
H	-4.493052	-1.087171	0.087387
H	-4.254882	0.394470	0.798941
H	-1.145065	0.457368	1.354651

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28		
Dimer 102 of the n...z	type	
C	2.808502 -0.082661 1.007589	
C	2.972719 -1.432220 0.301719	
N	1.652661 0.044660 1.899509	
H	0.887218 -0.545083 1.589763	
H	1.881410 -0.222611 2.849158	
H	3.714766 0.084985 1.599911	
C	2.789848 1.077939 -0.004816	
O	3.461928 1.099164 -1.010623	
O	1.972985 2.074844 0.335994	
H	1.531076 1.760311 1.165573	
H	3.909361 -1.457606 -0.252176	
S	2.980147 -2.230184 1.043739	
H	1.605445 -1.850713 -0.869107	
H	1.932774 -0.938011 -1.805908	
C	-3.129969 -0.532641 0.796491	
C	-1.729810 -0.596341 0.096221	
O	-3.990825 -1.318139 0.327526	
O	-3.216759 0.267586 1.745460	
H	-1.106703 -1.270604 0.687606	
C	-1.034282 0.749427 -0.045353	
N	-1.920856 -1.266197 -1.234786	
H	-1.104079 -1.800299 -1.532755	
H	-0.063405 0.638957 -0.526407	
H	-0.891290 1.163220 0.949382	
S	-1.964512 1.955732 -1.079792	
H	-2.750130 -1.872692 -1.120211	
H	-2.146708 -0.569470 -1.953150	
H	-3.030319 2.038232 -0.256420	
28		
Dimer 103 of the n...z	type	
C	-3.041141 -0.299208 -0.762752	
C	-2.133981 0.934792 -0.795876	
N	-4.447010 -0.072305 -0.418221	
H	-4.535317 0.679448 0.261171	
H	-4.997520 0.171684 -1.232571	
H	-3.007096 -0.753198 -1.759649	
C	-2.472882 -1.384397 0.169611	
O	-1.288638 -1.594969 0.311318	
O	-3.407669 -2.096845 0.796422	
H	-4.262264 -1.667203 0.534069	
H	-1.134395 0.663021 -1.128128	
H	-2.542589 1.663842 -1.496025	
S	-2.010514 1.820815 0.815688	
H	-1.383197 0.830207 1.480338	
C	3.234094 -1.199934 -0.217510	
C	2.679644 -0.188677 0.844717	
O	4.488003 -1.241951 -0.298877	
O	2.377303 -1.854585 -0.837864	
H	2.505270 -0.751053 1.764591	
C	1.395058 0.518379 0.439682	
N	3.786561 0.790219 1.137004	
H	3.770098 1.164043 2.085610	
H	1.067698 1.212923 1.214000	
H	0.621121 -0.230676 0.289000	
S	1.571047 1.533147 -1.090781	
H	4.661867 0.271728 0.950408	
H	3.745858 1.569589 0.470960	
H	1.841753 0.490542 -1.903438	
28		
Dimer 104 of the n...z	type	
C	3.011413 -0.117512 -0.899655	
C	1.584733 -0.665641 -0.783471	
N	4.099597 -1.088992 -0.769084	
H	3.873925 -1.803669 -0.081814	
H	4.298025 -1.549991 -1.648787	
H	3.097999 0.351289 -1.886449	
C	3.248637 1.034726 0.094122	

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O	2.399505 1.838898 0.402398	
O	4.494756 1.088756 0.567194	
H	4.943328 0.293289 0.184604	
H	0.863782 0.133047 -0.949659	
H	1.433179 -1.445738 -1.529119	
S	1.239871 -1.449077 0.855641	
H	0.986036 -0.295283 1.507147	
C	-1.448589 0.853088 0.020609	
C	-2.058512 -0.460088 -0.561566	
O	-1.247202 0.868456 1.256749	
O	-1.250591 1.742536 -0.831615	
H	-1.422847 -0.818030 -1.372662	
C	-3.469873 -0.238822 -1.100742	
N	-2.041421 -1.521283 0.502604	
H	-2.487655 -2.389521 0.202883	
H	-3.872398 -1.153783 -1.539289	
H	-3.414281 0.521843 -1.877147	
S	-4.701184 0.268562 0.176252	
H	-1.056269 -1.715871 0.757427	
H	-2.510860 -1.168247 1.341305	
H	-4.136767 1.457159 0.473047	
28		
Dimer 105 of the n...z	type	
C	-2.942380 -0.341817 0.894715	
C	-2.144909 0.944086 1.143541	
N	-2.177773 -1.541112 0.554193	
H	-1.407195 -1.325617 -0.072283	
H	-1.798882 -1.995398 1.376235	
H	-3.503073 -0.554330 1.812309	
C	-4.028232 -0.124849 -0.175028	
O	-4.614248 0.921914 -0.333232	
O	-4.290799 -1.210711 -0.903235	
H	-3.635364 -1.885670 -0.596922	
H	-2.814041 1.752151 1.434408	
H	-1.430136 0.777496 1.949850	
S	-1.144830 1.493462 -0.304263	
H	-2.178807 1.829974 -1.099993	
C	4.124618 0.008701 0.122412	
C	2.724968 0.521443 0.611083	
O	4.719221 0.780958 -0.670498	
O	4.489772 -1.084439 0.591160	
H	2.880262 1.027627 1.566022	
C	1.686153 -0.576837 0.786434	
N	2.274504 1.570925 -0.368958	
H	1.681304 2.294514 0.037897	
H	0.742483 -0.177316 1.155641	
H	2.065871 -1.289857 1.513887	
S	1.292622 -1.463879 -0.780978	
H	3.146626 1.968802 -0.757568	
H	1.767981 1.130338 -1.144911	
H	2.488299 -2.080863 -0.879865	
28		
Dimer 106 of the n...z	type	
C	2.272230 0.071064 0.957258	
C	1.593236 -1.247470 0.572657	
N	1.439658 1.275545 0.891323	
H	0.712034 1.193372 0.185856	
H	1.016754 1.492870 1.784573	
H	2.632819 -0.039064 1.985816	
C	3.548247 0.303670 0.125133	
O	4.323779 -0.577755 -0.171260	
O	3.736610 1.575131 -0.225965	
H	2.930646 2.042817 0.118108	
H	2.285106 -2.075579 0.720037	
H	0.707106 -1.401378 1.186030	
S	0.963991 -1.296725 -1.160389	
H	2.170644 -1.216031 -1.759765	
C	-2.386522 -1.253459 0.191660	
C	-3.035327 0.090766 0.670945	

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O -1.578199	-1.764539	1.009016	
O -2.764280	-1.669023	-0.916218	
H -4.006663	-0.160616	1.101385	
C -3.228171	1.126189	-0.427602	
N -2.180510	0.612198	1.793201	
H -2.701865	1.085996	2.530004	
H -3.720341	2.020997	-0.044367	
H -3.850972	0.684276	-1.201740	
S -1.646199	1.705886	-1.179481	
H -1.688303	-0.227477	2.153090	
H -1.471602	1.252757	1.422680	
H -1.260680	0.501633	-1.649984	
28			
Dimer 107 of the n...z type			
C -2.017388	-0.548083	0.750010	
C -1.595092	0.936187	0.710858	
N -1.009318	-1.430676	0.181232	
H -1.037150	-1.377648	-0.833677	
H -1.217051	-2.394722	0.421835	
H -2.145683	-0.795539	1.807223	
C -3.386531	-0.681431	0.079453	
O -3.562544	-1.127392	-1.031163	
O -4.369652	-0.190097	0.852507	
H -5.211146	-0.241028	0.370706	
H -2.383703	1.553051	1.140293	
H -0.684513	1.073563	1.295668	
S -1.170436	1.595756	-0.963309	
H -2.261033	1.152908	-1.622468	
C 2.034254	1.610242	0.535797	
C 1.857954	0.167537	-0.020351	
O 2.591029	2.429144	-0.235808	
O 1.614007	1.774532	1.699637	
H 0.877393	-0.223662	0.237195	
C 2.924494	-0.767381	0.534714	
N 1.923380	0.228534	-1.521100	
H 1.009269	0.520827	-1.884813	
H 2.879678	-0.723347	1.621457	
H 3.925597	-0.471543	0.215093	
S 2.705638	-2.515145	-0.028853	
H 2.605580	0.955898	-1.773492	
H 2.172481	-0.674761	-1.934499	
H 1.419745	-2.620711	0.368872	
28			
Dimer 108 of the n...z type			
C 2.322320	0.446627	1.001668	
C 2.849829	-0.810961	0.291931	
N 1.320497	0.123978	2.000053	
H 0.654437	-0.583400	1.687940	
H 0.786731	0.948088	2.255900	
H 3.190702	0.899173	1.500571	
C 1.882690	1.503499	-0.016040	
O 0.817498	2.077964	-0.007637	
O 2.845100	1.747370	-0.922638	
H 2.539724	2.435897	-1.534989	
H 3.811486	-0.611336	-0.174813	
H 2.980074	-1.599131	1.033237	
S 1.736488	-1.518094	-1.009108	
H 2.108097	-0.670219	-1.989613	
C -1.422228	-1.824054	0.416501	
C -1.481147	-0.371955	-0.143333	
O -1.984915	-2.699230	-0.281859	
O -0.846131	-1.936269	1.519219	
H -0.524263	0.119743	-0.015966	
C -2.569706	0.425262	0.566269	
N -1.743064	-0.454226	-1.619866	
H -0.870616	-0.623734	-2.123586	
H -2.336516	0.431994	1.629677	
H -3.550558	-0.034230	0.430194	
S -2.736624	2.157618	-0.049158	

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H -2.350501	-1.271893	-1.773642	
H -2.169757	0.404163	-1.983051	
H -1.451848	2.505057	0.170425	
28			
Dimer 109 of the n...z type			
C 2.834759	0.735681	0.947841	
C 1.356980	0.814717	0.536232	
N 3.531572	1.981428	0.669413	
H 3.572986	2.133202	-0.335499	
H 4.495101	1.917747	0.983031	
H 2.843573	0.565704	2.031034	
C 3.510556	-0.494859	0.328705	
O 4.547359	-0.471613	-0.290911	
O 2.808290	-1.618370	0.563661	
H 3.268990	-2.372218	0.161845	
H 0.807020	-0.049410	0.902341	
H 0.924875	1.722591	0.955701	
S 1.109174	0.932812	-1.296485	
H 1.102201	-0.395406	-1.534339	
C -1.233248	-1.451331	-0.066679	
C -2.096730	-0.150609	-0.007354	
O -1.012107	-1.911255	-1.211661	
O -0.881225	-1.882884	1.048748	
H -1.609560	0.577898	0.639161	
C -3.494489	-0.471182	0.513891	
N -2.161838	0.455454	-1.379207	
H -1.244539	0.877077	-1.596471	
H -3.393668	-0.926842	1.496756	
H -3.997101	-1.183203	-0.144034	
S -4.621937	0.986520	0.608875	
H -2.314224	-0.291452	-2.064887	
H -2.896163	1.166503	-1.446995	
H -3.908929	1.668780	1.528158	
28			
Dimer 110 of the n...z type			
C -2.317567	-0.739629	0.210870	
C -3.383858	-0.712095	-0.888902	
N -2.788504	-0.996166	1.573527	
H -3.717181	-0.607667	1.717738	
H -2.824376	-1.987579	1.776595	
H -1.594504	-1.519054	-0.049123	
C -1.482232	0.551503	0.206256	
O -1.148740	1.127399	-0.805484	
O -1.126731	0.970548	1.420109	
H -1.561105	0.327193	2.037629	
H -2.915148	-0.557284	-1.859555	
H -3.914164	-1.664372	-0.901871	
S -4.684364	0.574443	-0.639164	
H -3.881590	1.636796	-0.854160	
C 3.385903	1.080233	0.157816	
C 3.165127	0.008096	-0.964363	
O 4.512286	1.036079	0.714897	
O 2.436486	1.860262	0.349319	
H 3.386858	0.490293	-1.918982	
C 1.761464	-0.577387	-1.011699	
N 4.208773	-1.059051	-0.764290	
H 4.507706	-1.513922	-1.626591	
H 1.667021	-1.312267	-1.812476	
H 1.055065	0.229660	-1.188733	
S 1.285316	-1.453382	0.540924	
H 4.996878	-0.580573	-0.295020	
H 3.859760	-1.772414	-0.115115	
H 1.223180	-0.339119	1.298397	
28			
Dimer 111 of the n...z type			
C -2.955818	-0.443048	-0.750455	
C -1.485200	-0.249779	-0.355636	
N -3.262767	0.214634	-2.009611	
H -3.169824	1.221521	-1.902626	

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H -4.230525	0.044724	-2.264740	
H -3.095449	-1.523219	-0.876061	
C -3.885069	-0.035762	0.400039	
O -4.801570	0.744979	0.302932	
O -3.554554	-0.657286	1.548450	
H -4.167822	-0.380205	2.247946	
H -1.221803	-0.859378	0.505013	
H -0.851681	-0.544096	-1.191315	
S -1.028014	1.505927	0.007309	
H -1.658382	1.596337	1.197010	
C 1.459181	-1.513275	-0.033342	
C 2.257806	-0.169851	-0.070578	
O 1.035202	-1.856537	1.096938	
O 1.356881	-2.092056	-1.131135	
H 1.938275	0.426888	-0.923731	
C 3.752970	-0.465919	-0.152587	
N 1.930889	0.607610	1.169129	
H 1.021133	1.081464	1.035968	
H 3.935624	-1.054733	-1.049387	
H 4.075440	-1.048742	0.712841	
S 4.826884	1.034283	-0.156665	
H 1.814220	-0.067052	1.936044	
H 2.646989	1.305197	1.391443	
H 4.354129	1.555243	-1.307471	
28			
Dimer 112 of the n...z type			
C -1.850737	0.292540	-0.805691	
C -2.337464	0.789994	0.564331	
N -2.860369	0.487162	-1.832970	
H -3.673710	-0.088128	-1.628574	
H -2.508806	0.177183	-2.733372	
H -0.973598	0.902904	-1.044759	
C -1.357912	-1.151867	-0.715147	
O -1.710657	-2.060224	-1.421278	
O -0.444041	-1.323597	0.282479	
H -0.174478	-2.256914	0.307680	
H -1.515953	0.823830	1.273702	
H -2.719187	1.802735	0.441231	
S -3.735724	-0.182682	1.277563	
H -3.013038	-1.270171	1.616859	
C 1.495973	1.955070	-0.196547	
C 2.349412	0.812438	0.442559	
O 0.417372	2.215434	0.388161	
O 1.992173	2.469081	-1.217610	
H 3.269885	1.243705	0.838162	
C 2.667854	-0.283187	-0.569726	
N 1.596652	0.243513	1.616167	
H 1.311814	0.995098	2.245757	
H 3.203063	0.170358	-1.400197	
H 1.749236	-0.724628	-0.958557	
S 3.635256	-1.699748	0.110501	
H 0.737622	-0.215321	1.283217	
H 2.156762	-0.445833	2.124017	
H 4.762362	-1.006144	0.370744	
28			
Dimer 113 of the n...z type			
C -2.761584	-0.530811	0.425471	
C -1.296606	-0.777871	0.043859	
N -3.674620	-1.248280	-0.448577	
H -3.596544	-0.888896	-1.396532	
H -4.633889	-1.082550	-0.160509	
H -2.877642	-0.918217	1.445021	
C -3.057131	0.972021	0.524814	
O -4.000752	1.523574	0.011098	
O -2.131852	1.613927	1.264954	
H -2.363218	2.555150	1.317641	
H -0.632747	-0.362715	0.797943	
H -1.102448	-1.846618	-0.022577	
S -0.830897	-0.108739	-1.614901	

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H -0.845969	1.199240	-1.282982	
C 1.691042	-1.691730	0.836063	
C 2.553015	-0.573281	0.156063	
O 1.336770	-2.628965	0.083601	
O 1.467075	-1.521910	2.050624	
H 3.598730	-0.763558	0.405271	
C 2.160333	0.832353	0.593513	
N 2.432234	-0.720713	-1.335761	
H 2.602752	-1.695362	-1.593302	
H 2.236404	0.884063	1.676199	
H 1.128612	1.052260	0.319524	
S 3.156944	2.179002	-0.179974	
H 1.459379	-0.505592	-1.621187	
H 3.071507	-0.099657	-1.836628	
H 4.330695	1.854101	0.399554	
28			
Dimer 114 of the n...z type			
C -2.428640	0.723161	-0.064267	
C -1.819890	-0.118775	-1.201845	
N -1.415283	1.124495	0.900869	
H -1.107135	0.317344	1.436878	
H -1.796647	1.790069	1.565958	
H -2.842608	1.622866	-0.530716	
C -3.602725	-0.023335	0.573150	
O -3.639688	-0.394311	1.722160	
O -4.588905	-0.238295	-0.315746	
H -5.304334	-0.733431	0.114744	
H -2.584795	-0.373190	-1.933149	
H -1.048925	0.468182	-1.699822	
S -0.973331	-1.658818	-0.642385	
H -2.083541	-2.322310	-0.257159	
C 3.211469	-1.228561	0.204089	
C 2.246080	-0.013529	0.406018	
O 4.394502	-1.036767	0.588478	
O 2.710886	-2.220809	-0.352942	
H 1.310514	-0.335150	0.857271	
C 1.981417	0.651682	-0.947753	
N 2.922365	0.948018	1.344889	
H 2.665179	0.776725	2.316378	
H 1.400083	-0.044290	-1.550207	
H 2.921919	0.840249	-1.469243	
S 1.141030	2.291155	-0.845104	
H 3.934633	0.752375	1.249218	
H 2.692668	1.921943	1.112455	
H 0.069623	1.871247	-0.085024	
28			
Dimer 115 of the n...z type			
C 2.001269	-0.576908	-0.382300	
C 1.360644	0.772453	-0.757833	
N 1.247198	-1.284662	0.642618	
H 1.147776	-0.696495	1.466867	
H 1.761795	-2.107277	0.944747	
H 2.002743	-1.181300	-1.295995	
C 3.470623	-0.370458	-0.001012	
O 3.940938	-0.613483	1.085346	
O 4.181853	0.127861	-1.028190	
H 5.101109	0.258612	-0.745309	
H 1.949095	1.249635	-1.539354	
H 0.348870	0.628072	-1.131790	
S 1.148309	1.949074	0.647941	
H 2.444615	1.999197	1.022578	
C -2.542095	1.429095	-0.332245	
C -2.121191	0.040977	0.238578	
O -3.669777	1.848830	0.023849	
O -1.710839	1.934199	-1.111742	
H -1.119911	0.095014	0.658062	
C -2.180650	-1.012501	-0.865481	
N -3.053259	-0.330907	1.360688	
H -2.782772	0.121201	2.234549	

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H	-1.552340	-0.672770	-1.686427
H	-3.200280	-1.116774	-1.242058
S	-1.640106	-2.685060	-0.309436
H	-3.987672	0.024348	1.119213
H	-3.067698	-1.345594	1.512289
H	-0.403158	-2.246300	0.091063
28			
Dimer 116 of the n...z type			
C	2.048306	0.450176	-0.838414
C	2.062001	1.261937	0.467927
N	0.716647	-0.029048	-1.164706
H	0.408880	-0.739285	-0.499612
H	0.723136	-0.480329	-2.073838
H	2.373626	1.139387	-1.626884
C	3.101508	-0.662855	-0.801037
O	2.882246	-1.827892	-1.031966
O	4.319290	-0.185151	-0.477468
H	4.956175	-0.917583	-0.472206
H	3.029139	1.740774	0.606938
H	1.293586	2.031903	0.411453
S	1.656963	0.292044	1.984171
H	2.792300	-0.436014	2.019158
C	-2.368982	-1.637532	0.280879
C	-2.414016	-0.246122	-0.418632
O	-3.466983	-2.083248	0.690364
O	-1.222487	-2.122333	0.376454
H	-1.826251	-0.276794	-1.331925
C	-1.881619	0.831568	0.520850
N	-3.836022	0.066690	-0.807461
H	-4.108188	-0.432223	-1.655316
H	-0.954899	0.470932	0.957431
H	-2.587305	1.025333	1.331530
S	-1.569982	2.437489	-0.324345
H	-4.449444	-0.272157	-0.055466
H	-3.976285	1.068261	-0.969684
H	-0.610253	1.907719	-1.122137
28			
Dimer 117 of the n...z type			
C	3.244285	0.004255	0.897754
C	1.762473	0.397044	0.917343
N	4.208977	1.105258	0.964230
H	3.855948	1.925864	0.478104
H	4.413134	1.367644	1.920832
H	3.420431	-0.651395	1.757929
C	3.571334	-0.870665	-0.326853
O	2.819794	-1.707571	-0.773080
O	4.780393	-0.643648	-0.841855
H	5.140650	0.107451	-0.304152
H	1.137282	-0.494241	0.899115
H	1.549968	0.960840	1.825752
S	1.264098	1.487811	-0.483100
H	1.237951	0.513291	-1.414231
C	-3.673636	0.853822	-0.389141
C	-3.210244	0.060311	0.882097
O	-4.826818	0.564304	-0.798127
O	-2.862061	1.686906	-0.829524
H	-3.420081	0.689858	1.749397
C	-1.737221	-0.321418	0.883799
N	-4.102859	-1.146940	0.994291
H	-4.277882	-1.445005	1.953385
H	-1.466335	-0.855263	1.795951
H	-1.149431	0.591469	0.818822
S	-1.267097	-1.427444	-0.513142
H	-4.979437	-0.875050	0.515123
H	-3.699345	-1.930555	0.469263
H	-1.493717	-0.511376	-1.476890
28			
Dimer 118 of the n...z type			
C	1.360987	-0.090916	-0.032623

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C	1.793146	1.241005	-0.665788
N	0.732620	0.112186	1.260665
H	1.424703	0.416174	1.939100
H	0.338156	-0.765277	1.586331
H	0.628533	-0.531749	-0.716194
C	2.525583	-1.082085	-0.000568
O	2.952372	-1.621071	0.992973
O	3.032517	-1.288546	-1.232692
H	3.765190	-1.922102	-1.171399
H	2.143227	1.087501	-1.684779
H	0.932119	1.909194	-0.686457
S	3.090806	2.153290	0.280475
H	4.115991	1.330790	-0.023753
C	-1.559469	-1.740325	-0.374141
C	-2.657185	-0.642193	-0.199669
O	-1.119670	-2.242916	0.690571
O	-1.203234	-1.941061	-1.549723
H	-3.482338	-0.820857	-0.886046
C	-2.036308	0.734064	-0.438700
N	-3.192193	-0.736564	1.205257
H	-3.943170	-1.423625	1.275641
H	-1.627161	0.748439	-1.446952
H	-1.222946	0.905613	0.271161
S	-3.195756	2.145577	-0.206451
H	-2.414498	-1.076906	1.790788
H	-3.548600	0.164205	1.540853
H	-4.069398	1.798823	-1.174216
28			
Dimer 119 of the n...z type			
C	2.770743	0.463837	-0.290021
C	1.689689	-0.087006	-1.229909
N	4.053448	-0.178747	-0.511321
H	3.991892	-1.167476	-0.283447
H	4.753753	0.216379	0.108200
H	2.866345	1.529035	-0.534122
C	2.308003	0.430053	1.173641
O	2.957297	-0.002229	2.092512
O	1.072090	0.958306	1.320873
H	0.825572	0.946901	2.260147
H	0.787642	0.516716	-1.159933
H	2.055258	-0.037452	-2.255010
S	1.268855	-1.869344	-0.971681
H	0.934376	-1.785507	0.333474
C	-2.804233	-1.065776	0.791372
C	-1.840758	-0.113968	0.008745
O	-3.522902	-1.808348	0.075753
O	-2.764976	-0.948700	2.029550
H	-0.843301	-0.177571	0.432982
C	-2.350475	1.321781	0.088406
N	-1.782846	-0.595377	-1.414325
H	-0.981165	-1.230336	-1.547533
H	-2.426281	1.595670	1.138693
H	-3.342572	1.402964	-0.360147
S	-1.300836	2.549965	-0.803350
H	-2.652531	-1.141832	-1.548070
H	-1.704977	0.165643	-2.093539
H	-0.216416	2.410038	-0.014575
28			
Dimer 120 of the n...z type			
C	-1.601102	0.013046	-0.575840
C	-3.057567	0.407253	-0.889044
N	-1.304721	-1.344158	-0.982743
H	-1.900450	-1.988413	-0.469821
H	-0.339020	-1.598283	-0.762641
H	-0.982214	0.707954	-1.155033
C	-1.294637	0.302992	0.896771
O	-0.991938	-0.524014	1.722494
O	-1.384839	1.623116	1.169213
H	-1.196175	1.769635	2.110571

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H	-3.220776	1.463399	-0.681764	
H	-3.242204	0.221597	-1.946953	
S	-4.333188	-0.584547	0.003375	
H	-4.125061	-0.056227	1.227099	
C	2.507066	-1.641308	-0.080097	
C	2.203382	-0.155300	0.294379	
O	3.700298	-2.000321	0.038343	
O	1.517792	-2.279908	-0.494311	
H	1.345146	-0.115443	0.960028	
C	1.953057	0.642386	-0.984011	
N	3.387054	0.399572	1.039722	
H	3.332690	0.189377	2.036769	
H	1.134056	0.172520	-1.523787	
S	2.831967	0.607609	-1.631205	
S	1.620144	2.437161	-0.731875	
H	4.220930	-0.085572	0.675850	
H	3.467856	1.415828	0.931556	
H	0.513933	2.300900	0.027623	
28				
Dimer 121 of the n...z type				
C	-2.440849	-1.015203	-0.590604	
C	-2.958922	-0.746548	0.827035	
N	-1.454097	-2.085330	-0.615089	
H	-0.640173	-1.864357	-0.043396	
H	-1.108369	-2.216094	-1.560439	
H	-3.314180	-1.346856	-1.170056	
C	-1.984998	0.254521	-1.327764	
O	-1.159312	0.259175	-2.210716	
O	-2.625608	1.363828	-0.914776	
H	-2.294435	2.123862	-1.420572	
H	-3.814933	-0.075712	0.801316	
H	-3.271555	-1.694262	1.265098	
S	-1.713546	-0.055644	2.004000	
H	-1.667780	1.178951	1.462725	
C	2.418310	-1.435036	0.057794	
C	2.309899	0.066343	0.488978	
O	3.371642	-1.706208	-0.711747	
O	1.512273	-2.170333	0.494772	
H	2.199524	0.142684	1.568885	
C	1.110629	0.679791	-0.219013	
N	3.587974	0.756619	0.092837	
H	4.278859	0.736882	0.843373	
H	0.241928	0.111617	0.092407	
H	1.197455	0.593699	-1.302389	
S	0.815842	2.463731	0.111875	
H	3.970792	0.199368	-0.690173	
H	3.437639	1.733557	-0.174922	
H	0.694997	2.353339	1.451085	
28				
Dimer 122 of the n...z type				
C	-1.442266	-0.596294	0.217815	
C	-1.819839	0.624994	1.083325	
N	-0.668422	-0.210788	-0.946423	
H	-1.277695	0.039824	-1.717424	
H	-0.057936	-0.972356	-1.234545	
H	-0.827457	-1.244768	0.851115	
C	-2.699247	-1.399674	-0.119517	
O	-3.150132	-1.544426	-1.231357	
O	-3.272496	-1.905575	0.988671	
H	-4.081989	-2.380282	0.740415	
H	-2.377702	0.317437	1.966699	
H	-0.902293	1.117645	1.406489	
S	-2.762534	1.929854	0.186260	
H	-3.911730	1.237598	0.044370	
C	2.625107	-1.559542	-0.104226	
C	2.225603	-0.120580	0.337499	
O	3.756441	-1.954047	0.260748	
O	1.764150	-2.136490	-0.803000	
H	1.215889	-0.130611	0.733044	

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C	2.328116	0.851990	-0.833855	
N	3.130989	0.328203	1.455837	
H	2.893696	-0.138637	2.332236	
H	1.881621	0.384936	-1.707258	
H	3.372574	1.076797	-1.059650	
S	1.470808	2.452904	-0.522282	
H	4.092348	0.050641	1.227053	
H	3.075596	1.339348	1.608223	
H	0.246178	1.875351	-0.587041	
28				
Dimer 123 of the n...z type				
C	3.137503	0.180124	-0.083293	
C	2.643286	-1.041586	-0.881279	
N	3.769184	-0.227141	1.162817	
H	3.061840	-0.575437	1.805150	
H	4.190949	0.576348	1.618115	
H	3.887452	0.672800	-0.711221	
C	2.000396	1.185454	0.105601	
O	1.497870	1.463806	1.171176	
O	1.602821	1.713646	-1.063712	
H	0.839267	2.306263	-0.904456	
H	2.215750	-0.729676	-1.832488	
H	3.499625	-1.686707	-1.073997	
S	1.388493	-2.075320	0.012788	
H	0.299995	-1.724117	-0.700166	
C	-2.335784	-1.577505	-0.197848	
C	-2.646103	-0.042629	-0.205906	
O	-2.539934	-2.163294	0.891588	
O	-1.867925	-2.018223	-1.265682	
H	-3.273494	0.210974	-1.057466	
C	-1.325461	0.714242	-0.257272	
N	-3.404431	0.275461	1.055854	
H	-4.413456	0.243390	0.908744	
H	-0.798760	0.406173	-1.157618	
H	-0.701857	0.468691	0.603155	
S	-1.467722	2.552791	-0.233787	
H	-3.162447	-0.487088	1.714192	
H	-3.172099	1.194394	1.441451	
H	-2.144066	2.670153	-1.395079	
28				
Dimer 124 of the n...z type				
C	-3.075001	0.681195	0.769677	
C	-2.616801	-0.783857	0.921005	
N	-4.465671	0.757776	0.348169	
H	-4.553345	0.366943	-0.586616	
H	-4.758912	1.727744	0.282497	
H	-2.978413	1.140944	1.758822	
C	-2.109316	1.414602	-0.159931	
O	-2.361030	1.748229	-1.294362	
O	-0.916441	1.626805	0.427232	
H	-0.297779	1.927759	-0.257246	
H	-1.599422	-0.833355	1.306119	
H	-3.292771	-1.279276	1.618011	
S	-2.663951	-1.772694	-0.638174	
H	-1.458965	-1.341861	-1.096238	
C	0.932149	-0.670536	-0.134742	
C	2.220029	0.152287	0.192314	
O	0.621424	-1.535207	0.716187	
O	0.390231	-0.393653	-1.223808	
H	2.070381	1.210318	-0.011094	
C	3.380980	-0.393154	-0.637305	
N	2.494568	-0.007920	1.662977	
H	2.000051	0.692205	2.216479	
H	3.123549	-0.286219	-1.689168	
H	3.532702	-1.454315	-0.428451	
S	5.007199	0.406204	-0.299443	
H	2.105071	-0.931723	1.917318	
H	3.493460	0.057258	1.882611	
H	4.654431	1.645799	-0.697304	

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28		
Dimer 125 of the n...z	type	
C	2.046038 0.520998 -0.553058	
C	3.355937 -0.208791 -0.914327	
N	2.270985 1.648535 0.330178	
H	2.571051 1.319853 1.243412	
H	1.385772 2.136462 0.445940	
H	1.621062 0.889305 -1.488969	
C	1.061567 -0.503325 -0.000500	
O	0.830898 -0.703584 1.165669	
O	0.482254 -1.238732 -0.994112	
H	0.059601 -2.022171 -0.604156	
H	3.161509 -1.008012 -1.629274	
H	4.030817 0.514172 -1.372908	
S	4.301068 -0.891960 0.516438	
H	3.410376 -1.841807 0.868025	
C	-1.466574 1.799424 0.164351	
C	-2.505030 0.718303 -0.268614	
O	-0.517023 1.985667 -0.635044	
O	-1.697346 2.338086 1.262211	
H	-3.481050 1.188233 -0.391696	
C	-2.586226 -0.401678 0.764443	
N	-2.116570 0.177682 -1.621676	
H	-2.100394 0.929704 -2.311581	
H	-2.895207 0.041635 1.708253	
H	-1.607833 -0.858216 0.921107	
S	-3.717898 -1.785335 0.313273	
H	-1.166118 -0.212342 -1.593836	
H	-2.764617 -0.554184 -1.928268	
H	-4.861131 -1.070530 0.355504	
28		
Dimer 126 of the n...z	type	
C	-3.230396 0.689880 -0.224950	
C	-1.748589 0.468799 -0.560591	
N	-3.390250 1.538957 0.943744	
H	-3.019900 1.067501 1.765046	
H	-4.376356 1.694864 1.127774	
H	-3.665915 1.202194 -1.091130	
C	-3.974890 -0.647727 -0.121395	
O	-4.677223 -0.975350 0.804649	
O	-3.754462 -1.423411 -1.200463	
H	-4.250210 -2.252223 -1.103224	
H	-1.638005 -0.038318 -1.516557	
H	-1.246190 1.433227 -0.611023	
S	-0.824174 -0.490715 0.722518	
H	-1.326217 -1.703880 0.412569	
C	3.848651 -1.128298 0.302883	
C	3.049246 -0.018308 -0.464193	
O	3.566535 -2.309447 -0.021109	
O	4.690546 -0.711154 1.119380	
H	3.712938 0.384613 -1.230792	
C	2.562614 1.098530 0.448289	
N	1.910594 -0.688425 -1.183755	
H	1.666119 -0.231355 -2.061167	
H	3.428724 1.551958 0.923364	
H	1.916405 0.703617 1.233537	
S	1.556579 2.389474 -0.403410	
H	2.214138 -1.663282 -1.334312	
H	1.059200 -0.716369 -0.593148	
H	2.521405 2.811233 -1.246508	
28		
Dimer 127 of the n...z	type	
C	-2.765321 0.010812 -0.886149	
C	-1.302903 0.422684 -0.663010	
N	-3.595496 1.155567 -1.228999	
H	-3.607837 1.809948 -0.450273	
H	-4.557523 0.859830 -1.363133	
H	-2.764055 -0.685945 -1.733385	
C	-3.300874 -0.793447 0.304990	

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O	-4.348763 -0.576189 0.866083	
O	-2.464223 -1.788629 0.655994	
H	-2.849756 -2.277386 1.400663	
H	-0.652382 -0.449034 -0.606465	
H	-0.990223 1.045606 -1.501373	
S	-1.042009 1.465975 0.840626	
H	-1.136520 0.466649 1.741633	
C	2.048491 -1.838727 -0.387588	
C	2.210595 -0.440244 0.292709	
O	3.072287 -2.565543 -0.370675	
O	0.934698 -2.043909 -0.905235	
H	1.359971 -0.221066 0.933713	
C	2.352370 0.630787 -0.788183	
N	3.444230 -0.486538 1.153678	
H	3.237924 -0.847796 2.085103	
H	1.449583 0.622613 -1.394077	
H	3.199478 0.405948 -1.439246	
S	2.661570 2.329218 -0.142696	
H	4.083278 -1.159631 0.700887	
H	3.876580 0.437546 1.256123	
H	1.491233 2.429403 0.524249	
28		
Dimer 128 of the n...z	type	
C	-2.847069 -0.771612 0.707186	
C	-3.709436 0.493194 0.636022	
N	-1.723296 -0.768316 1.646540	
H	-1.232780 0.122703 1.610472	
H	-2.035955 -0.918611 2.598552	
H	-3.513029 -1.593449 0.998162	
C	-2.323305 -1.196234 -0.675053	
O	-2.864143 -0.928711 -1.721949	
O	-1.215041 -1.944018 -0.611782	
H	-0.966369 -1.936625 0.344471	
H	-4.517561 0.348259 -0.079958	
H	-4.143310 0.684241 1.617937	
S	-2.789691 2.029993 0.205299	
H	-2.420821 1.640609 -1.031669	
C	3.878671 0.433786 0.076781	
C	2.925770 -0.801153 -0.082741	
O	4.276178 0.644642 1.250096	
O	4.148143 1.043756 -0.973860	
H	3.546330 -1.652967 -0.369496	
C	1.820228 -0.617118 -1.113025	
N	2.372529 -1.110708 1.283155	
H	2.122398 -2.090567 1.415463	
H	1.202810 -1.511263 -1.202433	
H	2.286044 -0.408789 -2.073159	
S	0.645556 0.739354 -0.694913	
H	3.101201 -0.813390 1.951998	
H	1.545617 -0.530104 1.462704	
H	1.556706 1.733032 -0.752165	
28		
Dimer 129 of the n...z	type	
C	-3.259467 -0.862482 0.575386	
C	-2.201025 -0.010979 1.287139	
N	-2.779917 -1.797630 -0.443121	
H	-2.021187 -1.388320 -0.982147	
H	-2.447131 -2.661644 -0.032462	
H	-3.776281 -1.445585 1.346140	
C	-4.362911 0.017755 -0.039784	
O	-4.745568 1.055449 0.451092	
O	-4.888206 -0.482097 -1.159235	
H	-4.353721 -1.293680 -1.347621	
H	-2.671493 0.615543 2.043230	
H	-1.478408 -0.667343 1.773050	
S	-1.205136 1.052863 0.158425	
H	-2.213248 1.855463 -0.238292	
C	2.535095 1.307606 -0.348576	
C	2.171772 -0.022916 0.393881	

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O	1.969411	1.475112	-1.455474	
O	3.331738	2.048845	0.258159	
H	1.420354	0.219992	1.146858	
C	3.353973	-0.701969	1.072094	
N	1.511472	-0.936046	-0.603633	
H	0.893162	-1.626173	-0.177645	
H	3.047269	-1.618705	1.578344	
H	3.760731	-0.013197	1.808534	
S	4.688626	-1.195507	-0.102524	
H	0.995293	-0.331430	-1.259367	
H	2.229948	-1.428607	-1.146205	
H	5.001520	0.062161	-0.478022	
28				
Dimer 130 of the n...z type				
C	3.162303	0.540228	-0.163538	
C	2.717331	0.563753	1.308071	
N	2.383252	1.452309	-0.978858	
H	1.413415	1.146119	-1.056975	
H	2.747554	1.463732	-1.926261	
H	4.207766	0.873951	-0.165993	
C	3.197781	-0.896957	-0.698123	
O	2.684426	-1.267395	-1.726348	
O	3.888141	-1.715698	0.122803	
H	3.898208	-2.608895	-0.256729	
H	3.455154	0.076666	1.942028	
H	2.608017	1.601246	1.622158	
S	1.080189	-0.225333	1.634749	
H	1.476961	-1.504318	1.483073	
C	-1.191793	1.282732	-0.572666	
C	-2.035933	0.112659	0.019357	
O	-1.241217	2.363030	0.060370	
O	-0.591331	1.007085	-1.631261	
H	-1.445835	-0.800837	0.019612	
C	-3.314822	-0.062634	-0.794753	
N	-2.364215	0.447152	1.448394	
H	-1.571693	0.244505	2.060297	
H	-3.033960	-0.274164	-1.824536	
H	-3.907880	0.854356	-0.782877	
S	-4.443483	-1.379931	-0.166961	
H	-2.520372	1.463378	1.493851	
H	-3.181732	-0.071531	1.785347	
H	-3.595502	-2.411058	-0.358967	
28				
Dimer 131 of the n...z type				
C	2.068600	-0.602345	-0.346196	
C	1.764013	-0.304469	1.126264	
N	3.369576	-1.238416	-0.505455	
H	4.101499	-0.597565	-0.208224	
H	3.541844	-1.428941	-1.487688	
H	1.293822	-1.301386	-0.680556	
C	1.887013	0.634166	-1.229685	
O	2.618205	0.943863	-2.141634	
O	0.787842	1.340389	-0.895814	
H	0.691913	2.087711	-1.507369	
H	0.730233	0.002283	1.251574	
H	1.915830	-1.215694	1.702225	
S	2.871005	0.964084	1.890487	
H	2.345501	2.027564	1.248592	
C	-1.240728	-1.702123	-0.351816	
C	-2.514114	-0.833540	-0.090844	
O	-0.661610	-2.128388	0.677708	
O	-0.917924	-1.820944	-1.548108	
H	-3.330791	-1.155432	-0.733294	
C	-2.178699	0.634722	-0.335407	
N	-2.928208	-1.048025	1.341307	
H	-3.558932	-1.844087	1.437806	
H	-1.832040	0.736365	-1.360755	
H	-1.366571	0.957911	0.315959	
S	-3.564057	1.804761	-0.006659	

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H	-2.059235	-1.284502	1.849239	
H	-3.390610	-0.224828	1.739411	
H	-4.411817	1.306335	-0.930242	
28				
Dimer 132 of the n...z type				
C	-1.698019	-0.521151	-0.424714	
C	-3.093345	-0.535509	-1.082341	
N	-1.557136	-1.559973	0.576217	
H	-2.087071	-1.315185	1.407182	
H	-0.580871	-1.673580	0.846518	
H	-0.982036	-0.709899	-1.230635	
C	-1.413866	0.889473	0.097265	
O	-1.430274	1.212865	1.262284	
O	-1.142246	1.745104	-0.905588	
H	-0.938633	2.618442	-0.531819	
H	-3.147896	0.203814	-1.881100	
H	-3.259868	-1.525349	-1.507071	
S	-4.503208	-0.275137	0.079679	
H	-4.276392	1.030815	0.329715	
C	2.245778	-1.807086	0.195095	
C	2.829298	-0.363476	0.345741	
O	2.614331	-2.438231	-0.821936	
O	1.435855	-2.132259	1.087330	
H	3.251525	-0.225200	1.338756	
C	1.701123	0.632150	0.097421	
N	3.934988	-0.191660	-0.660917	
H	4.836961	-0.480744	-0.281608	
H	0.950404	0.458597	0.863210	
H	1.248060	0.463006	-0.880964	
S	2.177565	2.408501	0.095919	
H	3.717656	-0.829790	-1.442605	
H	4.019903	0.778762	-0.979801	
H	2.566451	2.467673	1.386019	
28				
Dimer 133 of the n...z type				
C	-3.336738	0.348169	0.661519	
C	-1.828078	0.534541	0.440753	
N	-3.604006	-0.510855	1.803262	
H	-3.272977	-1.452230	1.606952	
H	-4.605038	-0.588406	1.953240	
H	-3.743245	1.344708	0.871823	
C	-4.022744	-0.114739	-0.629891	
O	-4.761778	-1.066108	-0.715409	
O	-3.706168	0.678056	-1.672206	
H	-4.166549	0.359364	-2.465064	
H	-1.645140	1.293129	-0.316406	
H	-1.367616	0.853726	1.374674	
S	-0.946119	-1.013858	-0.047089	
H	-1.240976	-0.969018	-1.361235	
C	4.066514	-0.874352	-0.455162	
C	2.693552	-0.191946	-0.147193	
O	4.631198	-1.412832	0.529659	
O	4.452861	-0.765208	-1.633439	
H	1.952946	-0.467974	-0.894506	
C	2.877237	1.323386	-0.106767	
N	2.211027	-0.699579	1.183670	
H	1.652699	-1.546470	1.075025	
H	3.254076	1.644790	-1.075534	
H	3.607199	1.601983	0.656201	
S	1.345620	2.258672	0.318746	
H	3.058472	-0.944519	1.720358	
H	1.634026	-0.007935	1.672148	
H	0.613608	1.813261	-0.721111	
28				
Dimer 134 of the n...z type				
C	-2.142654	0.622548	0.080002	
C	-3.417016	0.619132	0.944296	
N	-2.360837	1.233563	-1.218384	
H	-2.970867	0.644057	-1.777926	

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H	-1.460530	1.279732	-1.689773	
H	-1.397824	1.213348	0.619897	
C	-1.591991	-0.800658	0.002426	
O	-1.696114	-1.542144	-0.946887	
O	-1.001159	-1.164563	1.160747	
H	-0.723278	-2.091933	1.093442	
H	-3.202388	0.223441	1.936623	
H	-3.767620	1.646603	1.044586	
S	-4.852107	-0.297906	0.228664	
H	-4.319728	-1.534327	0.313053	
C	1.193399	0.953943	-0.120438	
C	2.354913	-0.061023	0.136614	
O	0.646739	0.863537	-1.251016	
O	0.960559	1.745181	0.807833	
H	2.193506	-0.576299	1.080931	
C	3.686879	0.684799	0.146021	
N	2.315775	-1.079846	-0.973888	
H	1.827303	-1.931945	-0.699445	
H	3.648352	1.431979	0.935809	
H	3.842530	1.199333	-0.804795	
S	5.166791	-0.392560	0.361819	
H	1.761379	-0.622812	-1.723831	
H	3.249215	-1.349155	-1.296159	
H	4.819065	-0.889107	1.566819	
28				
Dimer 135 of the n...z type				
C	1.959249	0.605212	-0.058433	
C	2.686015	-0.189499	-1.159045	
N	2.731660	1.755998	0.370062	
H	3.582921	1.447794	0.832417	
H	2.208608	2.296726	1.051672	
H	1.024878	0.966594	-0.501723	
C	1.563049	-0.327626	1.088029	
O	1.943560	-0.244772	2.226172	
O	0.715866	-1.304373	0.663502	
H	0.507122	-1.899558	1.402359	
H	2.045590	-0.975502	-1.555411	
H	2.937194	0.497537	-1.966620	
S	4.291646	-0.934549	-0.636490	
H	3.772207	-1.910066	0.136900	
C	-3.579615	-1.123216	0.127315	
C	-2.339704	-0.169435	0.019505	
O	-3.665106	-1.994068	-0.777073	
O	-4.337769	-0.896129	1.085696	
H	-1.760702	-0.235734	0.939028	
C	-2.785220	1.267386	-0.224417	
N	-1.476757	-0.686844	-1.101307	
H	-0.616133	-1.104147	-0.732008	
H	-3.457815	1.555497	0.580369	
H	-3.329648	1.346636	-1.168083	
S	-1.400609	2.480733	-0.352658	
H	-2.064334	-1.424822	-1.542647	
H	-1.219350	0.028403	-1.783029	
H	-0.946493	2.325419	0.907757	
28				
Dimer 136 of the n...z type				
C	-2.761527	-0.937487	0.081505	
C	-1.340963	-0.396244	0.302920	
N	-2.935183	-1.431281	-1.275055	
H	-2.810665	-0.665711	-1.932963	
H	-3.885313	-1.764773	-1.404974	
H	-2.882517	-1.776089	0.777915	
C	-3.813886	0.096832	0.496889	
O	-4.729495	0.469461	-0.197788	
O	-3.601414	0.547552	1.749129	
H	-4.293351	1.189176	1.976141	
H	-1.177310	-0.170789	1.355159	
H	-0.617228	-1.143502	-0.024178	
S	-0.941024	1.108373	-0.691476	

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H	-1.674677	1.983020	0.027078	
C	2.293164	-1.796772	-0.079264	
C	2.314780	-0.312282	0.408217	
O	3.296969	-2.481348	0.234821	
O	1.297984	-2.107478	-0.761648	
H	1.359222	-0.036896	0.846089	
C	2.641334	0.602312	-0.770147	
N	3.364032	-0.183416	1.480316	
H	2.997909	-0.447427	2.395283	
H	1.873249	0.460297	-1.527241	
H	3.608159	0.339072	-1.204002	
S	2.759317	2.387654	-0.331379	
H	4.108734	-0.857336	1.247946	
H	3.728349	0.772938	1.544605	
H	1.461047	2.520834	0.015166	
28				
Dimer 137 of the n...z type				
C	-3.168408	0.584256	0.029000	
C	-2.680300	0.343600	-1.408854	
N	-2.373925	1.591427	0.706059	
H	-1.418764	1.267354	0.857369	
H	-2.756835	1.768532	1.629393	
H	-4.198806	0.951117	-0.060403	
C	-3.277781	-0.739148	0.797225	
O	-2.812132	-0.944839	1.892299	
O	-3.973871	-1.662429	0.101900	
H	-4.032352	-2.476464	0.627264	
H	-3.412390	-0.228159	-1.975138	
H	-2.532377	1.308822	-1.891938	
S	-1.056270	-0.524532	-1.535938	
H	-1.495585	-1.756581	-1.2111740	
C	1.186603	1.302534	0.421058	
C	2.066782	0.093962	-0.025888	
O	1.206047	2.297187	-0.341532	
O	0.591133	1.143620	1.505537	
H	1.506379	-0.830627	0.090020	
C	3.352282	0.059167	0.796601	
N	2.379474	0.264034	-1.487729	
H	1.604728	-0.062858	-2.067720	
H	3.079359	-0.025277	1.846583	
H	3.919421	0.982609	0.662688	
S	4.515463	-1.296866	0.337132	
H	2.469207	1.276607	-1.656705	
H	3.228795	-0.238673	-1.763344	
H	3.688797	-2.316810	0.645764	
28				
Dimer 138 of the n...z type				
C	2.392833	1.033060	-0.806549	
C	2.213908	1.706301	0.569463	
N	1.136441	0.943029	-1.532328	
H	0.576372	0.187087	-1.154359	
H	1.308846	0.706462	-2.504334	
H	3.080292	1.670297	-1.369781	
C	3.085373	-0.315607	-0.606766	
O	2.524925	-1.387770	-0.664605	
O	4.383538	-0.171048	-0.303374	
H	4.772644	-1.043838	-0.129867	
H	3.179898	1.833649	1.056734	
H	1.763072	2.686538	0.415997	
S	1.066930	0.842515	1.727823	
H	1.767075	-0.300906	1.867241	
C	-3.290644	0.819054	-0.616743	
C	-2.063294	0.102278	0.031951	
O	-4.313187	0.898699	0.108582	
O	-3.116967	1.187264	-1.793503	
H	-1.160429	0.679814	-0.138950	
C	-1.942122	-1.306438	-0.553998	
N	-2.283470	0.040061	1.518033	
H	-1.927090	0.875924	1.981842	

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H	-1.722630	-1.213718	-1.616059	
H	-2.890452	-1.837761	-0.452023	
S	-0.705240	-2.408220	0.259143	
H	-3.305252	0.013702	1.660604	
H	-1.819603	-0.774578	1.935108	
H	0.416614	-1.762076	-0.124486	
28				
Dimer 139 of the n...z type				
C	-3.033125	-0.169469	0.566020	
C	-1.848656	-1.060959	0.173592	
N	-4.268366	-0.622317	-0.053256	
H	-4.181813	-0.572658	-1.065425	
H	-5.034625	-0.006897	0.201071	
H	-3.138086	-0.256355	1.655287	
C	-2.750578	1.317986	0.322902	
O	-3.549746	2.110025	-0.104088	
O	-1.485564	1.679420	0.673342	
H	-1.390920	2.638982	0.549255	
H	-0.991149	-0.888155	0.818084	
H	-2.144152	-2.101697	0.304376	
S	-1.344852	-0.934325	-1.597174	
H	-0.960632	0.357813	-1.567481	
C	1.616282	-1.674075	0.531054	
C	1.935737	-0.228966	0.024969	
O	1.096931	-1.741796	1.673155	
O	1.948978	-2.585370	-0.247364	
H	1.502026	-0.081326	-0.961699	
C	3.449169	-0.026553	-0.018393	
N	1.299842	0.759637	0.963544	
H	0.313732	0.941333	0.742631	
H	3.868904	-0.768819	-0.693516	
H	3.885806	-0.178601	0.971188	
S	3.982200	1.664661	-0.526446	
H	1.314397	0.336525	1.901260	
H	1.793383	1.658025	0.954066	
H	3.447453	1.629198	-1.764422	
28				
Dimer 140 of the n...z type				
C	2.542424	-0.838973	-0.856031	
C	1.298508	-1.103985	0.006434	
N	3.632752	-1.730559	-0.500645	
H	3.932442	-1.541248	0.452429	
H	4.436858	-1.553401	-1.094273	
H	2.246994	-1.041323	-1.892511	
C	2.926945	0.644303	-0.821304	
O	4.019657	1.070491	-0.539543	
O	1.887081	1.439239	-1.160875	
H	2.182375	2.364387	-1.153948	
H	0.451413	-0.534835	-0.366146	
H	1.048706	-2.162245	-0.054296	
S	1.521097	-0.756377	1.804007	
H	1.470380	0.589269	1.716080	
C	-3.091952	-1.299695	-0.346521	
C	-2.377410	0.084282	-0.491676	
O	-4.346767	-1.258449	-0.365424	
O	-2.323526	-2.265065	-0.186567	
H	-1.560320	0.009476	-1.205804	
C	-1.874415	0.533937	0.876793	
N	-3.373602	1.074108	-1.034692	
H	-3.416626	1.044010	-2.053573	
H	-1.221697	-0.239562	1.277238	
H	-2.711000	0.657657	1.568133	
S	-0.997622	2.155183	0.871319	
H	-4.296303	0.773980	-0.682974	
H	-3.156983	2.035118	-0.752440	
H	-0.032044	1.804034	-0.002680	
28				
Dimer 141 of the n...z type				
C	1.723837	-0.175632	-0.506670	

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C	1.833416	0.708365	0.745464
N	0.899420	-1.345105	-0.252165
H	1.326431	-1.915473	0.473062
H	0.847001	-1.926410	-1.082781
H	1.236182	0.435727	-1.276153
C	3.108119	-0.508299	-1.072315
O	3.489299	-1.618885	-1.354612
O	3.858081	0.599536	-1.229337
H	4.718833	0.350479	-1.602465
H	2.293978	1.663397	0.503332
H	0.832431	0.890916	1.133501
S	2.753092	-0.067017	2.145903
H	3.982164	0.033154	1.598867
C	-3.558847	-1.127918	-0.093066
C	-3.096264	0.362141	0.020564
O	-3.276580	-1.852278	0.892812
O	-4.110260	-1.424167	-1.169484
H	-3.881417	1.034436	-0.319204
C	-1.819464	0.544356	-0.795941
N	-2.831131	0.660103	1.472861
H	-3.694957	0.865346	1.975686
H	-2.042720	0.303685	-1.833460
H	-1.042409	-0.141039	-0.444509
S	-1.074876	2.229259	-0.695137
H	-2.440350	-0.198622	1.886417
H	-2.194021	1.454603	1.591081
H	-2.099726	2.897217	-1.263754
28			
Dimer 142 of the n...z type			
C	2.202428	-0.833564	0.878269
C	1.526937	0.547199	0.817457
N	3.396922	-0.801776	1.701190
H	4.094629	-0.199903	1.271466
H	3.809194	-1.727333	1.761227
H	1.473710	-1.512172	1.336694
C	2.444576	-1.367411	-0.535696
O	3.517754	-1.643387	-1.005395
O	1.283982	-1.496507	-1.230754
H	1.478436	-1.830271	-2.122125
H	0.587130	0.492262	0.277946
H	1.323842	0.878288	1.835624
S	2.533943	1.885512	0.051778
H	2.381185	1.485970	-1.227583
C	-3.328824	-1.151479	0.523791
C	-2.154404	-0.183386	0.143931
O	-3.604482	-2.021533	-0.342202
O	-3.858981	-0.930536	1.625846
H	-1.408042	-0.212392	0.934844
C	-2.683090	1.236006	-0.044342
N	-1.535906	-0.714911	-1.122460
H	-0.615971	-1.146664	-0.978890
H	-3.170578	1.542844	0.878324
H	-3.425416	1.261166	-0.845244
S	-1.406409	2.478316	-0.527445
H	-2.212806	-1.445755	-1.429176
H	-1.419663	-0.000300	-1.843020
H	-0.715233	2.461325	0.629059
28			
Dimer 143 of the n...z type			
C	-2.416588	0.790390	0.112898
C	-3.806726	0.401879	0.652584
N	-2.475973	1.236175	-1.267179
H	-2.739452	0.460210	-1.868272
H	-1.553174	1.541577	-1.563420
H	-2.069379	1.618997	0.736037
C	-1.451736	-0.373896	0.341500
O	-1.091634	-1.151179	-0.511354
O	-1.059564	-0.451849	1.628859
H	-0.488866	-1.229504	1.741524

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H	-3.742068	0.140533	1.708406
H	-4.468605	1.261155	0.543918
S	-4.652114	-0.962363	-0.259188
H	-3.815282	-1.954619	0.107346
C	3.625943	-1.272653	-0.159743
C	2.904061	0.000535	0.395747
O	4.770042	-1.069630	-0.637371
O	2.959891	-2.321453	-0.099218
H	2.450730	-0.212026	1.361644
C	1.848104	0.453166	-0.607744
N	3.945068	1.071342	0.590588
H	4.381316	1.009521	1.510729
H	1.140800	-0.361161	-0.747789
H	2.305482	0.682235	-1.572650
S	0.947692	1.989045	-0.123036
H	4.680237	0.875749	-0.109311
H	3.559707	2.014585	0.482387
H	0.497421	1.529566	1.062411
28			
Dimer 144 of the n...z type			
C	-3.018788	-0.890141	0.721862
C	-1.538803	-0.847324	0.308985
N	-3.690467	-2.057089	0.174765
H	-3.705365	-1.995784	-0.840271
H	-4.660794	-2.072257	0.472796
H	-3.032239	-0.957903	1.816009
C	-3.710282	0.434793	0.377238
O	-4.711064	0.537988	-0.291446
O	-3.062073	1.486143	0.914133
H	-3.527441	2.303227	0.673784
H	-1.022199	-0.046407	0.833479
H	-1.073874	-1.798679	0.565960
S	-1.263165	-0.635997	-1.505226
H	-1.545739	0.682143	-1.548615
C	3.838782	-0.990973	0.483975
C	3.270242	0.446961	0.240963
O	4.141423	-1.627287	-0.556375
O	3.878572	-1.345297	1.675958
H	3.732190	1.160045	0.920289
C	1.755549	0.419311	0.428564
N	3.618849	0.846048	-1.168766
H	4.533321	1.295414	-1.217415
H	1.545189	0.106703	1.449325
H	1.298954	-0.299910	-0.253704
S	0.906196	2.015597	0.068404
H	3.682510	-0.037744	-1.701133
H	2.927782	1.485766	-1.573378
H	1.505454	2.730934	1.042353
28			
Dimer 145 of the n...z type			
C	2.739778	-0.858226	-0.451703
C	1.604733	-1.222356	0.519615
N	4.044869	-1.080738	0.149266
H	4.155743	-0.470453	0.955203
H	4.778338	-0.824810	-0.504304
H	2.632053	-1.524677	-1.315781
C	2.555872	0.561917	-0.999938
O	3.390958	1.432878	-0.959813
O	1.333356	0.732407	-1.544364
H	1.257051	1.640653	-1.878641
H	0.645069	-1.248297	0.006096
H	1.803128	-2.216088	0.921393
S	1.494574	-0.127563	2.003279
H	1.073190	0.984899	1.366564
C	-2.332211	-1.602455	-0.513168
C	-2.624534	-0.063993	-0.545858
O	-3.076992	-2.274601	0.241836
O	-1.358929	-1.962673	-1.201007
H	-2.693210	0.289452	-1.572529

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C	-1.501288	0.647303	0.198382
N	-3.952773	0.170700	0.123172
H	-4.721430	0.144352	-0.546847
H	-0.578445	0.426472	-0.326313
H	-1.419312	0.271952	1.219706
S	-1.673627	2.471953	0.359581
H	-4.082002	-0.627092	0.768733
H	-3.991870	1.068022	0.615521
H	-1.599353	2.748409	-0.958836
28			
Dimer 146 of the n...z type			
C	-1.562686	0.461647	0.091160
C	-1.300648	-0.930087	-0.508484
N	-1.126103	0.530238	1.474881
H	-1.656970	-0.130151	2.036375
H	-1.312161	1.451648	1.857845
H	-0.970746	1.174125	-0.496178
C	-3.021723	0.882037	-0.116035
O	-3.765385	1.250493	0.761357
O	-3.382015	0.795905	-1.411025
H	-4.306629	1.076468	-1.503085
H	-1.483359	-0.923720	-1.581292
H	-0.262657	-1.212289	-0.328284
S	-2.289975	-2.285764	0.259027
H	-3.478392	-1.942163	-0.279525
C	2.824730	-1.421863	0.139954
C	2.877503	0.067338	-0.335181
O	1.946338	-2.121468	-0.428858
O	3.607386	-1.719343	1.058467
H	3.902455	0.420736	-0.419105
C	2.088348	0.905031	0.676387
N	2.252110	0.127690	-1.702552
H	2.938966	-0.026873	-2.440449
H	2.664839	0.941313	1.598983
H	1.120070	0.454849	0.907169
S	1.663982	2.612734	0.135135
H	1.578741	-0.656102	-1.735009
H	1.790494	1.028823	-1.872421
H	2.925458	3.077005	0.015750
28			
Dimer 147 of the n...z type			
C	1.760781	-0.229865	0.122490
C	2.663087	-1.302500	0.756300
N	1.329099	-0.611189	-1.210645
H	2.144029	-0.797639	-1.789650
H	0.847990	0.168210	-1.648942
H	0.886274	-0.153080	0.775598
C	2.440546	1.140036	0.178386
O	2.762898	1.795233	-0.783792
O	2.651312	1.530476	1.450408
H	3.091613	2.395307	1.447823
H	2.875220	-1.051075	1.793742
H	2.139702	-2.258256	0.725720
S	4.256225	-1.599983	-0.128605
H	4.840434	-0.426375	0.189153
C	-3.676309	-1.368854	0.061418
C	-3.191091	0.046434	-0.400403
O	-4.447718	-1.371076	1.052591
O	-3.201676	-2.320627	-0.584082
H	-3.263376	0.138631	-1.482054
C	-1.751377	0.252786	0.061063
N	-4.103467	1.072584	0.218021
H	-4.929406	1.234706	-0.358785
H	-1.139441	-0.520717	-0.400460
H	-1.677659	0.150623	1.146058
S	-1.050879	1.918564	-0.310803
H	-4.430018	0.661631	1.107688
H	-3.633724	1.971475	0.365755
H	-1.208957	1.859210	-1.649283

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28		
Dimer 148 of the n...z	type	
C	-2.124499	0.128423
C	-1.580485	-1.204413
N	-3.013517	-0.075955
H	-3.833825	-0.596448
H	-3.352087	0.817564
H	-1.254598	0.703411
C	-2.746762	0.959157
O	-3.838214	1.471884
O	-1.913035	1.062643
H	-2.327803	1.612952
H	-0.802375	-1.031313
H	-1.158651	-1.767598
S	-2.860533	-2.308807
H	-3.044349	-1.593449
C	3.802045	-0.900489
C	2.442228	-0.206468
O	4.560731	-1.100439
O	3.983448	-1.127629
H	1.624443	-0.693570
C	2.527039	1.272524
N	2.204436	-0.358002
H	1.775791	-1.257004
H	2.722549	1.342403
H	3.353852	1.749439
S	1.033756	2.264859
H	3.136380	-0.350756
H	1.604321	0.384760
H	0.187507	1.676392
28		
Dimer 149 of the n...z	type	
C	-3.275450	0.909784
C	-4.030846	-0.428104
N	-3.789224	1.846044
H	-3.627356	1.479162
H	-3.281008	2.723151
H	-3.458566	1.324072
C	-1.760352	0.682860
O	-1.047465	1.259840
O	-1.320044	-0.176016
H	-0.319943	-0.323313
H	-3.734969	-1.071426
H	-5.099304	-0.227720
S	-3.826392	-1.360249
H	-2.570136	-1.795923
C	1.902700	-1.081249
C	2.242796	-0.116730
O	1.205507	-0.591000
O	2.361743	-2.225327
H	1.715664	-0.467770
C	3.739365	-0.069404
N	1.709226	1.254195
H	1.891078	1.904309
H	3.946971	0.590793
H	4.068658	-1.072690
S	4.769403	0.569938
H	0.677024	1.225784
H	2.156987	1.622079
H	4.599519	-0.490128
28		
Dimer 150 of the n...z	type	
C	-2.957711	0.171413
C	-3.840760	0.618590
N	-3.346417	-1.147424
H	-3.185135	-1.833507
H	-2.752054	-1.421810
H	-3.132464	0.895858
C	-1.467831	0.298439

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O	-0.684060	-0.630363
O	-1.149884	1.519971
H	-0.165488	1.593636
H	-3.634764	1.653841
H	-4.887335	0.529153
S	-3.679645	-0.419610
H	-2.456044	0.014305
C	2.168283	1.270557
C	3.403053	0.561358
O	1.309358	1.691232
O	2.144303	1.352239
H	4.272162	1.202810
C	3.667023	-0.809471
N	3.176553	0.455477
H	4.018492	0.603777
H	4.612700	-1.223742
H	3.718223	-0.683382
S	2.394497	-2.073166
H	2.450993	1.153117
H	2.785435	-0.471013
H	1.316603	-1.414939
28		
Dimer 151 of the n...z	type	
C	2.494109	0.979204
C	3.599493	-0.024966
N	2.975701	1.981906
H	3.236227	1.533242
H	2.229949	2.632749
H	2.222456	1.483625
C	1.217311	0.258159
O	0.640692	0.531045
O	0.811814	-0.656009
H	-0.042337	-1.106922
H	3.273347	-0.686642
H	4.476456	0.527556
S	4.193968	-1.052175
H	3.121407	-1.866853
C	-2.548554	-1.416880
C	-2.988714	-0.507617
O	-1.360030	-1.858283
O	-3.406483	-1.621234
H	-3.784990	-1.023095
C	-3.525634	0.844502
N	-1.845536	-0.349482
H	-2.103393	0.220578
H	-3.803575	1.466927
H	-4.420215	0.662405
S	-2.344966	1.859351
H	-1.554788	-1.267899
H	-0.993950	0.062434
H	-2.327779	1.061535
28		
Dimer 152 of the n...z	type	
C	-3.068110	0.761384
C	-3.376148	-0.739667
N	-3.489020	1.506883
H	-2.939659	1.205945
H	-3.285707	2.493891
H	-3.650223	1.109936
C	-1.588181	0.938295
O	-0.796621	1.541682
O	-1.275793	0.332743
H	-0.263998	0.222217
H	-3.212853	-1.258058
H	-4.419643	-0.856696
S	-2.401486	-1.594808
H	-1.210172	-1.601861
C	1.534074	-0.851609
C	2.984296	-0.721740

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O	0.801727	-1.696571	0.377275
O	1.256113	-0.079581	1.885360
H	3.655065	-1.203342	1.100675
C	3.424112	0.724591	0.169856
N	3.045098	-1.513209	-0.890738
H	3.937709	-1.982210	-1.042476
H	4.465937	0.769609	-0.149352
H	3.323614	1.254803	1.113711
S	2.463119	1.593488	-1.141443
H	2.271121	-2.196131	-0.840003
H	2.849524	-0.893718	-1.687949
H	1.256964	1.547314	-0.524303
28			
Dimer 153 of the n...z type			
C	3.266993	-0.834637	0.709391
C	4.164679	0.402978	0.563150
N	3.816057	-1.970911	-0.017970
H	3.838183	-1.754483	-1.011679
H	3.198879	-2.771299	0.079587
H	3.261702	-1.081011	1.778537
C	1.805404	-0.506990	0.355606
O	1.149168	-1.160585	-0.433829
O	1.353645	0.549034	1.015591
H	0.378827	0.753395	0.790364
H	3.826977	1.201978	1.218927
H	5.185917	0.132974	0.831951
S	4.284685	1.064599	-1.157998
H	3.045781	1.594989	-1.214113
C	-2.032021	0.547364	0.945407
C	-3.433525	0.956291	0.400998
O	-1.068919	1.218864	0.459023
O	-1.996242	-0.350238	1.792188
H	-3.868217	1.652537	1.121703
C	-4.387975	-0.214795	0.197811
N	-3.221062	1.726098	-0.875096
H	-3.944984	2.420944	-1.060355
H	-5.370182	0.133563	-0.123503
H	-4.496172	-0.735714	1.145927
S	-3.835434	-1.402347	-1.098227
H	-2.295022	2.172787	-0.794238
H	-3.178283	1.073961	-1.667919
H	-2.738953	-1.834836	-0.442079
28			
Dimer 154 of the n...z type			
C	3.064785	-0.768919	0.340320
C	3.382722	0.730463	0.191615
N	3.483292	-1.513629	-0.838624
H	2.934607	-1.209771	-1.639337
H	3.276972	-2.500220	-0.715394
H	3.643437	-1.123534	1.200887
C	1.583439	-0.938337	0.704175
O	0.789598	-1.535340	-0.002748
O	1.273135	-0.335092	1.839948
H	0.261502	-0.220991	1.926871
H	3.219656	1.248063	1.134457
H	4.427974	0.841182	-0.096643
S	2.418538	1.595192	-1.127510
H	1.229089	1.627133	-0.479414
C	-1.532842	0.852112	0.928996
C	-2.984468	0.726494	0.386905
O	-0.796900	1.689973	0.368906
O	-1.257292	0.083280	1.886064
H	-3.652624	1.210441	1.101821
C	-3.428585	-0.718926	0.172208
N	-3.045497	1.516938	-0.891094
H	-3.936355	1.990007	-1.040467
H	-4.471134	-0.761398	-0.145020
H	-3.327848	-1.248482	1.116423
S	-2.472330	-1.591544	-1.140038

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H	-2.268140	2.196231	-0.843515
H	-2.855225	0.895871	-1.688362
H	-1.264440	-1.545945	-0.526177
28			
Dimer 155 of the n...z type			
C	2.932645	-0.492350	1.047695
C	3.889395	0.650152	0.671679
N	3.542512	-1.791415	0.805515
H	3.717467	-1.903206	-0.190090
H	2.895334	-2.530274	1.062587
H	2.749403	-0.392348	2.124405
C	1.563527	-0.303418	0.375391
O	1.039189	-1.146022	-0.328701
O	1.021164	0.872441	0.662557
H	0.125870	1.002460	0.208756
H	3.478054	1.610329	0.974815
H	4.839179	0.496001	1.183496
S	4.324572	0.731587	-1.121632
H	3.137181	1.198975	-1.559081
C	-2.418104	1.421468	-0.099234
C	-2.768954	0.245655	0.864673
O	-3.351857	2.193970	-0.387782
O	-1.220391	1.479782	-0.477734
H	-2.337833	0.481202	1.839951
C	-2.257001	-1.118778	0.411880
N	-4.264810	0.243928	1.027200
H	-4.576648	-0.013372	1.963467
H	-2.488349	-1.881279	1.156832
H	-1.178311	-1.075537	0.284334
S	-3.019318	-1.719155	-1.154787
H	-4.575262	1.198190	0.777320
H	-4.687695	-0.397192	0.345088
H	-2.480265	-0.778197	-1.957404
28			
Dimer 156 of the n...z type			
C	3.094442	0.956039	-0.178858
C	3.498806	-0.395083	-0.788646
N	3.762921	1.180636	1.094446
H	3.459303	0.478376	1.764628
H	3.479708	2.076626	1.478850
H	3.435421	1.721639	-0.886566
C	1.565700	1.102772	-0.120918
O	0.957397	1.381288	0.896262
O	0.992467	0.898340	-1.299267
H	-0.015247	1.034726	-1.258543
H	3.093099	-0.501782	-1.792108
H	4.586271	-0.444722	-0.841485
S	3.004745	-1.870348	0.208231
H	1.695790	-1.858987	-0.112949
C	-2.431697	1.187829	-0.486866
C	-2.059991	0.331761	0.760808
O	-3.547929	1.739812	-0.465260
O	-1.554689	1.254846	-1.388221
H	-1.320736	0.898633	1.328787
C	-1.472866	-1.039687	0.438710
N	-3.302969	0.215618	1.598415
H	-3.124861	0.230620	2.602275
H	-1.169930	-1.553212	1.351955
H	-0.592461	-0.904178	-0.182314
S	-2.643252	-2.185495	-0.403644
H	-3.904855	1.007316	1.314209
H	-3.809399	-0.645957	1.361384
H	-2.759975	-1.475464	-1.545026
28			
Dimer 157 of the n...z type			
C	3.016249	1.046497	-0.220286
C	3.197279	-0.250374	-1.029592
N	3.957013	1.109158	0.887582
H	3.745387	0.371553	1.554604

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H	3.847667	1.985960	1.387530
H	3.239032	1.867266	-0.911340
C	1.547655	1.224756	0.188042
O	1.162782	1.242369	1.341424
O	0.748477	1.348884	-0.866857
H	-0.212536	1.475257	-0.601337
H	2.543537	-0.253904	-1.899721
H	4.231662	-0.305004	-1.368408
S	2.926220	-1.809138	-0.076396
H	1.574349	-1.784859	-0.079143
C	-2.859544	1.070742	-0.342577
C	-2.862355	0.029859	0.823131
O	-3.934801	1.184625	-0.962735
O	-1.796963	1.718965	-0.508497
H	-3.072436	0.586908	1.739398
C	-1.572134	-0.755543	1.011074
N	-4.038983	-0.877993	0.586428
H	-4.476571	-1.217319	1.443019
H	-1.656549	-1.437850	1.858121
H	-0.762042	-0.059797	1.218483
S	-1.132404	-1.826195	-0.423834
H	-4.706398	-0.322028	0.024655
H	-3.754049	-1.684128	0.018439
H	-0.907188	-0.829248	-1.304134
28			
Dimer 158 of the n...z type			
C	3.299084	-0.819986	0.709918
C	4.180183	0.429967	0.568217
N	3.874173	-1.952117	-0.003468
H	3.905383	-1.741635	-0.998181
H	3.268050	-2.761181	0.091770
C	3.283481	-1.060265	1.780346
C	1.837373	-0.516132	0.335886
O	1.201532	-1.181925	-0.460009
O	1.360585	0.534197	0.987176
H	0.382976	0.717168	0.756370
H	3.821104	1.228126	1.213588
H	5.201317	0.177231	0.853631
S	4.315409	1.082038	-1.155510
C	3.070139	1.594675	-1.232849
C	-2.022134	0.470395	0.934481
C	-3.444300	0.919357	0.484265
O	-1.076525	1.160928	0.439964
O	-1.955086	-0.472465	1.728377
H	-3.842733	1.559741	1.274295
C	-4.410991	-0.233679	0.239532
N	-3.286926	1.782254	-0.738852
H	-3.992761	2.514982	-0.814770
H	-5.406522	0.137379	-0.006451
H	-4.474198	-0.825417	1.149390
S	-3.924682	-1.317751	-1.169255
H	-2.339827	2.188861	-0.683299
H	-3.322739	1.198875	-1.584039
H	-2.795364	-1.793498	-0.605180
28			
Dimer 159 of the n...z type			
C	-3.580688	-0.354403	-0.578062
C	-3.232908	1.122189	-0.838796
N	-4.625884	-0.478207	0.428787
H	-4.281267	-0.114925	1.314238
H	-4.833240	-1.458972	0.591309
H	-3.961161	-0.754155	-1.525410
C	-2.296626	-1.133657	-0.256164
O	-2.121380	-1.733835	0.787301
O	-1.402884	-1.044863	-1.231973
H	-0.474061	-1.302244	-0.904271
H	-2.585095	1.209825	-1.708132
H	-4.153528	1.674747	-1.026006
S	-2.424998	1.983636	0.583392

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H	-1.220665	1.365818	0.496205
C	1.409158	-0.471963	0.277669
C	2.842461	-0.634811	0.861772
O	1.013477	-1.451441	-0.426297
O	0.800316	0.563152	0.574583
H	2.730883	-0.995649	1.886729
C	3.661740	0.650903	0.870254
N	3.532361	-1.726438	0.088546
H	4.212465	-2.249746	0.640700
H	4.630147	0.492259	1.346102
H	3.114302	1.401080	1.435491
S	4.036322	1.298258	-0.813666
H	2.789217	-2.349692	-0.262206
H	4.008426	-1.324995	-0.728749
H	2.762005	1.595213	-1.141891
28			
Dimer 160 of the n...z type			
C	3.584363	-0.354135	0.571331
C	3.240970	1.122398	0.837157
N	4.622531	-0.477718	-0.442951
H	4.273628	-0.108827	-1.324424
H	4.824066	-1.458665	-0.611621
H	3.970908	-0.756534	1.515170
C	2.297569	-1.132197	0.256739
O	2.119636	-1.739958	-0.781824
O	1.405303	-1.034581	1.233142
H	0.475760	-1.293753	0.908788
H	2.604074	1.210180	1.714479
H	4.164185	1.674305	1.013138
S	2.414947	1.984211	-0.574450
H	1.211974	1.365929	-0.471162
C	-1.408962	-0.475809	-0.279315
C	-2.844404	-0.643476	-0.856381
O	-1.012466	-1.446328	0.436511
O	-0.799352	0.553906	-0.592993
H	-2.736508	-1.013158	-1.878512
C	-3.663109	0.642582	-0.873540
N	-3.532224	-1.727991	-0.071268
H	-4.212052	-2.257962	-0.617458
H	-4.633550	0.479754	-1.343744
H	-3.117731	1.386958	-1.448347
S	-4.030571	1.306514	0.805373
H	-2.787725	-2.346456	0.285227
H	-4.007948	-1.319143	0.742485
H	-2.754765	1.605226	1.126117
28			
Dimer 161 of the n...z type			
C	-3.298366	0.967426	0.591869
C	-4.182729	-0.278387	0.739208
N	-3.938263	1.970339	-0.249209
H	-4.067366	1.590434	-1.184062
H	-3.322286	2.770479	-0.356156
H	-3.191410	1.384764	1.601331
C	-1.869778	0.598253	0.153273
O	-1.285534	1.166340	-0.750711
O	-1.355469	-0.381269	0.881577
H	-0.396994	-0.602180	0.607440
H	-3.769900	-0.958195	1.480607
H	-5.178267	0.029711	1.058667
S	-4.454720	-1.215079	-0.830569
H	-3.217875	-1.746290	-0.916571
C	2.024341	-0.578561	0.840519
C	3.411302	-1.062985	0.320107
O	1.034101	-1.085947	0.226828
O	2.021746	0.209430	1.790889
H	3.720504	-1.893465	0.958886
C	4.493530	0.009836	0.335315
N	3.208749	-1.628552	-1.059844
H	3.863996	-2.373959	-1.296686

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H	5.454582	-0.399981	0.022374
H	4.588992	0.384134	1.351584
S	4.156996	1.414908	-0.808661
H	2.236434	-1.971714	-1.091416
H	3.293685	-0.878519	-1.757004
H	3.067545	1.873099	-0.158355
28			
Dimer 162 of the n...z type			
C	3.577707	-0.885135	0.307846
C	3.833106	0.393228	1.119345
N	4.663888	-1.138335	-0.629443
H	4.710516	-0.376874	-1.302446
H	4.462045	-1.974523	-1.168998
H	3.553250	-1.706759	1.034710
C	2.180133	-0.867126	-0.337566
O	1.989699	-1.104888	-1.516089
O	1.227618	-0.581281	0.536156
H	0.295529	-0.575052	0.113250
H	3.099793	0.496355	1.915625
H	4.828352	0.339799	1.560562
S	3.837625	1.947281	0.119435
H	2.507187	2.003835	-0.095342
C	-2.097503	-0.924291	0.226461
C	-3.500449	-0.786436	-0.436323
O	-2.060145	-1.502652	1.328862
O	-1.146626	-0.451464	-0.448713
H	-3.594944	-1.597198	-1.162154
C	-3.744099	0.544150	-1.139583
N	-4.517022	-1.043047	0.641672
H	-5.366199	-1.496946	0.304746
H	-4.725225	0.558864	-1.615630
H	-2.983747	0.670815	-1.906115
S	-3.723037	1.995586	-0.005121
H	-4.039024	-1.630049	1.345416
H	-4.770503	-0.160020	1.101098
H	-2.416231	1.907489	0.317847
28			
Dimer 163 of the n...z type			
C	2.892366	1.064444	-0.430254
C	3.333144	-0.408539	-0.472981
N	3.199954	1.793126	0.803328
H	3.316989	1.154174	1.585957
H	4.036492	2.356782	0.715979
H	3.378863	1.569775	-1.271211
C	1.389057	1.205117	-0.711784
O	0.820359	0.629869	-1.623370
O	0.755082	2.021550	0.113385
H	1.472156	2.329830	0.738505
H	2.959402	-0.879996	-1.380511
H	4.422219	-0.450147	-0.484626
S	2.837353	-1.410511	0.992703
H	1.510536	-1.529031	0.731545
C	-1.153932	-1.711745	-0.170303
C	-1.798343	-0.294177	-0.054241
O	-1.375465	-2.315438	-1.245397
O	-0.510776	-2.090669	0.832626
H	-1.136499	0.373178	0.493979
C	-3.157215	-0.387884	0.635249
N	-1.934301	0.254681	-1.442594
H	-0.999802	0.584223	-1.749110
H	-3.016084	-0.802128	1.631839
H	-3.826565	-1.049200	0.081708
S	-4.057881	1.217363	0.755650
H	-2.210313	-0.523258	-2.054828
H	-2.612960	1.019605	-1.490326
H	-3.169623	1.836110	1.560248
28			
Dimer 164 of the n...z type			
C	2.697203	0.710480	-0.416193

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C	3.103932	-0.504421	-1.260170
N	3.746113	1.322587	0.401689
H	4.428096	0.628941	0.699131
H	4.233652	2.057683	-0.095999
H	2.313777	1.471003	-1.106498
C	1.503582	0.389121	0.494424
O	0.567598	-0.310012	0.145962
O	1.555873	0.960833	1.683647
H	2.435133	1.430297	1.689129
H	2.250215	-0.870090	-1.827979
H	3.885982	-0.208787	-1.959337
S	3.822328	-1.894282	-0.285326
H	2.673587	-2.285528	0.303206
C	-3.701166	-1.243643	-0.081992
C	-2.958412	0.084650	0.304248
O	-3.437109	-2.235526	0.645813
O	-4.484458	-1.161169	-1.045476
H	-3.698899	0.750824	0.748779
C	-2.300974	0.754646	-0.895357
N	-1.959529	-0.256388	1.377343
H	-1.968275	0.399698	2.155551
H	-3.055474	0.906585	-1.662718
H	-1.514551	0.120822	-1.307366
S	-1.469002	2.357343	-0.517200
H	-2.245142	-1.203443	1.690246
H	-0.988180	-0.309545	1.008018
H	-2.589449	3.061179	-0.256288
28			
Dimer 165 of the n...z type			
C	-3.178105	0.130183	0.743128
C	-2.462834	-1.228680	0.846523
N	-4.382110	0.034867	-0.069531
H	-4.126502	-0.219206	-1.020645
H	-4.829608	0.944238	-0.131557
H	-3.469150	0.401056	1.765175
C	-2.184068	1.205911	0.278994
O	-2.343920	1.891999	-0.710237
O	-1.126161	1.274049	1.081050
H	-0.345791	1.733593	0.639741
H	-1.657063	-1.175487	1.575117
H	-3.181128	-1.982930	1.167585
S	-1.777349	-1.866189	-0.747159
H	-0.810969	-0.930179	-0.916923
C	1.518618	1.008742	-0.653145
C	3.030370	0.646679	-0.575050
O	1.162449	1.977944	0.082618
O	0.824004	0.324541	-1.416621
H	3.533309	1.137565	-1.411001
C	3.302657	-0.852775	-0.631110
N	3.580197	1.261013	0.684456
H	4.569764	1.502176	0.623497
H	4.373474	-1.056375	-0.594473
H	2.907555	-1.238237	-1.567637
S	2.566456	-1.790540	0.775383
H	3.010408	2.099384	0.873631
H	3.444134	0.617926	1.473930
H	1.278445	-1.605655	0.416995
28			
Dimer 166 of the n...z type			
C	2.930773	-1.220587	-0.034033
C	3.453485	-0.082288	0.858719
N	3.219355	-1.098763	-1.465494
H	3.390419	-0.128691	-1.719804
H	4.019555	-1.653592	-1.743140
H	3.367675	-2.152353	0.340076
C	1.415373	-1.400370	0.138066
O	0.862142	-1.429133	1.224280
O	0.749911	-1.531724	-0.996048
H	1.459240	-1.459789	-1.697106

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H	3.096763	-0.221272	1.878022
H	4.543149	-0.109054	0.866043
S	3.020379	1.612019	0.276559
H	1.676523	1.568948	0.495865
C	-0.940449	1.324525	-0.350873
C	-1.945939	0.155065	-0.113200
O	-0.319449	1.725672	0.668241
O	-0.877645	1.737594	-1.522936
H	-1.725181	-0.644043	-0.819617
C	-3.384184	0.640894	-0.278992
N	-1.728579	-0.405756	1.261112
H	-0.823952	-0.920768	1.300026
H	-3.497072	1.050773	-1.280026
H	-3.610660	1.430619	0.440706
S	-4.666725	-0.652720	0.013206
H	-1.649286	0.367735	1.926963
H	-2.495331	-1.028257	1.532135
H	-4.339779	-1.440119	-1.032122
28			
Dimer 167 of the n...z type			
C	2.637144	1.092218	-0.683859
C	2.381448	-0.208574	-1.464368
N	3.863407	1.126723	0.118084
H	4.190555	0.185995	0.324455
H	4.607376	1.637597	-0.340810
H	2.662597	1.908459	-1.413084
C	1.450017	1.422596	0.233252
O	0.291092	1.404149	-0.146305
O	1.787760	1.747948	1.466761
H	2.785572	1.681943	1.462320
H	1.396500	-0.171921	-1.927688
H	3.130786	-0.304052	-2.250154
S	2.534449	-1.749119	-0.464042
H	1.413909	-1.602215	0.297536
C	-1.221531	-1.687954	0.650109
C	-2.304203	-0.562888	0.616597
O	-0.240964	-1.481081	1.411218
O	-1.454930	-2.670129	-0.078107
H	-3.207621	-0.945390	1.095203
C	-2.609337	-0.111707	-0.808683
N	-1.829375	0.599457	1.442654
H	-1.489413	0.260980	2.344079
H	-2.921748	-0.978590	-1.384676
H	-1.714846	0.306721	-1.272939
S	-3.886538	1.214737	-0.934642
H	-1.022174	1.056155	0.965993
H	-2.569758	1.289833	1.581573
H	-4.931413	0.472095	-0.514851
28			
Dimer 168 of the n...z type			
C	-3.155888	-0.759552	-0.566649
C	-3.649028	0.563819	-1.166931
N	-4.068778	-1.441954	0.352621
H	-4.651199	-0.773919	0.851865
H	-4.673347	-2.095821	-0.129674
H	-2.942725	-1.435612	-1.402743
C	-1.804722	-0.586292	0.142332
O	-0.912894	0.129652	-0.280483
O	-1.674021	-1.299739	1.246319
H	-2.560758	-1.741881	1.356535
H	-2.898767	0.974781	-1.840173
H	-4.561944	0.381258	-1.733655
S	-4.100300	1.839081	0.085478
H	-2.843371	2.115855	0.488713
C	2.648070	-1.712488	-0.322984
C	2.544113	-0.151693	-0.259697
O	2.284305	-2.316870	0.716443
O	3.113773	-2.170575	-1.384142
H	2.101023	0.227178	-1.179504

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C	3.935987	0.445155	-0.052153
N	1.628704	0.206430	0.871207
H	0.638700	0.208059	0.546955
H	4.565320	0.156789	-0.891266
H	4.388107	0.056954	0.863094
S	3.965780	2.278548	0.146653
H	1.727567	-0.543124	1.571190
H	1.850923	1.122745	1.269314
H	3.492808	2.579879	-1.080141
28			
Dimer 169 of the n...z type			
C	2.718210	-0.975525	0.439854
C	3.687896	0.083113	0.989983
N	3.367146	-1.824007	-0.547782
H	3.641006	-1.262115	-1.349992
H	2.708820	-2.513388	-0.897255
H	2.431042	-1.597999	1.295912
C	1.417468	-0.320800	-0.048603
O	0.985732	-0.445546	-1.179745
O	0.816785	0.377994	0.906450
H	-0.023488	0.826660	0.567793
H	3.229624	0.633370	1.808809
H	4.582836	-0.417703	1.358914
S	4.303617	1.289668	-0.265547
H	3.158787	1.990361	-0.399360
C	-2.489054	1.438664	-0.164913
C	-3.222755	0.393432	0.734905
O	-3.197791	2.007244	-1.018226
O	-1.276602	1.644133	0.090329
H	-3.465606	0.903415	1.669958
C	-2.445368	-0.879665	1.053227
N	-4.527739	0.083447	0.053484
H	-5.297519	-0.097645	0.697584
H	-3.017016	-1.512464	1.733544
H	-1.514270	-0.614919	1.548270
S	-2.093437	-1.933763	-0.416179
H	-4.724981	0.905603	-0.543817
H	-4.413502	-0.726956	-0.567114
H	-1.157834	-1.132685	-0.972740
28			
Dimer 170 of the n...z type			
C	-2.755807	0.211586	1.077952
C	-3.234301	-1.125098	0.494580
N	-3.879443	1.080365	1.399695
H	-4.393689	1.296004	0.548783
H	-3.537106	1.968248	1.753954
H	-2.233540	-0.033558	2.012027
C	-1.689728	0.872552	0.188389
O	-1.692689	2.051476	-0.101497
O	-0.754748	0.010040	-0.202817
H	-0.014525	0.461427	-0.716119
H	-2.406563	-1.824218	0.402664
H	-3.983090	-1.552006	1.161557
S	-4.074293	-0.986517	-1.144494
H	-2.963842	-0.744503	-1.870739
C	2.347924	1.105120	-0.614736
C	3.546558	0.107897	-0.625581
O	2.452956	2.088399	0.141830
O	1.403027	0.802723	-1.389491
H	4.135568	0.309143	-1.523020
C	3.132515	-1.361370	-0.616676
N	4.411148	0.446619	0.557788
H	5.406438	0.290328	0.399605
H	4.005762	-2.010910	-0.687611
H	2.493782	-1.541799	-1.477612
S	2.259521	-1.884756	0.921325
H	4.220109	1.439125	0.772258
H	4.112207	-0.101861	1.373672
H	1.121577	-1.189164	0.711136

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28		
Dimer 171 of the n...z	type	
C	3.183279 -0.902455 0.664912	
C	3.065155 0.535374 1.191012	
N	4.232848 -1.146541 -0.327214	
H	4.437054 -0.304990 -0.860413	
H	5.091253 -1.472899 0.099439	
H	3.362897 -1.552495 1.528367	
C	1.847243 -1.382979 0.079382	
O	0.769917 -1.150856 0.600367	
O	1.958965 -2.078835 -1.037598	
H	2.938547 -2.075018 -1.226906	
H	2.262238 0.602445 1.923025	
H	4.000727 0.818873 1.672846	
S	2.789091 1.798024 -0.124430	
H	1.504860 1.477018 -0.393233	
C	-3.827846 -0.894279 0.353815	
C	-2.494238 -0.082373 0.192654	
O	-3.905930 -1.941113 -0.340000	
O	-4.652833 -0.413248 1.151264	
H	-1.982969 -0.076723 1.155367	
C	-2.763921 1.346010 -0.265300	
N	-1.622218 -0.833689 -0.774135	
H	-0.728060 -1.125032 -0.333899	
H	-3.435665 1.815964 0.448875	
H	-3.250922 1.354131 -1.243043	
S	-1.253306 2.385729 -0.471261	
H	-2.197752 -1.658985 -1.035171	
H	-1.394988 -0.292476 -1.608586	
H	-0.873170 2.368382 0.822728	
28		
Dimer 172 of the n...z	type	
C	-3.013766 0.760874 0.656506	
C	-2.401902 -0.439733 1.392986	
N	-4.293485 0.530479 -0.016592	
H	-4.388625 -0.442535 -0.297234	
H	-5.081303 0.773125 0.571582	
H	-3.148058 1.558722 1.395161	
C	-2.023536 1.339528 -0.367813	
O	-0.833906 1.465457 -0.140629	
O	-2.574513 1.704453 -1.511464	
H	-3.534675 1.456659 -1.405923	
H	-1.447306 -0.160026 1.835318	
H	-3.075417 -0.756336 2.189202	
S	-2.168383 -1.936273 0.341397	
H	-1.198412 -1.434116 -0.449558	
C	3.106579 1.305460 0.627983	
C	2.131829 0.197259 0.104209	
O	3.451561 2.163000 -0.224248	
O	3.450056 1.191174 1.819373	
H	1.291886 0.094934 0.788747	
C	2.878732 -1.128282 -0.031524	
N	1.585475 0.659987 -1.215711	
H	0.672218 1.122925 -1.070240	
H	3.271895 -1.402991 0.944738	
H	3.719043 -1.029894 -0.722177	
S	1.866817 -2.514032 -0.706807	
H	2.264812 1.356697 -1.564927	
H	1.454208 -0.108047 -1.878247	
H	0.967667 -2.560801 0.297894	
28		
Dimer 173 of the n...z	type	
C	2.847322 -1.329995 -0.078543	
C	3.480349 -0.400633 0.966279	
N	3.325019 -1.186146 -1.455347	
H	3.642849 -0.236465 -1.633887	
H	4.084013 -1.823651 -1.662824	
H	3.033352 -2.359548 0.246891	
C	1.316744 -1.194770 -0.085285	

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O	0.652512 -1.076817 0.928602	
O	0.774383 -1.230577 -1.290328	
H	1.557962 -1.291686 -1.905729	
H	3.039949 -0.584269 1.944759	
H	4.550369 -0.599978 1.022882	
S	3.342577 1.393124 0.563495	
H	2.004909 1.495495 0.715865	
C	-3.883429 -0.542281 0.026861	
C	-2.743630 0.485294 0.364427	
O	-3.954475 -1.533391 0.799403	
O	-4.599460 -0.251087 -0.947655	
H	-3.225299 1.383392 0.752457	
C	-1.898168 0.827199 -0.854513	
N	-1.929167 -0.107040 1.482467	
H	-1.772954 0.542423 2.250995	
H	-2.559934 1.189340 -1.637229	
H	-1.375976 -0.054185 -1.229116	
S	-0.565500 2.066390 -0.550800	
H	-2.507780 -0.911227 1.797653	
H	-1.004924 -0.470339 1.176484	
H	-1.369543 3.086870 -0.187714	
28		
Dimer 174 of the n...z	type	
C	-2.971324 -0.930255 0.076873	
C	-3.207977 0.145527 -0.999389	
N	-3.638432 -0.585276 1.322454	
H	-3.214707 0.251841 1.714424	
H	-3.499225 -1.321889 2.007247	
H	-3.414129 -1.853576 -0.312626	
C	-1.466048 -1.193801 0.217244	
O	-0.833418 -0.950639 1.228279	
O	-0.939442 -1.685540 -0.896593	
H	0.063333 -1.747023 -0.838028	
H	-2.795335 -0.173801 -1.954254	
H	-4.281286 0.297701 -1.112312	
S	-2.536907 1.816818 -0.588630	
H	-1.227701 1.525013 -0.739105	
C	2.431387 -1.242280 -0.086591	
C	3.143957 0.114526 -0.377641	
O	1.661615 -1.649759 -1.012979	
O	2.698398 -1.779861 0.990919	
H	4.200463 -0.098319 -0.548576	
C	3.012556 1.117796 0.767364	
N	2.584077 0.668329 -1.660698	
H	3.278482 1.130579 -2.247151	
H	3.635161 1.995458 0.589731	
H	3.344603 0.632580 1.682177	
S	1.303086 1.773394 0.988242	
H	2.155435 -0.134550 -2.150337	
H	1.827621 1.331985 -1.447264	
H	0.696372 0.596551 1.265821	
28		
Dimer 175 of the n...z	type	
C	-2.957216 0.635609 0.711819	
C	-3.497242 -0.737808 1.131030	
N	-3.901713 1.538510 0.051515	
H	-4.588990 1.017059 -0.487416	
H	-4.393068 2.124186 0.715807	
H	-2.590725 1.129583 1.619196	
C	-1.713657 0.506904 -0.180535	
O	-0.853782 -0.340545 -0.011693	
O	-1.633886 1.414588 -1.136920	
H	-2.481448 1.931913 -1.053602	
H	-2.715052 -1.317178 1.618476	
H	-4.317124 -0.598882 1.835626	
S	-4.208105 -1.726188 -0.252989	
H	-3.038278 -2.011893 -0.860481	
C	2.486794 1.714785 0.242590	
C	2.447122 0.150605 0.184832	

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O	2.251036	2.297777	-0.845124
O	2.781962	2.197593	1.352482
H	1.883039	-0.235137	1.032597
C	3.873068	-0.398556	0.197474
N	1.719060	-0.245518	-1.064018
H	0.700664	-0.310386	-0.862941
H	4.357269	-0.080072	1.118063
H	4.445680	-0.003110	-0.644042
S	3.993533	-2.231539	0.031921
H	1.866411	0.521639	-1.736923
H	2.044357	-1.141520	-1.436223
H	3.343130	-2.538052	1.173252
28			
Dimer 176 of the n...z type			
C	-2.833138	-1.329974	0.098015
C	-3.431094	-0.430640	-0.992867
N	-3.338105	-1.131537	1.458222
H	-3.652078	-0.173728	1.595120
H	-4.106167	-1.755511	1.673299
H	-3.024337	-2.368252	-0.195078
C	-1.301844	-1.209902	0.132305
O	-0.616356	-1.136606	-0.871812
O	-0.784474	-1.204219	1.348424
H	-1.580725	-1.234829	1.949692
H	-2.974847	-0.657848	-1.954794
H	-4.502988	-0.614836	-1.063296
S	-3.270371	1.374294	-0.653423
H	-1.926717	1.446461	-0.767142
C	3.817133	-0.596231	-0.067419
C	2.725631	0.497395	-0.345754
O	3.891648	-1.506507	-0.932695
O	4.503550	-0.424938	0.956334
H	3.249495	1.385174	-0.703629
C	1.901335	0.835153	0.888357
N	1.874702	0.002106	-1.482552
H	1.629922	0.734029	-2.147159
H	2.577677	1.169149	1.670903
H	1.364056	-0.041089	1.253000
S	0.589755	2.104500	0.617110
H	2.455582	-0.728287	-1.932389
H	0.993640	-0.446751	-1.162624
H	1.408098	3.114978	0.257587
28			
Dimer 177 of the n...z type			
C	2.728038	-1.269214	0.388187
C	3.457690	0.052938	0.665780
N	3.028159	-1.925352	-0.886111
H	3.286616	-1.244842	-1.596535
H	3.778688	-2.599637	-0.798976
H	2.986352	-1.957693	1.200441
C	1.205412	-1.102722	0.493572
O	0.660445	-0.429789	1.351461
O	0.519988	-1.765299	-0.422341
H	1.222547	-2.186613	-0.992476
H	3.144295	0.460851	1.625131
H	4.530877	-0.133612	0.701036
S	3.233947	1.334794	-0.640565
H	1.958112	1.660061	-0.345792
C	-3.446974	-0.780673	-0.448382
C	-2.716732	0.424654	0.243451
O	-3.527041	-1.827792	0.244807
O	-3.883513	-0.558668	-1.592383
H	-3.477090	1.165170	0.493700
C	-1.649634	1.045161	-0.649109
N	-2.140687	-0.085876	1.537650
H	-2.331758	0.524252	2.329811
H	-2.113391	1.353014	-1.582549
H	-0.876264	0.313964	-0.885166
S	-0.764181	2.478653	0.102413

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H	-2.602856	-1.006912	1.664352
H	-1.113232	-0.240006	1.483959
H	-1.747277	3.386962	-0.060627
28			
Dimer 178 of the n...z type			
C	-2.895971	-0.434453	-0.757111
C	-2.206176	0.931229	-0.648733
N	-4.310894	-0.469835	-0.375275
H	-4.516883	0.232364	0.331128
H	-4.921396	-0.314674	-1.168383
H	-2.813664	-0.758840	-1.800763
C	-2.160141	-1.522721	0.044924
O	-0.947694	-1.633213	0.098678
O	-2.963111	-2.365724	0.667193
H	-3.876974	-2.013620	0.472243
H	-1.183533	0.896923	-1.019805
H	-2.756771	1.649708	-1.256603
S	-2.203645	1.642685	1.051735
H	-1.292189	0.799177	1.577235
C	1.568913	1.677590	-0.242235
C	2.043979	0.220676	0.078421
O	1.043964	1.834025	-1.373775
O	1.794142	2.516681	0.649118
H	1.666532	-0.081967	1.054389
C	3.571099	0.158900	0.054245
N	1.451268	-0.699424	-0.946749
H	0.512684	-1.027948	-0.649140
H	3.955810	0.835209	0.814120
H	3.954489	0.482349	-0.915823
S	4.276106	-1.526668	0.302714
H	1.331381	-0.140045	-1.803351
H	2.044679	-1.517495	-1.111832
H	3.805221	-1.714079	1.552802
28			
Dimer 179 of the n...z type			
C	2.824644	-1.168672	0.146192
C	2.539753	-0.382454	1.432336
N	4.085464	-0.865075	-0.534001
H	4.351141	0.106546	-0.391355
H	4.842298	-1.454728	-0.209314
H	2.828371	-2.231891	0.412886
C	1.682989	-1.041811	-0.877156
O	0.501056	-1.037831	-0.584532
O	2.091672	-0.977534	-2.131791
H	3.086221	-0.969458	-2.061635
H	1.588058	-0.691175	1.861420
H	3.322424	-0.598656	2.159406
S	2.563599	1.449433	1.231273
H	1.411659	1.565112	0.532838
C	-3.737024	-0.789534	0.309285
C	-2.618435	0.309253	0.405789
O	-3.559867	-1.794258	1.046242
O	-4.680504	-0.532835	-0.459309
H	-3.038366	1.146363	0.965297
C	-2.134524	0.776911	-0.959656
N	-1.503961	-0.267425	1.238447
H	-1.939438	-1.097307	1.686720
H	-2.993584	1.125337	-1.527040
H	-1.666704	-0.042972	-1.505754
S	-0.848487	2.097678	-0.909095
H	-0.708657	-0.589811	0.659377
H	-1.152874	0.381765	1.939825
H	-1.606137	3.042100	-0.314260
28			
Dimer 180 of the n...z type			
C	2.068460	-0.595580	-0.314030
C	1.864602	0.929273	-0.387044
N	1.365390	-1.177030	0.829768
H	1.797921	-0.851538	1.692686

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H	1.469329	-2.188319	0.825398
H	1.638196	-1.011113	-1.230858
C	3.556661	-0.948648	-0.328803
O	4.143085	-1.504108	0.568955
O	4.143024	-0.551593	-1.471124
H	5.085842	-0.781780	-1.440482
H	2.353736	1.329011	-1.273073
H	0.798416	1.148672	-0.454263
S	2.442422	1.859038	1.095349
H	3.766864	1.764540	0.856211
C	-1.999695	0.669594	-1.101576
C	-2.035153	-0.684137	-0.316985
O	-1.542637	1.654335	-0.464913
O	-2.439253	0.621137	-2.265128
H	-1.444169	-1.415715	-0.871002
C	-3.453594	-1.232603	-0.174961
N	-1.365128	-0.463935	1.007175
H	-0.346864	-0.772188	0.974169
H	-3.445249	-2.202729	0.325012
H	-3.867426	-1.365575	-1.172673
S	-4.594509	-0.188199	0.828335
H	-1.368691	0.560380	1.142898
H	-1.835744	-0.921195	1.787731
H	-4.612055	0.875315	-0.001234
28			
Dimer 181 of the n...z type			
C	1.930639	-0.135284	-0.826795
C	1.499320	1.215597	-0.233017
N	0.937606	-1.172399	-0.559817
H	0.770016	-1.245276	0.442196
H	1.286343	-2.079031	-0.860183
H	1.997780	0.008458	-1.911981
C	3.336268	-0.535155	-0.372482
O	3.623993	-1.594830	0.131241
O	4.230758	0.438838	-0.617910
H	5.108550	0.141147	-0.329506
H	2.186647	1.999652	-0.542639
H	0.499589	1.463122	-0.592155
S	1.361304	1.234223	1.606813
H	2.683602	1.247444	1.874855
C	-2.512979	1.201737	-0.495161
C	-2.735417	-0.270514	-0.974452
O	-1.666405	1.855540	-1.154300
O	-3.221654	1.574081	0.460855
H	-3.587643	-0.242038	-1.660499
C	-3.069597	-1.270752	0.125325
N	-1.551243	-0.681873	-1.799441
H	-1.753259	-1.483520	-2.396462
H	-3.130345	-2.283562	-0.276959
H	-4.045460	-1.009988	0.528881
S	-1.869406	-1.365445	1.520144
H	-1.308208	0.126266	-2.381957
H	-0.667687	-0.895295	-1.235944
H	-2.037777	-0.090728	1.926246
28			
Dimer 182 of the n...z type			
C	2.848688	0.745066	-0.595587
C	2.653407	-0.609291	-1.299046
N	3.733908	0.744080	0.572509
H	3.816474	-0.192393	0.961806
H	4.660761	1.084812	0.349012
C	3.245226	1.441044	-1.342221
C	1.497388	1.351684	-0.184464
O	0.530908	1.407918	-0.920074
O	1.475024	1.840370	1.049819
H	2.388969	1.643521	1.400673
H	1.866916	-0.518904	-2.046831
H	3.579479	-0.888129	-1.801938
S	2.283532	-2.022656	-0.174707

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H	1.113159	-1.564705	0.357780
C	-1.587825	-1.079080	1.029282
C	-2.471683	0.210383	1.072530
O	-0.397882	-0.911668	1.405171
O	-2.154228	-2.122701	0.659559
H	-2.953798	0.234119	2.053870
C	-3.553935	0.284466	0.003676
N	-1.553983	1.398217	1.025169
H	-2.014856	2.270148	1.286518
H	-4.134164	1.204005	0.096896
H	-4.225533	-0.559164	0.144840
S	-2.925350	0.270422	-1.727577
H	-0.764342	1.217328	1.655983
H	-1.117423	1.506906	0.091689
H	-2.398064	-0.969656	-1.669425
28			
Dimer 183 of the n...z type			
C	2.078351	0.314541	-0.980126
C	2.054646	-1.051996	-0.285421
N	3.386982	0.775057	-1.454045
H	4.134213	0.426628	-0.858330
H	3.570873	0.475307	-2.404007
H	1.406226	0.250048	-1.843852
C	1.472234	1.425907	-0.106075
O	0.490547	1.283135	0.601632
O	2.092388	2.587133	-0.208191
H	2.860956	2.396561	-0.815418
H	1.037466	-1.365885	-0.058434
H	2.484767	-1.792328	-0.960547
S	3.080249	-1.142035	1.243687
H	2.272457	-0.393359	2.022033
C	-1.822670	-1.946926	-0.555921
C	-2.402791	-0.729427	0.244104
O	-0.946260	-2.614004	0.051327
O	-2.312042	-2.133297	-1.684936
H	-3.374622	-1.035292	0.635904
C	-2.544015	0.530411	-0.599576
N	-1.509544	-0.494799	1.431512
H	-1.122647	-1.414908	1.682774
H	-3.177970	0.307962	-1.453590
H	-1.571005	0.853709	-0.972246
S	-3.211627	1.988072	0.313771
H	-0.711632	0.116300	1.174564
H	-1.999600	-0.072474	2.219318
H	-4.461083	1.510551	0.489667
28			
Dimer 184 of the n...z type			
C	-2.374372	-0.652203	0.581931
C	-2.055479	0.835713	0.817883
N	-1.347809	-1.303064	-0.229241
H	-1.360220	-0.912275	-1.169818
H	-1.560573	-2.292098	-0.330821
H	-2.387106	-1.126796	1.568737
C	-3.780355	-0.825927	0.000789
O	-4.026985	-1.337130	-1.065209
O	-4.717185	-0.333994	0.829409
H	-5.592473	-0.454184	0.426921
H	-2.816542	1.285934	1.451664
H	-1.096900	0.920178	1.328859
S	-1.864298	1.844663	-0.712746
H	-3.164673	1.864989	-1.071018
C	3.662170	-1.102115	-0.223408
C	2.200387	-0.606928	-0.491973
O	3.761629	-2.035732	0.611490
O	4.556893	-0.541541	-0.886728
H	1.841779	-1.143443	-1.375095
C	2.075460	0.889202	-0.754860
N	1.337516	-1.040275	0.651489
H	0.320320	-1.164972	0.375099

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H	1.052042	1.159937	-1.017209
H	2.727198	1.148703	-1.585222
S	2.501157	1.939625	0.699363
H	1.749839	-1.912918	1.007131
H	1.403753	-0.350734	1.407062
H	3.804197	1.593166	0.748238
28			
Dimer 185 of the n...z type			
C	2.145927	-0.619826	0.139176
C	1.920293	0.262224	-1.099249
N	1.423258	-0.108606	1.302628
H	1.717845	0.849475	1.487347
H	1.681379	-0.643135	2.128742
H	1.747411	-1.611036	-0.106754
C	3.637494	-0.826396	0.420837
O	4.170441	-0.623175	1.485278
O	4.285861	-1.282374	-0.664303
H	5.221751	-1.414493	-0.442606
H	2.400063	-0.178810	-1.969705
H	0.852257	0.331271	-1.299678
S	2.482073	2.008581	-0.915708
H	3.806243	1.765507	-1.000004
C	-3.303548	1.167095	0.353754
C	-1.993492	0.385989	-0.007963
O	-3.441736	1.438687	1.572875
O	-4.043729	1.455300	-0.606447
H	-1.282072	1.131112	-0.374841
C	-2.176712	-0.683682	-1.078581
N	-1.417796	-0.176930	1.253356
H	-0.357382	-0.173092	1.267605
H	-1.230458	-1.171354	-1.318835
H	-2.561999	-0.210583	-1.978191
S	-3.306949	-2.051401	-0.577730
H	-1.805509	0.407297	2.010422
H	-1.761989	-1.129944	1.403096
H	-4.414224	-1.288270	-0.470561
28			
Dimer 186 of the n...z type			
C	2.817600	-0.798306	0.715294
C	2.423947	0.661197	0.986717
N	4.166277	-1.002827	0.174955
H	4.482445	-0.190049	-0.347461
H	4.842630	-1.201339	0.901987
H	2.741502	-1.335032	1.667480
C	1.815562	-1.512908	-0.207753
O	0.607377	-1.451339	-0.077140
O	2.379961	-2.246018	-1.152645
H	3.358042	-2.113601	-1.004276
H	1.394720	0.734699	1.333680
H	3.080851	1.056502	1.761451
S	2.616674	1.783542	-0.469161
H	1.347425	1.691358	-0.931626
C	-1.129902	1.378816	-0.112443
C	-2.027676	0.102487	-0.119479
O	-0.829233	1.811045	1.026309
O	-0.823250	1.832601	-1.234779
H	-1.749790	-0.541372	-0.950919
C	-3.501484	0.493935	-0.197596
N	-1.735082	-0.652366	1.142637
H	-0.828158	-1.129580	1.023930
H	-3.668567	1.040978	-1.123719
H	-3.772285	1.144380	0.636351
S	-4.673929	-0.925858	-0.098625
H	-1.630448	0.038154	1.896680
H	-2.467486	-1.332266	1.365342
H	-4.300295	-1.521055	-1.249866
28			
Dimer 187 of the n...z type			
C	-2.592926	1.328222	0.457122

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C	-3.225619	0.042255	1.013970
N	-3.020674	1.732204	-0.886401
H	-3.370320	0.930403	-1.406899
H	-3.745818	2.438711	-0.858044
H	-2.830954	2.134615	1.158865
C	-1.056940	1.246309	0.479881
O	-0.404484	0.833584	1.408052
O	-0.487554	1.722356	-0.638302
H	-1.267088	1.965089	-1.217314
H	-2.729771	-0.231914	1.944027
H	-4.279836	0.223500	1.223879
S	-3.211812	-1.390770	-0.144947
H	-1.859765	-1.519351	-0.295632
C	0.963913	-1.736145	-0.150648
C	2.179544	-0.820742	-0.505054
O	-0.029512	-1.627918	-0.915492
O	1.124730	-2.484761	0.829138
H	2.956362	-1.451411	-0.941741
C	2.727241	-0.072022	0.704868
N	1.764198	0.145047	-1.582431
H	1.376485	-0.370996	-2.373610
H	2.998329	-0.802969	1.462330
H	1.961996	0.582873	1.123555
S	4.172828	1.014020	0.338259
H	1.011424	0.769509	-1.248770
H	2.554726	0.716190	-1.892451
H	5.046585	0.029637	0.042643
28			
Dimer 188 of the n...z type			
C	2.430461	0.805823	0.620501
C	2.261402	-0.543829	1.340291
N	1.198401	1.228014	-0.034831
H	0.985349	0.632159	-0.833853
H	1.304587	2.168123	-0.406590
H	2.680515	1.539018	1.394606
C	3.624398	0.770543	-0.338068
O	3.561617	0.968564	-1.527860
O	4.767847	0.486702	0.310854
H	5.498096	0.467241	-0.328481
H	3.176135	-0.807528	1.867198
H	1.459489	-0.453334	2.072610
S	1.761002	-1.946974	0.254355
H	2.941192	-2.101787	-0.380366
C	-1.766767	-0.578262	-0.969463
C	-1.993520	-0.287411	0.548189
O	-1.210690	0.326858	-1.634461
O	-2.183814	-1.693181	-1.347635
H	-1.419304	-1.015323	1.125048
C	-3.462650	-0.409003	0.949232
N	-1.448122	1.066266	0.893614
H	-1.560122	1.279345	1.885751
H	-3.597168	-0.218825	2.015516
H	-3.793586	-1.422455	0.734984
S	-4.582242	0.786953	0.100266
H	-0.414197	1.140465	0.637647
H	-1.945115	1.778799	0.353552
H	-4.467627	0.255763	-1.134338
28			
Dimer 189 of the n...z type			
C	-2.137982	-0.388667	0.190683
C	-1.617171	0.989273	0.613428
N	-1.715492	-0.874244	-1.124811
H	-1.610491	-0.098845	-1.775036
H	-0.821251	-1.362308	-1.053814
H	-1.758079	-1.095184	0.937556
C	-3.669979	-0.474967	0.284996
O	-4.331292	0.049123	1.155489
O	-4.214268	-1.220915	-0.677267
H	-3.434527	-1.468396	-1.247521

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H	-2.001756	1.251038	1.597925		
H	-0.530327	0.951257	0.667441		
S	-2.006835	2.353219	-0.564837		
H	-3.335632	2.391540	-0.335967		
C	1.346919	-1.436400	0.472386		
C	2.782836	-0.824547	0.412868		
O	0.977664	-2.024349	-0.580842		
O	0.711872	-1.223492	1.517200		
H	3.334406	-1.048166	1.323690		
C	2.670097	0.687410	0.203933		
N	3.501687	-1.466826	-0.742670		
H	3.999433	-2.311026	-0.458804		
H	2.153334	1.111568	1.062140		
H	2.084192	0.907814	-0.691022		
S	4.274020	1.553781	-0.054667		
H	2.759201	-1.751754	-1.404998		
H	4.178429	-0.830561	-1.176985		
H	4.804618	1.272974	1.153408		
28					
Dimer 190 of the n...z type					
C	1.766144	-0.414855	-0.096118		
C	2.223963	0.673800	-1.080883		
N	0.845742	0.120489	0.901254		
H	1.339005	0.777832	1.502599		
H	0.509599	-0.628966	1.499811		
H	1.232586	-1.166904	-0.687008		
C	2.960648	-1.140456	0.528378		
O	3.176741	-1.221446	1.713828		
O	3.748591	-1.689124	-0.413178		
H	4.492026	-2.139746	0.018888		
H	2.846460	0.242381	-1.861726		
H	1.345858	1.117481	-1.548785		
S	3.117825	2.088834	-0.306275		
H	4.285660	1.450453	-0.086397		
C	-3.750202	0.467542	0.471671		
C	-2.660607	0.780353	-0.609489		
O	-3.589392	1.043961	1.577469		
O	-4.665018	-0.296568	0.108829		
H	-3.106561	1.503212	-1.297431		
C	-2.221534	-0.430156	-1.425044		
N	-1.524874	1.481179	0.081012		
H	-1.192276	2.290992	-0.439881		
H	-1.395058	-0.174078	-2.089665		
H	-3.061487	-0.748442	-2.038251		
S	-1.641181	-1.875887	-0.438718		
H	-1.935995	1.789875	0.980874		
H	-0.682480	0.877224	0.311151		
H	-2.827544	-2.122085	0.153170		
28					
Dimer 191 of the n...z type					
C	2.899246	-1.056630	0.644467		
C	3.416219	0.390123	0.653217		
N	3.287668	-1.868795	-0.512924		
H	3.513920	-1.284064	-1.313651		
H	4.081668	-2.464430	-0.312429		
H	3.266454	-1.539457	1.555841		
C	1.366437	-1.082866	0.767835		
O	0.730567	-0.422496	1.555938		
O	0.779913	-1.919513	-0.099254		
H	1.547945	-2.306356	-0.612201		
H	3.030631	0.918738	1.523342		
H	4.504934	0.382623	0.703500		
S	3.013157	1.348460	-0.870743		
H	1.682452	1.456194	-0.662247		
C	-3.615490	-0.793771	0.002742		
C	-2.229144	-0.065216	0.042740		
O	-3.883083	-1.377600	-1.080043		
O	-4.298577	-0.698067	1.037963		
H	-1.649824	-0.422687	0.892016		

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C	-2.420714	1.445241	0.139388		
N	-1.487812	-0.455209	-1.208187		
H	-0.738557	-1.126637	-0.998724		
H	-2.986696	1.656612	1.043767		
H	-2.987302	1.824178	-0.714011		
S	-0.852797	2.419326	0.146923		
H	-2.212528	-0.913658	-1.796182		
H	-1.065497	0.341718	-1.688610		
H	-0.282246	1.780793	1.189315		
28					
Dimer 192 of the n...z type					
C	1.965815	-0.687015	0.115283		
C	3.465491	-0.844083	-0.190486		
N	1.110951	-0.361191	-1.031811		
H	1.531296	0.396848	-1.564647		
H	1.055081	-1.161151	-1.655115		
H	1.620166	-1.650601	0.504883		
C	1.698653	0.339970	1.232053		
O	2.520854	1.161891	1.592667		
O	0.499388	0.290937	1.793284		
H	-0.073548	-0.495350	1.487999		
H	4.027298	-1.009804	0.729087		
H	3.601050	-1.715635	-0.833071		
S	4.245011	0.541334	-1.125429		
H	4.112245	1.464864	-0.153692		
C	-1.901030	-1.669359	0.324827		
C	-2.079905	-0.296080	-0.379212		
O	-2.656620	-2.589880	-0.034792		
O	-1.010743	-1.698979	1.218758		
H	-1.096085	0.079027	-0.663832		
C	-2.807179	0.684539	0.540946		
N	-2.867743	-0.529947	-1.638995		
H	-2.256976	-0.785721	-2.416192		
H	-2.211788	0.819222	1.441441		
H	-3.786841	0.299827	0.832859		
S	-3.142249	2.325172	-0.227615		
H	-3.492461	-1.330824	-1.464647		
H	-3.397243	0.304737	-1.912642		
H	-1.852948	2.678835	-0.407881		
28					
Dimer 193 of the n...z type					
C	2.870393	-0.369761	0.611576		
C	3.071848	-0.107593	-0.888802		
N	2.569268	-1.754226	0.991329		
H	2.084355	-2.238581	0.239278		
H	3.407157	-2.275391	1.219721		
H	3.791781	-0.066987	1.121296		
C	1.784921	0.544972	1.202150		
O	1.645285	1.712309	0.932859		
O	0.988694	-0.082342	2.085773		
H	1.318186	-1.025455	2.079903		
H	3.221442	0.956227	-1.065521		
H	3.960929	-0.642060	-1.222913		
S	1.699923	-0.713538	-1.963457		
H	0.831645	0.322751	-1.791468		
C	-1.247260	1.693367	-0.585684		
C	-1.540025	0.288836	0.035475		
O	-1.692044	2.667909	0.062668		
O	-0.641300	1.676486	-1.678411		
H	-0.675526	-0.362920	-0.070838		
C	-2.750652	-0.337452	-0.654512		
N	-1.788093	0.483030	1.502634		
H	-0.901788	0.401194	2.018217		
H	-2.520090	-0.456671	-1.711285		
H	-3.625847	0.309037	-0.566079		
S	-3.273332	-1.955760	0.056038		
H	-2.147246	1.445570	1.606249		
H	-2.446588	-0.206620	1.877177		
H	-2.132529	-2.622078	-0.217105		

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28		
Dimer 194 of the n...z	type	
C	-2.885787	0.873054
C	-3.204629	0.382765
N	-3.083034	-0.091852
H	-2.880420	-1.039909
H	-4.031611	-0.070894
H	-3.531567	1.736623
C	-1.455826	1.426230
O	-0.879710	2.019433
O	-0.885286	1.194745
H	-1.541197	0.620046
H	-3.092209	1.193410
H	-4.236246	0.032858
S	-2.178587	-1.045763
H	-1.079530	-0.330528
C	3.155905	0.658652
C	1.960697	0.015108
O	3.759235	1.581315
O	3.356866	0.201500
H	1.043959	0.336573
C	2.042674	-1.504960
N	1.949769	0.631026
H	1.018581	0.982870
H	2.059169	-1.877107
H	2.966006	-1.826176
S	0.689680	-2.330127
H	2.646311	1.400606
H	2.252806	-0.018318
H	-0.325728	-1.981071
28		
Dimer 195 of the n...z	type	
C	1.704419	0.568771
C	1.993179	-0.608822
N	0.779562	0.187140
H	1.268600	-0.380713
H	0.453859	1.015493
H	1.223883	1.339302
C	3.004114	1.171061
O	3.327186	1.199954
O	3.762045	1.663755
H	4.583234	2.021498
H	2.672439	-0.301060
H	1.056786	-0.924641
S	2.659029	-2.119981
H	3.906085	-1.658016
C	-3.377008	0.192201
C	-2.784377	-0.904220
O	-2.974708	0.145819
O	-4.206801	0.964909
H	-3.495842	-1.735748
C	-2.585794	-0.476198
N	-1.524355	-1.428288
H	-1.229381	-2.320266
H	-2.118091	-1.272716
H	-3.564978	-0.274538
S	-1.520417	1.005115
H	-1.717668	-1.545121
H	-0.704902	-0.751377
H	-2.327244	1.861546
28		
Dimer 196 of the n...z	type	
C	-1.807302	-0.250966
C	-3.190749	-0.830020
N	-1.415089	-0.229478
H	-2.222279	-0.243172
H	-0.786264	-0.998444
H	-1.075279	-0.858317
C	-1.643048	1.165281

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O	-2.034459	1.499069
O	-0.985602	1.991256
H	-0.852834	1.437674
H	-3.379797	-0.794272
H	-3.229950	-1.869733
S	-4.584742	-0.001026
H	-4.513056	1.174310
C	1.440578	-1.714936
C	2.767755	-0.891525
O	0.943536	-1.913138
O	0.994903	-2.026421
H	3.501908	-1.353463
C	2.466746	0.541174
N	3.314521	-0.904441
H	3.939374	-1.695729
H	2.087948	0.508831
H	1.697817	0.989276
S	3.896569	1.696588
H	2.491060	-1.033476
H	3.827502	-0.044483
H	4.677697	1.069259
28		
Dimer 197 of the n...z	type	
C	2.659518	0.767445
C	3.765362	0.370350
N	2.985932	0.666694
H	3.655903	-0.079925
H	3.371769	1.530442
H	2.391202	1.808117
C	1.364163	-0.019613
O	0.932832	-0.294545
O	0.717810	-0.349669
H	1.317498	-0.019994
H	3.416181	0.490703
H	4.629779	1.016959
S	4.397391	-1.346561
H	3.298403	-1.981104
C	-3.841296	-1.114904
C	-3.047273	0.153330
O	-3.638069	-2.157577
O	-4.586724	-0.944363
H	-3.770911	0.870734
C	-2.237015	0.775199
N	-2.182927	-0.286322
H	-2.337130	0.261065
H	-2.914050	0.993720
H	-1.471428	0.084740
S	-1.307291	2.299012
H	-2.485697	-1.273949
H	-1.173309	-0.274367
H	-2.378406	3.049421
28		
Dimer 198 of the n...z	type	
C	-1.566437	-0.256689
C	-2.799428	-0.559900
N	-1.365484	-1.108895
H	-2.215512	-1.591208
H	-0.605031	-1.767512
H	-0.690630	-0.362956
C	-1.537792	1.218023
O	-1.807591	2.154286
O	-1.143172	1.365337
H	-1.054167	0.415738
H	-2.857786	0.139017
H	-2.723374	-1.571475
S	-4.397841	-0.530662
H	-4.419820	0.796103
C	2.059709	-1.377706
C	3.165534	-0.725589

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O	1.216943	-2.077347	-0.053386	
O	2.143434	-1.155854	1.791823	
H	4.059531	-1.346333	-0.230485	
C	3.515434	0.708448	0.059799	
N	2.699111	-0.833960	-1.746865	
H	3.447822	-1.016306	-2.414701	
H	4.332155	1.087880	-0.555504	
H	3.830091	0.718504	1.100408	
S	2.129654	1.901205	-0.173615	
H	2.006431	-1.605944	-1.734809	
H	2.202789	0.020372	-2.024854	
H	1.344077	1.424508	0.813588	
28				
Dimer 199 of the n...z type				
C	2.881409	1.010790	-0.258808	
C	3.066335	-0.310317	-1.033105	
N	3.692589	1.033999	0.945565	
H	3.376820	0.310214	1.585916	
H	3.583426	1.919691	1.429238	
H	3.219336	1.810053	-0.927479	
C	1.391166	1.252170	-0.017595	
O	0.873839	1.270507	1.086438	
O	0.709750	1.409842	-1.147837	
H	-0.251418	1.519798	-0.945513	
H	2.531060	-0.275500	-1.980114	
H	4.129115	-0.439390	-1.236015	
S	2.560799	-1.827922	-0.112228	
H	1.218739	-1.705788	-0.252289	
C	-2.005932	-1.529455	-0.238520	
C	-2.486855	-0.637566	0.954497	
O	-0.878451	-2.063973	-0.082776	
O	-2.804560	-1.634185	-1.186863	
H	-3.151196	-1.260945	1.558321	
C	-3.255694	0.619630	0.566615	
N	-1.295296	-0.343198	1.822343	
H	-1.543512	-0.171764	2.796689	
H	-3.394355	1.275326	1.427301	
H	-4.239078	0.324749	0.208488	
S	-2.495115	1.672750	-0.745571	
H	-0.685215	-1.169965	1.748776	
H	-0.719504	0.449546	1.483972	
H	-2.653414	0.772093	-1.738060	
28				
Dimer 200 of the n...z type				
C	3.221901	-0.517867	-0.490810	
C	1.793166	0.005887	-0.664576	
N	3.418555	-1.551096	0.529659	
H	2.795117	-1.409639	1.320611	
H	3.252692	-2.479868	0.160603	
H	3.525904	-0.938597	-1.456181	
C	4.220474	0.628173	-0.239311	
O	4.144367	1.714526	-0.767951	
O	5.206801	0.305345	0.597404	
H	4.986812	-0.614186	0.896832	
H	1.753408	0.749027	-1.459039	
H	1.117249	-0.811188	-0.917499	
S	1.080525	0.748389	0.869840	
H	1.727015	1.929762	0.804160	
C	-1.827521	-1.529471	-0.175894	
C	-2.552845	-0.193335	0.195016	
O	-1.147338	-1.495523	-1.231504	
O	-2.034165	-2.476821	0.605081	
H	-2.406302	0.025580	1.251633	
C	-4.042554	-0.297687	-0.128394	
N	-1.916884	0.917909	-0.588544	
H	-1.022289	1.190666	-0.149102	
H	-4.464601	-1.114534	0.452925	
H	-4.192333	-0.519071	-1.187121	
S	-5.003822	1.246113	0.177410	

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H	-1.683985	0.543024	-1.517387	
H	-2.528916	1.736571	-0.659591	
H	-4.831743	1.278299	1.514925	
28				
Dimer 201 of the n...z type				
C	-2.026652	-0.397380	-0.001042	
C	-2.100092	0.949170	0.728236	
N	-1.984085	-0.345512	-1.463523	
H	-2.517310	0.449174	-1.808212	
H	-1.015393	-0.254372	-1.773380	
H	-1.106312	-0.890101	0.335401	
C	-3.155705	-1.349577	0.432232	
O	-3.574549	-1.437634	1.566052	
O	-3.615607	-2.104891	-0.564933	
H	-3.111300	-1.773469	-1.359193	
H	-2.097722	0.797402	1.806536	
H	-1.228993	1.543640	0.451444	
S	-3.562717	1.976063	0.272067	
H	-4.494211	1.208707	0.874554	
C	1.367401	0.529550	-0.688782	
C	2.517760	0.007384	0.230166	
O	0.947347	-0.305748	-1.535204	
O	1.018036	1.706036	-0.503252	
H	2.339046	0.299576	1.262992	
C	3.856481	0.556956	-0.264704	
N	2.505321	-1.495801	0.158350	
H	1.884299	-1.903115	0.858086	
H	3.828837	1.641958	-0.189776	
H	4.016281	0.291478	-1.311797	
S	5.332639	-0.097343	0.622558	
H	2.115635	-1.726099	-0.771806	
H	3.440924	-1.893884	0.292070	
H	5.021839	0.400055	1.837344	
28				
Dimer 202 of the n...z type				
C	3.030114	-0.279249	-0.065024	
C	2.928171	1.204514	-0.449163	
N	2.658038	-1.240853	-1.106296	
H	2.001490	-0.830490	-1.765058	
H	3.464111	-1.570315	-1.623248	
H	4.072048	-0.462993	0.218466	
C	2.229853	-0.584353	1.216468	
O	2.262653	0.109977	2.207094	
O	1.524052	-1.713941	1.153835	
H	1.692145	-2.057360	0.236402	
H	3.153935	1.826730	0.415376	
H	3.654859	1.421755	-1.232208	
S	1.302426	1.716675	-1.153673	
H	0.549523	1.621295	-0.025476	
C	-2.117451	1.160786	0.622520	
C	-2.753754	-0.263921	0.736293	
O	-2.791007	2.001499	-0.021981	
O	-1.023802	1.304077	1.204183	
H	-3.132345	-0.368515	1.754760	
C	-1.785203	-1.406651	0.446775	
N	-3.943447	-0.286434	-0.185441	
H	-4.753812	-0.775741	0.192373	
H	-2.246195	-2.371864	0.660327	
H	-0.909536	-1.288775	1.080272	
S	-1.249189	-1.510206	-1.313741	
H	-4.150306	0.715708	-0.361868	
H	-3.682754	-0.707995	-1.085125	
H	-0.532627	-0.363570	-1.336468	
28				
Dimer 203 of the n...z type				
C	-2.317742	-0.538974	0.206644	
C	-1.717417	0.584026	1.062437	
N	-1.557476	-0.944064	-0.976913	
H	-1.151470	-0.124159	-1.423914	

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H	-0.785750	-1.560261	-0.718907
H	-2.405952	-1.416794	0.858695
C	-3.764591	-0.230249	-0.217301
O	-4.564640	0.364653	0.470427
O	-4.076766	-0.717118	-1.419806
H	-3.223435	-1.106916	-1.749454
H	-2.383428	0.824443	1.889736
H	-0.763507	0.246219	1.467630
S	-1.336829	2.129022	0.131494
H	-2.612272	2.512007	-0.084015
C	1.458781	-1.530739	0.795822
C	2.756200	-0.771538	0.369933
O	0.957742	-2.270189	-0.094088
O	1.038136	-1.275547	1.935720
H	3.518733	-0.857522	1.141680
C	2.416891	0.697235	0.107623
N	3.276464	-1.428173	-0.880276
H	3.926293	-2.185771	-0.668128
H	2.057275	1.134376	1.036412
H	1.623887	0.782892	-0.638137
S	3.806562	1.702906	-0.561348
H	2.449226	-1.850947	-1.335738
H	3.753881	-0.761344	-1.495749
H	4.619370	1.585638	0.508917
28			
Dimer 204 of the n...z type			
C	2.321123	0.527656	0.410819
C	3.408612	0.731833	-0.648435
N	2.778629	0.243882	1.774128
H	3.661324	-0.261385	1.766866
H	2.900375	1.092302	2.314021
H	1.703780	1.432550	0.443574
C	1.316657	-0.555419	-0.003411
O	0.900344	-0.718721	-1.125288
O	0.876297	-1.292817	1.030598
H	1.403957	-0.952557	1.806742
H	2.956220	0.938497	-1.616943
H	4.029982	1.582359	-0.367657
S	4.577476	-0.685239	-0.818953
H	3.709954	-1.538307	-1.401046
C	-1.322878	1.430135	-0.054708
C	-2.190578	0.131599	-0.125539
O	-0.694676	1.609216	1.016725
O	-1.360122	2.138844	-1.079063
H	-1.839493	-0.476748	-0.958513
C	-3.671139	0.464866	-0.289841
N	-1.969343	-0.680498	1.122296
H	-1.022340	-1.085392	1.132503
H	-3.788994	1.059308	-1.192435
H	-4.033066	1.054888	0.555066
S	-4.783411	-1.005906	-0.359486
H	-2.025421	-0.067550	1.940083
H	-2.662680	-1.431548	1.198817
H	-4.309161	-1.507963	-1.518112
28			
Dimer 205 of the n...z type			
C	3.072263	0.389528	-0.749473
C	2.646785	1.785331	-0.274183
N	2.220732	-0.319096	-1.695926
H	1.247170	-0.387518	-1.397262
H	2.262068	0.085087	-2.623426
H	4.046298	0.531778	-1.235891
C	3.382036	-0.551681	0.428621
O	3.777617	-0.178654	1.509853
O	3.209431	-1.842838	0.138951
H	2.836791	-1.850674	-0.777856
H	3.422159	2.206254	0.364424
H	2.520328	2.437211	-1.138827
S	1.046968	1.894686	0.631400

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H	1.327481	1.003958	1.603887
C	-1.113569	-1.435284	0.097468
C	-2.090126	-0.220744	0.201140
O	-0.432279	-1.490282	-0.958213
O	-1.143675	-2.221059	1.060874
H	-1.952981	0.275403	1.161712
C	-3.538021	-0.679456	0.039915
N	-1.727252	0.770928	-0.865704
H	-0.849000	1.247613	-0.603600
H	-3.756216	-1.408241	0.817275
H	-3.684302	-1.160094	-0.929677
S	-4.781087	0.681923	0.092577
H	-1.537826	0.259672	-1.734132
H	-2.467407	1.465545	-1.006325
H	-4.567977	1.041931	1.374842
28			
Dimer 206 of the n...z type			
C	2.544024	0.137036	-0.860092
C	2.781470	1.368776	0.021050
N	1.378294	0.172711	-1.748285
H	0.615467	0.769704	-1.413696
H	1.629404	0.489243	-2.676964
H	3.439971	0.017709	-1.480828
C	2.485287	-1.156702	-0.023658
O	3.190890	-1.380956	0.934311
O	1.587807	-2.030590	-0.482199
H	1.166546	-1.538037	-1.244580
H	3.749713	1.296905	0.513686
H	2.779292	2.261696	-0.604040
S	1.496324	1.664327	1.312369
H	1.898716	0.688004	2.150603
C	-2.012999	1.547689	-0.563407
C	-1.816425	0.229730	0.249310
O	-3.063819	2.185527	-0.318437
O	-1.108864	1.793946	-1.388369
H	-0.806399	0.202884	0.651392
C	-2.086423	-0.981835	-0.640778
N	-2.771035	0.259543	1.412276
H	-2.357320	0.721255	2.223054
H	-1.404847	-0.940518	-1.487964
H	-3.107182	-0.960097	-1.028361
S	-1.923900	-2.606427	0.215396
H	-3.573384	0.835410	1.109223
H	-3.061924	-0.680549	1.698153
H	-0.595351	-2.527363	0.441140
28			
Dimer 207 of the n...z type			
C	2.690580	-0.902530	0.012860
C	3.343157	0.371639	-0.542191
N	1.890029	-1.682457	-0.930164
H	1.440115	-1.082176	-1.616637
H	2.452300	-2.363478	-1.425979
H	3.496912	-1.544148	0.385681
C	1.842143	-0.584517	1.255059
O	2.156967	0.210853	2.107712
O	0.702274	-1.286823	1.329031
H	0.641918	-1.831845	0.499975
H	3.958775	0.848115	0.218629
H	3.977116	0.109339	-1.389046
S	2.136631	1.606976	-1.193651
H	1.702994	2.044720	0.005789
C	-2.231990	-1.545333	-0.680019
C	-2.501659	-0.220368	0.106187
O	-1.551986	-2.412614	-0.082084
O	-2.719697	-1.570331	-1.827274
H	-3.576835	-0.044984	0.148212
C	-1.801826	0.959729	-0.564689
N	-2.032438	-0.368520	1.529239
H	-2.577131	-1.080819	2.015501

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H	-2.174114	1.040527	-1.583111	
H	-0.723436	0.801361	-0.614569	
S	-2.003542	2.574560	0.303059	
H	-1.046072	-0.676867	1.555109	
H	-2.121162	0.519461	2.033605	
H	-3.326820	2.712648	0.080477	
28				
Dimer 208 of the n...z type				
C	-2.986892	0.153228	0.604759	
C	-2.852265	-1.328977	0.228658	
N	-3.461860	1.046456	-0.457061	
H	-3.159847	0.715969	-1.370591	
H	-4.471833	1.123697	-0.463157	
H	-3.693150	0.214114	1.440605	
C	-1.672826	0.718841	1.168919	
O	-0.943220	0.116947	1.924395	
O	-1.414168	1.966722	0.769541	
H	-2.161819	2.180628	0.147673	
H	-2.461800	-1.896491	1.071741	
H	-3.838527	-1.718491	-0.023322	
S	-1.789130	-1.643718	-1.247213	
H	-0.588650	-1.742293	-0.610571	
C	2.245816	-1.598542	0.190131	
C	1.989731	-0.065025	0.329125	
O	3.439669	-1.961271	0.316282	
O	1.236941	-2.288714	-0.066496	
H	1.141766	0.117443	0.985818	
C	1.744307	0.545793	-1.052460	
N	3.213313	0.538698	0.964314	
H	3.139202	0.559790	1.981559	
H	0.833829	0.112799	-1.461931	
H	2.568181	0.313632	-1.730321	
S	1.613386	2.383849	-1.062579	
H	3.994514	-0.094814	0.722469	
H	3.378087	1.496947	0.637503	
H	0.510782	2.457518	-0.286126	
28				
Dimer 209 of the n...z type				
C	3.305099	0.601799	0.303241	
C	1.819454	0.417684	0.631423	
N	3.617598	1.345033	-0.919455	
H	2.925865	1.170366	-1.644132	
H	3.654745	2.343610	-0.753223	
H	3.752491	1.140678	1.146343	
C	4.048505	-0.747796	0.272085	
O	3.800689	-1.668450	1.017831	
O	5.020773	-0.802539	-0.637721	
H	4.959957	0.061759	-1.119780	
H	1.699389	-0.115094	1.572923	
H	1.337314	1.391028	0.716698	
S	0.871734	-0.473177	-0.678681	
H	1.365379	-1.703627	-0.430072	
C	-4.026399	-1.066214	-0.302378	
C	-3.137017	-0.017874	0.457352	
O	-3.733815	-2.269804	-0.080433	
O	-4.931116	-0.591473	-1.011043	
H	-3.743405	0.391843	1.265997	
C	-2.641690	1.102373	-0.446959	
N	-2.005875	-0.779700	1.096580	
H	-2.322328	-1.768908	1.052548	
H	-3.505326	1.588142	-0.893465	
H	-2.024116	0.705689	-1.254763	
S	-1.583187	2.357467	0.393060	
H	-1.124464	-0.702325	0.559933	
H	-1.816865	-0.496532	2.056705	
H	-2.517412	2.805694	1.256689	
28				
Dimer 210 of the n...z type				
C	3.035945	0.361236	-0.722133	

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C	1.541072	0.121649	-0.489059	
N	3.688479	-0.481557	-1.727258	
H	3.285343	-1.415096	-1.742149	
H	3.607744	-0.088472	-2.657437	
H	3.142655	1.404978	-1.039600	
C	3.834304	0.276746	0.593494	
O	3.413641	0.660378	1.661625	
O	5.056190	-0.234472	0.444648	
H	5.099816	-0.498178	-0.510460	
H	1.146894	0.819687	0.247096	
H	1.000736	0.263165	-1.425031	
S	1.132223	-1.599300	0.045771	
H	1.659727	-1.510646	1.284612	
C	-1.590643	1.553880	-0.099835	
C	-2.372872	0.199354	-0.158124	
O	-1.067654	1.821736	1.010325	
O	-1.600588	2.216929	-1.153410	
H	-2.113452	-0.341048	-1.067366	
C	-3.877156	0.463035	-0.105751	
N	-1.938385	-0.636945	1.009435	
H	-1.044471	-1.113378	0.797875	
H	-4.150448	1.073100	-0.964017	
H	-4.141232	1.011427	0.800880	
S	-4.920508	-1.056922	-0.063558	
H	-1.751708	0.011064	1.787588	
H	-2.641091	-1.338427	1.262484	
H	-4.575214	-1.521065	-1.282179	
28				
Dimer 211 of the n...z type				
C	-2.378823	-0.395081	0.861905	
C	-3.854425	0.046465	0.844407	
N	-1.511958	0.650979	1.359438	
H	-1.555037	1.465150	0.753575	
H	-0.543433	0.333418	1.404889	
H	-2.324766	-1.249971	1.546982	
C	-1.975957	-0.954150	-0.507108	
O	-1.061289	-0.542912	-1.194326	
O	-2.751946	-1.974521	-0.887016	
H	-2.455505	-2.299179	-1.753299	
H	-4.507254	-0.783270	0.581813	
H	-4.115459	0.396753	1.842551	
S	-4.218068	1.470732	-0.272012	
H	-4.170139	0.790513	-1.435896	
C	2.051537	-1.017358	0.635983	
C	2.289159	-0.381565	-0.767938	
O	1.286861	-0.387059	1.408462	
O	2.675751	-2.075911	0.838496	
H	2.011102	-1.107722	-1.533397	
C	3.748172	0.019888	-0.978788	
N	1.370240	0.795652	-0.939112	
H	1.530613	1.291690	-1.817454	
H	3.904922	0.418900	-1.982467	
H	4.363170	-0.870225	-0.864487	
S	4.354479	1.335721	0.162466	
H	0.385622	0.468574	-0.919968	
H	1.505885	1.447078	-0.161796	
H	4.306736	0.602643	1.293714	
28				
Dimer 212 of the n...z type				
C	-2.891668	0.873172	0.338878	
C	-2.992594	-0.450528	1.113655	
N	-3.532725	0.898952	-0.979052	
H	-3.606952	-0.040667	-1.362324	
H	-4.458968	1.306868	-0.944143	
H	-3.345326	1.648227	0.965821	
C	-1.424485	1.314647	0.186835	
O	-0.621527	1.295462	1.096272	
O	-1.116228	1.751002	-1.030368	
H	-1.963869	1.646710	-1.543347	

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H	-2.389074	-0.392835	2.018244
H	-4.030823	-0.619873	1.399937
S	-2.521317	-1.947140	0.147304
H	-1.202661	-1.678022	-0.047034
C	1.796232	-1.826393	-0.416269
C	2.027166	-0.460193	0.299018
O	2.804989	-2.566909	-0.507081
O	0.641101	-2.008906	-0.853560
H	1.224095	-0.252234	1.001534
C	2.116208	0.657951	-0.740580
N	3.316647	-0.562755	1.068978
H	3.168737	-0.933872	2.007685
H	1.169125	0.706087	-1.272669
H	2.912165	0.455599	-1.460124
S	2.494167	2.314233	-0.028753
H	3.898148	-1.245528	0.555893
H	3.780420	0.347872	1.155362
H	1.340084	2.407671	0.667557
28			
Dimer 213 of the n...z type			
C	2.838900	-0.721407	0.196388
C	2.285595	-0.804289	-1.232810
N	1.834642	-0.993639	1.233146
H	1.003145	-1.450218	0.849620
H	2.214888	-1.597997	1.953451
H	3.671840	-1.431919	0.240396
C	3.459941	0.667814	0.437890
O	4.367753	1.116760	-0.226254
O	2.893990	1.343960	1.435638
H	2.186604	0.729920	1.769832
H	3.094975	-0.663712	-1.946557
H	1.843268	-1.786967	-1.394556
S	0.943003	0.390174	-1.656037
H	1.693111	1.511493	-1.637453
C	-1.879987	-1.814677	0.159711
C	-2.302395	-0.382123	0.617470
O	-0.646147	-2.055803	0.140720
O	-2.828343	-2.561311	-0.141453
H	-2.914049	-0.472687	1.515878
C	-3.082207	0.343358	-0.478044
N	-1.089301	0.419053	0.998966
H	-0.580140	-0.016687	1.768858
H	-3.944838	-0.262940	-0.742145
H	-2.468468	0.468599	-1.372430
S	-3.627483	2.046534	-0.025655
H	-0.422987	0.473895	0.203518
H	-1.354817	1.371167	1.269838
H	-4.505334	1.681929	0.931194
28			
Dimer 214 of the n...z type			
C	3.006381	0.248329	-0.377674
C	1.926931	-0.396529	-1.252074
N	4.205047	-0.548239	-0.109225
H	3.986867	-1.540235	-0.060156
H	4.912226	-0.416213	-0.822440
H	3.318554	1.165612	-0.889909
C	2.426707	0.740800	0.964139
O	1.312998	1.205058	1.089426
O	3.273049	0.633127	1.982303
H	4.066701	0.176398	1.597909
H	1.113430	0.308024	-1.412808
H	2.350790	-0.661236	-2.220452
S	1.251247	-1.983058	-0.585739
H	0.930213	-1.529726	0.644478
C	-3.269209	-0.797005	0.871489
C	-2.107294	-0.076972	0.104991
O	-3.879889	-1.676962	0.210609
O	-3.465270	-0.401901	2.034082
H	-1.192672	-0.142344	0.692322

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C	-2.455435	1.387906	-0.149591
N	-1.894102	-0.827674	-1.182052
H	-1.045415	-1.411881	-1.144094
H	-2.604000	1.872492	0.812758
H	-3.381839	1.474423	-0.721453
S	-1.190368	2.306811	-1.127575
H	-2.730826	-1.442009	-1.253726
H	-1.809571	-0.209865	-1.992566
H	-0.160716	2.094154	-0.276952
28			
Dimer 215 of the n...z type			
C	-1.789440	0.387136	0.291721
C	-1.619434	-0.370380	-1.030443
N	-1.957046	-0.430093	1.495013
H	-2.463585	-1.284657	1.275968
H	-1.037419	-0.679130	1.864888
H	-0.883114	0.988373	0.431141
C	-2.930989	1.416620	0.223398
O	-3.186213	2.086887	-0.753613
O	-3.604973	1.528049	1.367899
H	-3.190231	0.832225	1.950082
H	-1.459029	0.327374	-1.850837
H	-0.755126	-1.029228	-0.946335
S	-3.032168	-1.478325	-1.453542
H	-3.926317	-0.504962	-1.722775
C	1.472231	-1.119545	1.006765
C	2.818691	-0.470335	0.552948
O	1.056599	-2.056769	0.284405
O	0.939513	-0.595795	2.006304
H	3.483350	-0.339037	1.404331
C	2.533832	0.871417	-0.123800
N	3.471829	-1.422536	-0.411952
H	4.079089	-2.089119	0.065712
H	2.060878	1.526630	0.604418
H	1.846648	0.741017	-0.962532
S	4.012447	1.697828	-0.847384
H	2.696263	-1.960386	-0.836256
H	4.030659	-0.933672	-1.118858
H	4.681238	1.872483	0.310950
28			
Dimer 216 of the n...z type			
C	-1.624025	-0.869618	-0.271452
C	-1.973742	0.400379	-1.058590
N	-2.563675	-1.986435	-0.402784
H	-3.507733	-1.654075	-0.583740
H	-2.296989	-2.616157	-1.149881
H	-0.636220	-1.211561	-0.611033
C	-1.420581	-0.566675	1.220859
O	-0.824842	0.408019	1.634753
O	-1.915176	-1.494862	2.032628
H	-2.348308	-2.146009	1.417473
H	-1.232327	1.177722	-0.883828
H	-1.989819	0.171181	-2.124207
S	-3.642527	1.093715	-0.688283
H	-3.359228	1.530328	0.556050
C	2.464889	-1.415416	-0.582667
C	2.219017	-0.085701	0.201965
O	3.668134	-1.748810	-0.712772
O	1.434584	-1.968038	-1.014940
H	1.450178	-0.231072	0.956962
C	1.810703	1.021750	-0.765946
N	3.501862	0.272305	0.905053
H	3.534630	-0.108995	1.850902
H	0.959144	0.670675	-1.344061
H	2.617569	1.241355	-1.468127
S	1.403838	2.623484	0.047363
H	4.249082	-0.190610	0.356950
H	3.645554	1.283824	0.969666
H	0.407011	2.128337	0.813357

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28		
Dimer 217 of the n...z	type	
C	2.670222	-0.910239
C	3.315801	0.402381
N	1.796346	-1.579111
H	1.300294	-0.902734
H	2.316132	-2.193995
H	3.483711	-1.599053
C	1.907044	-0.703991
O	2.286630	0.006345
O	0.764465	-1.400996
H	0.640990	-1.869953
H	3.975266	0.799434
H	3.903158	0.212207
S	2.100120	1.706638
H	1.721242	2.031529
C	-2.263490	-1.533978
C	-2.487733	-0.214021
O	-1.544846	-2.402569
O	-2.822630	-1.554119
H	-3.558717	-0.037984
C	-1.826439	0.971635
N	-1.943195	-0.369953
H	-2.487260	-1.053435
H	-2.248397	1.053352
H	-0.750056	0.823257
S	-1.997458	2.581601
H	-0.970534	-0.718749
H	-1.968441	0.525525
H	-3.333420	2.702233
28		
Dimer 218 of the n...z	type	
C	1.438853	-0.250052
C	2.090539	1.046971
N	0.621920	-0.008060
H	1.200606	0.268633
H	0.111917	-0.846462
H	0.772065	-0.604027
C	2.476667	-1.355613
O	2.678094	-1.949703
O	3.152094	-1.606030
H	3.794247	-2.314870
H	2.614186	0.874126
H	1.306398	1.784844
S	3.248027	1.850291
H	4.266193	0.976157
C	-2.070375	-1.395533
C	-3.176022	-0.362738
O	-2.108537	-1.801344
O	-1.280157	-1.708769
H	-3.855313	-0.861723
C	-2.625090	0.902062
N	-3.952410	-0.046373
H	-4.963213	-0.037525
H	-3.428570	1.475682
H	-1.927223	0.591122
S	-1.799951	2.073167
H	-3.658156	-0.780731
H	-3.643930	0.861666
H	-0.784385	1.235007
28		
Dimer 219 of the n...z	type	
C	-2.864078	0.726569
C	-2.333378	-0.440356
N	-4.042454	0.443889
H	-4.077028	-0.540569
H	-4.904020	0.681562
H	-3.113826	1.538639
C	-1.759289	1.317258

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O	-0.625158	1.514689
O	-2.168637	1.629480
H	-3.121839	1.346200
H	-1.418615	-0.141855
H	-3.077139	-0.702584
S	-2.035908	-1.997129
H	-0.947031	-1.604834
C	1.796158	-1.640437
C	1.938647	-0.399029
O	2.771322	-2.428822
O	0.744290	-1.683355
H	1.005776	-0.191354
C	2.357498	0.816667
N	2.989628	-0.722487
H	2.593574	-1.206184
H	1.563823	1.025416
H	3.281236	0.614811
S	2.690346	2.330585
H	3.646167	-1.373961
H	3.464303	0.122511
H	1.415515	2.507125
28		
Dimer 220 of the n...z	type	
C	-2.825878	-0.227087
C	-3.407163	-0.863702
N	-1.790162	-1.058438
H	-1.021631	-1.229938
H	-1.395502	-0.624372
H	-3.658494	-0.159002
C	-2.407657	1.218325
O	-1.267550	1.633023
O	-3.464720	1.994433
H	-3.157755	2.894242
H	-4.293031	-0.325663
H	-3.686317	-1.891620
S	-2.229681	-0.982787
H	-2.368107	0.285272
C	1.868961	-1.141745
C	1.743085	0.392099
O	1.013283	-1.855922
O	2.764410	-1.479487
H	1.135603	0.813383
C	3.066090	1.142102
N	0.936794	0.553167
H	0.247591	1.303953
H	2.903914	2.210857
H	3.590736	0.995746
S	4.152810	0.614275
H	0.437608	-0.347374
H	1.542200	0.699583
H	4.338677	-0.648307
28		
Dimer 221 of the n...z	type	
C	2.799161	0.507619
C	1.301290	0.539548
N	3.677068	1.248846
H	3.330444	1.215662
H	3.762015	2.221460
H	2.919305	0.933058
C	3.319980	-0.937004
O	2.677368	-1.842295
O	4.566142	-1.098365
H	4.813464	-0.212830
H	0.743961	-0.004458
H	0.939396	1.566590
S	0.878941	-0.147692
H	1.038270	-1.450653
C	-1.895749	1.759332
C	-2.726874	0.589035

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O	-1.353464	2.536062	-0.156504	
O	-1.887588	1.792609	1.911101	
H	-3.783515	0.849212	0.123427	
C	-2.461440	-0.757899	0.698057	
N	-2.424226	0.524890	-1.435641	
H	-2.489709	1.465752	-1.830873	
H	-2.662257	-0.663076	1.761714	
H	-1.417136	-1.051015	0.577918	
S	-3.432871	-2.161305	-0.003563	
H	-1.446347	0.215935	-1.583039	
H	-3.050527	-0.117125	-1.926481	
H	-4.642255	-1.748576	0.428029	
28				
Dimer 222 of the n...z type				
C	1.726713	-0.198494	0.425420	
C	3.054865	-0.780101	0.923366	
N	1.053028	-0.937089	-0.643707	
H	1.710943	-1.486674	-1.188718	
H	0.313594	-1.539364	-0.274361	
H	1.055102	-0.161844	1.291138	
C	1.883865	1.274560	-0.006323	
O	2.525985	2.097412	0.607134	
O	1.206503	1.565745	-1.117835	
H	0.839965	0.676178	-1.394888	
H	3.458407	-0.162960	1.724307	
H	2.885762	-1.785526	1.309100	
S	4.337050	-0.977023	-0.388075	
H	4.580290	0.336953	-0.571617	
C	-2.422759	-1.802114	0.208750	
C	-2.393997	-0.341334	-0.346844	
O	-3.557536	-2.323218	0.294384	
O	-1.308813	-2.263623	0.538162	
H	-1.582303	-0.229380	-1.061354	
C	-2.242174	0.646554	0.809927	
N	-3.688792	-0.100164	-1.073384	
H	-3.639140	-0.404521	-2.046556	
H	-1.335702	0.400314	1.358253	
H	-3.082366	0.559124	1.502133	
S	-2.207728	2.419580	0.309838	
H	-4.394940	-0.689526	-0.603579	
H	-3.955512	0.889330	-1.064771	
H	-1.041080	2.372793	-0.368202	
28				
Dimer 223 of the n...z type				
C	2.006353	-1.034198	0.287636	
C	3.272192	-1.346655	-0.532843	
N	0.821655	-0.704464	-0.513407	
H	1.058378	0.006237	-1.205457	
H	0.549908	-1.525007	-1.050774	
H	1.769374	-1.934292	0.865122	
C	2.325016	0.029203	1.349609	
O	3.295555	-0.076921	2.063583	
O	1.507644	1.078565	1.480552	
H	0.765080	1.086873	0.842488	
H	4.085210	-1.646835	0.125197	
H	3.058605	-2.167624	-1.217914	
S	3.835372	0.044782	-1.602539	
H	4.348755	0.808697	-0.616682	
C	-3.936923	-0.868948	-0.150532	
C	-2.819273	0.108601	0.369061	
O	-3.689354	-2.092673	0.007645	
O	-4.935007	-0.324141	-0.652835	
H	-3.242860	0.701699	1.179234	
C	-2.327781	1.018981	-0.749179	
N	-1.716910	-0.741895	0.939322	
H	-1.551172	-0.564123	1.928215	
H	-3.186526	1.540431	-1.164472	
H	-1.864318	0.439528	-1.550141	
S	-1.049928	2.254107	-0.256061	

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H	-2.083631	-1.710091	0.818299
H	-0.806443	-0.649392	0.428887
H	-1.748896	2.835651	0.740129
28			
Dimer 224 of the n...z type			
C	-2.652261	-0.485714	-0.997420
C	-3.160270	-1.128684	0.296331
N	-1.573844	-1.190029	-1.699260
H	-0.996786	-1.727472	-1.059016
H	-1.935838	-1.829758	-2.396481
H	-3.510083	-0.425263	-1.676962
C	-2.233381	0.980291	-0.780104
O	-2.793956	1.740545	-0.025612
O	-1.193291	1.352461	-1.532131
H	-0.924114	0.522971	-2.007118
H	-4.034616	-0.595216	0.664400
H	-3.443069	-2.162253	0.098654
S	-1.933488	-1.208645	1.675425
H	-1.972303	0.103021	1.987354
C	2.881621	-1.224443	-0.533327
C	1.858435	-0.164349	0.001383
O	3.253260	-2.080417	0.310822
O	3.217867	-1.086295	-1.722373
H	0.978514	-0.169439	-0.637644
C	2.479980	1.229921	0.020382
N	1.439627	-0.604067	1.377064
H	0.478762	-0.972488	1.388173
H	2.762229	1.489498	-0.997353
H	3.380619	1.243390	0.637656
S	1.388600	2.538192	0.726801
H	2.107320	-1.367903	1.609343
H	1.480667	0.152751	2.063649
H	0.370648	2.371583	-0.144016
28			
Dimer 225 of the n...z type			
C	-2.083132	-0.762451	0.301763
C	-1.773697	0.333537	1.331853
N	-1.216363	-0.837534	-0.872310
H	-0.951688	0.095739	-1.177820
H	-0.368277	-1.381904	-0.692538
H	-2.011645	-1.720480	0.830653
C	-3.550291	-0.692552	-0.167265
O	-4.478412	-0.384842	0.547512
O	-3.710849	-1.039770	-1.443846
H	-2.781819	-1.191561	-1.767572
H	-2.517527	0.320057	2.126760
H	-0.796036	0.151964	1.778666
S	-1.670484	2.037448	0.635756
H	-2.969462	2.156058	0.292247
C	2.306905	-1.820335	0.147105
C	2.234543	-0.269391	0.332530
O	3.393559	-2.350639	0.470423
O	1.279872	-2.342394	-0.335923
H	1.302473	0.003336	0.819497
C	2.358685	0.427334	-1.022233
N	3.362583	0.136397	1.241265
H	3.087245	0.102412	2.223396
H	1.561353	0.070380	-1.669998
H	3.309750	0.176950	-1.496566
S	2.322371	2.267209	-0.943977
H	4.103597	-0.571399	1.104089
H	3.698307	1.083777	1.040954
H	1.048551	2.382431	-0.510748
28			
Dimer 226 of the n...z type			
C	-2.772788	-0.959652	0.213897
C	-3.462286	0.412681	0.253500
N	-2.010998	-1.326813	1.404172
H	-1.598011	-0.509800	1.846043

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H	-2.590299	-1.795165	2.090170
H	-3.558367	-1.709815	0.068152
C	-1.885460	-1.089604	-1.037794
O	-2.227113	-0.691953	-2.131226
O	-0.715362	-1.692169	-0.846816
H	-0.617498	-1.882755	0.118356
H	-4.033172	0.581799	-0.657690
H	-4.142854	0.447323	1.104364
S	-2.298739	1.823939	0.502237
H	-1.771165	1.816728	-0.738402
C	2.230248	-1.515121	0.431736
C	2.520087	0.022571	0.507573
O	2.889484	-2.138633	-0.435712
O	1.351387	-1.929349	1.210883
H	2.670517	0.330777	1.540229
C	1.358905	0.792927	-0.119856
N	3.797546	0.272640	-0.248617
H	4.614576	0.227136	0.360759
H	0.465700	0.610785	0.472085
H	1.165717	0.442568	-1.135149
S	1.623376	2.607708	-0.279237
H	3.868061	-0.512112	-0.921857
H	3.798721	1.185037	-0.715779
H	1.708645	2.874367	1.040469
28			
Dimer 227 of the n...z type			
C	2.533773	-0.376474	-0.793419
C	3.029889	0.808358	0.044538
N	1.547432	-0.094808	-1.837905
H	0.871696	0.635503	-1.592887
H	1.990316	0.163746	-2.711123
H	3.417424	-0.806593	-1.280410
C	1.992947	-1.518751	0.087919
O	2.450637	-1.828634	1.163945
O	0.965417	-2.163941	-0.473148
H	0.821843	-1.666038	-1.328011
H	3.880173	0.508390	0.654955
H	3.354092	1.604474	-0.625604
S	1.769764	1.575997	1.154200
H	1.826166	0.635012	2.117999
C	-1.513360	1.772147	-0.592146
C	-1.570612	0.405518	0.162900
O	-2.251670	2.672778	-0.128622
O	-0.763936	1.795284	-1.589696
H	-0.563659	0.028169	0.317276
C	-2.411482	-0.600108	-0.620538
N	-2.169758	0.661204	1.518058
H	-1.454757	0.921801	2.198521
H	-1.960676	-0.731769	-1.602140
H	-3.428861	-0.230198	-0.762038
S	-2.596129	-2.235298	0.211026
H	-2.793977	1.476534	1.399920
H	-2.670241	-0.157071	1.879669
H	-1.281927	-2.545948	0.213831
28			
Dimer 228 of the n...z type			
C	2.921888	0.627662	0.434379
C	1.870198	-0.290452	1.068219
N	2.366918	1.574534	-0.543203
H	1.347389	1.635272	-0.510311
H	2.731837	2.508063	-0.390504
H	3.417820	1.146085	1.262152
C	4.012189	-0.217529	-0.253311
O	4.710072	-1.015386	0.334515
O	4.106125	0.001346	-1.561776
H	3.404457	0.693461	-1.729703
H	2.336369	-0.926626	1.816999
H	1.102463	0.314334	1.550073
S	0.988855	-1.389054	-0.140212

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H	1.695178	-2.511595	0.091978
C	-1.229022	1.131211	0.428345
C	-2.231252	0.046941	-0.078184
O	-1.114086	1.206173	1.674019
O	-0.658679	1.800664	-0.458931
H	-1.888746	-0.370068	-1.023069
C	-3.630039	0.643580	-0.219104
N	-2.231146	-1.065135	0.931973
H	-1.371024	-1.620135	0.831310
H	-3.593813	1.446724	-0.952937
H	-3.964815	1.063705	0.731286
S	-4.932506	-0.571650	-0.694759
H	-2.206620	-0.633134	1.865064
H	-3.049763	-1.673595	0.830071
H	-4.443932	-0.857878	-1.918942
28			
Dimer 229 of the n...z type			
C	-1.607171	-0.131744	0.352101
C	-2.385283	1.194232	0.419389
N	-0.715390	-0.169207	-0.791748
H	-1.244041	-0.177369	-1.658856
H	-0.126274	-0.999648	-0.756605
H	-0.997112	-0.173820	1.262167
C	-2.557782	-1.330238	0.432210
O	-2.654392	-2.199450	-0.400963
O	-3.290477	-1.303497	1.562903
H	-3.879023	-2.075372	1.574887
H	-2.968837	1.253572	1.335728
H	-1.668103	2.014592	0.408887
S	-3.494890	1.511200	-1.020100
H	-4.458153	0.627171	-0.688017
C	2.531429	-1.273375	-0.426037
C	3.282857	-0.306637	0.548429
O	3.007144	-1.342362	-1.586589
O	1.561116	-1.884011	0.063719
H	3.860099	-0.927723	1.236263
C	2.370170	0.616117	1.355582
N	4.266335	0.471837	-0.282243
H	5.168784	0.620419	0.167353
H	2.934024	1.128951	2.135411
H	1.607473	0.001090	1.828309
S	1.571668	1.949300	0.362077
H	4.360040	-0.082249	-1.155223
H	3.857013	1.380824	-0.536092
H	0.676600	1.147583	-0.310511
28			
Dimer 230 of the n...z type			
C	2.497439	-0.609668	-0.346599
C	2.090977	0.730665	-0.973638
N	1.499837	-1.327210	0.446771
H	1.002291	-0.688110	1.062234
H	0.806694	-1.778696	-0.146200
H	2.776270	-1.262405	-1.183219
C	3.791792	-0.490168	0.480554
O	4.686033	0.287628	0.236200
O	3.861083	-1.363920	1.487237
H	2.985780	-1.828354	1.475440
H	2.941516	1.161391	-1.499552
H	1.276348	0.570809	-1.680910
S	1.422870	1.987044	0.198332
H	2.430585	1.980738	1.094455
C	-1.318803	-0.644458	-1.294079
C	-2.106602	-0.169597	-0.030077
O	-1.111079	0.238105	-2.159484
O	-0.996433	-1.850237	-1.297044
H	-1.657900	-0.585393	0.870397
C	-3.572578	-0.588532	-0.134199
N	-1.988612	1.326762	0.049820
H	-1.085391	1.602679	0.453465

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H -3.617464	-1.674489	-0.184946	
H -4.024932	-0.185860	-1.042540	
S -4.638178	0.018189	1.241646	
H -2.000909	1.680017	-0.917377	
H -2.743922	1.739287	0.607573	
H -4.032796	-0.674260	2.228354	
28			
Dimer 231 of the n...z type			
C 2.921623	-0.633613	-0.427157	
C 1.865680	0.277788	-1.063527	
N 2.373215	-1.571801	0.562035	
H 1.354468	-1.645323	0.528023	
H 2.749818	-2.503131	0.424561	
H 3.413829	-1.158251	-1.253288	
C 4.014027	0.219619	0.247157	
O 4.711804	1.008543	-0.352700	
O 4.109473	0.019265	1.558515	
H 3.407871	-0.670028	1.737277	
H 2.328101	0.908050	-1.819608	
H 1.096794	-0.331679	-1.537396	
S 0.988589	1.386063	0.139048	
H 1.691888	2.507469	-0.107580	
C -1.229627	-1.129410	-0.429466	
C -2.232642	-0.046276	0.077862	
O -1.121269	-1.208958	-1.675441	
O -0.651845	-1.793097	0.457257	
H -1.890283	0.370766	1.022782	
C -3.631099	-0.643567	0.218543	
N -2.233010	1.066147	-0.931936	
H -1.371569	1.619371	-0.832421	
H -3.594668	-1.446984	0.952100	
H -3.965597	-1.063483	-0.732027	
S -4.934059	0.570955	0.694681	
H -2.211335	0.634814	-1.865347	
H -3.050419	1.675882	-0.828137	
H -4.445900	0.856543	1.919174	
28			
Dimer 232 of the n...z type			
C 2.125599	0.785292	0.254334	
C 1.746366	-0.191250	1.377489	
N 1.246753	0.840141	-0.911713	
H 0.938998	-0.095758	-1.164949	
H 0.419603	1.419902	-0.745010	
H 2.143271	1.786009	0.702885	
C 3.572436	0.557746	-0.225898	
O 4.481427	0.207873	0.493533	
O 3.744193	0.820359	-1.521871	
H 2.829973	1.034708	-1.847976	
H 2.514069	-0.188527	2.149474	
H 0.807198	0.122909	1.833096	
S 1.454732	-1.926605	0.827442	
H 2.714945	-2.187464	0.423535	
C -2.237230	1.827582	0.151535	
C -2.159064	0.272043	0.293717	
O -3.301441	2.349756	0.553761	
O -1.240951	2.361823	-0.379655	
H -1.196741	-0.017801	0.706808	
C -2.378223	-0.393132	-1.064762	
N -3.225529	-0.150856	1.266564	
H -2.883685	-0.150122	2.228312	
H -1.622235	-0.027161	-1.756099	
H -3.357616	-0.128367	-1.468162	
S -2.349894	-2.234809	-1.020012	
H -3.964444	0.569894	1.200324	
H -3.585596	-1.088043	1.060040	
H -1.068837	-2.360711	-0.609745	
28			
Dimer 233 of the n...z type			
C 3.258892	0.682883	-0.216794	

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C 1.760609	0.677283	0.106726	
N 3.624307	0.617222	-1.633358	
H 2.964133	0.048348	-2.157669	
H 3.654594	1.536839	-2.057366	
H 3.666952	1.614550	0.191823	
C 4.005902	-0.429492	0.544727	
O 3.725462	-0.779260	1.669050	
O 5.019818	-0.958126	-0.139606	
H 4.979073	-0.516678	-1.026470	
H 1.601501	0.753793	1.180476	
H 1.280410	1.526361	-0.378393	
S 0.865625	-0.809649	-0.523314	
H 1.404837	-1.699257	0.335849	
C -3.955981	-1.066014	-0.324255	
C -3.139049	0.022142	0.459692	
O -3.698767	-2.254873	-0.002548	
O -4.780700	-0.631797	-1.147550	
H -3.812440	0.459785	1.198129	
C -2.571772	1.108598	-0.443080	
N -2.060876	-0.699818	1.223056	
H -2.390144	-1.683880	1.249325	
H -3.394039	1.573261	-0.980744	
H -1.887954	0.682933	-1.179977	
S -1.591561	2.398532	0.438763	
H -1.155807	-0.688465	0.722574	
H -1.910306	-0.332354	2.161126	
H -2.607953	2.900863	1.169362	
28			
Dimer 234 of the n...z type			
C 2.019480	-1.096327	0.100278	
C 3.305451	-1.210044	-0.740767	
N 0.835065	-0.658167	-0.647958	
H 1.064249	0.159602	-1.213013	
H 0.581181	-1.385177	-1.313677	
H 1.806164	-2.095220	0.494991	
C 2.294382	-0.243585	1.348246	
O 3.238018	-0.482771	2.066549	
O 1.472862	0.770065	1.636216	
H 0.756741	0.902438	0.980976	
H 4.120339	-1.602155	-0.135261	
H 3.128351	-1.894560	-1.570812	
S 3.833008	0.374286	-1.521708	
H 4.302273	0.959589	-0.400607	
C -3.967565	-0.787472	-0.239920	
C -2.797609	0.060708	0.380358	
O -3.749872	-2.025092	-0.308469	
O -4.970272	-0.141224	-0.589375	
H -3.170182	0.537184	1.286247	
C -2.311745	1.113892	-0.607484	
N -1.711064	-0.903608	0.770747	
H -1.535273	-0.911785	1.773883	
H -3.166265	1.712060	-0.914232	
H -1.888816	0.648332	-1.500010	
S -0.987848	2.235586	0.017239	
H -2.106975	-1.824984	0.485222	
H -0.800538	-0.745509	0.276268	
H -1.662079	2.723801	1.078368	
28			
Dimer 235 of the n...z type			
C 2.236892	0.048867	-0.789432	
C 3.688041	-0.451454	-0.884343	
N 2.048773	1.492278	-0.841617	
H 2.707981	1.958911	-0.223877	
H 2.207667	1.842234	-1.779629	
H 1.701381	-0.381588	-1.646237	
C 1.523963	-0.547344	0.435498	
O 1.889765	-1.577365	0.965102	
O 0.447154	0.092446	0.878590	
H 0.188854	0.899246	0.354259	

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H	3.723529	-1.539564	-0.894023
H	4.128366	-0.080368	-1.810372
S	4.792979	0.168316	0.455612
H	4.253655	-0.570738	1.445678
C	-2.355029	1.729870	0.034791
C	-2.633317	0.238390	0.411917
O	-3.368851	2.440314	-0.145512
O	-1.147358	2.038173	-0.079694
H	-2.010822	-0.058623	1.252428
C	-2.363075	-0.663842	-0.792108
N	-4.075654	0.143629	0.831833
H	-4.187528	0.277987	1.837097
H	-1.327792	-0.533355	-1.094802
H	-2.999578	-0.387631	-1.635365
S	-2.700657	-2.449669	-0.493348
H	-4.555342	0.928587	0.358026
H	-4.492481	-0.759908	0.587778
H	-1.777402	-2.620358	0.475494
28			
Dimer 236 of the n...z type			
C	1.460260	-0.374127	-0.177774
C	1.935032	0.908709	-0.881790
N	0.618306	-0.068495	0.968154
H	1.176784	0.273572	1.744822
H	0.117127	-0.897117	1.277231
H	0.843427	-0.917859	-0.901288
C	2.638918	-1.285031	0.161071
O	2.933429	-1.662291	1.271204
O	3.331636	-1.629267	-0.942933
H	4.071731	-2.201152	-0.683450
H	2.491294	0.671086	-1.786418
H	1.058447	1.495284	-1.155998
S	2.950385	2.039415	0.166272
H	4.092165	1.321578	0.134448
C	-1.994218	-1.414283	-0.344318
C	-3.168729	-0.389462	-0.468260
O	-1.901848	-2.000964	0.766919
O	-1.291474	-1.546635	-1.361582
H	-3.897386	-0.815461	-1.159401
C	-2.734811	0.985774	-0.983950
N	-3.824178	-0.299553	0.882425
H	-4.842483	-0.316419	0.854473
H	-3.600604	1.573472	-1.290838
H	-2.096626	0.826637	-1.850634
S	-1.863552	2.027207	0.263699
H	-3.442434	-1.112395	1.405036
H	-3.507432	0.557269	1.358694
H	-0.804887	1.175656	0.520997
28			
Dimer 237 of the n...z type			
C	3.213369	0.609593	-0.432549
C	1.700380	0.622350	-0.188408
N	3.660282	0.188974	-1.762327
H	3.047426	-0.524953	-2.148413
H	3.688920	0.965546	-2.412313
H	3.568661	1.633055	-0.267824
C	3.950491	-0.227444	0.630975
O	3.619117	-0.278627	1.794063
O	5.015619	-0.873875	0.158598
H	5.009405	-0.685528	-0.814976
H	1.477568	0.980171	0.814593
H	1.222863	1.285617	-0.909166
S	0.890250	-1.018666	-0.431313
H	1.426948	-1.623684	0.648704
C	-3.987529	-1.008328	-0.249598
C	-3.117201	0.083915	0.468749
O	-3.770525	-2.189166	0.126161
O	-4.808984	-0.582593	-1.080684
H	-3.759762	0.574665	1.201447

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C	-2.533965	1.110698	-0.491075
N	-2.047991	-0.640076	1.242041
H	-1.855505	-0.226324	2.152846
H	-3.351824	1.580982	-1.030590
H	-1.883490	0.630577	-1.224648
S	-1.491670	2.402615	0.314552
H	-2.415173	-1.606108	1.333883
H	-1.155981	-0.697011	0.720152
H	-2.478453	2.976925	1.032808
28			
Dimer 238 of the n...z type			
C	2.801166	0.453980	0.838878
C	2.058132	-0.765350	1.397924
N	1.988068	1.599043	0.432044
H	1.065630	1.350294	0.068680
H	1.854062	2.253584	1.192747
H	3.488166	0.790608	1.624641
C	3.724064	0.061949	-0.331808
O	4.361444	-0.967763	-0.375252
O	3.779629	0.984696	-1.290163
H	3.130785	1.678258	-0.985994
H	2.767740	-1.505271	1.764498
H	1.424934	-0.451184	2.227879
S	0.921713	-1.583162	0.199892
H	1.873274	-2.141108	-0.574680
C	-1.935344	1.846958	-0.199004
C	-2.277135	0.403004	0.295632
O	-2.889262	2.661874	-0.167626
O	-0.767965	2.008581	-0.603812
H	-1.507433	0.042442	0.974183
C	-2.416211	-0.530592	-0.906614
N	-3.573539	0.485500	1.056645
H	-3.420310	0.652805	2.051303
H	-1.460321	-0.560666	-1.423938
H	-3.171743	-0.155381	-1.599870
S	-2.952830	-2.243836	-0.491441
H	-4.060273	1.315350	0.673074
H	-4.133729	-0.367471	0.961601
H	-1.853409	-2.580906	0.214617
28			
Dimer 239 of the n...z type			
C	2.801162	-0.581352	-0.378361
C	1.320945	-0.298513	-0.100376
N	3.506216	-1.390707	0.620324
H	3.131401	-1.223477	1.551165
H	3.429917	-2.381277	0.422461
H	2.851520	-1.109272	-1.337608
C	3.593417	0.719157	-0.613226
O	3.156089	1.675342	-1.213668
O	4.830742	0.688550	-0.117695
H	4.888375	-0.189024	0.342997
H	0.895245	0.296240	-0.906731
H	0.770386	-1.236432	-0.033468
S	0.999975	0.549944	1.504904
H	1.525875	1.745185	1.166630
C	-1.857047	-1.701600	-0.613541
C	-2.953499	-0.617319	-0.341974
O	-1.401917	-2.264976	0.414993
O	-1.530882	-1.844611	-1.804501
H	-3.796265	-0.752800	-1.016657
C	-2.345090	0.776328	-0.505282
N	-3.441311	-0.819917	1.067647
H	-4.243941	-1.448396	1.106614
H	-2.015237	0.886259	-1.535958
H	-1.478100	0.893646	0.148721
S	-3.464481	2.167076	-0.050516
H	-2.656327	-1.286544	1.557507
H	-3.706997	0.063055	1.515458
H	-4.409675	1.930232	-0.983612

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28		
Dimer 240 of the n...z	type	
C	-2.292152	-0.333964
C	-2.011379	1.169253
N	-3.637271	-0.775766
H	-4.328553	-0.062058
H	-3.701159	-0.986940
H	-1.573324	-0.851546
C	-1.973316	-0.860305
O	-1.034596	-0.477366
O	-2.805828	-1.810697
H	-3.480507	-1.882980
H	-0.984557	1.387586
H	-2.155709	1.482096
S	-3.146758	2.230765
H	-2.662601	1.887309
C	3.340532	1.345035
C	3.080984	-0.192174
O	3.492461	1.737529
O	3.327394	1.997628
H	3.707649	-0.604397
C	1.601429	-0.426982
N	3.468023	-0.843412
H	4.438042	-1.158955
H	1.358479	0.068657
H	0.976735	-0.004993
S	1.095020	-2.196597
H	3.389629	-0.087257
H	2.875042	-1.647708
H	1.841343	-2.533189
28		
Dimer 241 of the n...z	type	
C	3.164620	-0.019483
C	1.739103	0.223955
N	4.090742	1.114188
H	3.606709	1.994691
H	4.553823	1.165581
C	3.581372	-0.830357
C	3.170212	-0.577451
O	2.338152	-1.345586
O	4.201971	-0.157136
H	4.676026	0.487133
H	1.142723	-0.685989
H	1.773433	0.564759
S	0.841990	1.558557
H	0.726951	0.896102
C	-1.690169	-1.842598
C	-2.636439	-0.593653
O	-0.849450	-1.919444
O	-1.903791	-2.629057
H	-3.588876	-0.928622
C	-2.856573	0.064654
N	-2.065598	0.384076
H	-1.715093	-0.152591
H	-3.240260	-0.684726
H	-1.916364	0.441036
S	-3.986216	1.523880
H	-1.244898	0.877466
H	-2.749867	1.081610
H	-5.113644	0.844310
28		
Dimer 242 of the n...z	type	
C	-2.414700	0.175370
C	-1.833617	1.535860
N	-1.512993	-0.971486
H	-0.846430	-1.007697
H	-0.997617	-1.012199
H	-2.828571	0.311131
C	-3.639383	-0.199897

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O	-4.424845	0.604384
O	-3.778162	-1.513825
H	-2.973702	-1.902523
H	-2.602593	2.302940
H	-1.015792	1.795372
S	-1.102745	1.623471
H	-2.208929	1.279878
C	1.762086	-1.954488
C	2.609507	-0.653643
O	0.606542	-1.911581
O	2.320541	-2.868217
H	3.616238	-0.904963
C	2.657609	0.108923
N	1.991617	0.203667
H	2.139552	-0.196743
H	3.130555	-0.528711
H	1.650594	0.345595
S	3.529236	1.731776
H	0.970341	0.260488
H	2.390851	1.148903
H	4.759652	1.240461
28		
Dimer 243 of the n...z	type	
C	-2.525350	-0.811411
C	-1.649704	-1.337643
N	-3.968002	-0.764928
H	-4.154728	-0.605752
H	-4.428876	-1.623596
H	-2.353370	-1.463963
C	-2.067723	0.580986
O	-0.903369	0.908317
O	-3.067389	1.396911
H	-3.885169	0.872020
H	-0.601780	-1.386170
H	-1.972267	-2.347089
S	-1.807541	-0.383534
H	-1.242875	0.761705
C	2.560935	-1.544225
C	2.152137	-0.043382
O	3.782898	-1.787103
O	1.631654	-2.315696
H	1.269413	0.048480
C	1.880653	0.558958
N	3.295519	0.668984
H	3.185078	0.689469
H	1.099387	-0.026653
H	2.770746	0.511814
S	1.399611	2.338945
H	4.130473	0.092516
H	3.400497	1.634325
H	0.361690	2.188793
28		
Dimer 244 of the n...z	type	
C	-2.550737	-0.413277
C	-1.319324	0.471678
N	-2.342501	-1.457129
H	-1.354408	-1.692667
H	-2.822961	-2.311146
H	-2.804023	-0.825064
C	-3.752323	0.458916
O	-4.239837	1.308632
O	-4.202740	0.197550
H	-3.602277	-0.526639
H	-1.560270	1.241370
H	-0.497281	-0.134757
S	-0.787314	1.337479
H	-0.372480	2.476506
C	1.347490	-1.749245
C	2.489675	-0.783914

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O	0.520246	-2.056106	-0.707274		
O	1.382306	-2.108540	1.379835		
H	3.379650	-1.383821	-0.467449		
C	2.802805	0.298539	0.759765		
N	2.083445	-0.166813	-1.576845		
H	1.825842	-0.903493	-2.236445		
H	3.064656	-0.183643	1.697568		
H	1.928569	0.927047	0.937690		
S	4.139361	1.465773	0.255426		
H	1.233120	0.408600	-1.434814		
H	2.825509	0.419454	-1.966998		
H	5.151666	0.575344	0.295579		
28					
Dimer 245 of the n...z type					
C	-3.141368	-0.527163	0.766163		
C	-3.942454	0.773437	0.527281		
N	-1.938249	-0.404511	1.569875		
H	-1.297395	0.306690	1.217668		
H	-2.180057	-0.155030	2.522713		
H	-3.825103	-1.202086	1.294244		
C	-2.905221	-1.226143	-0.582062		
O	-3.851279	-1.479834	-1.306673		
O	-1.677469	-1.548489	-0.956769		
H	-0.910277	-1.279819	-0.367215		
H	-4.889675	0.554674	0.036113		
H	-4.150252	1.239327	1.491371		
S	-3.052657	2.063441	-0.444901		
H	-3.147658	1.455956	-1.645411		
C	1.231562	-0.055135	0.461190		
C	2.780564	-0.109229	0.599955		
O	0.709080	-1.098434	-0.026085		
O	0.686743	1.004707	0.800805		
H	3.085733	0.291065	1.564713		
C	3.422286	0.683565	-0.541330		
N	3.203049	-1.552789	0.542490		
H	3.152263	-1.998061	1.459909		
H	3.097612	1.718890	-0.461895		
H	3.094813	0.297285	-1.508788		
S	5.261239	0.603161	-0.590843		
H	2.526973	-2.034924	-0.068869		
H	4.162326	-1.652020	0.192159		
H	5.480975	1.233919	0.581230		
28					
Dimer 246 of the n...z type					
C	3.282601	0.501967	0.473944		
C	3.328614	-0.956256	-0.022627		
N	3.033288	0.565139	1.902340		
H	2.113787	0.185883	2.112199		
H	3.032180	1.528613	2.221257		
H	4.273109	0.925351	0.271684		
C	2.299370	1.319695	-0.367021		
O	1.318095	1.882392	0.074672		
O	2.641489	1.342893	-1.660899		
H	1.998742	1.871607	-2.161032		
H	3.608595	-0.997870	-1.073191		
H	4.079792	-1.488007	0.560491		
S	1.766648	-1.908780	0.220568		
H	1.084609	-1.433609	-0.843512		
C	-1.677588	-1.217619	-0.485772		
C	-1.544491	0.146906	0.270070		
O	-1.239614	-1.206114	-1.668037		
O	-2.154992	-2.161676	0.165706		
H	-0.634498	0.078665	0.870808		
C	-2.714327	0.488835	1.181870		
N	-1.292684	1.202894	-0.768765		
H	-0.512234	1.820928	-0.517660		
H	-2.528501	1.415131	1.727569		
H	-2.835746	-0.319601	1.898824		
S	-4.305630	0.757627	0.290025		

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H	-1.044474	0.653120	-1.616039		
H	-2.139354	1.741871	-0.968534		
H	-4.421423	-0.500986	-0.181690		
28					
Dimer 247 of the n...z type					
C	-2.596564	0.243201	0.816377		
C	-2.855895	1.175015	-0.372884		
N	-1.440333	0.575252	1.655627		
H	-0.725900	1.106520	1.155769		
H	-1.713130	1.115634	2.467749		
H	-3.495333	0.265599	1.443417		
C	-2.481138	-1.225663	0.362129		
O	-3.183098	-1.726297	-0.488527		
O	-1.545836	-1.909939	1.019021		
H	-1.132055	-1.226666	1.613210		
H	-3.782097	0.899323	-0.874050		
H	-2.949154	2.199619	-0.012750		
S	-1.496675	1.211436	-1.619921		
H	-1.767822	0.012710	-2.174775		
C	2.007157	1.730680	0.202055		
C	2.544325	0.261260	0.256247		
O	1.133735	2.008677	1.065797		
O	2.473416	2.436024	-0.707294		
H	3.626703	0.247799	0.146750		
C	1.879036	-0.563390	-0.847517		
N	2.209728	-0.301752	1.612205		
H	2.939018	-0.097943	2.296349		
H	2.191802	-0.160373	-1.808398		
H	0.792907	-0.480581	-0.789744		
S	2.224207	-2.371290	-0.782540		
H	1.351856	0.182515	1.922866		
H	2.077404	-1.319085	1.576870		
H	3.552249	-2.296238	-1.009137		
28					
Dimer 248 of the n...z type					
C	-2.099400	-0.047470	0.597019		
C	-3.575825	-0.127253	1.004002		
N	-1.478774	1.279136	0.647347		
H	-2.152370	2.004463	0.411448		
H	-1.108075	1.484316	1.567825		
H	-1.539509	-0.706918	1.269978		
C	-1.866805	-0.655266	-0.798051		
O	-2.419975	-1.654173	-1.197274		
O	-0.956544	-0.003827	-1.526655		
H	-0.712843	0.783682	-0.976438		
H	-3.928732	-1.154992	0.938215		
H	-3.685183	0.212862	2.033871		
S	-4.691456	0.958398	0.015630		
H	-4.618204	0.256449	-1.133783		
C	3.480268	1.404993	-0.159210		
C	2.920352	-0.044018	-0.366975		
O	4.637552	1.460483	0.329320		
O	2.701438	2.323536	-0.467999		
H	2.500915	-0.144624	-1.366111		
C	1.864225	-0.341693	0.694406		
N	4.083864	-0.992151	-0.242803		
H	4.499332	-1.209672	-1.148819		
H	1.064357	0.388120	0.591092		
H	2.283674	-0.239188	1.697426		
S	1.179136	-2.051845	0.638612		
H	4.788795	-0.465544	0.308020		
H	3.824637	-1.875969	0.205387		
H	0.708023	-1.990641	-0.624083		
28					
Dimer 249 of the n...z type					
C	-1.699584	0.184812	-0.305784		
C	-2.913578	1.073438	-0.592480		
N	-1.448376	-0.902814	-1.257325		
H	-2.320880	-1.271880	-1.628306		

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H	-0.880282	-0.595117	-2.037473
H	-0.814952	0.836435	-0.285938
C	-1.744236	-0.400936	1.113407
O	-2.161175	0.194285	2.081612
O	-1.222875	-1.628823	1.199734
H	-1.030911	-1.877025	0.257717
H	-2.997417	1.852539	0.163376
H	-2.792600	1.547351	-1.566851
S	-4.516675	0.164003	-0.695942
H	-4.610662	-0.137575	0.615225
C	2.118593	1.818277	0.168257
C	2.454910	0.435296	-0.484217
O	3.114105	2.514196	0.484708
O	0.904592	2.045954	0.328638
H	1.838792	0.275646	-1.366245
C	2.242476	-0.681603	0.535864
N	3.894112	0.484034	-0.923112
H	3.987055	0.822886	-1.881060
H	1.208528	-0.654678	0.871266
H	2.881799	-0.531658	1.408219
S	2.651976	-2.368071	-0.080722
H	4.341190	1.182232	-0.302219
H	4.351950	-0.430697	-0.865749
H	1.724777	-2.402513	-1.060091
28			
Dimer 250 of the n...z type			
C	-2.864851	0.737489	0.127441
C	-3.280875	-0.730846	-0.016894
N	-2.496141	1.433526	-1.109013
H	-2.068943	0.795264	-1.775366
H	-3.300162	1.860157	-1.553799
H	-3.713238	1.270619	0.571977
C	-1.727020	0.907527	1.151340
O	-1.626253	0.256941	2.166339
O	-0.862287	1.872069	0.830736
H	-1.162521	2.186366	-0.061770
H	-3.568206	-1.139567	0.950226
H	-4.136315	-0.797094	-0.689080
S	-1.989451	-1.821820	-0.755274
H	-1.186074	-1.912378	0.324520
C	2.260426	-1.754685	0.341580
C	2.377219	-0.428907	-0.480598
O	1.157904	-2.348824	0.254981
O	3.267131	-2.041867	1.016048
H	3.326955	-0.400493	-1.011838
C	2.254094	0.768660	0.462396
N	1.282055	-0.399536	-1.513125
H	1.542908	-0.922553	-2.349636
H	3.077834	0.729262	1.171574
H	1.316181	0.731988	1.016917
S	2.225887	2.409685	-0.375607
H	0.447040	-0.862473	-1.120252
H	1.061159	0.563107	-1.793464
H	3.473081	2.352050	-0.887367
28			
Dimer 251 of the n...z type			
C	1.956274	-0.737392	0.251716
C	3.437091	-0.626150	0.653788
N	1.791869	-1.323154	-1.064812
H	2.164175	-0.692667	-1.769610
H	0.796001	-1.441774	-1.259588
H	1.475553	-1.395544	0.981303
C	1.258482	0.614351	0.416168
O	0.784996	1.270862	-0.484929
O	1.235345	1.016547	1.701286
H	0.791657	1.878417	1.751157
H	3.536117	-0.276838	1.680135
H	3.889259	-1.614721	0.575508
S	4.467076	0.447232	-0.441335

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H	3.975287	1.634076	-0.029922
C	-1.657661	-1.357065	-0.180488
C	-3.127626	-0.845454	-0.017807
O	-1.043212	-1.573774	0.894672
O	-1.267654	-1.515031	-1.352527
H	-3.787780	-1.678663	-0.264952
C	-3.476778	0.346056	-0.906250
N	-3.320814	-0.539533	1.442178
H	-4.218008	-0.843899	1.817440
H	-4.545800	0.559270	-0.870864
H	-3.203133	0.094219	-1.928283
S	-2.658951	1.920932	-0.408925
H	-2.527214	-1.025913	1.906249
H	-3.207588	0.468491	1.607720
H	-1.380404	1.528822	-0.604491
28			
Dimer 252 of the n...z type			
C	-2.874304	-1.276319	0.281708
C	-3.684394	-0.445963	-0.723476
N	-3.065213	-0.950764	1.697407
H	-3.303394	0.031093	1.816212
H	-3.797140	-1.509885	2.118686
H	-3.151555	-2.325362	0.130965
C	-1.369337	-1.221656	-0.041342
O	-0.918669	-1.261389	-1.163580
O	-0.591615	-1.138673	1.040793
H	-1.234573	-1.102196	1.799058
H	-3.450056	-0.757196	-1.740005
H	-4.748487	-0.603638	-0.546977
S	-3.439109	1.375846	-0.574872
H	-2.157056	1.411186	-0.996495
C	3.527548	-0.923125	-0.353074
C	2.545870	0.053750	0.377525
O	4.719621	-0.524544	-0.417921
O	3.012412	-1.956337	-0.814981
H	1.911014	-0.488676	1.074503
C	1.686090	0.782516	-0.653901
N	3.392594	1.027051	1.155039
H	3.551910	0.713561	2.112578
H	1.066586	0.045390	-1.159717
H	2.309728	1.288330	-1.393726
S	0.610509	2.105512	0.049228
H	4.307374	1.026160	0.665864
H	2.973729	1.961776	1.191699
H	-0.074969	1.306047	0.891402
28			
Dimer 253 of the n...z type			
C	-2.961979	0.449065	-0.493238
C	-3.172515	-1.021420	-0.877308
N	-2.026668	1.204783	-1.330816
H	-1.310086	0.610999	-1.738154
H	-2.500494	1.684179	-2.086722
H	-3.939866	0.939017	-0.548434
C	-2.532093	0.573563	0.981084
O	-3.032264	-0.057082	1.882741
O	-1.537841	1.446078	1.180374
H	-1.345259	1.822820	0.280127
H	-3.988927	-1.454450	-0.303097
H	-3.421755	-1.083089	-1.936097
S	-1.688486	-2.105827	-0.642637
H	-1.920439	-2.399176	0.652876
C	3.199561	-1.272692	0.054864
C	2.098729	-0.184448	-0.197953
O	3.086255	-1.902076	1.137764
O	4.070236	-1.364574	-0.828702
H	1.686814	-0.302869	-1.198938
C	2.698040	1.208983	-0.026701
N	0.997963	-0.432643	0.793951
H	0.247000	-1.001289	0.378438

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H	3.531568	1.309432	-0.718407
H	3.079788	1.342286	0.987877
S	1.511732	2.597400	-0.280036
H	1.444302	-0.988719	1.547286
H	0.564239	0.422755	1.154421
H	1.232582	2.330893	-1.572239
28			
Dimer 254 of the n...z type			
C	2.856779	0.020552	-0.949028
C	1.753920	1.068272	-0.736385
N	2.383011	-1.363250	-0.811874
H	1.359982	-1.420042	-0.812673
H	2.726040	-1.938797	-1.572916
H	3.281185	0.209544	-1.941128
C	4.000375	0.253561	0.057390
O	4.654257	1.273732	0.109103
O	4.187174	-0.770834	0.884157
H	3.494420	-1.430340	0.581750
H	2.146427	2.063576	-0.935835
H	0.934111	0.864937	-1.424264
S	0.980974	1.067105	0.940635
H	1.962416	1.744327	1.571143
C	-1.378871	-1.466165	-0.164835
C	-2.756810	-0.747939	-0.338398
O	-1.252217	-2.148943	0.877689
O	-0.551967	-1.241880	-1.072852
H	-3.158637	-0.944429	-1.330490
C	-2.591338	0.754920	-0.113242
N	-3.698427	-1.339085	0.676297
H	-4.229253	-2.121058	0.292477
H	-1.900888	1.137041	-0.861443
H	-2.163227	0.954115	0.870816
S	-4.162430	1.715950	-0.155008
H	-3.089081	-1.716011	1.424302
H	-4.366605	-0.649220	1.033790
H	-4.487983	1.437997	-1.434290
28			
Dimer 255 of the n...z type			
C	2.785252	-0.194407	1.037099
C	2.104713	-1.454121	0.486701
N	1.973103	1.022474	1.090166
H	1.317604	1.075258	0.312704
H	1.442948	1.085505	1.951051
H	3.108965	-0.426819	2.058407
C	4.092656	0.116175	0.282611
O	4.856900	-0.732259	-0.119987
O	4.327507	1.420214	0.137446
H	3.524032	1.857783	0.523730
H	2.789935	-2.299184	0.525769
H	1.230895	-1.687287	1.095755
S	1.462237	-1.282607	-1.232932
H	2.660933	-1.214368	-1.846858
C	-3.695961	-1.168029	0.297159
C	-3.212260	0.145059	-0.408789
O	-4.487350	-0.990558	1.258042
O	-3.211097	-2.221732	-0.150424
H	-3.279199	0.041879	-1.489715
C	-1.777602	0.449796	0.017996
N	-4.141987	1.248756	0.020443
H	-4.922076	1.363153	-0.627167
H	-1.144152	-0.369527	-0.313208
H	-1.704226	0.519668	1.105202
S	-1.100569	2.044244	-0.608293
H	-4.531714	0.926916	0.926403
H	-3.665242	2.151796	0.103033
H	-1.101679	1.718268	-1.917048
28			
Dimer 256 of the n...z type			
C	-2.966565	0.534590	-0.283596

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C	-1.874929	1.403315	0.356816
N	-3.977457	-0.013894	0.624323
H	-3.596204	-0.134010	1.559827
H	-4.793205	0.583149	0.686814
H	-3.474216	1.157744	-1.028140
C	-2.352588	-0.614503	-1.107134
O	-1.390570	-0.478993	-1.830536
O	-3.001198	-1.770516	-0.982836
H	-3.721037	-1.575738	-0.325882
H	-1.148785	1.696025	-0.400211
H	-2.325771	2.308251	0.764591
S	-1.011196	0.625849	1.787672
H	-0.436899	-0.430389	1.146587
C	1.982197	-1.710106	0.316140
C	2.324670	-0.185985	0.366875
O	2.923368	-2.464248	-0.025828
O	0.797902	-1.991400	0.592441
H	1.952478	0.246026	1.293138
C	1.719394	0.524395	-0.839817
N	3.825204	-0.054596	0.361577
H	4.209784	-0.061043	1.306833
H	0.667182	0.261590	-0.917144
H	2.204149	0.198065	-1.762644
S	1.908320	2.356614	-0.802412
H	4.173310	-0.903272	-0.117147
H	4.145464	0.800169	-0.101407
H	1.226453	2.544484	0.347684
28			
Dimer 257 of the n...z type			
C	2.101884	-0.870171	0.519284
C	1.873370	0.565566	1.007589
N	3.428489	-1.438896	0.777576
H	4.143382	-0.715450	0.754104
H	3.471977	-1.897181	1.679960
H	1.361156	-1.504980	1.019442
C	1.785223	-1.017994	-0.981193
O	0.857764	-0.464820	-1.530281
O	2.609445	-1.842788	-1.624656
H	3.272270	-2.112707	-0.936010
H	0.853949	0.892915	0.811839
H	2.046684	0.606938	2.083348
S	3.036783	1.799787	0.283151
C	2.501476	1.809189	-0.954630
H	-1.829058	1.809432	0.019026
C	-2.728222	0.556108	0.295225
O	-1.857069	2.235881	-1.162518
O	-1.163905	2.208328	0.992181
H	-3.349917	0.722603	1.172893
C	-1.840956	-0.674096	0.484791
N	-3.632887	0.386853	-0.896097
H	-4.531306	0.849943	-0.760051
H	-1.234292	-0.515838	1.373745
H	-1.169110	-0.796063	-0.366625
S	-2.743195	-2.272963	0.623653
H	-3.144973	0.875300	-1.670028
H	-3.813779	-0.599041	-1.109949
H	-3.417463	-1.986381	1.756602
28			
Dimer 258 of the n...z type			
C	-1.982788	-0.559247	0.805100
C	-3.506033	-0.351381	0.696956
N	-1.324515	0.567453	1.438639
H	-1.391377	1.390736	0.847107
H	-0.338950	0.336571	1.546015
H	-1.837666	-1.441546	1.434699
C	-1.418747	-0.919030	-0.570535
O	-0.804126	-0.167814	-1.295296
O	-1.726754	-2.180625	-0.921021
H	-1.378356	-2.352921	-1.810710

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H	-3.987395	-1.237201	0.284807		
H	-3.897542	-0.176560	1.699162		
S	-4.034817	1.126942	-0.272028		
H	-3.700915	0.663978	-1.493996		
C	2.045091	-1.180180	0.478827		
C	3.140579	-0.066815	0.601970		
O	2.256305	-2.037214	-0.414265		
O	1.112057	-1.112705	1.301350		
H	3.765784	-0.332292	1.456920		
C	2.600720	1.345872	0.805072		
N	4.002558	-0.169103	-0.626388		
H	4.996493	-0.024578	-0.453147		
H	3.409511	2.042807	1.028506		
H	1.919318	1.329276	1.652552		
S	1.753402	2.050363	-0.671541		
H	3.814324	-1.123813	-0.989750		
H	3.681774	0.504060	-1.333606		
H	0.728554	1.167694	-0.727688		
28					
Dimer 259 of the n...z type					
C	-1.843643	-0.594305	-0.389188		
C	-1.812693	0.839203	-0.931855		
N	-3.003846	-1.407320	-0.764011		
H	-3.835645	-0.831836	-0.872504		
H	-2.847256	-1.906644	-1.631382		
H	-0.940419	-1.100820	-0.751514		
C	-1.689905	-0.619294	1.139352		
O	-0.955300	0.124073	1.754032		
O	-2.409725	-1.567755	1.737313		
H	-2.925374	-1.983918	0.997790		
H	-0.915645	1.353261	-0.591233		
H	-1.806059	0.813932	-2.021742		
S	-3.283719	1.857276	-0.480250		
H	-2.993490	1.979182	0.831306		
C	2.023000	-1.772156	-0.304872		
C	2.696330	-0.364179	-0.435772		
O	1.060602	-1.973137	-1.093192		
O	2.487025	-2.509178	0.580314		
H	3.779165	-0.463921	-0.475396		
C	2.278090	0.512364	0.747055		
N	2.232091	0.226860	-1.740695		
H	2.892475	0.047938	-2.497166		
H	2.685559	0.070439	1.653844		
H	1.191732	0.543657	0.850541		
S	2.794977	2.275544	0.622974		
H	1.355897	-0.283564	-1.960692		
H	2.086696	1.239710	-1.679870		
H	4.126626	2.058867	0.621324		
28					
Dimer 260 of the n...z type					
C	3.178042	0.418412	0.665843		
C	1.906177	-0.420712	0.837035		
N	3.058712	1.616141	-0.170159		
H	2.398805	1.462630	-0.929095		
H	2.741825	2.416314	0.364184		
H	3.490135	0.737651	1.667051		
C	4.353406	-0.432968	0.148692		
O	4.552433	-1.579618	0.481818		
O	5.162456	0.222169	-0.684342		
H	4.732424	1.108775	-0.799837		
H	2.097606	-1.273754	1.485435		
H	1.129318	0.196896	1.287847		
S	1.181684	-1.021513	-0.748720		
H	2.116455	-1.957529	-1.010074		
C	-4.031369	-1.167540	0.043139		
C	-3.210126	0.078311	-0.436275		
O	-5.165773	-0.902680	0.516681		
O	-3.450772	-2.261391	-0.066357		
H	-2.784926	-0.103726	-1.421297		

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C	-2.107830	0.384111	0.576532
N	-4.172079	1.231578	-0.542068
H	-4.561455	1.318369	-1.480882
H	-1.436047	-0.470946	0.611214
H	-2.528345	0.529391	1.573614
S	-1.154374	1.924833	0.236754
H	-4.949637	0.985137	0.098754
H	-3.735710	2.125525	-0.295655
H	-0.670396	1.552600	-0.966406
28			
Dimer 261 of the n...z type			
C	-3.101773	0.272863	-0.818881
C	-1.649494	0.114964	-0.354155
N	-3.787504	1.497725	-0.398003
H	-3.456950	1.804436	0.513966
H	-3.644778	2.253608	-1.057086
H	-3.093041	0.250798	-1.914655
C	-3.959663	-0.942231	-0.416064
O	-3.558073	-2.084204	-0.431825
O	-5.208732	-0.625592	-0.074720
H	-5.231635	0.365620	-0.118275
H	-1.229812	-0.814573	-0.735158
H	-1.056475	0.947935	-0.731324
S	-1.430485	0.167224	1.476060
H	-1.985196	-1.034603	1.734154
C	3.606405	-1.495437	0.013165
C	3.352246	0.020753	0.316769
O	4.406615	-1.718293	-0.931032
O	2.959804	-2.294122	0.713010
H	3.407620	0.209328	1.386934
C	1.985306	0.425451	-0.231768
N	4.450853	0.798256	-0.358345
H	5.243542	0.956627	0.263953
H	1.226152	-0.157193	0.285943
H	1.917303	0.208208	-1.299653
S	1.591364	2.218852	-0.084014
H	4.774193	0.181500	-1.127189
H	4.131250	1.709184	-0.701606
H	1.585238	2.269563	1.263811
28			
Dimer 262 of the n...z type			
C	3.697139	-0.429164	-0.534492
C	2.471098	-0.718404	-1.412593
N	4.150335	-1.531630	0.319232
H	3.372842	-2.137804	0.570350
H	4.859927	-2.094214	-0.134428
H	4.518368	-0.155867	-1.206295
C	3.482440	0.824002	0.336987
O	2.974583	1.845055	-0.069003
O	3.944924	0.697217	1.580996
H	4.289115	-0.234147	1.617880
H	2.189335	0.175365	-1.966891
H	2.719028	-1.505884	-2.124442
S	1.004907	-1.343657	-0.486262
H	0.640706	-0.177112	0.101082
C	-1.507997	1.439225	0.091165
C	-2.897486	0.779286	0.375306
O	-1.406535	2.021364	-1.015029
O	-0.648219	1.263380	0.977290
H	-3.251554	1.053254	1.367016
C	-2.773156	-0.740235	0.249937
N	-3.867355	1.325213	-0.638110
H	-4.365925	2.142155	-0.284947
H	-2.081657	-1.087862	1.014086
H	-2.366191	-1.015499	-0.725175
S	-4.364391	-1.658571	0.379013
H	-3.279562	1.637527	-1.432611
H	-4.563720	0.629022	-0.922845
H	-4.660079	-1.292759	1.643451

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28		
Dimer 263 of the n...z	type	
C	2.700788	-0.620794 0.403260
C	3.293981	0.505832 -0.456681
N	2.006771	-1.694400 -0.295605
H	1.397551	-1.357923 -1.040027
H	2.651285	-2.371265 -0.684900
H	3.538299	-1.069628 0.951536
C	1.784400	-0.059282 1.503921
O	2.002856	0.975770 2.094605
O	0.721692	-0.815919 1.781521
H	0.735490	-1.574525 1.145571
H	3.854383	1.203184 0.164073
H	3.973749	0.071478 -1.189966
S	2.055694	1.452475 -1.441437
H	1.535813	2.146058 -0.408740
C	-1.377081	-1.618246 -0.773384
C	-2.393895	-0.454335 -0.526042
O	-1.281166	-2.447849 0.166537
O	-0.744676	-1.555741 -1.843345
H	-3.019961	-0.301084 -1.402881
C	-1.625118	0.819132 -0.175203
N	-3.276974	-0.869986 0.619817
H	-4.114910	-1.355090 0.298547
H	-0.981128	1.071504 -1.014334
H	-0.991721	0.650654 0.697215
S	-2.679256	2.260228 0.274066
H	-2.710829	-1.549518 1.160244
H	-3.571103	-0.072122 1.191890
H	-3.316600	2.371812 -0.909534
28		
Dimer 264 of the n...z	type	
C	2.086738	-0.003759 -0.587709
C	3.543690	0.001730 -1.065898
N	1.428948	1.302095 -0.485930
H	2.089834	2.019048 -0.194476
H	1.030944	1.589848 -1.372435
H	1.513246	-0.613957 -1.295223
C	1.934501	-0.744548 0.752685
O	2.542580	-1.750088 1.038984
O	1.028256	-0.201023 1.570291
H	0.731557	0.621586 1.104603
H	3.925151	-1.016180 -1.125253
H	3.594604	0.450968 -2.057753
S	4.677335	1.010140 -0.017789
H	4.685291	0.181659 1.046516
C	-3.497678	1.409239 0.175296
C	-2.945769	-0.044339 0.371800
O	-4.635277	1.475863 -0.356130
O	-2.731369	2.320721 0.532871
H	-2.549694	-0.164933 1.378110
C	-1.864819	-0.323727 -0.670148
N	-4.106812	-0.987804 0.202767
H	-4.552686	-1.209193 1.093280
H	-1.062506	0.396366 -0.525581
H	-2.257207	-0.192022 -1.680730
S	-1.191571	-2.039238 -0.641397
H	-4.792396	-0.457929 -0.368182
H	-3.833315	-1.869461 -0.241478
H	-0.723497	-2.001625 0.623444
28		
Dimer 265 of the n...z	type	
C	2.012628	-0.703561 0.433185
C	3.530603	-0.702132 0.695167
N	1.655034	-1.537092 -0.699795
H	1.972335	-1.103967 -1.562375
H	0.639617	-1.592541 -0.734743
H	1.542247	-1.123194 1.326052
C	1.508006	0.735456 0.320332

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O	1.192317	1.285165 -0.710131
O	1.485767	1.353790 1.517830
H	1.194240	2.271086 1.390441
H	3.765804	-0.138393 1.596962
H	3.853495	-1.733767 0.835168
S	4.573070	-0.073510 -0.692184
H	4.260396	1.232735 -0.568321
C	-2.236197	-1.330914 0.424022
C	-2.755496	-0.571819 -0.843653
O	-3.119407	-1.939232 1.077317
O	-1.008954	-1.264346 0.626828
H	-2.561472	-1.214179 -1.705632
C	-2.107695	0.785205 -1.078786
N	-4.250936	-0.467569 -0.703946
H	-4.757443	-0.547098 -1.585447
H	-2.493939	1.252369 -1.985741
H	-1.035243	0.647524 -1.186655
S	-2.421425	1.999186 0.272732
H	-4.502882	-1.233369 -0.050942
H	-4.503189	0.418237 -0.251616
H	-1.737841	1.329942 1.223912
28		
Dimer 266 of the n...z	type	
C	2.989102	0.500240 0.289860
C	3.036356	-1.001285 0.602816
N	2.408836	1.361394 1.324429
H	1.692550	0.863751 1.848037
H	3.109593	1.688482 1.978721
H	4.021353	0.826325 0.118139
C	2.275779	0.777644 -1.047147
O	2.396376	0.086544 -2.032901
O	1.530013	1.884389 -1.034599
H	1.601175	2.216850 -0.101147
H	3.455447	-1.545112 -0.242178
H	3.673895	-1.165579 1.471703
S	1.407708	-1.740276 1.051495
H	0.842012	-1.703447 -0.176503
C	-1.781884	-1.604634 -0.631516
C	-2.500517	-0.222957 -0.479739
O	-2.084599	-2.461541 0.235024
O	-0.952351	-1.675323 -1.558392
H	-2.914654	0.098656 -1.433161
C	-1.501413	0.805502 0.049511
N	-3.637766	-0.417259 0.487494
H	-4.514129	-0.624556 0.008301
H	-0.720323	0.938995 -0.693824
H	-1.031846	0.447725 0.967942
S	-2.222472	2.441647 0.487736
H	-3.375436	-1.254541 1.040633
H	-3.787159	0.406261 1.079276
H	-2.633802	2.775708 -0.752867
28		
Dimer 267 of the n...z	type	
C	-2.374196	-0.508027 -0.781072
C	-1.467473	-1.219793 0.230821
N	-1.869157	0.735836 -1.367114
H	-1.304904	1.262099 -0.705079
H	-1.325954	0.573464 -2.205969
H	-2.550882	-1.214986 -1.599755
C	-3.776106	-0.244940 -0.194117
O	-4.349579	-1.009776 0.548428
O	-4.323482	0.898947 -0.605649
H	-3.619604	1.324404 -1.159993
H	-1.960783	-2.116578 0.602084
H	-0.525483	-1.509196 -0.238724
S	-0.968294	-0.180190 1.669312
H	-2.192896	-0.024164 2.212118
C	2.754013	-1.492879 -0.420563
C	2.497103	-0.117904 0.282892

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O	3.956924	-1.743845	-0.679169		
O	1.728307	-2.152370	-0.671220		
H	1.853896	-0.256695	1.148830		
C	1.864568	0.850482	-0.713166		
N	3.824583	0.399999	0.768517		
H	4.012448	0.116255	1.730724		
H	0.957533	0.389391	-1.096795		
H	2.530894	1.024240	-1.560828		
S	1.487606	2.522314	-0.038423		
H	4.529236	-0.063320	0.166056		
H	3.891133	1.420629	0.723114		
H	0.623564	2.104353	0.912270		
28					
Dimer 268 of the n...z type					
C	-2.913739	0.623747	0.190477		
C	-2.960786	-0.047570	-1.189186		
N	-2.339408	1.972075	0.234120		
H	-1.644514	2.094973	-0.498568		
H	-3.047055	2.688162	0.123353		
H	-3.945668	0.682044	0.554318		
C	-2.194685	-0.261768	1.227790		
O	-2.338854	-1.460926	1.302279		
O	-1.419243	0.423342	2.069340		
H	-1.491660	1.363288	1.756432		
H	-3.353353	-1.058960	-1.099322		
H	-3.620586	0.523721	-1.842380		
S	-1.343133	-0.101823	-2.072587		
H	-0.740953	-1.063996	-1.333394		
C	1.524262	-1.782662	0.384579		
C	2.472028	-0.555045	0.176224		
O	0.976248	-2.206792	-0.668480		
O	1.388227	-2.163503	1.557788		
H	3.348047	-0.634094	0.816009		
C	1.698017	0.732101	0.457814		
N	2.931508	-0.576509	-1.257581		
H	3.770903	-1.143755	-1.380039		
H	1.330255	0.702261	1.481124		
H	0.837828	0.807821	-0.209795		
S	2.650320	2.281736	0.167556		
H	2.167474	-1.029898	-1.786491		
H	3.128990	0.365066	-1.612085		
H	3.598984	2.066005	1.101965		
28					
Dimer 269 of the n...z type					
C	1.550614	-0.272718	-0.230986		
C	2.748669	-1.109626	-0.693247		
N	1.171103	0.851440	-1.094836		
H	2.001002	1.322215	-1.451631		
H	0.646087	0.530164	-1.900616		
H	0.687488	-0.949545	-0.155967		
C	1.739086	0.235824	1.204429		
O	2.275518	-0.402227	2.080680		
O	1.211209	1.444932	1.432718		
H	0.889928	1.759738	0.554929		
H	2.922815	-1.932279	-0.001813		
H	2.538990	-1.524103	-1.679617		
S	4.312620	-0.150906	-0.893491		
H	4.536609	0.056680	0.420147		
C	-2.248132	-1.773078	0.180358		
C	-2.341723	-0.353939	-0.473338		
O	-3.345299	-2.359132	0.343552		
O	-1.096044	-2.132039	0.489700		
H	-1.598644	-0.259230	-1.261346		
C	-2.145938	0.722958	0.590733		
N	-3.702998	-0.232386	-1.103843		
H	-3.701245	-0.549039	-2.074028		
H	-1.205932	0.536948	1.104366		
H	-2.943616	0.677621	1.335222		
S	-2.173431	2.446360	-0.058565		

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H	-4.308351	-0.880036	-0.568578		
H	-4.059507	0.727204	-1.087144		
H	-1.087902	2.314211	-0.851163		
28					
Dimer 270 of the n...z type					
C	-1.629311	-0.224903	-0.533348		
C	-3.044477	-0.227283	-1.125057		
N	-1.206143	-1.566592	-0.166040		
H	-1.795838	-1.921535	0.582520		
H	-0.256796	-1.550553	0.194500		
H	-0.954435	0.148900	-1.313156		
C	-1.471301	0.798382	0.595083		
O	-0.843744	0.608084	1.614999		
O	-2.083013	1.962773	0.324910		
H	-1.905978	2.586170	1.047791		
H	-3.301743	0.749287	-1.528646		
H	-3.080698	-0.959643	-1.930930		
S	-4.367329	-0.745873	0.056014		
H	-4.389893	0.393237	0.777707		
C	2.107734	0.949040	-1.094187		
C	2.928050	0.788743	0.231541		
O	1.035435	1.593994	-0.976884		
O	2.619306	0.443181	-2.109637		
H	3.682593	1.579124	0.240615		
C	3.622630	-0.555624	0.395155		
N	1.992747	1.079729	1.370901		
H	2.456923	1.449604	2.200121		
H	4.157321	-0.610287	1.344634		
H	4.341451	-0.671521	-0.412142		
S	2.476199	-1.999604	0.381805		
H	1.301016	1.750645	1.002220		
H	1.454269	0.246814	1.633421		
H	2.139829	-1.888941	-0.920008		
28					
Dimer 271 of the n...z type					
C	1.925580	0.695036	-0.447320		
C	3.245643	0.124902	-1.000610		
N	2.149287	1.740640	0.534755		
H	2.605302	1.350341	1.354948		
H	1.240734	2.094355	0.827458		
H	1.401591	1.132673	-1.300557		
C	1.048525	-0.445022	0.069593		
O	0.951845	-0.784198	1.223999		
O	0.392190	-1.080175	-0.934200		
H	-0.178017	-1.769922	-0.540471		
H	3.047933	-0.608199	-1.782018		
H	3.816425	0.946716	-1.433561		
S	4.380094	-0.619186	0.249020		
H	3.641073	-1.712855	0.525372		
C	-1.905203	1.350062	0.556123		
C	-2.819169	0.762636	-0.572551		
O	-0.857407	1.909661	0.144109		
O	-2.329497	1.221505	1.717655		
H	-3.558680	1.530949	-0.812940		
C	-3.568120	-0.513786	-0.213815		
N	-1.970835	0.612420	-1.808677		
H	-2.513254	0.515600	-2.668124		
H	-4.133927	-0.892349	-1.066328		
H	-4.272794	-0.273301	0.578734		
S	-2.528203	-1.925111	0.361307		
H	-1.374063	1.448001	-1.853622		
H	-1.324695	-0.181533	-1.725640		
H	-2.097632	-1.320459	1.487944		
28					
Dimer 272 of the n...z type					
C	2.900128	-0.918592	0.662478		
C	2.639120	-1.707029	-0.626649		
N	1.817147	-0.923586	1.650339		
H	0.911192	-1.025447	1.202169		

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H	1.921936	-1.675009	2.321418
H	3.790464	-1.352194	1.131247
C	3.291952	0.540325	0.356278
O	4.019664	0.862107	-0.556394
O	2.772722	1.424084	1.206989
H	2.201063	0.879062	1.809041
H	3.521326	-1.696562	-1.264026
H	2.403792	-2.741118	-0.375138
S	1.197279	-1.100379	-1.606914
H	1.798363	-0.000798	-2.105139
C	-3.370347	-0.973572	0.551237
C	-2.375136	-0.045217	-0.220926
O	-4.579272	-0.840486	0.231150
O	-2.852685	-1.706170	1.413208
H	-1.524251	-0.618121	-0.582349
C	-1.906593	1.086777	0.693309
N	-3.110173	0.506014	-1.413945
H	-2.965340	-0.065081	-2.246511
H	-1.387452	0.647608	1.542451
H	-2.757784	1.654858	1.074219
S	-0.824727	2.332882	-0.127436
H	-4.113498	0.443998	-1.159585
H	-2.825165	1.465139	-1.635780
H	0.157532	1.474214	-0.471169
28			
Dimer 273 of the n...z type			
C	2.742014	0.994994	-0.015409
C	3.171959	-0.044508	1.034503
N	1.815693	1.969002	0.529642
H	0.893099	1.564278	0.687323
H	1.678624	2.724336	-0.134155
H	3.662596	1.516346	-0.307071
C	2.246977	0.316660	-1.298957
O	1.194655	0.552902	-1.847990
O	3.132225	-0.581361	-1.770031
H	2.778642	-0.973308	-2.584897
H	3.959411	-0.685150	0.642727
H	3.555282	0.487999	1.904444
S	1.815874	-1.106225	1.693615
H	1.627522	-1.857637	0.589015
C	-2.237403	1.304260	0.328928
C	-2.909613	-0.064505	0.686748
O	-2.843571	1.986783	-0.535582
O	-1.201991	1.574402	0.963932
H	-3.382888	0.058017	1.662814
C	-1.942702	-1.243014	0.750373
N	-4.010195	-0.286433	-0.315351
H	-4.865945	-0.669834	0.083901
H	-2.434440	-2.131373	1.148357
H	-1.119641	-0.970792	1.407710
S	-1.270367	-1.755983	-0.885773
H	-4.167880	0.654919	-0.727243
H	-3.682312	-0.902899	-1.068730
H	-0.546597	-0.642682	-1.129439
28			
Dimer 274 of the n...z type			
C	1.676738	0.121581	0.375659
C	2.881643	1.078942	0.444625
N	1.650978	-0.805902	1.490638
H	2.431451	-1.452727	1.420154
H	0.791507	-1.347518	1.430505
H	0.786356	0.752317	0.432221
C	1.635236	-0.555451	-0.995350
O	1.980598	-1.689375	-1.229623
O	1.195637	0.292219	-1.951026
H	1.222533	-0.161171	-2.808940
H	2.838147	1.809571	-0.362095
H	2.841371	1.609007	1.396309
S	4.539958	0.270309	0.435497

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H	4.524685	-0.145593	-0.847472
C	-2.297759	-1.242896	0.410515
C	-2.903150	-0.298374	-0.682981
O	-3.139063	-1.789924	1.164964
O	-1.058131	-1.359910	0.388998
H	-2.946205	-0.869242	-1.612822
C	-2.110031	0.979082	-0.922505
N	-4.323935	-0.014898	-0.275735
H	-4.976132	0.049337	-1.057129
H	-2.560775	1.578903	-1.714469
H	-1.102972	0.707371	-1.227377
S	-2.035396	2.092988	0.545148
H	-4.570128	-0.796942	0.360353
H	-4.369713	0.853143	0.269685
H	-1.400803	1.225013	1.360146
28			
Dimer 275 of the n...z type			
C	2.599835	0.621669	0.923218
C	3.190158	-0.734850	0.501769
N	1.555344	0.464895	1.917487
H	0.763199	-0.074513	1.566258
H	1.189205	1.371962	2.187807
H	3.427203	1.184672	1.373538
C	2.182202	1.434236	-0.308667
O	1.078536	1.886629	-0.504530
O	3.208180	1.599471	-1.167145
H	2.902402	2.123984	-1.924611
H	4.107014	-0.597482	-0.067147
H	3.418895	-1.303413	1.402590
S	2.048741	-1.806029	-0.479454
H	2.245050	-1.201285	-1.668805
C	-1.536730	-1.322849	0.411830
C	-1.457321	-0.144404	-0.610405
O	-1.983929	-2.403121	-0.049018
O	-1.123560	-1.065919	1.559093
H	-0.413202	-0.056985	-0.913272
C	-1.919798	1.198753	-0.063966
N	-2.242296	-0.564759	-1.823565
H	-1.824005	-0.276280	-2.707140
H	-1.777640	1.989789	-0.800465
H	-1.316624	1.435466	0.807283
S	-3.708663	1.250396	0.379359
H	-2.293567	-1.598993	-1.745553
H	-3.201427	-0.203896	-1.772964
H	-3.642988	0.344325	1.376670
28			
Dimer 276 of the n...z type			
C	3.057573	-0.269556	-0.327549
C	3.102219	0.108750	1.158116
N	2.752820	0.811144	-1.268208
H	2.102635	1.482893	-0.867546
H	3.587621	1.309074	-1.553095
H	4.044506	-0.669979	-0.586579
C	2.087509	-1.438866	-0.582508
O	1.947682	-2.374571	0.172485
O	1.422755	-1.341360	-1.734336
H	1.712876	-0.471447	-2.113974
H	3.398503	-0.749043	1.759168
H	3.833539	0.903854	1.304026
S	1.514776	0.776318	1.821145
H	0.868027	-0.404423	1.902162
C	-3.021556	-1.191308	0.095647
C	-2.738134	0.337404	-0.096489
O	-2.761453	-1.635202	1.242970
O	-3.427684	-1.789951	-0.915839
H	-3.558738	0.818561	-0.624470
C	-1.423025	0.509593	-0.857230
N	-2.637360	0.947240	1.275443
H	-3.543215	1.272546	1.613608

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H	-1.540422	0.086649	-1.852256	
H	-0.621206	-0.030909	-0.354609	
S	-0.815881	2.244013	-0.979962	
H	-2.334076	0.172355	1.892544	
H	-1.985298	1.738197	1.299837	
H	-1.793199	2.700266	-1.790548	
28				
Dimer 277 of the n...z type				
C	2.811258	-0.237707	0.859191	
C	3.019263	-1.293151	-0.240476	
N	1.816592	-0.657254	1.827339	
H	0.877370	-0.676709	1.429247	
H	1.780351	0.002825	2.597391	
H	3.777722	-0.147188	1.371091	
C	2.550126	1.146215	0.250446	
O	1.610587	1.858617	0.516446	
O	3.511708	1.496089	-0.627396	
H	3.311041	2.379142	-0.977140	
H	3.878527	-1.043734	-0.859361	
H	3.199533	-2.255082	0.238397	
S	1.564948	-1.571027	-1.341566	
H	1.695778	-0.448137	-2.077211	
C	-2.183035	-1.015623	0.882699	
C	-1.995982	-0.558038	-0.601951	
O	-3.262145	-1.614719	1.121323	
O	-1.236501	-0.761428	1.650849	
H	-1.352005	-1.296552	-1.082782	
C	-1.370219	0.819210	-0.769325	
N	-3.347497	-0.649361	-1.257532	
H	-3.319572	-0.953938	-2.230157	
H	-1.214662	1.053048	-1.823741	
H	-0.407260	0.827704	-0.267600	
S	-2.406180	2.192801	-0.108414	
H	-3.875179	-1.317761	-0.664451	
H	-3.827503	0.256180	-1.202792	
H	-2.325762	1.824218	1.186867	
28				
Dimer 278 of the n...z type				
C	2.920323	0.489381	0.603545	
C	3.256768	-1.014022	0.535335	
N	1.987855	0.805270	1.672839	
H	1.021933	0.711009	1.372789	
H	2.091849	1.777079	1.945398	
H	3.872311	0.984367	0.821389	
C	2.478428	0.989239	-0.774326	
O	1.375842	1.409168	-1.038075	
O	3.463919	0.875362	-1.683075	
H	3.134035	1.173464	-2.546338	
H	4.097524	-1.187095	-0.134315	
H	3.530311	-1.347245	1.535551	
S	1.892877	-2.145568	0.017367	
H	1.883566	-1.826751	-1.293280	
C	-1.723683	1.287656	0.496166	
C	-1.525681	-0.070882	-0.255233	
O	-1.298844	1.290509	1.684232	
O	-2.237283	2.210184	-0.157230	
H	-0.611129	0.040670	-0.841339	
C	-2.665079	-0.464343	-1.184028	
N	-1.249818	-1.111727	0.795552	
H	-0.404084	-1.661890	0.596271	
H	-2.428633	-1.380718	-1.727048	
H	-2.810943	0.338276	-1.903052	
S	-4.257211	-0.806274	-0.319661	
H	-1.098854	-0.547688	1.657637	
H	-2.054391	-1.726455	0.943354	
H	-4.435941	0.443680	0.155386	
28				
Dimer 279 of the n...z type				
C	1.991936	-0.667384	0.550191	

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C	3.423271	-0.218119	0.899284	
N	1.974496	-1.705485	-0.463750	
H	2.284140	-1.322912	-1.352820	
H	1.007613	-2.006636	-0.576256	
H	1.565376	-1.078552	1.469265	
C	1.139306	0.551513	0.194925	
O	0.814263	0.873663	-0.925474	
O	0.807017	1.264692	1.289760	
H	0.282808	2.035329	1.016847	
H	3.411232	0.508001	1.711200	
H	3.986136	-1.093404	1.223886	
S	4.402874	0.468958	-0.505468	
H	3.732272	1.632169	-0.633171	
C	-1.810599	-1.417639	-0.403107	
C	-3.048864	-0.756859	0.292621	
O	-0.898199	-1.782678	0.386335	
O	-1.877898	-1.538103	-1.636350	
H	-3.823010	-1.524543	0.353890	
C	-3.615935	0.456355	-0.434706	
N	-2.637510	-0.435506	1.703803	
H	-3.363212	-0.610853	2.398001	
H	-4.543078	0.794422	0.029985	
H	-3.825170	0.165048	-1.461364	
S	-2.508544	1.929838	-0.426458	
H	-1.803863	-1.034826	1.865441	
H	-2.338208	0.543961	1.772126	
H	-1.477367	1.371202	-1.095997	
28				
Dimer 280 of the n...z type				
C	-2.827620	-1.235122	0.207667	
C	-3.385059	-0.258585	-0.841349	
N	-3.056113	-0.873970	1.610238	
H	-3.168095	0.133018	1.706586	
H	-3.880095	-1.325330	1.988414	
H	-3.296256	-2.207136	0.019479	
C	-1.323495	-1.498140	-0.005559	
O	-0.826968	-1.718643	-1.087290	
O	-0.617969	-1.512042	1.126147	
H	-1.289375	-1.305281	1.830270	
H	-3.034809	-0.546622	-1.831478	
H	-4.474129	-0.308092	-0.832303	
S	-2.990636	1.515817	-0.536880	
H	-1.641446	1.475217	-0.750905	
C	1.007565	1.627632	-0.036213	
C	2.399721	0.946658	-0.237847	
O	0.773923	2.040234	1.124231	
O	0.276385	1.645798	-1.047848	
H	2.859229	1.288896	-1.162856	
C	2.230087	-0.571438	-0.237249	
N	3.277290	1.373528	0.908595	
H	3.775045	2.240985	0.706691	
H	1.561708	-0.851849	-1.047606	
H	1.763149	-0.904497	0.690549	
S	3.806398	-1.517837	-0.352665	
H	2.631489	1.561685	1.694378	
H	3.970841	0.657159	1.146815	
H	4.172145	-1.081538	-1.575782	
28				
Dimer 281 of the n...z type				
C	3.045016	0.443654	1.059060	
C	3.628038	-0.953949	0.811411	
N	1.622962	0.526737	1.386796	
H	1.040440	-0.159695	0.900016	
H	1.462259	0.427888	2.381661	
H	3.607097	0.872768	1.897600	
C	3.337144	1.395435	-0.116922	
O	4.372969	1.395661	-0.746276	
O	2.347025	2.251559	-0.361267	
H	1.635377	1.978625	0.281301	

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H	4.709667	-0.894826	0.699389
H	3.404470	-1.589948	1.668146
S	2.931812	-1.836291	-0.649779
H	3.544883	-1.084910	-1.586481
C	-1.307009	-0.384345	-0.440967
C	-2.866724	-0.480185	-0.513926
O	-0.781260	-1.043741	0.495728
O	-0.774221	0.359601	-1.279660
H	-3.190665	-0.634415	-1.540919
C	-3.479669	0.796629	0.062267
N	-3.279996	-1.678403	0.297931
H	-3.344054	-2.522441	-0.271869
H	-3.155071	1.636764	-0.547743
H	-3.130535	0.961621	1.083713
S	-5.317902	0.782412	0.187422
H	-2.510998	-1.815502	0.979479
H	-4.184225	-1.540342	0.760651
H	-5.568848	0.680084	-1.134051
28			
Dimer 282 of the n...z type			
C	2.747317	-0.995565	-0.035031
C	3.167583	0.081802	-1.050857
N	1.803811	-1.939698	-0.601877
H	0.883034	-1.522143	-0.731840
H	1.669127	-2.718588	0.034382
H	3.668698	-1.534154	0.219705
C	2.280488	-0.359597	1.280311
O	1.215518	-0.568017	1.816118
O	3.209374	0.467216	1.796066
H	2.873492	0.836956	2.628659
H	3.961086	0.706050	-0.644298
H	3.540167	-0.418989	-1.944249
S	1.806478	1.168637	-1.657378
H	1.627160	1.878800	-0.524280
C	-2.252941	-1.296361	-0.350494
C	-2.925445	0.080827	-0.673935
O	-2.870944	-2.007980	0.481983
O	-1.208019	-1.544331	-0.979396
H	-3.403403	-0.020004	-1.650241
C	-1.961238	1.262039	-0.713932
N	-4.022383	0.278914	0.336896
H	-4.874629	0.684655	-0.047281
H	-2.458214	2.160224	-1.082631
H	-1.142970	1.010597	-1.385605
S	-1.275341	1.727724	0.930657
H	-4.188997	-0.673934	0.717074
H	-3.686108	0.866414	1.109150
H	-0.538657	0.613864	1.129321
28			
Dimer 283 of the n...z type			
C	-1.758738	-0.762498	-0.245626
C	-1.971602	0.426335	-1.190107
N	-2.691466	-1.843256	-0.533801
H	-3.641945	-1.544190	-0.330034
H	-2.502873	-2.634770	0.073084
H	-0.743847	-1.130502	-0.439419
C	-1.745320	-0.346253	1.226626
O	-2.249304	-0.973445	2.128170
O	-1.076201	0.810320	1.429993
H	-1.056912	0.995816	2.382676
H	-1.179844	1.163538	-1.076694
H	-1.957984	0.058230	-2.215634
S	-3.601793	1.276590	-1.007200
H	-3.320418	1.912352	0.148454
C	1.819955	-1.345571	-0.083993
C	3.165058	-0.547704	-0.162944
O	1.352031	-1.703378	-1.197798
O	1.374130	-1.554228	1.056659
H	3.968957	-1.247754	0.074013

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C	3.250119	0.645743	0.781719
N	3.344212	-0.141341	-1.600039
H	4.311361	-0.158470	-1.921811
H	4.245147	1.091840	0.760810
H	3.046047	0.295356	1.790661
S	2.091991	2.016376	0.359071
H	2.750744	-0.807362	-2.130546
H	2.957612	0.799177	-1.745896
H	0.949470	1.357001	0.647035
28			
Dimer 284 of the n...z type			
C	2.054038	-0.462665	0.755568
C	1.633563	1.011436	0.733172
N	3.325505	-0.768009	1.419297
H	3.982829	0.001017	1.312577
H	3.200495	-0.942248	2.409337
H	1.264069	-1.015127	1.276923
C	2.078163	-1.068921	-0.660872
O	1.266324	-0.806521	-1.520737
O	3.064918	-1.943038	-0.852668
H	3.577897	-1.923526	-0.002539
H	0.666052	1.142373	0.248950
H	1.559016	1.376230	1.758283
S	2.853223	2.126655	-0.086634
H	2.610212	1.720929	-1.349662
C	-2.375732	1.658961	-0.246380
C	-2.319195	0.249251	0.434053
O	-3.533485	2.105859	-0.445337
O	-1.272031	2.149987	-0.544051
H	-1.590362	0.245955	1.242322
C	-1.971558	-0.807405	-0.613543
N	-3.677067	-0.013569	1.028596
H	-3.737671	0.309925	1.993998
H	-0.978634	-0.595843	-1.004866
H	-2.683765	-0.775595	-1.440807
S	-2.035513	-2.546413	-0.005078
H	-4.332121	0.559340	0.466226
H	-3.920267	-1.009216	1.011644
H	-1.041666	-2.441287	0.900119
28			
Dimer 285 of the n...z type			
C	2.833667	0.340869	0.939067
C	3.574601	-1.002270	0.902350
N	1.416338	0.285573	1.297367
H	0.995415	-0.573471	0.951864
H	1.282704	0.318761	2.301117
H	3.344572	0.970590	1.676936
C	2.995345	1.104303	-0.388419
O	4.012268	1.092331	-1.046250
O	1.929147	1.818861	-0.746799
H	1.229220	1.632404	-0.073466
H	4.621831	-0.851727	0.646325
H	3.518704	-1.470139	1.885331
S	2.842079	-2.232373	-0.260962
H	3.214856	-1.611868	-1.398960
C	-3.343795	-1.478475	-0.316163
C	-3.188618	0.078100	-0.422966
O	-3.984840	-1.877580	0.689609
O	-2.785972	-2.131729	-1.214637
H	-3.432480	0.414326	-1.428605
C	-1.761488	0.476793	-0.051152
N	-4.179656	0.686743	0.533700
H	-5.059221	0.921372	0.073364
H	-1.081261	0.012144	-0.761632
H	-1.508390	0.118404	0.948158
S	-1.459572	2.292916	0.011818
H	-4.373239	-0.068220	1.219986
H	-3.822645	1.535643	0.982191
H	-1.730046	2.545906	-1.285467

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28		
Dimer 286 of the n...z	type	
C	-1.466196	0.092636
C	-2.536424	-0.945315
N	-1.618730	1.336345
H	-2.450656	1.825137
H	-0.812623	1.923414
H	-0.504320	-0.349279
C	-1.439167	0.266410
O	-1.832043	1.236383
O	-0.940603	-0.830180
H	-0.944476	-0.684136
H	-2.352989	-1.893748
H	-2.482763	-1.105599
S	-4.280583	-0.429045
H	-4.259539	-0.536491
C	1.940335	1.274346
C	3.126050	0.491602
O	1.227743	1.927071
O	1.852631	1.188571
H	4.022960	1.100147
C	3.376304	-0.894795
N	2.845206	0.447790
H	3.673445	0.549426
H	4.262059	-1.350877
H	3.539190	-0.790976
S	2.006577	-2.093183
H	2.176604	1.228610
H	2.364607	-0.424762
H	1.100034	-1.508222
28		
Dimer 287 of the n...z	type	
C	3.270936	0.475301
C	2.845686	-0.636825
N	4.162008	-0.035272
H	3.670538	-0.715960
H	4.452266	0.714689
H	3.814099	1.214911
C	2.031107	1.193741
O	1.652678	1.159502
O	1.392183	1.866916
H	0.556559	2.238924
H	2.217024	-0.226246
H	3.744064	-1.054470
S	1.994460	-2.082403
H	0.801236	-1.507705
C	-2.317528	-1.255434
C	-2.711405	-0.487837
O	-3.288129	-1.646471
O	-1.096196	-1.406522
H	-2.692465	-1.211975
C	-1.797009	0.674873
N	-4.143929	-0.057411
H	-4.684805	-0.074773
H	-2.110931	1.162054
H	-0.790677	0.287827
S	-1.763868	2.010327
H	-4.530184	-0.717576
H	-4.192796	0.884143
H	-1.284974	1.237843
28		
Dimer 288 of the n...z	type	
C	-2.506059	-0.375114
C	-3.576319	-0.715529
N	-1.439276	-1.353678
H	-0.932559	-1.360348
H	-0.733312	-1.131108
H	-3.018715	-0.403904
C	-2.034656	1.075968

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O	-0.884831	1.430154
O	-3.065774	1.943308
H	-2.719773	2.846008
H	-4.441294	-0.063301
H	-3.894163	-1.746200
S	-2.987026	-0.656622
H	-2.936425	0.686657
C	1.830447	-1.352389
C	3.189109	-0.709554
O	1.708140	-1.546656
O	1.037719	-1.615974
H	3.795506	-1.503833
C	3.042529	0.423165
N	3.884158	-0.260601
H	4.887897	-0.437235
H	4.016542	0.751029
H	2.460225	0.050425
S	2.249438	1.938092
H	3.396725	-0.783460
H	3.715059	0.740491
H	1.059173	1.385261
28		
Dimer 289 of the n...z	type	
C	-2.060747	0.062802
C	-3.499184	0.609861
N	-2.014904	-1.371368
H	-2.432694	-1.853069
H	-1.037483	-1.650266
H	-1.508938	0.548326
C	-1.388823	0.518175
O	-1.121333	-0.192087
O	-1.144078	1.845478
H	-0.777580	2.103729
H	-3.503514	1.695941
H	-3.928023	0.327302
S	-4.663369	-0.084511
H	-4.180197	0.576257
C	1.703622	-1.238998
C	2.132065	-0.251389
O	2.174282	-2.398899
O	0.919103	-0.775071
H	1.322724	-0.249553
C	2.387671	1.176060
N	3.337380	-0.851492
H	3.386071	-0.674190
H	2.626414	1.827250
H	1.484547	1.544879
S	3.807327	1.335751
H	3.268992	-1.866050
H	4.195544	-0.504458
H	3.252072	0.619658
28		
Dimer 290 of the n...z	type	
C	-2.781903	0.399351
C	-1.546211	1.286511
N	-3.962013	0.968107
H	-3.843335	0.973682
H	-4.777447	0.395749
H	-2.938901	0.379720
C	-2.495964	-1.047191
O	-3.014824	-1.616124
O	-1.588760	-1.635587
H	-1.433171	-2.534991
H	-0.688827	0.910922
H	-1.774148	2.290358
S	-1.066883	1.494750
H	-0.536338	0.256903
C	1.780914	-0.962666
C	2.681712	-0.994948

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O	0.620329	-1.434741	0.979338
O	2.303706	-0.488623	2.154326
H	3.406580	-1.799630	-0.011701
C	3.429830	0.309751	-0.404673
N	1.794480	-1.374207	-1.300673
H	2.192809	-2.079316	-1.919392
H	4.146935	0.195585	-1.218439
H	3.967422	0.576016	0.502242
S	2.342990	1.707014	-0.921197
H	0.923429	-1.717482	-0.847244
H	1.550946	-0.541253	-1.849336
H	1.585204	1.763962	0.198053
28			
Dimer 291 of the n...z type			
C	-2.568153	0.272629	1.094718
C	-2.539525	1.584710	0.293975
N	-1.318945	0.060706	1.805270
H	-0.555904	-0.040915	1.141826
H	-1.356220	-0.807110	2.330665
H	-3.372559	0.383179	1.832038
C	-2.985048	-0.904095	0.203407
O	-2.351686	-1.921779	0.054498
O	-4.167781	-0.673644	-0.400443
H	-4.397667	-1.443123	-0.945735
H	-3.526033	1.819241	-0.099756
H	-2.226877	2.388555	0.959650
S	-1.329122	1.615999	-1.101259
H	-2.051199	0.869670	-1.962189
C	2.667948	1.165611	0.082517
C	3.266777	-0.282170	0.149747
O	2.233949	1.609869	1.177648
O	2.718539	1.716313	-1.030226
H	4.352901	-0.181999	0.106721
C	2.807338	-1.202276	-0.977646
N	2.922449	-0.831508	1.507687
H	3.683487	-1.334701	1.961359
H	3.360166	-2.142591	-0.965621
S	2.996440	-0.697921	-1.922426
H	1.032949	-1.689600	-0.870500
H	2.644949	0.014215	2.048411
H	2.101438	-1.444946	1.443576
H	0.501122	-0.460853	-1.063210
28			
Dimer 292 of the n...z type			
C	1.737743	0.033683	-0.172009
C	2.755998	0.949690	-0.873973
N	1.029130	0.729828	0.886156
H	1.676723	0.984001	1.626695
H	0.333216	0.105116	1.286372
H	1.016610	-0.260646	-0.942017
C	2.408193	-1.265950	0.284395
O	2.524514	-1.625986	1.431950
O	2.870790	-1.977641	-0.763227
H	3.294812	-2.785288	-0.431410
H	3.208762	0.443004	-1.724197
H	2.230387	1.834255	-1.233186
S	4.095019	1.606201	0.213446
H	4.805430	0.464440	0.318851
C	-1.619838	-0.822858	-0.523062
C	-2.067052	0.672521	-0.401626
O	-1.685275	-1.305055	-1.681060
O	-1.210668	-1.349459	0.529584
H	-1.154833	1.273119	-0.390081
C	-2.878352	0.988392	0.848060
N	-2.813176	1.010833	-1.662857
H	-2.658959	1.963180	-1.992496
H	-3.111353	2.052364	0.908224
H	-2.286538	0.713146	1.717510
S	-4.505835	0.125780	0.916222

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H	-2.482480	0.312761	-2.354800
H	-3.820045	0.861076	-1.531419
H	-4.005402	-1.124608	0.995479
28			
Dimer 293 of the n...z type			
C	-2.147059	-0.155768	0.767518
C	-2.262168	-1.061537	-0.471736
N	-3.091573	-0.548505	1.799007
H	-4.043488	-0.370465	1.490190
H	-2.947628	0.003494	2.638355
H	-1.126920	-0.286716	1.147246
C	-2.248744	1.315683	0.366202
O	-3.090699	2.094879	0.737275
O	-1.253390	1.674084	-0.488071
H	-1.367843	2.608075	-0.729201
H	-1.492374	-0.822322	-1.202365
H	-2.129844	-2.094820	-0.152335
S	-3.906179	-1.030189	-1.310948
H	-3.776738	0.180238	-1.892032
C	1.781091	-0.862541	0.749431
C	2.115010	-0.412735	-0.710039
O	1.028181	-0.096310	1.396786
O	2.295943	-1.944231	1.093147
H	1.550601	-1.048864	-1.395458
C	3.599249	-0.509595	-1.048853
N	1.613074	0.991188	-0.916316
H	1.582921	1.253017	-1.903137
H	3.792818	-0.213321	-2.080866
H	3.910320	-1.543010	-0.919058
S	4.667021	0.583146	-0.015157
H	0.671933	1.097554	-0.511229
H	2.231888	1.647787	-0.428295
H	4.455819	-0.065149	1.148789
28			
Dimer 294 of the n...z type			
C	2.718083	-0.411230	-0.871687
C	1.348415	0.026743	-0.329088
N	2.882755	-1.852986	-0.793150
H	2.861063	-2.148805	0.179376
H	3.790841	-2.124224	-1.156813
H	2.733514	-0.116169	-1.927790
C	3.851598	0.378924	-0.206559
O	4.784651	-0.108267	0.387208
O	3.692962	1.707566	-0.368914
H	4.432839	2.166855	0.059862
H	1.190504	1.090513	-0.496180
H	0.564191	-0.536176	-0.833344
S	1.070012	-0.338772	1.457955
H	1.874214	0.622899	1.958242
C	-2.513960	-1.337170	-0.090426
C	-3.279376	-0.169524	-0.802367
O	-3.108151	-1.835524	0.900279
O	-1.427397	-1.656597	-0.603390
H	-3.690745	-0.575682	-1.728468
C	-2.413162	1.041767	-1.137123
N	-4.441809	0.192535	0.081227
H	-5.309593	0.373472	-0.421600
H	-2.955834	1.747906	-1.766805
H	-1.538764	0.691834	-1.681031
S	-1.883626	2.021931	0.331501
H	-4.532337	-0.624602	0.718679
H	-4.205179	1.010578	0.655836
H	-1.089611	1.079738	0.894233
28			
Dimer 295 of the n...z type			
C	-1.872489	-0.073452	-0.768724
C	-1.969228	1.259504	-0.009943
N	-2.746894	-0.084293	-1.930083
H	-3.719392	-0.063521	-1.634342

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H -2.622014	-0.944196	-2.454445	
H -0.834159	-0.165274	-1.113071	
C -2.079112	-1.263232	0.172277	
O -2.863002	-2.165890	-0.002107	
O -1.252043	-1.205991	1.239438	
H -1.400317	-1.989029	1.793569	
H -1.232988	1.310009	0.789523	
H -1.779117	2.070934	-0.712024	
S -3.632974	1.626164	0.703065	
H -3.564133	0.761673	1.736324	
C 1.946620	-1.211523	-0.452431	
C 1.937071	-0.185283	0.730872	
O 2.637821	-2.241512	-0.251592	
O 1.249338	-0.907140	-1.438256	
H 1.033008	-0.386371	1.309406	
C 1.946687	1.276790	0.304751	
N 3.110736	-0.523319	1.607836	
H 2.947793	-0.364672	2.601624	
H 1.882610	1.939831	1.168670	
H 1.085203	1.454542	-0.333784	
S 3.477059	1.780070	-0.590303	
H 3.301175	-1.523256	1.409451	
H 3.935339	0.013057	1.313973	
H 3.280521	0.987247	-1.664011	
28			
Dimer 296 of the n...z type			
C -2.485662	0.197308	1.013977	
C -2.428993	1.467162	0.147177	
N -1.167874	-0.221874	1.451673	
H -0.609773	-0.583052	0.677826	
H -1.251016	-0.985448	2.115259	
H -3.075337	0.470095	1.898202	
C -3.291272	-0.908024	0.318059	
O -2.903575	-2.035738	0.124765	
O -4.514495	-0.476273	-0.052875	
H -4.990052	-1.208540	-0.476983	
H -3.429615	1.855516	-0.030971	
H -1.849423	2.220948	0.679541	
S -1.573752	1.279412	-1.475726	
H -2.500027	0.501061	-2.072335	
C 2.175946	-1.379554	-0.492393	
C 3.008586	-0.658767	0.622956	
O 2.828289	-1.691881	-1.520474	
O 0.979038	-1.592117	-0.225621	
H 3.247934	-1.410191	1.378326	
C 2.307076	0.514673	1.296750	
N 4.307783	-0.244624	-0.013587	
H 5.119301	-0.329862	0.597299	
H 2.917354	0.918658	2.105721	
H 1.360743	0.172284	1.709352	
S 1.983587	1.935841	0.169716	
H 4.388709	-0.861066	-0.845815	
H 4.239796	0.721894	-0.352463	
H 1.066536	1.310413	-0.598936	
28			
Dimer 297 of the n...z type			
C 3.466803	-0.816737	0.023770	
C 3.864332	0.583759	0.525912	
N 3.942251	-1.045771	-1.330283	
H 3.471438	-0.412226	-1.971057	
H 3.707360	-1.986585	-1.630686	
C 3.958373	-1.531740	0.692828	
C 1.958630	-1.027683	0.202487	
O 1.176710	-1.204142	-0.705532	
O 1.600061	-0.972699	1.493133	
H 0.622153	-1.056619	1.571418	
H 3.603544	0.703314	1.575473	
H 4.942522	0.698011	0.416012	
S 3.140464	1.985499	-0.433236	

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H 1.875600	1.868136	0.020276	
C -3.462489	-0.233503	-1.122215	
C -2.799733	0.940217	-0.318384	
O -4.718353	-0.263718	-1.060755	
O -2.680578	-0.976172	-1.740158	
H -2.612267	1.748917	-1.028044	
C -1.493301	0.584289	0.372555	
N -3.842243	1.443240	0.644936	
H -3.816290	2.450872	0.799365	
H -1.077296	1.441401	0.904070	
H -0.779243	0.254068	-0.378269	
S -1.661736	-0.747697	1.639198	
H -4.741071	1.147575	0.215782	
H -3.763375	0.967514	1.549086	
H -1.979321	-1.727968	0.767531	
28			
Dimer 298 of the n...z type			
C -2.231694	0.774568	0.483583	
C -1.637056	-0.569223	0.937501	
N -3.472805	1.068795	1.179884	
H -4.177380	0.378753	0.932216	
H -3.836358	1.970343	0.887603	
H -1.492308	1.538673	0.751581	
C -2.352158	0.830151	-1.043446	
O -3.374697	1.022579	-1.656607	
O -1.157752	0.642843	-1.643787	
H -1.273644	0.692081	-2.606324	
H -0.656424	-0.744522	0.499174	
H -1.540377	-0.549655	2.023092	
S -2.695021	-2.039612	0.579230	
H -2.401012	-2.140165	-0.733408	
C 2.384241	-1.241434	-0.489471	
C 3.088583	-0.407556	0.635534	
O 3.028642	-1.329200	-1.566073	
O 1.288155	-1.741013	-0.180441	
H 3.509454	-1.119755	1.347821	
C 2.164441	0.549324	1.380507	
N 4.242726	0.307254	-0.013149	
H 5.091289	0.332737	0.551172	
H 2.681595	1.025734	2.214448	
H 1.328735	-0.024668	1.773718	
S 1.534308	1.938791	0.346915	
H 4.389842	-0.214904	-0.900605	
H 3.972681	1.266539	-0.259566	
H 0.812933	1.192966	-0.516365	
28			
Dimer 299 of the n...z type			
C -3.580555	0.221897	1.004070	
C -2.488349	-0.832083	0.783143	
N -4.964031	-0.261277	0.980320	
H -5.064617	-1.046383	0.341496	
H -5.275231	-0.557279	1.897681	
H -3.397797	0.673523	1.985830	
C -3.444569	1.392567	0.011010	
O -2.383214	1.857026	-0.339728	
O -4.613407	1.877125	-0.408661	
H -5.290069	1.285944	0.012927	
H -1.502944	-0.372823	0.836878	
H -2.561154	-1.593590	1.559785	
S -2.630150	-1.748480	-0.809703	
H -2.229634	-0.737980	-1.608163	
C 4.998500	0.508201	0.163817	
C 3.761405	-0.405234	-0.135522	
O 5.222382	0.711445	1.384255	
O 5.585999	0.953987	-0.837529	
H 4.010022	-1.147899	-0.890835	
C 2.586955	0.459900	-0.594140	
N 3.420782	-1.127424	1.140047	
H 3.913804	-2.017544	1.213587	

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H	2.866060	0.950338	-1.524110
H	2.368079	1.232154	0.146198
S	0.997446	-0.446534	-0.810338
H	3.771559	-0.513926	1.897562
H	2.415367	-1.310487	1.223794
H	1.408168	-1.271065	-1.795510
28			
Dimer 300 of the n...z type			
C	-2.732823	-0.880138	-0.123699
C	-1.448490	-0.051452	0.049657
N	-3.001130	-1.152154	-1.525402
H	-3.176225	-0.279798	-2.017380
H	-3.841894	-1.712810	-1.621487
H	-2.549792	-1.832539	0.387551
C	-3.904851	-0.227086	0.618211
O	-4.938725	0.135222	0.107953
O	-3.648399	-0.101268	1.935625
H	-4.411724	0.316094	2.366060
H	-1.208286	0.064462	1.104883
H	-0.623335	-0.561396	-0.448529
S	-1.494462	1.619398	-0.733553
H	-2.271344	2.226322	0.187339
C	2.325986	-1.347352	-0.519044
C	2.351510	-0.533602	0.821689
O	3.160375	-2.285827	-0.581228
O	1.471757	-0.992073	-1.350753
H	1.547708	-0.923470	1.449975
C	2.172000	0.969756	0.657827
N	3.647492	-0.874676	1.506859
H	3.582519	-0.927826	2.522920
H	2.153963	1.471200	1.626598
H	1.225104	1.155993	0.157529
S	3.528532	1.779337	-0.290756
H	3.920781	-1.787131	1.093296
H	4.370220	-0.191918	1.251908
H	3.272599	1.161688	-1.462528
28			
Dimer 301 of the n...z type			
C	-1.420202	-0.100336	0.571674
C	-2.264656	-1.170815	-0.143388
N	-1.820510	0.056706	1.958127
H	-2.754586	0.454277	2.008815
H	-1.199111	0.704178	2.432509
H	-0.392550	-0.476471	0.547931
C	-1.431666	1.204556	-0.225157
O	-1.894057	2.253690	0.145101
O	-0.862746	1.047993	-1.450159
H	-0.909214	1.892486	-1.927723
H	-1.893176	-1.343775	-1.151629
H	-2.183106	-2.099009	0.421205
S	-4.074000	-0.817946	-0.222064
H	-4.023497	0.130508	-1.179928
C	2.296609	-1.515275	0.362892
C	2.767340	-0.577645	-0.799841
O	1.272141	-2.199766	0.111055
O	2.994787	-1.487000	1.392107
H	3.603136	-1.075132	-1.297787
C	3.219518	0.805854	-0.352572
N	1.649252	-0.518275	-1.806883
H	1.971605	-0.377022	-2.764204
H	3.460786	1.435620	-1.210115
H	4.116565	0.692717	0.251372
S	1.962709	1.741736	0.618851
H	1.154816	-1.420150	-1.713681
H	0.955717	0.209392	-1.582811
H	1.989409	0.925358	1.692258
28			
Dimer 302 of the n...z type			
C	-2.220102	-0.641312	0.535377

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C	-3.639657	-1.162932	0.279172
N	-2.072267	0.337274	1.616899
H	-2.914164	0.899093	1.719281
H	-1.876587	-0.108521	2.505079
H	-1.595923	-1.509462	0.775079
C	-1.594979	-0.059113	-0.747221
O	-1.725137	-0.548205	-1.845603
O	-0.854521	1.030339	-0.527686
H	-0.966467	1.205016	0.445940
H	-3.633482	-1.883644	-0.536725
H	-4.009602	-1.657192	1.177503
S	-4.873550	0.156610	-0.089187
H	-4.400676	0.479901	-1.310229
C	3.195503	-1.586344	-0.196797
C	2.369658	-0.280208	0.053210
O	3.752418	-2.064522	0.824507
O	3.233437	-1.974717	-1.377664
H	1.398738	-0.340979	-0.432443
C	3.145905	0.929746	-0.466805
N	2.147410	-0.170614	1.538224
H	1.274056	-0.612932	1.825000
H	3.276869	0.812174	-1.540302
H	4.134488	0.983465	-0.006041
S	2.357975	2.557235	-0.105545
H	2.924801	-0.708502	1.963786
H	2.129127	0.804063	1.855146
H	1.194476	2.307203	-0.741266
28			
Dimer 303 of the n...z type			
C	2.398778	-0.431592	-0.735466
C	1.661906	0.896627	-0.483814
N	1.633545	-1.563405	-0.239425
H	1.611901	-1.545975	0.776804
H	2.080517	-2.435409	-0.504123
H	2.490623	-0.524455	-1.823410
C	3.830283	-0.367361	-0.191949
O	4.279376	-1.080979	0.674071
O	4.546908	0.600926	-0.796027
H	5.440228	0.614518	-0.416493
H	2.206057	1.728464	-0.926977
H	0.671341	0.838324	-0.937129
S	1.340401	1.276193	1.293449
H	2.594291	1.636518	1.636202
C	-2.442815	1.076007	-0.878399
C	-2.284473	0.509614	0.574562
O	-3.491711	1.741541	-1.073881
O	-1.506957	0.828250	-1.660196
H	-1.614832	1.185763	1.110627
C	-1.727422	-0.905418	0.649909
N	-3.634650	0.622407	1.230713
H	-3.599313	0.860249	2.221558
H	-1.596110	-1.219771	1.686501
H	-0.758421	-0.935752	0.156701
S	-2.825397	-2.174946	-0.111945
H	-4.124505	1.353326	0.679666
H	-4.157028	-0.253245	1.113701
H	-2.715560	-1.720672	-1.377512
28			
Dimer 304 of the n...z type			
C	-1.564014	-0.030286	-0.165270
C	-2.419190	1.164223	-0.615378
N	-1.425787	-1.012536	-1.228357
H	-2.333228	-1.414183	-1.449211
H	-0.834712	-1.779409	-0.921106
H	-0.575328	0.388480	0.061685
C	-2.078368	-0.613953	1.152798
O	-2.362751	-1.774227	1.339541
O	-2.162345	0.327145	2.115430
H	-2.475093	-0.089642	2.934302

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H	-2.417736	1.946418	0.140617
H	-1.993541	1.565738	-1.534713
S	-4.168518	0.750833	-1.042003
H	-4.608951	0.569059	0.220017
C	2.464089	1.369498	0.389971
C	2.989305	0.514173	-0.815225
O	3.352389	1.744436	1.195329
O	1.240529	1.598848	0.398832
H	3.105899	1.193146	-1.662668
C	2.081262	-0.636570	-1.224619
N	4.368285	0.042520	-0.438686
H	5.024655	0.006304	-1.218299
H	2.486682	-1.170983	-2.084944
H	1.108965	-0.233980	-1.498676
S	1.869073	-1.919389	0.083238
H	4.677830	0.718007	0.286565
H	4.319821	-0.883390	0.000595
H	1.327302	-1.100690	1.008669
28	Dimer 305 of the n...z type		
C	2.740201	0.401273	0.946245
C	1.382315	0.996242	0.531572
N	3.832180	1.314224	0.659191
H	3.933235	1.433516	-0.345028
H	4.709971	0.934018	0.998589
H	2.684491	0.252674	2.029931
C	2.909339	-0.993367	0.331837
O	3.729640	-1.290439	-0.504341
O	2.012098	-1.863733	0.832887
H	2.130867	-2.724662	0.400449
H	0.570528	0.323891	0.803835
H	1.244242	1.946498	1.046543
S	1.230019	1.409002	-1.261013
H	1.189985	0.142933	-1.725180
C	-2.978198	0.311119	1.124841
C	-3.077968	0.361377	-0.439166
O	-2.496574	1.344264	1.655450
O	-3.408422	-0.725925	1.661593
H	-4.101991	0.657977	-0.680266
C	-2.778152	-0.954947	-1.143382
N	-2.192170	1.487163	-0.898360
H	-2.546271	1.977902	-1.718731
H	-2.819844	-0.837253	-2.227395
H	-3.536378	-1.676461	-0.848083
S	-1.112691	-1.654392	-0.782351
H	-2.140638	2.120539	-0.079825
H	-1.222337	1.188691	-1.094266
H	-1.332343	-1.867235	0.531055
28	Dimer 306 of the n...z type		
C	3.355222	-0.116539	-0.705667
C	2.146453	-1.044045	-0.913850
N	4.509659	-0.848747	-0.216277
H	4.309716	-1.238979	0.700924
H	5.300556	-0.223272	-0.100182
H	3.596454	0.292711	-1.694198
C	2.976384	1.096152	0.155377
O	3.551016	1.442600	1.159083
O	1.912778	1.754034	-0.351663
H	1.717419	2.519547	0.212812
H	1.334019	-0.507546	-1.398978
H	2.448021	-1.869269	-1.558264
S	1.518039	-1.857015	0.618884
H	1.083232	-0.742884	1.242927
C	-3.417167	-0.860540	0.514997
C	-2.065765	-0.572719	-0.223723
O	-4.329611	-1.320960	-0.218993
O	-3.425835	-0.629436	1.736800
H	-1.405410	-1.422816	-0.036218

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C	-1.359081	0.702044	0.216816
N	-2.369068	-0.572006	-1.697618
H	-1.632587	-0.977308	-2.274491
H	-0.403490	0.826352	-0.292972
H	-1.175857	0.637229	1.286800
S	-2.298687	2.244828	-0.146376
H	-3.252512	-1.113308	-1.771763
H	-2.562436	0.381741	-2.022587
H	-3.333963	1.982046	0.677810
28	Dimer 307 of the n...z type		
C	2.308735	-1.019654	0.108599
C	3.130382	-0.192563	1.110907
N	3.162681	-1.868860	-0.703847
H	3.777449	-1.292675	-1.273201
H	2.601952	-2.417231	-1.348317
H	1.650930	-1.661900	0.707840
C	1.367432	-0.126890	-0.708623
O	1.273398	-0.132340	-1.911371
O	0.623994	0.678728	0.083102
H	-0.037103	1.173956	-0.456083
H	2.479111	0.334176	1.804879
H	3.769364	-0.870657	1.675711
S	4.284196	1.023219	0.337768
H	3.351060	1.928468	-0.021423
C	-2.929555	-1.256117	-0.085210
C	-2.886435	-0.186692	1.060369
O	-2.114884	-2.202082	0.049111
O	-3.781571	-1.062771	-0.972311
H	-3.656125	-0.476021	1.780242
C	-3.170353	1.249823	0.637962
N	-1.573746	-0.358520	1.779444
H	-1.608370	-0.079777	2.759884
H	-2.996301	1.943375	1.462020
H	-4.219983	1.313001	0.360520
S	-2.184756	1.906995	-0.778590
H	-1.356679	-1.364728	1.688874
H	-0.797381	0.136195	1.320239
H	-2.600230	0.982348	-1.669476
28	Dimer 308 of the n...z type		
C	-2.743561	-0.286308	0.875460
C	-1.893876	0.953415	0.569525
N	-2.077861	-1.584031	0.741185
H	-1.376926	-1.565301	0.004607
H	-1.631703	-1.873803	1.602950
H	-3.090096	-0.190641	1.910698
C	-4.036539	-0.300119	0.035537
O	-4.677794	0.692447	-0.227195
O	-4.408145	-1.518840	-0.355214
H	-3.681763	-2.113351	-0.033806
H	-2.481646	1.858744	0.709370
H	-1.041238	0.986615	1.247626
S	-1.168131	0.968763	-1.125329
H	-2.309541	1.231964	-1.793014
C	3.162024	-1.559841	-0.481104
C	2.314794	-0.340956	0.017044
O	3.777548	-2.181745	0.421392
O	3.154377	-1.744084	-1.711309
H	1.328325	-0.356305	-0.441258
C	3.042905	0.963141	-0.311903
N	2.145027	-0.488805	1.504751
H	1.311478	-1.028311	1.738218
H	3.128800	1.043069	-1.393293
H	4.049779	0.957484	0.110657
S	2.251713	2.482893	0.369102
H	2.965577	-1.035957	1.819703
H	2.079147	0.418894	1.977565
H	1.099949	2.392041	-0.330677

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28		
Dimer 309 of the n...z	type	
C	-3.324704	-0.218370
C	-2.376389	0.963134
N	-4.619942	0.245157
H	-4.518412	0.701941
H	-5.246970	-0.540759
H	-3.461670	-0.728000
C	-2.665486	-1.247311
O	-3.069133	-1.560363
O	-1.562382	-1.787308
H	-1.193768	-2.446600
H	-1.440428	0.613343
H	-2.859111	1.626404
S	-2.009171	2.029318
H	-1.148535	1.189381
C	3.868822	0.641832
C	2.782067	-0.263909
O	4.937562	0.047347
O	3.562200	1.838039
H	2.852821	-0.101743
C	1.354253	0.011952
N	3.188156	-1.690913
H	2.984457	-2.325667
H	0.641934	-0.617896
H	1.125393	1.055264
S	1.053193	-0.334890
H	4.207704	-1.633764
H	2.737368	-2.043447
H	1.859991	0.635308
28		
Dimer 310 of the n...z	type	
C	-1.980938	0.129761
C	-2.246785	-1.377242
N	-2.028036	0.875932
H	-2.698522	0.463896
H	-1.119510	0.903278
H	-0.979757	0.256532
C	-2.915484	0.809609
O	-3.256065	0.302604
O	-3.292261	2.036238
H	-2.899358	2.155887
H	-2.159411	-1.838608
H	-1.513421	-1.832365
S	-3.885067	-1.812232
H	-4.634643	-1.393174
C	4.205240	-0.795374
C	2.800308	-0.172093
O	4.492588	-1.816363
O	4.878488	-0.189392
H	2.261573	0.027837
C	2.976974	1.108797
N	2.032437	-1.203218
H	1.446172	-1.780498
H	3.587692	1.798377
H	3.495161	0.901943
S	1.408009	1.943464
H	2.769382	-1.815579
H	1.434883	-0.793488
H	0.994001	2.251822
28		
Dimer 311 of the n...z	type	
C	-2.972770	-0.910317
C	-3.668262	0.447852
N	-2.286112	-0.985783
H	-1.575660	-0.260826
H	-1.801556	-1.873291
H	-3.769621	-1.664908
C	-2.083722	-1.254952

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O	-0.939960	-1.638805
O	-2.736182	-1.104864
H	-2.143544	-1.357896
H	-4.298123	0.445566
H	-4.293079	0.635269
S	-2.522738	1.893536
H	-2.101188	1.687032
C	2.996828	-1.136942
C	1.771102	-0.335982
O	3.868713	-1.427896
O	2.961178	-1.418308
H	0.962753	-1.050096
C	1.257199	0.762936
N	2.180309	0.199053
H	1.431665	0.208131
H	0.370515	1.239443
H	0.987544	0.310986
S	2.462223	2.129158
H	2.959900	-0.422840
H	2.560125	1.147437
H	3.386896	1.383428
28		
Dimer 312 of the n...z	type	
C	2.135313	-0.312086
C	1.551923	0.847143
N	2.647477	0.153989
H	3.451648	0.757750
H	2.974662	-0.630594
H	1.294441	-0.992566
C	3.153123	-1.109671
O	4.289715	-1.345931
O	2.628260	-1.540732
H	3.304110	-2.046003
H	1.069899	0.470295
H	0.808795	1.356632
S	2.764314	2.153294
H	3.412973	1.441785
C	-1.454355	-0.410436
C	-2.181583	0.333769
O	-0.975923	-1.533544
O	-1.396365	0.204890
H	-1.473418	1.058568
C	-3.455460	1.063070
N	-2.427892	-0.689034
H	-2.334150	-0.328197
H	-3.878635	1.613704
H	-3.205398	1.768548
S	-4.799958	-0.055646
H	-1.731679	-1.434264
H	-3.360957	-1.101995
H	-4.158369	-0.498924
28		
Dimer 313 of the n...z	type	
C	-3.337181	0.633889
C	-3.513099	-0.515773
N	-3.551238	0.182571
H	-2.855824	-0.517896
H	-3.431604	0.953032
H	-4.108985	1.372774
C	-2.003689	1.358243
O	-1.128600	1.474587
O	-1.926675	1.887080
H	-1.083300	2.357088
H	-3.386996	-0.148103
H	-4.524326	-0.908820
S	-2.408043	-1.967498
H	-1.235693	-1.407013
C	1.218182	-0.652746
C	1.993756	0.684412

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O	0.635675	-0.730694	1.221421
O	1.223787	-1.464543	-0.834744
H	1.287349	1.359591	-0.615217
C	3.254398	0.560853	-0.969433
N	2.277974	1.262914	1.232889
H	2.266050	2.282211	1.259865
H	3.712856	1.535601	-1.140853
H	2.981916	0.130668	-1.930001
S	4.569167	-0.472264	-0.190887
H	1.542285	0.863455	1.843668
H	3.186452	0.930219	1.575467
H	3.876968	-1.629717	-0.226335
28			
Dimer 314 of the n...z type			
C	-2.146430	0.647754	-1.004405
C	-3.327450	-0.334752	-0.939424
N	-0.944041	0.010366	-1.506741
H	-0.572242	-0.663528	-0.838392
H	-0.214475	0.700385	-1.651607
H	-2.446155	1.429312	-1.714499
C	-1.954983	1.382003	0.329864
O	-0.898881	1.526365	0.901995
O	-3.112955	1.883724	0.799438
H	-2.936910	2.357429	1.628418
H	-4.255084	0.188059	-0.716660
H	-3.422760	-0.818701	-1.910949
S	-3.122925	-1.716324	0.266455
H	-3.340214	-0.992525	1.383786
C	1.760733	-1.291521	0.808909
C	3.091009	-0.828039	0.123556
O	0.967103	-1.918298	0.056328
O	1.650917	-1.013373	2.013601
H	3.888125	-1.474414	0.494892
C	3.461093	0.625668	0.402552
N	2.945294	-1.101106	-1.349352
H	3.775568	-1.501788	-1.783539
H	4.453462	0.857374	0.013729
H	3.465052	0.771527	1.480199
S	2.336276	1.854498	-0.386938
H	2.134764	-1.751145	-1.402801
H	2.685757	-0.240990	-1.846274
H	1.209419	1.529403	0.286867
28			
Dimer 315 of the n...z type			
C	3.564264	0.518399	-0.018757
C	3.347937	-0.654318	-0.994553
N	4.210760	0.074253	1.204733
H	3.608569	-0.586716	1.688634
H	4.349336	0.857595	1.835277
H	4.231852	1.221735	-0.529851
C	2.253561	1.279173	0.209311
O	1.678605	1.379308	1.267699
O	1.812355	1.849796	-0.928140
H	0.965436	2.286535	-0.747125
H	2.924930	-0.293986	-1.930628
H	4.316867	-1.108010	-1.201858
S	2.290974	-2.020760	-0.346404
H	1.086334	-1.396039	-0.494734
C	-1.294603	-0.306996	0.220036
C	-2.319711	0.875515	0.176631
O	-0.590140	-0.423149	-0.820791
O	-1.267414	-0.973525	1.265399
H	-1.851443	1.720872	0.685776
C	-3.660658	0.574496	0.832910
N	-2.473848	1.265630	-1.268858
H	-2.601718	2.266043	-1.418322
H	-4.309756	1.451089	0.823355
H	-3.478072	0.286448	1.865218
S	-4.615996	-0.754124	-0.015300

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H	-1.606917	0.923870	-1.724243
H	-3.263582	0.760489	-1.687483
H	-3.741855	-1.748002	0.245312
28			
Dimer 316 of the n...z type			
C	2.159412	-0.770087	-0.068587
C	2.114083	0.511726	-0.909513
N	1.658849	-0.662779	1.304800
H	1.826694	0.267739	1.680063
H	0.666052	-0.853828	1.361505
H	1.557116	-1.521368	-0.591759
C	3.578368	-1.371413	-0.033516
O	4.327305	-1.384279	-0.984832
O	3.901345	-1.910525	1.141629
H	3.119960	-1.716231	1.722852
H	2.494767	0.320102	-1.911139
H	1.083615	0.858028	-0.983389
S	3.031460	1.931047	-0.173880
H	4.271886	1.437788	-0.367932
C	-4.273792	-0.938745	0.021713
C	-2.845434	-0.312299	0.177689
O	-4.529139	-1.391286	-1.123598
O	-4.993478	-0.882974	1.033776
H	-2.370655	-0.681299	1.084375
C	-2.950370	1.212240	0.203612
N	-2.033219	-0.769557	-1.004600
H	-1.508577	-1.620612	-0.801461
H	-3.547599	1.499323	1.066206
H	-3.451853	1.579623	-0.694381
S	-1.333383	2.097001	0.240411
H	-2.739316	-1.001668	-1.729884
H	-1.369809	-0.057120	-1.322651
H	-0.922797	1.631093	1.437517
28			
Dimer 1 of the z...z type			
C	0.530028	1.668862	0.134520
C	1.957368	1.067280	0.296421
O	-0.200790	1.632448	1.169871
O	0.251790	2.131120	-0.980426
H	2.658713	1.899597	0.382312
C	2.338715	0.178390	-0.885099
N	2.023015	0.293664	1.579754
H	2.969956	-0.047006	1.757614
H	2.250889	0.765865	-1.795382
H	1.662984	-0.674686	-0.962503
S	4.029303	-0.548593	-0.765922
H	1.711331	0.877062	2.356586
H	1.361384	-0.525531	1.512435
H	4.709835	0.611811	-0.866752
C	-0.530268	-1.668942	0.136022
C	-1.957364	-1.066883	0.297460
O	0.201191	-1.630510	1.170895
O	-0.252723	-2.133844	-0.977999
H	-2.658927	-1.898919	0.384507
C	-2.338773	-0.179170	-0.884970
N	-2.022545	-0.291825	1.579901
H	-1.711974	-0.874687	2.357525
H	-2.251108	-0.767683	-1.794605
H	-1.662791	0.673674	-0.963223
S	-4.029183	0.548130	-0.766278
H	-1.360364	0.526665	1.511921
H	-2.969295	0.049850	1.757080
H	-4.709809	-0.612420	-0.864774
28			
Dimer 2 of the z...z type			
C	1.784535	-0.844415	0.700633
C	2.206667	-0.447138	-0.740482
O	1.057240	-0.014331	1.323216
O	2.246209	-1.916590	1.112500

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H	1.905085	-1.244798	-1.421229
C	3.720390	-0.257443	-0.840848
N	1.468585	0.785158	-1.162852
H	1.763784	1.111020	-2.083820
H	4.015637	-0.019287	-1.864142
H	4.199443	-1.190503	-0.550930
S	4.381080	1.121781	0.192261
H	0.434215	0.569675	-1.192972
H	1.630048	1.532975	-0.484395
H	4.097516	0.567210	1.388810
C	-1.784601	-0.844317	-0.700762
C	-2.206723	-0.447211	0.740402
O	-1.057305	-0.014161	-1.323249
O	-2.246281	-1.916441	-1.112757
H	-1.905134	-1.244952	1.421052
C	-3.720446	-0.257533	0.840801
N	-1.468640	0.785037	1.162910
H	-1.763844	1.110803	2.083912
H	-4.015689	-0.019513	1.864128
H	-4.199500	-1.190555	0.550763
S	-4.381143	1.121827	-0.192121
H	-0.434271	0.569545	1.193014
H	-1.630094	1.532928	0.484534
H	-4.097572	0.567422	-1.388745
28			
Dimer 3 of the z...z type			
C	-0.677447	-0.835422	-0.555541
C	-1.943423	-0.177344	0.059582
O	-0.424157	-0.547156	-1.738667
O	-0.039067	-1.608985	0.212143
H	-1.815985	-0.081385	1.135794
C	-3.175770	-1.011557	-0.277233
N	-2.051082	1.210402	-0.491459
H	-1.248060	1.755987	-0.079113
H	-3.035571	-2.020447	0.108709
H	-3.306541	-1.073787	-1.359328
S	-4.755691	-0.316461	0.373373
H	-1.933349	1.179004	-1.507937
H	-2.947574	1.643775	-0.259017
H	-4.451671	-0.448819	1.680623
C	1.267567	1.780473	0.109856
C	2.318938	0.736933	0.587166
O	0.190582	1.814154	0.778631
O	1.586559	2.470698	-0.866996
H	3.147865	1.280036	1.044365
C	2.820801	-0.113069	-0.578703
N	1.717457	-0.135656	1.652907
H	2.430477	-0.706877	2.109149
H	3.246598	0.551149	-1.326488
H	1.990473	-0.657037	-1.030776
S	4.056031	-1.394802	-0.099266
H	1.238110	0.441973	2.344289
H	0.998855	-0.773197	1.218604
H	5.040978	-0.543162	0.253634
28			
Dimer 4 of the z...z type			
C	1.169207	-0.763937	-0.286567
C	2.025578	0.512208	-0.503020
O	0.864636	-1.027956	0.915231
O	0.871655	-1.392712	-1.311826
H	1.538285	1.113745	-1.271390
C	3.444673	0.168124	-0.950122
N	2.021520	1.336153	0.751504
H	2.614907	2.162042	0.667306
H	4.018145	1.074221	-1.152673
H	3.378358	-0.410004	-1.870358
S	4.434321	-0.762097	0.298833
H	1.029935	1.635269	0.953132
H	2.349332	0.767967	1.536144

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H	3.665637	-1.870456	0.314318
C	-1.130562	1.368793	-0.135271
C	-2.013882	0.094595	-0.034592
O	-0.635687	1.785522	0.955331
O	-0.987389	1.838023	-1.272969
H	-1.697231	-0.595897	-0.816088
C	-3.487827	0.455787	-0.195742
N	-1.753980	-0.588014	1.273785
H	-0.756885	-0.932589	1.269283
H	-3.612919	0.976399	-1.143322
H	-3.809589	1.121931	0.607603
S	-4.629842	-0.990059	-0.121080
H	-1.839428	0.085639	2.037850
H	-2.402988	-1.364147	1.423340
H	-4.168851	-1.603047	-1.230467
28			
Dimer 5 of the z...z type			
C	1.278344	-0.310986	0.933931
C	2.088404	-0.682882	-0.335573
O	0.325575	0.507293	0.762703
O	1.656726	-0.840966	1.986978
H	2.050281	-1.767122	-0.449344
C	3.546612	-0.243350	-0.218264
N	1.433652	-0.097337	-1.551422
H	0.493204	-0.555654	-1.706211
H	4.116816	-0.547428	-1.097680
H	3.977379	-0.725384	0.657196
S	3.775683	1.583466	-0.091495
H	1.278175	0.902835	-1.407794
H	2.003799	-0.224335	-2.388464
H	3.184001	1.727929	1.112172
C	-1.324762	-1.609157	-0.556383
C	-2.407639	-0.648386	0.028167
O	-0.945054	-2.517730	0.201898
O	-0.935512	-1.365232	-1.733686
H	-3.368341	-1.166519	0.000219
C	-2.494970	0.682784	-0.705909
N	-2.059682	-0.432273	1.473308
H	-1.955756	-1.336436	1.937150
H	-2.722315	0.490687	-1.751004
H	-1.536130	1.197741	-0.653511
S	-3.735272	1.854502	-0.000522
H	-1.120917	0.050684	1.492273
H	-2.763240	0.131127	1.953604
H	-4.831135	1.126607	-0.298498
28			
Dimer 6 of the z...z type			
C	1.062653	1.632276	0.421462
C	2.430553	0.902083	0.548807
O	0.318522	1.543840	1.443925
O	0.833920	2.228814	-0.639978
H	3.131044	1.611889	0.998410
C	3.019298	0.426237	-0.773198
N	2.272946	-0.224933	1.530937
H	3.146062	-0.732091	1.675699
H	3.982582	-0.061273	-0.612270
H	3.179192	1.300117	-1.401101
S	1.986422	-0.795628	-1.682852
H	1.960192	0.156492	2.425387
H	1.515068	-0.902500	1.244471
H	0.975471	0.054607	-1.945973
C	-0.751345	-1.932098	0.322019
C	-1.911615	-0.898203	0.419214
O	0.145749	-1.842055	1.210484
O	-0.841826	-2.738569	-0.612927
H	-2.849108	-1.452430	0.477211
C	-1.921520	0.026452	-0.796201
N	-1.785434	-0.096910	1.681286
H	-1.631837	-0.714301	2.478324

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H -1.954928	-0.587610	-1.693461	
H -1.021391	0.641168	-0.826480	
S -3.310200	1.239660	-0.810584	
H -0.955974	0.555366	1.620736	
H -2.622927	0.465175	1.843049	
H -4.304643	0.337072	-0.939231	
28			
Dimer 7 of the z...z type			
C 0.949153	-0.956933	0.512871	
C 2.127717	-0.269580	-0.225469	
O 0.542804	-0.358739	1.554609	
O 0.522115	-2.012979	0.024722	
H 2.011615	-0.423326	-1.296879	
C 3.454064	-0.849748	0.262058	
N 2.055148	1.206680	0.016427	
H 1.183834	1.576992	-0.449491	
H 3.447979	-1.925180	0.091149	
H 3.577154	-0.672927	1.332599	
S 4.941573	-0.103957	-0.532999	
H 1.956382	1.379596	1.020222	
H 2.887937	1.685396	-0.334906	
H 4.678271	-0.536267	-1.783135	
C -1.213385	1.499290	-0.108747	
C -2.043828	0.184516	-0.069095	
O -1.454613	2.323919	0.790315	
O -0.376257	1.587373	-1.051168	
H -1.517966	-0.604147	-0.603336	
C -3.431782	0.416226	-0.655194	
N -2.120405	-0.244640	1.365551	
H -1.133006	-0.462338	1.674604	
H -3.329799	0.762828	-1.683000	
H -3.958985	1.184035	-0.085726	
S -4.521598	-1.072164	-0.613970	
H -2.468096	0.533542	1.931945	
H -2.730608	-1.055951	1.485491	
H -3.791554	-1.817803	-1.468251	
28			
Dimer 8 of the z...z type			
C 1.550327	0.568701	1.115026	
C 2.346021	-0.664181	0.606709	
O 0.437668	0.782842	0.547322	
O 2.099738	1.225797	2.009272	
H 2.510894	-1.334664	1.451922	
C 3.701239	-0.257349	0.028835	
N 1.528950	-1.419278	-0.395977	
H 2.026445	-2.236156	-0.752154	
H 4.266772	-1.131727	-0.297644	
H 4.265141	0.248672	0.809807	
S 3.585694	0.837199	-1.453225	
H 0.607781	-1.736224	0.018187	
H 1.307780	-0.807427	-1.185638	
H 3.061774	1.902985	-0.813629	
C -1.846721	-1.843355	-0.135081	
C -2.575954	-0.530064	0.266326	
O -0.858822	-2.174764	0.588780	
O -2.298969	-2.423265	-1.131526	
H -3.613341	-0.769176	0.503222	
C -2.505571	0.484043	-0.875618	
N -1.944486	0.045632	1.498187	
H -1.851451	-0.668933	2.219703	
H -2.930113	0.029073	-1.767254	
H -1.464732	0.745373	-1.074765	
S -3.352132	2.083879	-0.522366	
H -0.973254	0.383677	1.252913	
H -2.488145	0.830935	1.860073	
H -4.606747	1.590202	-0.478734	
28			
Dimer 9 of the z...z type			
C -1.127110	-0.853063	0.102293	

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C -2.105324	-0.065985	1.009242	
O -0.901335	-0.336515	-1.033405	
O -0.668456	-1.909223	0.562257	
H -1.765947	-0.154921	2.040902	
C -3.529399	-0.616459	0.908912	
N -2.042393	1.387572	0.650845	
H -2.709616	1.946191	1.183271	
H -4.184017	-0.114628	1.623843	
H -3.500707	-1.676400	1.159912	
S -4.342613	-0.379234	-0.730184	
H -1.058513	1.734043	0.826705	
H -2.238204	1.499596	-0.347322	
H -3.398528	-1.000142	-1.467179	
C 1.218406	1.550377	-0.001075	
C 1.954415	0.180462	-0.020500	
O 1.343568	2.251175	-1.019937	
O 0.572979	1.805888	1.055334	
H 1.492530	-0.500293	0.691804	
C 3.435459	0.375103	0.282983	
N 1.745739	-0.413490	-1.380888	
H 0.708603	-0.592929	-1.477195	
H 3.537761	0.843459	1.261306	
H 3.889384	1.033541	-0.460232	
S 4.425236	-1.181495	0.240943	
H 2.019950	0.268838	-2.092614	
H 2.283885	-1.273770	-1.504207	
H 3.825314	-1.772699	1.294032	
28			
Dimer 10 of the z...z type			
C 0.930377	-1.270077	-0.045592	
C 2.032710	-0.174851	-0.066355	
O 0.467694	-1.564910	1.097746	
O 0.610981	-1.734481	-1.148415	
H 1.769003	0.552147	-0.834056	
C 3.395267	-0.798957	-0.356648	
N 2.031105	0.559417	1.240877	
H 1.133041	1.105127	1.313163	
H 3.329331	-1.343308	-1.296780	
H 3.671733	-1.504266	0.429934	
S 4.780734	0.415924	-0.433449	
H 2.040322	-0.112195	2.011766	
H 2.837277	1.184721	1.315906	
H 4.336174	1.084254	-1.517274	
C -0.930999	1.271400	-0.042595	
C -2.032685	0.175563	-0.065817	
O -0.464719	1.559951	1.100864	
O -0.615608	1.742253	-1.143822	
H -1.768953	-0.548891	-0.835875	
C -3.395966	0.799444	-0.353167	
N -2.029436	-0.562926	1.239101	
H -1.130416	-1.107182	1.309752	
H -3.330964	1.347220	-1.291362	
H -3.672799	1.501741	0.435989	
S -4.780355	-0.416443	-0.433720	
H -2.040108	0.105961	2.012314	
H -2.834312	-1.190145	1.312049	
H -4.336092	-1.079965	-1.520609	
28			
Dimer 11 of the z...z type			
C 0.997443	-1.242935	-0.402620	
C 2.222384	-0.290620	-0.374129	
O 0.096580	-0.992188	0.453641	
O 1.009501	-2.150639	-1.247106	
H 2.663765	-0.244860	-1.368432	
C 3.243574	-0.786300	0.646927	
N 1.746545	1.089164	-0.040104	
H 1.070759	1.409275	-0.780428	
H 3.540057	-1.800995	0.384404	
H 2.800632	-0.806263	1.644630	

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S	4.743956	0.276324	0.791574
H	1.201700	1.073940	0.826990
H	2.525535	1.743227	0.061028
H	5.212145	0.047257	-0.452336
C	-1.191791	1.498634	-0.639913
C	-2.432622	0.562097	-0.547200
O	-0.424925	1.283362	-1.626181
O	-1.040723	2.346011	0.254142
H	-3.225361	0.981792	-1.170124
C	-2.912930	0.376750	0.887133
N	-2.050050	-0.763970	-1.137744
H	-1.631988	-0.622879	-2.059223
H	-3.141617	1.351702	1.308614
H	-2.120346	-0.075840	1.484759
S	-4.372081	-0.739769	1.056928
H	-1.300587	-1.170449	-0.519683
H	-2.846846	-1.398987	-1.202686
H	-5.253132	0.053721	0.414229
28			
Dimer 12 of the z...z type			
C	1.557567	1.792990	0.559417
C	2.573927	0.617165	0.518294
O	0.506386	1.596814	1.242289
O	1.869817	2.794680	-0.098698
H	3.509793	0.953460	0.966492
C	2.802865	0.165085	-0.924039
N	2.060238	-0.531373	1.333950
H	1.763176	-0.209885	2.255100
H	3.123557	1.023880	-1.508397
H	1.871078	-0.217972	-1.345001
S	4.022326	-1.207361	-1.102813
H	1.211643	-0.939913	0.850413
H	2.769321	-1.259451	1.435857
H	5.104445	-0.506395	-0.706213
C	-1.182686	-1.378463	0.553596
C	-2.216206	-0.239723	0.330346
O	-0.090365	-1.264288	-0.082684
O	-1.536174	-2.282131	1.321907
H	-2.555787	0.110176	1.305130
C	-3.400916	-0.750411	-0.487884
N	-1.548016	0.918417	-0.340390
H	-0.795449	1.310962	0.291191
H	-3.823790	-1.614045	0.021603
H	-3.074282	-1.064770	-1.481721
S	-4.716630	0.508399	-0.780691
H	-1.073585	0.598985	-1.187638
H	-2.222975	1.646612	-0.585484
H	-5.088446	0.641964	0.508913
28			
Dimer 13 of the z...z type			
C	2.293215	0.611617	1.324520
C	2.957951	-0.456789	0.413265
O	1.177551	0.290665	1.833594
O	2.919077	1.673514	1.441239
H	3.892784	-0.767921	0.885004
C	3.278743	0.087628	-0.976045
N	2.086767	-1.676980	0.336465
H	2.560536	-2.451131	-0.130579
H	3.600643	-0.711188	-1.645808
H	4.094572	0.800452	-0.881392
S	1.875718	0.936184	-1.827677
H	1.838316	-1.976528	1.280818
H	1.162843	-1.524426	-0.149731
H	1.913383	2.047834	-1.063804
C	-1.473083	-1.763793	-0.083843
C	-2.017068	-0.380702	0.376436
O	-0.378205	-1.745479	-0.720464
O	-2.192141	-2.736021	0.185058
H	-2.268691	-0.434321	1.435402

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C	-3.258198	-0.020857	-0.441823
N	-0.956015	0.659296	0.221267
H	-0.183223	0.536598	0.925703
H	-3.990787	-0.816223	-0.322660
H	-3.007056	0.059368	-1.501869
S	-4.014634	1.601444	0.002302
H	-0.499951	0.565333	-0.694157
H	-1.346249	1.601167	0.311411
H	-4.359347	1.268664	1.263066
28			
Dimer 14 of the z...z type			
C	1.482743	-1.559222	0.193762
C	2.625679	-0.926219	-0.654555
O	0.435086	-1.833325	-0.469796
O	1.704372	-1.772515	1.390798
H	3.183717	-1.765416	-1.079335
C	3.608855	-0.062754	0.126845
N	2.012550	-0.196702	-1.820549
H	2.718917	0.226199	-2.423402
H	4.509623	0.116201	-0.462470
H	3.885007	-0.625016	1.016867
S	3.010168	1.613819	0.603236
H	1.458302	-0.857885	-2.367268
H	1.332672	0.543931	-1.511476
H	1.756736	1.272501	1.004564
C	-0.643528	0.911483	-0.061999
C	-1.932158	0.062385	-0.234744
O	-0.246469	1.046146	1.115459
O	-0.128807	1.367462	-1.114862
H	-1.971339	-0.339677	-1.245250
C	-3.166886	0.902960	0.073665
N	-1.813888	-1.104792	0.696363
H	-0.967917	-1.659877	0.372659
H	-3.195588	1.755366	-0.604219
H	-3.117639	1.281314	1.096560
S	-4.757726	-0.024319	-0.037029
H	-1.620325	-0.764219	1.641675
H	-2.661874	-1.674929	0.703424
H	-4.701689	-0.263987	-1.362994
28			
Dimer 15 of the z...z type			
C	-1.254991	0.873123	-0.334329
C	-1.865395	-0.496214	-0.752325
O	-0.746430	0.924984	0.816413
O	-1.366485	1.779477	-1.179776
H	-1.516205	-0.744142	-1.755426
C	-3.392629	-0.426457	-0.769504
N	-1.364833	-1.563602	0.168266
H	-0.353129	-1.795975	-0.074571
H	-3.820757	-1.364804	-1.127382
H	-3.686610	0.368474	-1.453137
S	-4.165922	-0.146286	0.882404
H	-1.391117	-1.205639	1.126845
H	-1.919334	-2.418031	0.114428
H	-3.569436	1.036472	1.137179
C	2.211296	-1.737066	-0.213836
C	2.151127	-0.320171	0.414569
O	3.336365	-2.256263	-0.317165
O	1.101896	-2.194972	-0.603582
H	1.282167	-0.210983	1.059435
C	2.105337	0.733599	-0.694198
N	3.382351	-0.119452	1.255823
H	3.300854	-0.586089	2.159828
H	1.221673	0.556292	-1.304064
H	2.985717	0.655095	-1.335117
S	2.068573	2.461255	-0.059633
H	4.180540	-0.543175	0.766334
H	3.548276	0.880430	1.420820
H	0.841075	2.327260	0.502487

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28		
Dimer 16 of the z...z type		
C	-1.260857	0.898511 -0.252013
C	-1.840057	-0.461292 -0.740612
O	-0.732423	0.900921 0.890416
O	-1.409301	1.846678 -1.044560
H	-1.455323	-0.665585 -1.740735
C	-3.366320	-0.411260 -0.806379
N	-1.355486	-1.559304 0.152877
H	-0.341399	-1.790743 -0.081047
H	-3.769072	-1.341550 -1.211450
H	-3.649396	0.404447 -1.469490
S	-4.194796	-0.200157 0.828478
H	-1.394616	-1.232820 1.122081
H	-1.912239	-2.409306 0.062985
H	-3.667082	1.006938 1.118507
C	2.224295	-1.741044 -0.208582
C	2.161644	-0.319232 0.408370
O	3.350007	-2.259060 -0.310362
O	1.114941	-2.203906 -0.592481
H	1.301813	-0.212166 1.065880
C	2.086333	0.722559 -0.710291
N	3.403872	-0.099945 1.228056
H	3.338118	-0.555138 2.139247
H	1.190216	0.532906 -1.298035
H	2.951630	0.640499 -1.371099
S	2.059729	2.457736 -0.097351
H	4.197283	-0.526088 0.732905
H	3.566621	0.903008 1.377170
H	0.849799	2.332551 0.501457
28		
Dimer 17 of the z...z type		
C	1.876896	1.935511 0.158696
C	2.146970	0.459515 -0.236867
O	2.871621	2.657830 0.345639
O	0.659577	2.235051 0.301954
H	1.475368	0.136244 -1.029930
C	1.985715	-0.433506 0.997579
N	3.552983	0.356428 -0.762842
H	3.620379	0.717292 -1.715179
H	0.958450	-0.352041 1.349148
H	2.644596	-0.091994 1.798364
S	2.390021	-2.208168 0.714524
H	4.167620	0.935190 -0.178418
H	3.870749	-0.619518 -0.763510
H	1.210392	-2.515565 0.113225
C	-0.900505	-1.205487 -0.709089
C	-1.822186	-0.144037 -0.037925
O	-0.368518	-0.876063 -1.794290
O	-0.798596	-2.282610 -0.081087
H	-1.553793	-0.052692 1.014377
C	-3.282360	-0.574047 -0.170769
N	-1.581892	1.185955 -0.673895
H	-0.660290	1.592332 -0.328967
H	-3.393242	-1.560293 0.275478
H	-3.566805	-0.638535 -1.223133
S	-4.490170	0.595839 0.588250
H	-1.504926	1.059013 -1.686555
H	-2.337512	1.841600 -0.459733
H	-4.066075	0.448185 1.860141
28		
Dimer 18 of the z...z type		
C	0.508626	1.877653 -0.285686
C	1.834015	1.181039 0.168927
O	-0.237381	2.257124 0.653270
O	0.327887	1.985478 -1.513037
H	2.587184	1.964929 0.274803
C	2.320893	0.113527 -0.802254
N	1.605086	0.595715 1.530971

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H	1.083550	1.276332 2.089067
H	2.433960	0.562599 -1.785216
H	1.596557	-0.697683 -0.875696
S	3.896235	-0.701988 -0.291893
H	1.014892	-0.279104 1.432993
H	2.480625	0.350697 1.993805
H	4.682700	0.386518 -0.419225
C	-0.689894	-2.026183 0.340592
C	-1.472623	-0.844593 -0.292795
O	-1.103271	-3.171939 0.094025
O	0.274499	-1.685728 1.078405
H	-0.793245	-0.135086 -0.759526
C	-2.318257	-0.145188 0.773240
N	-2.354755	-1.377171 -1.389755
H	-1.814149	-1.594437 -2.228011
H	-1.647311	0.221211 1.546674
H	-3.025857	-0.845688 1.220832
S	-3.300373	1.271627 0.125242
H	-2.785235	-2.254795 -1.077214
H	-3.076111	-0.690772 -1.639133
H	-2.214118	2.074245 -0.009711
28		
Dimer 19 of the z...z type		
C	1.163191	0.684012 0.549316
C	1.855600	-0.696515 0.385935
O	0.670086	1.184458 -0.496059
O	1.194668	1.158459 1.701148
H	1.373163	-1.389205 1.074595
C	3.348464	-0.622843 0.694056
N	1.600562	-1.219542 -0.993670
H	0.551807	-1.364780 -1.139601
H	3.817462	-1.604299 0.602363
H	3.467723	-0.277998 1.719409
S	4.309179	0.479763 -0.434905
H	1.912199	-0.530322 -1.680820
H	2.089098	-2.098593 -1.164404
H	3.711200	1.632061 -0.068855
C	-1.568068	-1.334845 -0.139614
C	-3.034825	-0.825775 -0.139851
O	-1.057553	-1.595246 0.967924
O	-1.049781	-1.446884 -1.280087
H	-3.660366	-1.635134 -0.519951
C	-3.249491	0.424437 -0.993511
N	-3.431600	-0.582494 1.290293
H	-4.415005	-0.774449 1.480349
H	-4.313158	0.646688 -1.086148
H	-2.844794	0.225641 -1.983310
S	-2.482789	1.946148 -0.288723
H	-2.817787	-1.169587 1.874442
H	-3.227984	0.399083 1.527798
H	-1.169578	1.571211 -0.395787
28		
Dimer 20 of the z...z type		
C	-1.781512	1.964145 -0.286069
C	-2.149542	0.578089 0.308049
O	-2.728855	2.721287 -0.560893
O	-0.549110	2.155090 -0.477226
H	-1.441757	0.270648 1.074633
C	-2.184651	-0.466439 -0.810025
N	-3.507326	0.684229 0.947891
H	-3.456233	1.128285 1.865448
H	-1.201367	-0.511570 -1.274793
H	-2.913212	-0.185466 -1.573210
S	-2.655582	-2.147548 -0.227054
H	-4.096344	1.280670 0.353148
H	-3.930374	-0.244602 1.060056
H	-1.534408	-2.308105 0.518557
C	0.935279	-1.366576 0.090777
C	1.907720	-0.172698 -0.149858

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O	0.276449	-1.331425	1.163570
O	0.932683	-2.236290	-0.798829
H	1.817105	0.160686	-1.183170
C	3.338606	-0.625189	0.138649
N	1.509753	0.972099	0.723851
H	0.657639	1.455766	0.306049
H	3.569941	-1.472151	-0.504411
H	3.434817	-0.945867	1.178312
S	4.611455	0.692257	-0.081843
H	1.249008	0.604751	1.643510
H	2.269802	1.650415	0.819047
H	4.419690	0.869600	-1.405142
28			
Dimer 21 of the z...z type			
C	-0.937372	1.368891	0.103222
C	-1.906610	0.174049	-0.145865
O	-0.273930	1.325528	1.172801
O	-0.941591	2.247535	-0.777603
H	-1.812779	-0.153537	-1.180787
C	-3.339355	0.621764	0.141101
N	-1.508637	-0.974752	0.722576
H	-0.655319	-1.456290	0.304600
H	-3.570287	1.472243	-0.497395
H	-3.439543	0.935799	1.182428
S	-4.608657	-0.696952	-0.091517
H	-1.249692	-0.612073	1.644565
H	-2.268178	-1.654314	0.812947
H	-4.411659	-0.866387	-1.415073
C	1.784906	-1.965084	-0.282405
C	2.151210	-0.576427	0.306586
O	2.732868	-2.722699	-0.553667
O	0.552739	-2.157568	-0.473646
H	1.444855	-0.268771	1.074420
C	2.179632	0.464975	-0.814628
N	3.511190	-0.676648	0.942639
H	3.464093	-1.117570	1.861923
H	1.194327	0.506287	-1.275436
H	2.905466	0.183352	-1.580192
S	2.649991	2.148758	-0.239084
H	4.100240	-1.273484	0.348408
H	3.931803	0.253849	1.050261
H	1.532313	2.310411	0.511292
28			
Dimer 22 of the z...z type			
C	1.653368	-1.333730	-0.384011
C	1.652223	0.200955	-0.662148
O	0.533481	-1.791191	-0.000911
O	2.702581	-1.956685	-0.591226
H	1.128795	0.333996	-1.611855
C	3.028487	0.845132	-0.760327
N	0.796190	0.892320	0.362500
H	0.200986	1.598410	-0.093047
H	2.943290	1.895768	-1.042317
S	3.596455	0.321760	-1.526156
H	3.979757	0.826948	0.820000
H	0.142535	0.216724	0.792333
H	1.368694	1.297578	1.108181
H	4.035682	-0.517610	0.912814
C	-2.335905	1.150001	-0.820960
C	-2.818496	-0.328622	-0.748421
O	-1.218498	1.341443	-1.375762
O	-3.101239	1.978570	-0.301332
H	-3.694832	-0.424957	-1.393296
C	-3.211510	-0.746797	0.665943
N	-1.766367	-1.240260	-1.313808
H	-2.142550	-2.165646	-1.523087
H	-3.367466	-1.824847	0.726957
H	-4.144427	-0.251617	0.924101
S	-1.969898	-0.334846	1.972211

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H	-1.405933	-0.831633	-2.178745
H	-0.921014	-1.372012	-0.688566
H	-2.228661	0.989217	1.978898
28			
Dimer 23 of the z...z type			
C	-1.186871	0.840402	0.217784
C	-1.775277	-0.228929	-0.746000
O	-0.797177	0.432427	1.336008
O	-1.180290	2.006524	-0.235699
H	-1.285222	-0.136572	-1.716680
C	-3.278512	-0.030332	-0.943153
N	-1.457693	-1.591717	-0.217472
H	-0.415491	-1.791981	-0.312881
H	-3.674615	-0.750396	-1.661575
H	-3.438738	0.972067	-1.336490
S	-4.288337	-0.266599	0.582410
H	-1.692710	-1.624716	0.777451
H	-1.973410	-2.324267	-0.705029
H	-3.764001	0.762679	1.278943
C	2.194200	-1.764796	-0.147853
C	2.138626	-0.306110	0.374136
O	3.299584	-2.333320	-0.119902
O	1.101770	-2.209217	-0.597746
H	1.272488	-0.157746	1.015867
C	2.089481	0.659905	-0.813199
N	3.367381	-0.043155	1.201845
H	3.304596	-0.501116	2.111989
H	1.189519	0.448785	-1.388233
H	2.949869	0.501261	-1.466511
S	2.113057	2.442846	-0.349921
H	4.185398	-0.439606	0.725796
H	3.495468	0.963774	1.353459
H	0.802526	2.509814	0.001893
28			
Dimer 24 of the z...z type			
C	1.515773	1.472560	-0.211910
C	2.989456	1.115537	0.122560
O	0.750309	1.621081	0.791585
O	1.230739	1.598475	-1.408907
C	3.585826	2.011630	-0.057262
C	3.540793	-0.036808	-0.716709
N	3.080352	0.808109	1.592763
H	3.980581	1.054597	2.003269
H	4.617802	-0.132996	-0.575109
H	3.342154	0.189118	-1.762187
S	2.834361	-1.682281	-0.276079
H	2.312635	1.310336	2.059182
H	2.915432	-0.199795	1.729374
H	1.533221	-1.441641	-0.626590
C	-0.978200	-1.329254	0.147878
C	-2.030627	-0.196627	0.348589
O	-0.333900	-1.272670	-0.933386
O	-0.916151	-2.181050	1.052905
H	-2.093619	0.059833	1.405218
C	-3.385720	-0.676669	-0.167500
N	-1.570443	1.019726	-0.384588
H	-0.750407	1.447911	0.129262
H	-3.661713	-1.586566	0.363052
H	-3.324849	-0.903927	-1.233853
S	-4.742815	0.564420	-0.010345
H	-1.186519	0.738565	-1.293810
H	-2.321417	1.701903	-0.507148
H	-4.740059	0.622831	1.337144
28			
Dimer 25 of the z...z type			
C	1.578701	-1.405293	0.285170
C	3.011601	-0.814758	0.197897
O	1.038814	-1.698522	-0.827263
O	1.109980	-1.557401	1.419701

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H	3.697830	-1.589426	0.544017
C	3.201928	0.444482	1.044824
N	3.333362	-0.548472	-1.248309
H	4.323269	-0.657734	-1.469409
H	4.259034	0.702698	1.115653
H	2.824799	0.231790	2.042926
S	2.371443	1.939289	0.354400
H	2.757157	-1.184067	-1.816055
H	3.046110	0.415325	-1.475834
H	1.073520	1.503349	0.444845
C	-1.213952	0.865409	-0.714735
C	-2.054089	-0.422437	-0.953207
O	-0.705500	0.968508	0.434659
O	-1.176325	1.672722	-1.660652
H	-1.933321	-0.738489	-1.989506
C	-3.539960	-0.161391	-0.695152
N	-1.518163	-1.515196	-0.086789
H	-2.130830	-2.328632	-0.042142
H	-4.135455	-1.037235	-0.960494
H	-3.852852	0.667602	-1.329466
S	-3.978438	0.192591	1.062897
H	-0.554635	-1.787357	-0.435007
H	-1.357781	-1.151934	0.858502
H	-3.069742	1.171028	1.257731
28			
Dimer 26 of the z...z type			
C	1.222057	-1.059108	0.607197
C	2.766454	-1.079891	0.743071
O	0.750000	-1.663867	-0.398112
O	0.615681	-0.432982	1.489926
H	3.024280	-1.620389	1.654559
C	3.346364	0.333858	0.805855
N	3.352962	-1.846642	-0.413799
H	4.271680	-2.239743	-0.205067
H	4.421807	0.309500	0.985653
H	2.863236	0.857260	1.628074
S	3.131584	1.287927	-0.759552
H	2.701999	-2.590245	-0.685961
H	3.439882	-1.219969	-1.224646
H	1.780782	1.313603	-0.754001
C	-3.697045	-0.696593	0.092457
C	-2.271928	-0.057202	0.027059
O	-3.994987	-1.469319	-0.855228
O	-4.378922	-0.375098	1.085674
H	-1.692026	-0.414386	0.877744
C	-2.346532	1.464305	0.065473
N	-1.579463	-0.561428	-1.204603
H	-0.691421	-1.069255	-0.945203
H	-2.866718	1.753517	0.975561
H	-2.909631	1.849743	-0.787743
S	-0.700405	2.305842	-0.006039
H	-2.261232	-1.200915	-1.647135
H	-1.338025	0.185294	-1.855723
H	-0.108378	1.540087	0.937418
28			
Dimer 27 of the z...z type			
C	-1.338553	0.895831	1.080615
C	-2.798154	0.725330	0.588688
O	-0.710581	1.897028	0.674532
O	-0.927168	-0.006410	1.853484
H	-3.456818	0.942559	1.431609
C	-3.107876	-0.673141	0.053159
N	-3.051126	1.776998	-0.457376
H	-4.023983	2.080171	-0.501933
H	-4.174741	-0.773875	-0.148420
H	-2.826336	-1.395753	0.815785
S	-2.255457	-1.076442	-1.532947
H	-2.427304	2.569709	-0.252636
H	-2.771808	1.410822	-1.377184

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H	-1.032281	-1.421719	-1.036692
C	1.344373	-1.830308	0.239120
C	1.608432	-0.304642	0.087452
O	1.868719	-2.377756	1.233955
O	0.661048	-2.347358	-0.676630
H	0.764404	0.175441	-0.402532
C	2.884010	-0.077415	-0.717545
N	1.706080	0.290259	1.454699
H	0.737033	0.238562	1.872253
H	2.777382	-0.561890	-1.687171
H	3.744606	-0.514883	-0.207471
S	3.308745	1.702553	-0.962552
H	2.351044	-0.265780	2.021055
H	2.005598	1.266432	1.418739
H	2.206386	2.023663	-1.670321
28			
Dimer 28 of the z...z type			
C	-0.551869	1.862251	-0.076682
C	-1.900989	1.081988	-0.223398
O	-0.063344	2.275789	-1.152162
O	-0.106033	1.996783	1.085129
H	-2.697712	1.828686	-0.250770
C	-2.166151	0.071083	0.883288
N	-1.880482	0.401978	-1.559938
H	-1.563488	1.074217	-2.262358
H	-2.084004	0.572218	1.843881
H	-1.433101	-0.734537	0.849340
S	-3.800985	-0.776075	0.743857
H	-1.180283	-0.387171	-1.518561
H	-2.796203	0.028139	-1.812127
H	-4.560871	0.319463	0.947999
C	0.834098	-1.992368	-0.554205
C	1.494114	-0.866271	0.287389
O	1.376927	-3.111030	-0.511722
O	-0.170749	-1.640440	-1.227288
H	0.748761	-0.305245	0.846458
C	2.280404	0.080230	-0.620583
N	2.416258	-1.499076	1.294802
H	1.898988	-1.880247	2.087849
H	1.590243	0.512769	-1.341555
H	3.061541	-0.463088	-1.156048
S	3.118537	1.439775	0.298025
H	2.899016	-2.286263	0.845189
H	3.093381	-0.811801	1.646572
H	1.960406	2.003057	0.733461
28			
Dimer 29 of the z...z type			
C	-3.427950	-0.779506	0.006225
C	-1.865928	-0.728237	-0.068480
O	-4.018761	-0.863478	-1.098368
O	-3.910849	-0.758243	1.157157
H	-1.508838	-1.748813	0.093836
C	-1.224122	0.182743	0.970897
N	-1.453188	-0.348127	-1.456436
H	-0.485360	-0.685655	-1.684456
H	-0.141330	0.200643	0.867345
H	-1.479947	-0.189338	1.959765
S	-1.755074	1.943264	0.834475
H	-2.169313	-0.705553	-2.097512
H	-1.423399	0.672030	-1.544901
H	-3.029290	1.718438	1.217318
C	1.596724	0.260172	-1.214819
C	3.058289	0.338310	-0.688605
O	0.936672	1.321022	-1.168785
O	1.219636	-0.865598	-1.625830
H	3.706198	0.525912	-1.547886
C	3.533547	-0.912861	0.038763
N	3.139054	1.557237	0.191045
H	4.070006	1.972797	0.225026

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H	4.553486	-0.786813	0.404214
H	3.515118	-1.743495	-0.662638
S	2.507520	-1.342020	1.511570
H	2.451505	2.231605	-0.178444
H	2.847920	1.322821	1.146702
H	1.419905	-1.705388	0.803279
28			
Dimer 30 of the z...z type			
C	1.501587	1.673546	-0.055359
C	2.391662	0.652197	0.720067
O	0.477390	2.067182	0.562584
O	1.909268	2.000948	-1.184754
H	3.200206	1.233119	1.173197
C	3.025447	-0.430253	-0.145669
N	1.596806	0.077386	1.855493
H	2.194525	-0.342731	2.566692
H	3.518823	-1.180447	0.474526
H	3.779766	0.037133	-0.774455
S	1.868110	-1.361096	-1.242438
H	1.061954	0.843526	2.274619
H	0.869421	-0.649527	1.571243
H	1.636937	-0.326434	-2.076166
C	-1.160534	-1.843610	0.583062
C	-1.434627	-0.518060	-0.173327
O	-1.826596	-2.835427	0.235046
O	-0.311985	-1.757756	1.510497
H	-0.502597	-0.008784	-0.391341
C	-2.337968	0.395609	0.652037
N	-2.079628	-0.845261	-1.491076
H	-1.387744	-1.168361	-2.168754
H	-1.846011	0.581186	1.604662
H	-3.303196	-0.077004	0.843171
S	-2.684287	2.004542	-0.179168
H	-2.742967	-1.616212	-1.345982
H	-2.554692	-0.022797	-1.879948
H	-1.383845	2.401171	-0.148543
28			
Dimer 31 of the z...z type			
C	0.935559	1.188082	-0.398375
C	2.476551	1.324026	-0.551128
O	0.455783	1.636973	0.688226
O	0.334304	0.682530	-1.351214
H	2.659754	2.137509	-1.254948
C	3.142052	0.048380	-1.065170
N	3.051462	1.744136	0.774983
H	3.870640	2.345658	0.689822
H	4.188463	0.231028	-1.312528
H	2.615303	-0.259073	-1.965872
S	3.156164	-1.327143	0.163152
H	2.297455	2.217516	1.293064
H	3.309116	0.900490	1.306771
H	1.802352	-1.467110	0.324411
C	-0.946984	-1.740906	0.164921
C	-2.123879	-0.778671	0.520734
O	0.037395	-1.701242	0.950045
O	-1.127064	-2.474707	-0.823954
H	-2.900893	-1.384628	0.993215
C	-2.690967	-0.062644	-0.698909
N	-1.656861	0.211574	1.545553
H	-1.249262	-0.286501	2.336920
H	-2.980114	-0.812094	-1.431441
H	-1.923761	0.573682	-1.139887
S	-4.125763	1.039436	-0.331507
H	-0.883531	0.829475	1.156628
H	-2.427515	0.799193	1.868777
H	-4.983982	0.070147	0.047723
28			
Dimer 32 of the z...z type			
C	-0.890969	-0.466303	-1.536894

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C	-1.613316	0.070743	-0.265072
O	-0.584830	0.383601	-2.400640
O	-0.701891	-1.704973	-1.546104
H	-1.177320	-0.390824	0.619732
C	-3.100778	-0.270830	-0.337113
N	-1.395237	1.545818	-0.161534
H	-0.387679	1.771901	0.098517
H	-3.201141	-1.348746	-0.448641
H	-3.561720	0.209608	-1.202745
S	-4.078963	0.300275	1.118602
H	-1.564452	1.968011	-1.078369
H	-2.022169	1.963808	0.530557
H	-3.463388	-0.481140	2.029528
C	2.216018	1.644521	0.303579
C	2.091641	0.137406	-0.049536
O	3.363264	2.106159	0.419579
O	1.112290	2.229526	0.477711
H	1.386949	0.012011	-0.868102
C	1.653324	-0.647388	1.188031
N	3.422484	-0.367428	-0.535189
H	3.594068	-0.094300	-1.503957
H	0.740274	-0.197823	1.572490
H	2.409234	-0.567290	1.972081
S	1.411309	-2.449078	0.896694
H	4.163816	0.061786	0.031155
H	3.471169	-1.390711	-0.475239
H	0.457906	-2.307573	-0.067021
28			
Dimer 33 of the z...z type			
C	-1.229055	1.047289	0.619280
C	-2.768478	1.044872	0.778295
O	-0.788403	1.583512	-0.436753
O	-0.597630	0.484375	1.527718
H	-3.031393	1.530758	1.718237
C	-3.320206	-0.382313	0.768474
N	-3.385766	1.855768	-0.331923
H	-4.374795	2.052097	-0.167160
H	-4.395768	-0.387729	0.949480
H	-2.828929	-0.934937	1.566943
S	-3.087827	-1.260375	-0.838579
H	-2.881218	2.736591	-0.452896
H	-3.297875	1.337501	-1.214613
H	-1.737173	-1.294609	-0.816112
C	3.700146	0.700962	0.064677
C	2.272394	0.065445	0.021524
O	3.981324	1.480425	-0.882615
O	4.399046	0.374601	1.044444
H	1.699858	0.448599	0.866364
C	2.335391	-1.454671	0.099453
N	1.573045	0.543798	-1.216393
H	2.235052	1.207421	-1.652840
H	2.857339	-1.724078	1.014542
H	2.892287	-1.866683	-0.745319
S	0.682879	-2.285206	0.056760
H	1.370245	-0.210448	-1.871758
H	0.662400	1.017749	-0.965404
H	0.102319	-1.492699	0.985281
28			
Dimer 34 of the z...z type			
C	2.000785	1.459883	-0.321542
C	2.079794	-0.057126	-0.651224
O	2.969754	2.162363	-0.661765
O	0.939936	1.819979	0.256848
H	1.373269	-0.261030	-1.458162
C	1.732224	-0.951537	0.535420
N	3.462677	-0.349312	-1.167058
H	3.486001	-1.109000	-1.847459
H	1.724996	-2.002049	0.245087
H	0.738099	-0.691213	0.883797

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S	2.915799	-0.814244	1.942593
H	3.821879	0.522449	-1.580656
H	4.085188	-0.584033	-0.384354
H	2.644232	0.475356	2.232342
C	-1.208735	-1.292791	-0.892911
C	-1.947238	-0.227183	-0.021172
O	-0.721167	-0.871220	-1.971302
O	-1.206713	-2.445744	-0.421788
H	-1.635365	-0.325696	1.018160
C	-3.456196	-0.437856	-0.134684
N	-1.555365	1.141273	-0.480540
H	-0.576828	1.386211	-0.160059
H	-3.685897	-1.454016	0.179604
H	-3.781752	-0.315968	-1.170023
S	-4.468162	0.761009	0.836557
H	-1.538260	1.143596	-1.504842
H	-2.208687	1.850761	-0.138578
H	-4.018535	0.389297	2.052654
28			
Dimer 35 of the z...z type			
C	1.622609	0.330185	-1.205770
C	3.071486	0.343135	-0.640991
O	0.978400	1.396711	-1.106860
O	1.236870	-0.761251	-1.694930
H	3.747157	0.550761	-1.473579
C	3.487661	-0.956830	0.036204
N	3.163230	1.516656	0.297994
H	4.101131	1.912224	0.364430
H	4.498813	-0.881143	0.438194
H	3.466133	-1.750629	-0.706537
S	2.403891	-1.425231	1.454817
H	2.493706	2.220969	-0.048607
H	2.852987	1.244543	1.237448
H	1.323404	-1.706239	0.698848
C	-3.374359	-0.818867	-0.023711
C	-1.815521	-0.697473	-0.099010
O	-3.963088	-0.894202	-1.130190
O	-3.855415	-0.852888	1.127405
H	-1.413719	-1.706196	0.030922
C	-1.213026	0.207259	0.969014
N	-1.427014	-0.256660	-1.475996
H	-0.457204	-0.570479	-1.730560
H	-0.131471	0.266279	0.873487
H	-1.461870	-0.200549	1.945523
S	-1.802521	1.951173	0.874030
H	-2.147332	-0.604438	-2.118717
H	-1.418337	0.766331	-1.526190
H	-3.076069	1.672100	1.222001
28			
Dimer 36 of the z...z type			
C	-1.215820	-0.922499	-0.296173
C	-2.716130	-1.289911	-0.472933
O	-0.674251	-1.383619	0.749671
O	-0.704348	-0.236617	-1.194633
H	-2.758045	-2.162210	-1.128274
C	-3.558289	-0.169274	-1.071408
N	-3.248251	-1.725875	0.866309
H	-4.028633	-2.379613	0.797754
H	-4.594447	-0.485283	-1.199701
H	-3.144794	0.082444	-2.045033
S	-3.616817	1.345414	-0.020575
H	-2.464077	-2.152298	1.379484
H	-3.551590	-0.904939	1.403536
H	-2.314808	1.661750	-0.166444
C	3.789496	-0.612834	-0.462934
C	2.397710	-0.028027	-0.057807
O	4.163521	-1.625432	0.183906
O	4.364166	-0.028100	-1.402839
H	1.686905	-0.275567	-0.847896

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C	2.434155	1.482511	0.132534
N	1.913463	-0.738050	1.171450
H	0.898763	-1.015015	1.067884
H	2.765759	1.933366	-0.799496
H	3.143720	1.758312	0.916107
S	0.811091	2.206460	0.646972
H	2.527647	-1.562665	1.262214
H	2.014790	-0.168974	2.011319
H	0.074498	1.518535	-0.254634
28			
Dimer 37 of the z...z type			
C	3.750963	-0.087621	0.142392
C	2.389227	0.377707	0.747724
O	4.124377	0.509288	-0.897968
O	4.296633	-1.032478	0.747949
H	2.536757	0.628999	1.798336
C	1.336627	-0.726279	0.663407
N	1.934303	1.617096	0.030652
H	2.273385	2.454289	0.501279
H	0.407939	-0.393443	1.124977
H	1.709242	-1.591072	1.209046
S	0.897413	-1.238441	-1.053437
H	2.391769	1.588542	-0.890930
H	0.882455	1.686777	-0.076709
H	2.072335	-1.838131	-1.336720
C	-1.554421	1.265858	0.475614
C	-2.974218	0.971690	-0.092677
O	-0.729784	1.706493	-0.379342
O	-1.371525	1.048453	1.680002
H	-3.578457	1.867629	0.064588
C	-3.663024	-0.223762	0.554974
N	-2.838508	0.792613	-1.580969
H	-3.688697	1.019293	-2.097571
H	-4.669366	-0.358275	0.156851
H	-3.730167	-0.036944	1.624100
S	-2.786999	-1.819485	0.261675
H	-2.056063	1.390256	-1.883909
H	-2.577315	-0.179559	-1.786286
H	-1.679542	-1.499117	0.959617
28			
Dimer 38 of the z...z type			
C	-1.492786	-1.123750	0.980632
C	-2.387896	0.150905	1.101188
O	-0.337161	-0.996045	1.463716
O	-2.011245	-2.126671	0.455028
H	-2.837252	0.123573	2.098472
C	-3.515203	0.243322	0.081417
N	-1.497114	1.353694	1.061200
H	-2.004185	2.223491	1.220606
H	-4.118884	1.137245	0.250031
H	-4.151095	-0.630397	0.207213
S	-2.969931	0.337882	-1.676173
H	-0.753748	1.263242	1.760730
H	-0.950491	1.417077	0.155874
H	-2.340232	-0.854632	-1.677251
C	1.389921	1.365911	-0.069080
C	2.710714	0.807163	-0.666862
O	1.442479	1.817144	1.096656
O	0.401352	1.323324	-0.840933
H	3.067129	1.536686	-1.396049
C	2.547525	-0.551586	-1.348814
N	3.722969	0.747990	0.443049
H	4.675748	0.949179	0.141150
H	3.446573	-0.810026	-1.909406
H	1.710786	-0.475966	-2.039825
S	2.281457	-1.949465	-0.176381
H	3.409521	1.419523	1.160938
H	3.695261	-0.191609	0.865872
H	1.120063	-1.512254	0.406494

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28		
Dimer 39 of the z...z type		
C	-3.338612 -1.222257 0.595688	
C	-2.023056 -0.429760 0.326263	
O	-3.452598 -2.310360 -0.021436	
O	-4.122970 -0.702590 1.418890	
H	-1.303561 -0.693269 1.103990	
C	-2.176540 1.084287 0.341403	
N	-1.416687 -0.882933 -0.965021	
H	-0.393300 -0.601777 -1.030869	
H	-1.213048 1.562375 0.163551	
H	-2.543192 1.385083 1.319503	
S	-3.326754 1.725484 -0.953034	
H	-1.540739 -1.896062 -1.035954	
H	-1.925935 -0.465407 -1.748543	
H	-4.424751 1.116249 -0.459475	
C	1.499302 0.423352 0.057303	
C	2.908879 1.081509 0.080363	
O	0.868841 0.420905 1.132259	
O	1.134739 -0.020243 -1.062198	
H	2.790422 2.112513 -0.260411	
C	3.945172 0.379122 -0.788850	
N	3.342413 1.144699 1.519672	
H	3.990886 1.907302 1.716475	
H	4.908601 0.887552 -0.734541	
H	3.594625 0.400356 -1.817882	
S	4.263616 -1.365815 -0.285041	
H	2.485220 1.240694 2.083857	
H	3.784097 0.257866 1.789509	
H	3.027810 -1.816072 -0.585513	
28		
Dimer 40 of the z...z type		
C	-2.042228 0.262512 -1.376646	
C	-2.451669 -0.882491 -0.398290	
O	-0.974249 0.081234 -2.017019	
O	-2.822210 1.232798 -1.415011	
H	-3.295642 -1.402752 -0.857558	
C	-2.890977 -0.372101 0.970375	
N	-1.327604 -1.870069 -0.303341	
H	-1.656633 -2.828130 -0.197185	
H	-3.049364 -1.201846 1.661323	
H	-3.832083 0.159424 0.849088	
S	-1.679292 0.750999 1.794451	
H	-0.767796 -1.788017 -1.163981	
H	-0.631179 -1.680903 0.465935	
H	-1.770701 1.737408 0.879756	
C	1.670651 -1.334124 0.304999	
C	2.742634 -0.249616 0.594288	
O	1.694499 -1.877874 -0.820809	
O	0.862437 -1.529685 1.244849	
H	3.362472 -0.599486 1.420021	
C	2.107633 1.093109 0.972315	
N	3.618576 -0.132480 -0.624558	
H	4.614085 -0.081515 -0.413060	
H	2.857515 1.775966 1.372641	
H	1.354022 0.899284 1.733298	
S	1.346388 1.992307 -0.443751	
H	3.405152 -0.960584 -1.205422	
H	3.343308 0.695744 -1.170537	
H	0.456398 1.044844 -0.828556	
28		
Dimer 41 of the z...z type		
C	1.261246 1.403371 -0.515665	
C	2.706544 1.047404 -0.065089	
O	0.585821 2.084665 0.285705	
O	0.922947 0.952438 -1.636875	
H	3.382438 1.784474 -0.503829	
C	3.156056 -0.353844 -0.464678	
N	2.763220 1.238203 1.427373	

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H	3.699601 1.446065 1.775415	
H	4.168134 -0.550640 -0.108224	
H	3.151534 -0.417015 -1.549921	
S	2.099836 -1.701389 0.225027	
H	2.113229 2.003254 1.657940	
H	2.413244 0.397638 1.901533	
H	1.060115 -1.536164 -0.615279	
C	-1.509875 -1.994590 0.272041	
C	-1.574372 -0.459723 -0.015384	
O	-1.195388 -2.708245 -0.717805	
O	-1.724664 -2.335477 1.449012	
H	-0.674847 -0.029606 0.422466	
C	-2.791108 0.225223 0.587096	
N	-1.477968 -0.250477 -1.501043	
H	-1.336734 -1.199192 -1.889102	
H	-2.771137 0.060718 1.661717	
H	-3.715557 -0.200750 0.191711	
S	-2.861843 2.038146 0.213941	
H	-2.318705 0.169975 -1.895589	
H	-0.645922 0.348321 -1.726585	
H	-1.530734 2.266629 0.339704	
28		
Dimer 42 of the z...z type		
C	1.165643 -0.871418 0.979944	
C	2.587943 -1.168352 0.429751	
O	0.266765 -1.685163 0.607325	
O	1.037118 0.110501 1.723883	
H	3.111964 -1.752377 1.189635	
C	3.401783 0.076997 0.099619	
N	2.434439 -2.060807 -0.773385	
H	3.253476 -2.642591 -0.952274	
H	4.397902 -0.195420 -0.251140	
H	3.500039 0.669335 1.006181	
S	2.658200 1.116618 -1.230059	
H	1.601897 -2.644889 -0.613153	
H	2.247380 -1.491101 -1.606923	
H	1.641507 1.605735 -0.489498	
C	-3.118843 -0.782659 -0.713369	
C	-2.469266 0.301343 0.209414	
O	-3.276909 -1.915503 -0.200956	
O	-3.436321 -0.380146 -1.853119	
H	-3.261770 0.986519 0.516411	
C	-1.354473 1.071516 -0.488383	
N	-1.939808 -0.359229 1.446467	
H	-2.676688 -0.895908 1.902112	
H	-1.728084 1.430637 -1.443299	
H	-0.505803 0.416496 -0.682580	
S	-0.703609 2.505466 0.483573	
H	-1.161035 -1.020821 1.178613	
H	-1.537550 0.319527 2.096715	
H	-1.621056 3.399696 0.062482	
28		
Dimer 43 of the z...z type		
C	1.549606 0.106802 1.357526	
C	2.803336 -0.419687 0.605922	
O	0.851437 -0.784549 1.934589	
O	1.348498 1.325150 1.329374	
H	3.662225 -0.273670 1.264444	
C	3.063333 0.275413 -0.727647	
N	2.644098 -1.906228 0.422791	
H	3.531583 -2.401766 0.332607	
H	4.008658 -0.061736 -1.153976	
H	3.124530 1.345281 -0.542657	
S	1.776782 -0.055139 -2.009081	
H	2.108147 -2.258351 1.227345	
H	2.079606 -2.084168 -0.417650	
H	0.826503 0.825539 -1.573521	
C	-1.252641 1.780710 -0.194314	
C	-1.501505 0.268057 0.086639	

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O	-1.726304	2.576460	0.646350
O	-0.658412	2.027989	-1.269496
H	-0.639224	-0.319053	-0.221206
C	-2.739606	-0.179325	-0.685763
N	-1.664728	0.077429	1.561244
H	-0.724563	-0.182427	1.962198
H	-2.576448	0.016735	-1.744119
H	-3.618929	0.381049	-0.361748
S	-3.174420	-1.956349	-0.443834
H	-1.988563	0.974582	1.945156
H	-2.326098	-0.669784	1.782838
H	-2.017701	-2.459061	-0.922025
28			
Dimer 44 of the z...z type			
C	2.978560	-0.477051	-0.979131
C	1.581523	-0.410139	-0.287938
O	3.609634	-1.549375	-0.818033
O	3.299295	0.534172	-1.639807
H	0.837632	-0.725087	-1.023563
C	1.196376	0.966567	0.237553
N	1.509374	-1.425599	0.812314
H	0.511643	-1.533159	1.136474
H	0.218203	0.934721	0.717328
H	1.159027	1.660984	-0.597923
S	2.358042	1.623849	1.512277
H	1.900486	-2.306766	0.473809
H	2.087400	-1.121667	1.600012
H	3.420839	1.700829	0.684491
C	-1.706962	-1.271155	0.304917
C	-3.113117	-0.610506	0.256272
O	-1.119428	-1.214873	1.425862
O	-1.292332	-1.775808	-0.747758
H	-3.856116	-1.404062	0.360313
C	-3.370664	0.161820	-1.032674
N	-3.255909	0.279438	1.463578
H	-4.226056	0.413156	1.751372
H	-4.356430	0.627644	-1.018745
H	-3.324749	-0.536622	-1.864575
S	-2.162251	1.527906	-1.316913
H	-2.708640	-0.143090	2.225346
H	-2.841423	1.198878	1.272692
H	-1.105956	0.720731	-1.536322
28			
Dimer 45 of the z...z type			
C	-1.422196	-0.307533	-0.239643
C	-2.746110	-0.128866	-1.034772
O	-0.960698	-1.487696	-0.222882
O	-0.929094	0.711144	0.266951
H	-2.471458	0.188913	-2.043069
C	-3.701155	0.890235	-0.426043
N	-3.390332	-1.483264	-1.165744
H	-3.981000	-1.572766	-1.993077
H	-4.602247	0.991863	-1.032083
H	-3.192415	1.850587	-0.388960
S	-4.273668	0.434149	1.266402
H	-2.629826	-2.177590	-1.187539
H	-3.958369	-1.679029	-0.332919
H	-3.058152	0.527322	1.844198
C	3.873630	-0.710023	0.243827
C	2.401578	-0.715197	-0.282264
O	4.043732	-1.206308	1.384497
O	4.721023	-0.236838	-0.542063
H	2.298685	-1.593039	-0.925960
C	2.020768	0.520775	-1.088023
N	1.463130	-0.917130	0.865765
H	0.549321	-1.324152	0.544910
H	0.977501	0.475827	-1.396484
H	2.657893	0.570843	-1.967313
S	2.184645	2.094959	-0.139566

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H	1.944608	-1.491362	1.564888
H	1.234036	-0.014179	1.291855
H	3.530559	2.047929	-0.055615
28			
Dimer 46 of the z...z type			
C	1.174906	-1.175549	-0.408195
C	2.719096	-1.293504	-0.234960
O	0.759048	-1.016395	-1.571522
O	0.519588	-1.273631	0.659592
H	2.960238	-2.358055	-0.201406
C	3.258102	-0.614478	1.018287
N	3.352968	-0.739161	-1.481101
H	4.257232	-1.158137	-1.698438
H	4.334350	-0.764388	1.111798
H	2.763787	-1.056975	1.879652
S	3.001257	1.211942	1.027202
H	2.683963	-0.895437	-2.249598
H	3.473877	0.276548	-1.382690
H	1.651955	1.174695	0.982725
C	-3.706678	-0.593234	0.130992
C	-2.606139	0.496663	0.365061
O	-3.762692	-1.503181	0.996203
O	-4.425891	-0.417686	-0.872526
H	-3.116314	1.388276	0.734151
C	-1.831564	0.819032	-0.904838
N	-1.692558	0.020689	1.455494
H	-2.246568	-0.623365	2.034598
H	-2.533687	1.162344	-1.660290
H	-1.310678	-0.062807	-1.278533
S	-0.490869	2.066461	-0.677319
H	-0.869572	-0.522345	1.070515
H	-1.323597	0.785647	2.017122
H	-1.280815	3.082411	-0.270520
28			
Dimer 47 of the z...z type			
C	-3.574482	-0.255966	0.793611
C	-2.076130	-0.341827	0.373777
O	-4.305003	-1.193632	0.390261
O	-3.877624	0.723729	1.508831
H	-1.524807	-0.830378	1.179962
C	-1.412214	1.001662	0.103609
N	-1.932652	-1.241465	-0.816441
H	-0.912764	-1.474087	-0.975555
H	-0.375738	0.860379	-0.203532
H	-1.435678	1.591415	1.016235
S	-2.207184	1.963100	-1.257277
H	-2.503213	-2.076125	-0.668807
H	-2.297982	-0.771978	-1.648951
H	-3.384470	2.129699	-0.619216
C	1.262463	-1.361168	0.075959
C	2.728410	-0.858122	0.119711
O	0.745224	-1.414115	-1.080181
O	0.728836	-1.588659	1.169112
H	3.312003	-1.456600	0.816317
C	2.732820	0.613413	0.538709
N	3.344235	-1.013181	-1.244692
H	3.606044	-1.982727	-1.428983
H	2.252475	0.688949	1.512280
H	2.163645	1.216144	-0.172352
S	4.407255	1.378565	0.594614
H	2.641896	-0.753103	-1.947716
H	4.181278	-0.427335	-1.342361
H	4.898436	0.595099	1.576785
28			
Dimer 48 of the z...z type			
C	1.374079	0.715665	-0.978441
C	1.330288	-0.152758	0.311401
O	1.982489	0.218368	-1.953623
O	0.853109	1.849672	-0.870005

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H	0.366342	-0.032343	0.802121
C	2.421330	0.282263	1.290627
N	1.452356	-1.593972	-0.080392
H	0.487644	-2.015049	-0.076649
H	2.320134	-0.250546	2.237868
H	2.293799	1.347338	1.481467
S	4.148802	-0.060149	0.736036
H	1.844358	-1.595356	-1.032677
H	2.066960	-2.128355	0.533063
H	4.028690	0.480909	-0.494437
C	-1.660962	-1.210881	-0.577973
C	-3.037504	-0.610059	-0.186497
O	-1.193684	-2.079275	0.221958
O	-1.148491	-0.794826	-1.623216
H	-3.795282	-1.111972	-0.791803
C	-3.134033	0.898251	-0.403639
N	-3.317811	-0.972180	1.248613
H	-4.313229	-0.994474	1.472682
H	-4.151329	1.244941	-0.219312
H	-2.876235	1.104559	-1.439762
S	-2.042293	1.887756	0.708628
H	-2.883307	-1.886236	1.430420
H	-2.855538	-0.292847	1.865742
H	-0.876609	1.761649	0.007625
28			
Dimer 49 of the z...z type			
C	1.798859	-1.315579	0.375055
C	2.683684	-0.089257	0.750022
O	2.211020	-2.043709	-0.549322
O	0.772494	-1.438005	1.087508
H	3.160613	-0.317233	1.704456
C	1.889769	1.208883	0.881490
N	3.773786	0.025160	-0.280796
H	4.669410	0.327144	0.101366
H	2.506249	2.002121	1.306023
H	1.051017	1.012324	1.545961
S	1.273087	1.873250	-0.722756
H	3.853047	-0.904873	-0.722164
H	3.481082	0.687809	-1.011649
H	0.528789	0.799389	-1.101279
C	-1.858263	0.010465	-1.442285
C	-2.582339	-0.840125	-0.355996
O	-0.790744	-0.476192	-1.895967
O	-2.414382	1.085119	-1.737761
H	-3.444096	-1.314569	-0.833754
C	-3.096385	-0.010213	0.814623
N	-1.673894	-1.949953	0.086110
H	-2.138115	-2.590815	0.730284
H	-3.566786	-0.642820	1.569506
H	-3.846576	0.674657	0.425263
S	-1.811880	0.959847	1.711144
H	-1.373209	-2.474956	-0.736581
H	-0.769880	-1.621037	0.526722
H	-1.421008	1.697918	0.650627
28			
Dimer 50 of the z...z type			
C	-1.216786	-1.343003	0.101630
C	-2.580240	-1.043400	0.790522
O	-0.222677	-1.304242	0.889036
O	-1.216056	-1.596136	-1.110742
H	-2.884814	-1.963714	1.294371
C	-3.695317	-0.593529	-0.142627
N	-2.316646	-0.034358	1.877657
H	-3.036374	-0.029768	2.601835
H	-4.635702	-0.490100	0.400089
H	-3.816373	-1.356624	-0.908439
S	-3.396309	1.038238	-0.943658
H	-1.401604	-0.257951	2.290206
H	-2.259091	0.908190	1.471662

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H	-2.265860	0.666551	-1.578758
C	3.930030	-0.204860	-0.025388
C	2.534981	0.326320	-0.502826
O	4.172843	-1.409312	-0.288363
O	4.655998	0.639267	0.536762
H	2.714199	0.957464	-1.374766
C	1.815264	1.117956	0.581870
N	1.708058	-0.843023	-0.948055
H	2.367008	-1.589167	-1.203551
H	2.466009	1.917442	0.925494
H	1.578227	0.473189	1.429007
S	0.193205	1.816419	0.047838
H	1.084138	-1.184293	-0.170455
H	1.075384	-0.631687	-1.719134
H	0.676179	2.854113	-0.664289
28			
Dimer 51 of the z...z type			
C	1.089383	-0.523344	0.046518
C	2.117191	0.521957	-0.476405
O	0.541671	-0.222711	1.149541
O	0.871995	-1.494219	-0.686318
H	1.603561	1.107813	-1.241488
C	3.375752	-0.094724	-1.072910
N	2.436028	1.468399	0.649518
H	2.695339	2.402449	0.331010
H	4.048545	0.675473	-1.451930
H	3.076609	-0.736851	-1.898175
S	4.358957	-1.072095	0.143006
H	1.600705	1.508707	1.251761
H	3.200751	1.088342	1.219100
H	3.426698	-2.027945	0.336556
C	-3.583083	-1.039413	-0.258820
C	-2.845715	0.231223	0.290893
O	-3.577619	-2.040403	0.501987
O	-4.112170	-0.904426	-1.378695
H	-3.612161	0.960906	0.553595
C	-1.891831	0.820211	-0.739494
N	-2.134555	-0.156898	1.557828
H	-2.252775	0.529719	2.299632
H	-2.457665	1.059217	-1.635994
H	-1.130697	0.089192	-1.012733
S	-0.986775	2.328447	-0.171155
H	-2.557007	-1.060383	1.828537
H	-1.100747	-0.298204	1.411246
H	-1.967569	3.218042	-0.422977
28			
Dimer 52 of the z...z type			
C	-3.825513	-0.715135	0.074962
C	-2.454783	-0.419215	0.765971
O	-3.866091	-1.746673	-0.641435
O	-4.731837	0.105080	0.324223
H	-2.571904	-0.666396	1.823318
C	-2.023789	1.039021	0.658054
N	-1.422585	-1.352316	0.201369
H	-0.853160	-1.771454	0.936281
H	-1.018952	1.168933	1.058474
H	-2.714966	1.646324	1.237802
S	-1.984230	1.685820	-1.070231
H	-1.946660	-2.063137	-0.330170
H	-0.723196	-0.862230	-0.404721
H	-3.324476	1.697108	-1.226740
C	1.364284	0.042895	0.422985
C	2.677678	0.874322	0.464014
O	0.967416	-0.419714	1.517752
O	0.815992	-0.048029	-0.700285
H	2.388130	1.922786	0.562532
C	3.563605	0.708143	-0.763954
N	3.403972	0.502672	1.728019
H	3.995663	1.250772	2.090205

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H	4.464027	1.317979	-0.681832
H	2.999152	1.031152	-1.635419
S	4.143479	-1.023931	-1.016585
H	2.683753	0.241524	2.417851
H	3.984726	-0.328196	1.564412
H	2.918333	-1.536800	-1.254202
28			
Dimer 53 of the z...z type			
C	1.630112	-1.221826	0.751690
C	2.051274	-0.876967	-0.705912
O	0.644864	-0.601825	1.225695
O	2.356144	-2.068335	1.307175
H	2.084454	-1.802851	-1.281818
C	3.431993	-0.221451	-0.741145
N	1.025545	0.000805	-1.354536
H	1.255607	0.190351	-2.330676
H	3.746903	-0.024471	-1.767543
H	4.145087	-0.903524	-0.282799
S	3.503520	1.415419	0.111241
H	0.072387	-0.458903	-1.312182
H	0.978979	0.897322	-0.862144
H	3.226477	0.957068	1.349282
C	-2.239302	-1.169004	-0.432380
C	-3.059412	0.154897	-0.542904
O	-2.636581	-1.988906	0.414902
O	-1.301590	-1.288627	-1.262008
H	-3.741286	0.018493	-1.384706
C	-2.231372	1.414220	-0.776636
N	-3.905212	0.267652	0.694550
H	-4.810473	0.708563	0.532792
H	-2.879261	2.262911	-0.999699
H	-1.595658	1.241583	-1.642858
S	-1.227188	1.940732	0.678130
H	-4.022081	-0.695233	1.049012
H	-3.398177	0.806774	1.408664
H	-0.492931	0.796056	0.838281
28			
Dimer 54 of the z...z type			
C	3.579267	1.195762	0.569272
C	2.233245	0.465229	0.274541
O	3.787219	2.239547	-0.098285
O	4.291261	0.679698	1.457750
H	1.491254	0.822442	0.991792
C	2.289672	-1.050655	0.396205
N	1.727710	0.868131	-1.075088
H	0.682770	0.687187	-1.166937
H	1.310213	-1.480271	0.186143
H	2.574841	-1.305565	1.413783
S	3.473906	-1.844997	-0.776469
H	1.956089	1.856817	-1.211666
H	2.224827	0.343777	-1.799885
H	4.575526	-1.265972	-0.255075
C	-1.341953	-0.117419	-0.121550
C	-2.845957	-0.501417	-0.140029
O	-0.745993	-0.224058	0.966919
O	-0.900510	0.306092	-1.221480
H	-3.068726	-1.117567	-1.008764
C	-3.694675	0.770695	-0.149654
N	-3.135911	-1.316615	1.090791
H	-2.869687	-2.294097	0.965389
H	-3.443412	1.337935	-1.043582
H	-3.467938	1.386505	0.722935
S	-5.510671	0.470117	-0.077133
H	-2.558864	-0.943814	1.856710
H	-4.131946	-1.283915	1.335077
H	-5.602731	-0.189383	-1.250143
28			
Dimer 55 of the z...z type			
C	-1.583561	1.335964	0.284714

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C	-1.388380	-0.131211	-0.214867
O	-1.045963	1.592065	1.392577
O	-2.200398	2.098489	-0.483764
H	-0.456908	-0.135961	-0.787373
C	-2.505943	-0.661874	-1.100304
N	-1.145451	-1.022599	0.963375
H	-0.469175	-1.773168	0.716043
H	-2.291541	-1.679228	-1.431413
H	-2.589308	-0.017443	-1.972023
S	-4.142704	-0.743798	-0.251365
H	-0.701655	-0.446175	1.691849
H	-2.023495	-1.398361	1.328434
H	-4.241677	0.586310	-0.047620
C	1.869966	-1.239084	0.672782
C	3.118974	-0.702418	-0.081787
O	1.180863	-2.095684	0.045002
O	1.659880	-0.767853	1.801204
H	3.988432	-1.255266	0.279478
C	3.347268	0.792357	0.113289
N	2.957238	-1.048205	-1.539132
H	3.844487	-1.159778	-2.030452
H	4.223870	1.127338	-0.442713
H	3.514426	0.974384	1.171997
S	1.937477	1.832985	-0.465315
H	2.404541	-1.916725	-1.581382
H	2.409146	-0.321019	-2.012392
H	1.084978	1.505186	0.531645
28			
Dimer 56 of the z...z type			
C	-2.486332	-1.418852	0.099031
C	-2.797870	-0.181698	-0.802872
O	-3.474174	-1.999570	0.585737
O	-1.270900	-1.709207	0.232009
H	-2.775946	-0.525232	-1.839205
C	-1.840332	0.991696	-0.644979
N	-4.215765	0.230605	-0.508256
H	-4.693644	0.647056	-1.307510
H	-2.160155	1.832790	-1.262174
H	-0.850015	0.707544	-0.985279
S	-1.749703	1.653884	1.072010
H	-4.703812	-0.622104	-0.191074
H	-4.233351	0.898181	0.270894
H	-1.361599	0.499431	1.651341
C	1.820900	1.235113	-0.342042
C	1.615198	-0.173232	0.306729
O	1.428733	1.341394	-1.533380
O	2.341942	2.091506	0.394937
H	0.801970	-0.081674	1.028086
C	2.850832	-0.681429	1.037989
N	1.138783	-1.117771	-0.758507
H	0.171237	-1.449843	-0.522011
H	2.660641	-1.651720	1.499986
H	3.100381	0.034753	1.817558
S	4.317782	-0.929497	-0.053358
H	1.109096	-0.547881	-1.621421
H	1.768066	-1.906536	-0.905435
H	4.437562	0.362636	-0.422397
28			
Dimer 57 of the z...z type			
C	-1.457499	1.476152	0.184829
C	-1.989064	0.241678	0.977436
O	-2.051142	2.550780	0.390860
O	-0.467113	1.269811	-0.560750
H	-1.388037	0.164461	1.886411
C	-1.942370	-1.086267	0.236364
N	-3.392060	0.573998	1.413007
H	-3.675119	0.095523	2.268491
H	-2.409247	-1.871253	0.833964
H	-0.909082	-1.381075	0.073256

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S	-2.853178	-1.076490	-1.366185
H	-3.427056	1.597057	1.537501
H	-4.055949	0.335770	0.667962
H	-2.065983	-0.159610	-1.965678
C	1.847361	-1.931439	0.562869
C	2.323837	-0.688786	-0.260875
O	0.956260	-2.632839	0.019623
O	2.425422	-2.102338	1.653270
H	3.296211	-0.942589	-0.686920
C	2.432650	0.570390	0.589981
N	1.375340	-0.476273	-1.406076
H	1.021153	-1.396410	-1.687516
H	3.106643	0.373165	1.419318
H	1.456205	0.843036	0.990679
S	2.998169	2.059097	-0.342649
H	0.559952	0.113532	-1.093868
H	1.818988	-0.004401	-2.192866
H	4.271602	1.653308	-0.525561
28			
Dimer 58 of the z...z type			
C	1.248306	-0.025310	0.624098
C	2.395968	0.725102	-0.104463
O	1.103896	0.221600	1.839561
O	0.540938	-0.767488	-0.103958
H	1.953275	1.633062	-0.520608
C	3.066204	-0.067435	-1.217905
N	3.382554	1.163836	0.943133
H	3.911147	1.996146	0.680017
H	3.845587	0.521909	-1.702346
H	2.307829	-0.319371	-1.955424
S	3.885446	-1.610436	-0.628415
H	2.844168	1.335167	1.804901
H	4.043618	0.403703	1.141858
H	2.746817	-2.218732	-0.236396
C	-3.762803	-0.991539	-0.115529
C	-2.790604	0.168144	0.292471
O	-3.677937	-2.039731	0.570878
O	-4.537852	-0.728407	-1.057080
H	-3.387878	0.905366	0.832383
C	-2.117223	0.815010	-0.911480
N	-1.772195	-0.373407	1.249357
H	-2.214329	-1.135264	1.773831
H	-2.886760	1.127033	-1.612532
H	-1.458617	0.101597	-1.408298
S	-1.029879	2.249005	-0.498976
H	-0.938564	-0.756623	0.732238
H	-1.388955	0.332736	1.878187
H	-2.010346	3.091542	-0.115326
28			
Dimer 59 of the z...z type			
C	-3.894020	-0.507369	-0.082529
C	-2.642486	-0.317177	0.831756
O	-3.968634	-1.605991	-0.681476
O	-4.685893	0.459083	-0.101362
H	-2.956249	-0.485440	1.865333
C	-2.020666	1.072465	0.741887
N	-1.627985	-1.375809	0.518431
H	-2.042747	-2.301906	0.615652
H	-1.145526	1.149248	1.386798
H	-2.767252	1.798489	1.053908
S	-1.422045	1.515573	-0.946052
H	-1.310086	-1.293712	-0.452107
H	-0.763689	-1.264745	1.092542
H	-2.641580	1.547432	-1.521724
C	1.282808	-0.402912	0.199494
C	2.233775	0.788868	-0.102265
O	0.779056	-0.409067	1.361131
O	1.065780	-1.193422	-0.731257
H	1.628037	1.554469	-0.592443

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C	3.415014	0.431905	-0.994240
N	2.682945	1.367174	1.212850
H	2.925993	2.356553	1.157472
H	4.034556	1.307561	-1.192380
H	3.024832	0.057115	-1.937553
S	4.536582	-0.828072	-0.248858
H	1.914362	1.220139	1.882462
H	3.496842	0.847752	1.562337
H	3.627890	-1.825057	-0.244710
28			
Dimer 60 of the z...z type			
C	-1.102841	-0.841680	0.220059
C	-1.861361	0.509241	0.377216
O	-0.996209	-1.288950	-0.945641
O	-0.709492	-1.344492	1.295278
H	-1.288806	1.153774	1.043264
C	-3.256071	0.291851	0.960311
N	-1.913097	1.201601	-0.951161
H	-2.529730	2.013841	-0.946122
H	-3.760791	1.244278	1.133807
H	-3.145030	-0.216956	1.916759
S	-4.407581	-0.664212	-0.121800
H	-0.927947	1.499859	-1.209646
H	-2.234498	0.536337	-1.658747
H	-3.645793	-1.773008	-0.222722
C	1.284711	1.608509	-0.261805
C	2.584483	0.764154	-0.253298
O	0.920714	2.095342	0.825861
O	0.695738	1.641338	-1.373799
H	3.195721	0.991189	-1.124366
C	2.202352	-0.716342	-0.220134
N	3.378742	1.122953	0.974501
H	3.908136	1.986053	0.843263
H	1.575800	-0.930657	-1.083091
H	1.606060	-0.940776	0.666723
S	3.638066	-1.865663	-0.157737
H	2.714653	1.289185	1.741948
H	4.037151	0.376129	1.222189
H	4.154147	-1.543426	-1.361724
28			
Dimer 61 of the z...z type			
C	-3.660277	-1.119843	0.505331
C	-2.258022	-0.483470	0.264676
O	-3.925213	-2.131398	-0.190157
O	-4.357790	-0.570233	1.385711
H	-1.564037	-0.900440	0.997375
C	-2.213042	1.031482	0.406635
N	-1.734881	-0.896464	-1.075706
H	-0.692716	-0.694891	-1.153485
H	-1.200366	1.396177	0.233571
H	-2.515090	1.293456	1.417476
S	-3.298156	1.920871	-0.793983
H	-1.945896	-1.886929	-1.215271
H	-2.226892	-0.380296	-1.809583
H	-4.454530	1.414306	-0.317476
C	1.315271	0.014513	-0.017170
C	2.796694	0.474831	0.011290
O	0.743155	-0.125920	1.079860
O	0.863475	-0.204499	-1.171745
H	2.950260	1.291308	-0.691998
C	3.706427	-0.706952	-0.329707
N	3.103744	0.995655	1.389203
H	2.770148	1.952725	1.509390
H	3.445694	-1.055056	-1.327004
H	3.546047	-1.527880	0.372255
S	5.507973	-0.332310	-0.237564
H	2.598198	0.416885	2.071877
H	4.112591	0.980170	1.576213
H	5.526155	0.582181	-1.228750

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28		
Dimer 62 of the z...z type		
C	-3.409144 1.554955 -0.473299	
C	-2.501983 0.348762 -0.069069	
O	-3.440835 2.511898 0.343439	
O	-3.983143 1.447824 -1.575647	
H	-1.623498 0.358369 -0.715646	
C	-3.217495 -0.987886 -0.213792	
N	-1.993637 0.568095 1.324918	
H	-0.950907 0.385420 1.376148	
H	-3.519458 -1.097871 -1.252494	
H	-4.115928 -1.016917 0.406996	
S	-2.198024 -2.440002 0.312299	
H	-2.217980 1.552290 1.540116	
H	-2.464937 -0.025895 2.006203	
H	-1.055672 -2.030019 -0.286869	
C	1.130712 -0.353869 0.224406	
C	2.677978 -0.461437 0.196990	
O	0.524564 -0.702403 -0.810556	
O	0.664027 0.119187 1.289798	
H	3.038274 -0.931990 1.109765	
C	3.282659 0.934550 0.036321	
N	3.073475 -1.340615 -0.957991	
H	2.975448 -2.330040 -0.727462	
H	2.955938 1.542149 0.877707	
H	2.925711 1.402659 -0.883505	
S	5.120669 0.954321 -0.085916	
H	2.432206 -1.151389 -1.738759	
H	4.045712 -1.169752 -1.237976	
H	5.360652 0.469024 1.149550	
28		
Dimer 63 of the z...z type		
C	-3.618281 0.174954 0.163839	
C	-2.283048 -0.360039 0.771521	
O	-3.897134 -0.258968 -0.984750	
O	-4.222273 1.011988 0.859906	
H	-2.429483 -0.588024 1.826578	
C	-1.181801 0.695332 0.670160	
N	-1.899483 -1.630277 0.071463	
H	-0.855958 -1.819156 0.069473	
H	-0.265605 0.336489 1.137202	
H	-1.527620 1.576640 1.207846	
S	-0.723860 1.202680 -1.056461	
H	-2.375892 -2.427605 0.490828	
H	-2.250553 -1.552366 -0.891306	
H	-1.875898 0.836325 -1.660227	
C	1.625817 -1.394456 0.508105	
C	2.786518 -0.874651 -0.391158	
O	0.728479 -2.016426 -0.134881	
O	1.683512 -1.161451 1.721755	
H	3.468914 -1.712076 -0.557737	
C	3.579039 0.293513 0.177549	
N	2.191640 -0.545161 -1.736665	
H	2.895756 -0.290441 -2.430763	
H	4.377356 0.586787 -0.505970	
H	4.031548 -0.033247 1.111437	
S	2.593594 1.818332 0.491373	
H	1.658474 -1.356035 -2.064170	
H	1.509133 0.222591 -1.649440	
H	1.888853 1.302909 1.517742	
28		
Dimer 64 of the z...z type		
C	3.594856 -1.124374 -0.063674	
C	2.202504 -0.423999 -0.053317	
O	3.909121 -1.726765 0.991349	
O	4.233688 -1.030761 -1.134806	
H	1.478305 -1.113585 -0.493721	
C	2.144868 0.887239 -0.827248	
N	1.743642 -0.211680 1.356264	

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H	0.721713 0.070335 1.349847	
H	1.145834 1.322144 -0.763945	
H	2.384281 0.687589 -1.868602	
S	3.299316 2.176809 -0.182791	
H	1.901289 -1.067332 1.890689	
H	2.299586 0.526349 1.794734	
H	4.425638 1.493011 -0.473477	
C	-1.298721 -0.337305 0.203972	
C	-2.683163 0.016234 -0.398996	
O	-0.851617 -1.478805 -0.017690	
O	-0.780863 0.583814 0.888188	
H	-2.615530 0.952250 -0.951403	
C	-3.726623 0.124255 0.713185	
N	-3.068628 -1.058170 -1.379705	
H	-2.563212 -0.957291 -2.260732	
H	-3.399769 0.895783 1.406945	
H	-3.802183 -0.818038 1.259889	
S	-5.433324 0.483672 0.118907	
H	-2.802854 -1.970956 -0.992971	
H	-4.075345 -1.033085 -1.577224	
H	-5.163664 1.701928 -0.393645	
28		
Dimer 65 of the z...z type		
C	-2.144390 -1.569320 -0.011624	
C	-2.791625 -0.345058 -0.730892	
O	-2.934225 -2.377990 0.508444	
O	-0.888353 -1.624435 -0.043203	
H	-2.860817 -0.592795 -1.792462	
C	-2.043801 0.971825 -0.568991	
N	-4.203498 -0.230037 -0.219066	
H	-4.841121 0.209251 -0.883565	
H	-2.597481 1.786971 -1.037831	
H	-1.076710 0.915739 -1.060215	
S	-1.809074 1.477570 1.186709	
H	-4.515000 -1.184994 0.011340	
H	-4.215996 0.307841 0.654865	
H	-1.007678 0.445351 1.519789	
C	1.536807 1.732036 -0.266633	
C	1.880257 0.226026 -0.012546	
O	1.018747 1.990533 -1.382669	
O	1.846046 2.503753 0.659857	
H	1.402280 -0.096667 0.912182	
C	3.394550 0.057012 0.088306	
N	1.306256 -0.594509 -1.126236	
H	0.364036 -0.970837 -0.839516	
H	3.757465 0.693150 0.892166	
H	3.875501 0.368884 -0.841502	
S	3.951360 -1.681421 0.358873	
H	1.188207 0.039601 -1.927717	
H	1.903267 -1.387794 -1.369429	
H	3.299657 -1.870275 1.524548	
28		
Dimer 66 of the z...z type		
C	3.720036 -0.076522 0.226714	
C	2.418656 -0.876357 -0.087182	
O	3.828883 0.362812 1.395517	
O	4.497593 0.045754 -0.743233	
H	2.692133 -1.896507 -0.362718	
C	1.625538 -0.265993 -1.239953	
N	1.563969 -0.970301 1.143428	
H	0.619500 -1.371635 0.907549	
H	0.742591 -0.867771 -1.458502	
H	2.267802 -0.236300 -2.117035	
S	0.986378 1.430627 -0.894701	
H	2.024200 -1.537215 1.854153	
H	1.461184 -0.036341 1.546418	
H	2.183331 2.034389 -0.748448	
C	-1.932714 -1.801801 0.006064	
C	-2.236520 -0.314653 -0.346248	

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O	-2.902799 -2.578412 0.020436	
O	-0.726336 -2.048729 0.263874	
H	-1.560123 0.034010 -1.123875	
C	-2.110328 0.559797 0.901958	
N	-3.630385 -0.234919 -0.906142	
H	-3.653818 -0.521447 -1.885580	
H	-1.087296 0.495043 1.263996	
H	-2.775947 0.201483 1.689507	
S	-2.558467 2.326254 0.641815	
H	-4.223700 -0.896657 -0.390729	
H	-4.004033 0.718771 -0.837835	
H	-1.554217 2.608394 -0.212599	
28		
Dimer 67 of the z...z type		
C	3.811210 -0.244423 0.162187	
C	2.435067 0.084565 0.823801	
O	4.422857 0.732438 -0.331943	
O	4.157217 -1.443672 0.222555	
H	2.610038 0.195972 1.897452	
C	1.370238 -0.986273 0.619906	
N	1.943468 1.412793 0.336832	
H	1.098384 1.724733 0.870443	
H	0.431325 -0.681287 1.080726	
H	1.710637 -1.906577 1.087318	
S	0.990279 -1.328718 -1.153506	
H	2.707363 2.089906 0.363995	
H	1.625326 1.344240 -0.635668	
H	2.171433 -1.924573 -1.417702	
C	-1.154552 1.509951 0.148017	
C	-2.573641 0.881681 0.162976	
O	-0.666680 1.767829 -0.972868	
O	-0.612894 1.622089 1.276196	
H	-3.197033 1.369249 0.909808	
C	-2.453123 -0.615798 0.455356	
N	-3.202543 1.105345 -1.185057	
H	-3.617450 2.035492 -1.255498	
H	-1.990497 -0.731708 1.433213	
H	-1.818182 -1.102318 -0.287878	
S	-4.047137 -1.535256 0.400100	
H	-2.455615 1.054284 -1.891345	
H	-3.933972 0.411625 -1.376990	
H	-4.633675 -0.890121 1.429215	
28		
Dimer 68 of the z...z type		
C	2.687178 -1.356502 -0.087673	
C	1.999929 0.007510 -0.391586	
O	2.593621 -1.778178 1.088862	
O	3.278891 -1.865553 -1.065017	
H	1.235741 -0.141171 -1.155993	
C	2.994211 1.051099 -0.891049	
N	1.271229 0.482227 0.825619	
H	0.844734 1.396158 0.668035	
H	2.492726 1.993365 -1.119819	
H	3.456044 0.672925 -1.800654	
S	4.313305 1.484316 0.326679	
H	0.475402 -0.179748 1.008971	
H	1.901481 0.510889 1.627939	
H	4.901171 0.270458 0.348296	
C	-1.556941 -0.288090 -0.184881	
C	-2.951275 -0.796851 -0.649618	
O	-0.999726 -0.987632 0.711220	
O	-1.118328 0.730768 -0.742166	
H	-2.793228 -1.411813 -1.538480	
C	-3.936094 0.319178 -0.973893	
N	-3.489233 -1.710071 0.419792	
H	-4.169278 -2.386234 0.070497	
H	-4.890393 -0.088374 -1.309435	
H	-3.512013 0.924130 -1.771646	
S	-4.322448 1.395858 0.473158	

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H	-2.686042 -2.192446 0.844720	
H	-3.933203 -1.151029 1.158030	
H	-3.075647 1.895713 0.598581	
28		
Dimer 69 of the z...z type		
C	4.037869 0.451727 -0.498397	
C	2.854915 -0.230296 0.276548	
O	4.243970 1.657337 -0.214538	
O	4.662611 -0.291958 -1.280250	
H	3.306261 -0.843954 1.058493	
C	1.985300 -1.088789 -0.631680	
N	2.054148 0.839421 0.954573	
H	1.560348 0.516881 1.787288	
H	2.631749 -1.768896 -1.179612	
H	1.443624 -0.466389 -1.345104	
S	0.674312 -2.062009 0.231785	
H	2.700054 1.604072 1.180070	
H	1.304656 1.213821 0.320823	
H	1.489001 -2.798544 1.013244	
C	-0.957746 0.857230 0.451716	
C	-2.185789 0.026310 0.001573	
O	-0.818838 1.032448 1.680135	
O	-0.220518 1.268833 -0.479868	
H	-1.904779 -0.638789 -0.812305	
C	-3.320102 0.956223 -0.423619	
N	-2.608314 -0.831252 1.161128	
H	-1.958909 -1.611153 1.285629	
H	-2.962457 1.577145 -1.243126	
H	-3.606706 1.610190 0.402295	
S	-4.867071 0.086193 -0.920938	
H	-2.557669 -0.265002 2.017037	
H	-3.554825 -1.203593 1.030984	
H	-4.351516 -0.537633 -1.999866	
28		
Dimer 70 of the z...z type		
C	0.690865 -1.200923 0.706090	
C	2.213090 -1.017186 0.472956	
O	0.065499 -1.877761 -0.131290	
O	0.239915 -0.555846 1.687629	
H	2.766284 -1.187703 1.394454	
C	2.456493 0.400360 -0.050523	
N	2.668232 -2.036899 -0.534332	
H	2.823621 -2.947904 -0.100789	
H	2.104807 1.101763 0.702507	
H	1.887698 0.574215 -0.966516	
S	4.206384 0.764013 -0.489923	
H	1.916630 -2.158976 -1.225415	
H	3.538219 -1.744465 -0.993575	
H	4.707439 0.631362 0.755325	
C	-3.321340 -0.640606 -0.622945	
C	-2.646686 0.606024 0.044975	
O	-3.744967 -1.515302 0.173841	
O	-3.399843 -0.607888 -1.867178	
H	-3.402993 1.393016 0.076439	
C	-1.425300 1.093847 -0.722117	
N	-2.316144 0.254657 1.465422	
H	-2.987920 -0.475859 1.736215	
H	-1.737291 1.376843 -1.723935	
H	-0.696163 0.291788 -0.816632	
S	-0.536557 2.503000 0.071569	
H	-1.335463 -0.145025 1.559339	
H	-2.384918 1.056571 2.088993	
H	-1.469373 3.443126 -0.185009	
28		
Dimer 71 of the z...z type		
C	1.525651 0.352699 1.133997	
C	2.436294 0.637853 -0.098199	
O	1.923886 0.802872 2.223270	
O	0.466381 -0.275610 0.876591	

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H	2.129528	1.610098	-0.489767
C	2.359426	-0.395293	-1.212591
N	3.841975	0.804211	0.410982
H	4.428243	1.373854	-0.200129
H	3.017091	-0.124834	-2.039478
H	1.336735	-0.423472	-1.580246
S	2.869790	-2.086261	-0.686120
H	3.775147	1.234521	1.344096
H	4.284439	-0.115259	0.523350
H	1.848808	-2.258049	0.178713
C	-3.586985	-0.890729	0.162607
C	-2.740120	0.422277	0.045532
O	-3.683223	-1.372674	1.319587
O	-4.095461	-1.293484	-0.902005
H	-3.444577	1.246679	-0.075858
C	-1.771609	0.383916	-1.129481
N	-2.021124	0.635344	1.348259
H	-2.556501	0.106290	2.051209
H	-2.338617	0.227120	-2.043232
H	-1.063958	-0.435523	-1.010345
S	-0.726148	1.895800	-1.293156
H	-1.041654	0.246503	1.310272
H	-1.958344	1.618690	1.603939
H	-1.689182	2.710702	-1.769541
28			
Dimer 72 of the z...z type			
C	-1.309959	1.466355	0.178024
C	-1.826626	0.211348	0.947979
O	-1.796660	2.558099	0.525305
O	-0.436959	1.251789	-0.700883
H	-1.111363	0.006688	1.748323
C	-2.002622	-1.042734	0.102260
N	-3.119537	0.606442	1.611570
H	-3.309921	0.087702	2.469109
H	-2.443937	-1.844475	0.696958
H	-1.030739	-1.393531	-0.232654
S	-3.126667	-0.809637	-1.339540
H	-3.055840	1.618163	1.801293
H	-3.902954	0.469331	0.963548
H	-2.337789	0.078382	-1.979127
C	1.688361	-1.974459	0.548439
C	2.285896	-0.773157	-0.258619
O	0.833957	-2.663714	-0.064465
O	2.147841	-2.131641	1.695805
H	3.263571	-1.091642	-0.625635
C	2.425445	0.490534	0.580646
N	1.420133	-0.525697	-1.460404
H	1.058526	-1.433447	-1.770436
H	3.047296	0.267796	1.443488
H	1.449810	0.823507	0.933949
S	3.115429	1.933976	-0.339499
H	0.603257	0.086309	-1.196207
H	1.928864	-0.064471	-2.213460
H	4.368454	1.451479	-0.471151
28			
Dimer 73 of the z...z type			
C	-1.914779	-1.355391	0.492624
C	-2.915697	-0.878034	-0.600310
O	-2.364069	-1.508182	1.643496
O	-0.746131	-1.539671	0.066973
H	-3.133163	-1.730936	-1.245381
C	-2.372282	0.269850	-1.447871
N	-4.200150	-0.497705	0.085258
H	-5.028862	-0.655294	-0.488240
H	-3.066422	0.529876	-2.247903
H	-1.430366	-0.052813	-1.885336
S	-2.115942	1.829615	-0.496750
H	-4.249229	-1.042433	0.958163
H	-4.167792	0.493810	0.353690

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H	-1.211672	1.337666	0.373910
C	3.114318	-1.206739	-0.638717
C	2.084197	-0.170953	-0.079941
O	3.467210	-2.111555	0.158597
O	3.489480	-0.993497	-1.808596
H	1.262599	-0.068211	-0.787267
C	2.774671	1.172707	0.135502
N	1.508313	-0.713946	1.192035
H	0.598993	-1.194989	0.959007
H	3.224830	1.483318	-0.805010
H	3.566481	1.084408	0.882600
S	1.661343	2.506061	0.760738
H	2.187581	-1.399796	1.550317
H	1.317399	0.014221	1.882337
H	0.851582	2.546489	-0.317235
28			
Dimer 74 of the z...z type			
C	1.209018	1.621828	0.015778
C	2.362037	0.898029	0.782738
O	0.134029	1.709244	0.667682
O	1.486854	2.088055	-1.102201
H	2.874590	1.680699	1.349445
C	3.405868	0.204454	-0.085698
N	1.750124	-0.029318	1.795544
H	2.454897	-0.563788	2.303191
H	4.304514	-0.009366	0.496003
H	3.666039	0.899108	-0.882216
S	2.901698	-1.415746	-0.807681
H	1.202998	0.521466	2.457767
H	1.053576	-0.691613	1.350651
H	1.620697	-1.080223	-1.136518
C	-0.853242	-1.179557	-0.230849
C	-2.404321	-1.265605	-0.290394
O	-0.334974	-1.477549	0.884224
O	-0.287611	-0.863569	-1.287540
H	-2.650531	-2.201719	-0.795093
C	-3.051850	-0.100637	-1.036210
N	-2.921251	-1.370747	1.118353
H	-3.770982	-1.928628	1.200566
H	-4.113472	-0.290345	-1.198790
H	-2.557723	-0.011520	-2.001203
S	-2.965065	1.501079	-0.126723
H	-2.159915	-1.771581	1.685725
H	-3.110710	-0.422359	1.473486
H	-1.600222	1.577237	0.009576
28			
Dimer 75 of the z...z type			
C	-1.464775	-0.732398	0.233866
C	-3.012247	-0.899531	0.212713
O	-0.955152	-0.684283	1.395267
O	-0.890359	-0.680421	-0.859244
H	-3.220910	-1.967622	0.120956
C	-3.697018	-0.151079	-0.923902
N	-3.541753	-0.468305	1.554473
H	-4.430008	-0.907274	1.798580
H	-4.775707	-0.311296	-0.903726
H	-3.302907	-0.528573	-1.864420
S	-3.453421	1.676192	-0.848498
H	-2.820283	-0.698582	2.251756
H	-3.663816	0.551174	1.566739
H	-2.121100	1.637690	-1.057498
C	2.427708	-1.592311	-0.646262
C	2.146440	-0.159277	-0.096401
O	2.504199	-2.507995	0.210755
O	2.581565	-1.657900	-1.883483
H	1.324499	0.271115	-0.664359
C	3.408413	0.690376	-0.218434
N	1.697619	-0.265736	1.325750
H	0.652532	-0.459914	1.371716

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H	3.717276	0.701081	-1.261620
H	4.220284	0.266557	0.377117
S	3.218233	2.423149	0.392392
H	2.183797	-1.065741	1.744673
H	1.891624	0.590544	1.849400
H	2.243528	2.779774	-0.469025
28			
Dimer 76 of the z...z type			
C	-0.815054	1.417838	-0.067363
C	-1.874087	0.273821	-0.008303
O	-0.502473	1.940125	1.028478
O	-0.413703	1.697487	-1.217395
H	-1.549619	-0.542155	-0.651228
C	-3.230593	0.814041	-0.450555
N	-1.930253	-0.268411	1.386199
H	-1.052433	-0.834134	1.560619
H	-3.125035	1.235679	-1.448377
H	-3.569243	1.604439	0.222763
S	-4.588541	-0.437772	-0.449448
H	-1.923512	0.516485	2.043659
H	-2.760129	-0.846963	1.533176
H	-4.057319	-1.238983	-1.395417
C	0.963781	-1.549335	0.395152
C	2.416880	-1.041015	0.209880
O	0.386855	-1.989767	-0.617215
O	0.502873	-1.384185	1.554848
H	3.047200	-1.369604	1.033825
C	2.389767	0.484201	0.109042
N	2.971620	-1.630462	-1.059460
H	3.281018	-2.593967	-0.925832
H	1.914033	0.882160	1.002707
H	1.783735	0.799969	-0.742538
S	4.042678	1.253261	-0.144385
H	2.214091	-1.650421	-1.754362
H	3.765051	-1.081140	-1.407359
H	4.583835	0.856328	1.025664
28			
Dimer 77 of the z...z type			
C	1.634621	1.358613	-0.111092
C	2.923489	0.867576	-0.829795
O	1.772204	2.228976	0.767599
O	0.575748	0.811953	-0.515354
H	2.970183	1.363754	-1.801095
C	2.970339	-0.643642	-1.031767
N	4.101438	1.352083	-0.028969
H	4.940496	1.498039	-0.590916
H	3.883160	-0.940387	-1.549851
H	2.114617	-0.930921	-1.638482
S	2.957542	-1.594373	0.548505
H	3.815220	2.226632	0.433524
H	4.314875	0.676921	0.714985
H	1.720856	-1.212751	0.932646
C	-3.940501	0.714915	-0.221021
C	-2.509498	0.080726	-0.172448
O	-4.088149	1.766460	0.451634
O	-4.763732	0.122089	-0.945767
H	-2.025874	0.301766	-1.126248
C	-2.547294	-1.425371	0.041924
N	-1.694736	0.785818	0.869259
H	-2.190313	1.669161	1.058738
H	-3.097048	-1.868620	-0.784559
H	-3.069825	-1.671017	0.969209
S	-0.880267	-2.216145	0.194601
H	-1.636776	0.258648	1.740048
H	-0.721445	0.942159	0.485911
H	-0.256943	-1.463127	-0.735355
28			
Dimer 78 of the z...z type			
C	-1.171545	-0.269341	-0.298230

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C	-2.477377	-0.096220	-1.125253
O	-0.765687	-1.433961	-0.125971
O	-0.646566	0.805861	0.091361
H	-2.182013	0.136429	-2.150491
C	-3.404393	0.996457	-0.606123
N	-3.163204	-1.435051	-1.160923
H	-3.739840	-1.572457	-1.991309
H	-4.301055	1.073938	-1.222176
H	-2.868862	1.941865	-0.645366
S	-3.994345	0.697004	1.115352
H	-2.423721	-2.151009	-1.108748
H	-3.751626	-1.548129	-0.327035
H	-2.778509	0.806559	1.689868
C	2.936998	1.632591	-0.420728
C	2.746606	0.318517	0.408818
O	2.465589	2.673083	0.098082
O	3.574893	1.505786	-1.487279
H	3.677180	0.153646	0.957363
C	2.429567	-0.896886	-0.452999
N	1.664891	0.534230	1.422651
H	1.833733	1.415636	1.909267
H	3.194558	-0.987632	-1.219232
H	1.459806	-0.784903	-0.935379
S	2.307729	-2.477469	0.496094
H	0.720903	0.619415	0.931852
H	1.622558	-0.235779	2.091478
H	3.625970	-2.591247	0.762215
28			
Dimer 79 of the z...z type			
C	4.056946	-0.706436	-0.005055
C	2.532982	-0.654430	-0.351070
O	4.350650	-1.312102	1.054830
O	4.814572	-0.163529	-0.836120
H	2.339340	-1.473148	-1.049461
C	2.080349	0.648911	-0.997783
N	1.733794	-0.948326	0.879409
H	0.780485	-1.321312	0.637187
H	1.007216	0.638076	-1.182270
H	2.609334	0.771360	-1.939588
S	2.380364	2.133848	0.055630
H	2.285679	-1.584343	1.463748
H	1.573067	-0.084285	1.405533
C	3.726023	2.067068	-0.019029
H	-1.249618	-0.255861	0.161536
C	-2.672623	-0.016545	-0.405681
O	-0.802290	-1.434726	0.043556
O	-0.702205	0.721967	0.693505
H	-2.671847	0.878509	-1.025369
C	-3.670060	0.127560	0.744047
N	-3.051072	-1.174523	-1.290292
H	-2.571206	-1.125386	-2.190160
H	-3.346430	0.958437	1.367755
H	-3.681979	-0.776115	1.357049
S	-5.414677	0.380102	0.207930
H	-2.748746	-2.046867	-0.842163
H	-4.062624	-1.193974	-1.461845
H	-5.222032	1.576655	-0.384294
28			
Dimer 80 of the z...z type			
C	-2.476739	1.763535	-0.321611
C	-2.339628	0.227943	-0.085277
O	-2.581972	2.471969	0.709110
O	-2.502395	2.107722	-1.522356
H	-1.558626	-0.175673	-0.726833
C	-3.673835	-0.453306	-0.378894
N	-1.902332	-0.013401	1.323210
H	-0.871160	0.221618	1.390095
H	-3.963736	-0.219670	-1.401554
H	-4.451720	-0.083765	0.292804

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S	-3.659090	-2.284713	-0.140501
H	-2.421098	0.614763	1.942639
H	-2.043778	-0.988202	1.596739
H	-2.725004	-2.552070	-1.075915
C	1.122311	-0.210268	0.213864
C	2.530866	0.093589	-0.359194
O	0.695307	0.620908	1.070404
O	0.572127	-1.243001	-0.191491
H	2.529952	-0.048963	-1.437948
C	3.558880	-0.825573	0.302701
N	2.865563	1.537096	-0.090109
H	2.415723	2.156632	-0.765337
H	3.277021	-1.855130	0.091051
H	3.557384	-0.684528	1.385382
S	5.297638	-0.522485	-0.225865
H	2.496931	1.785040	0.836755
H	3.878751	1.696502	-0.130717
H	5.124302	-0.853545	-1.521893
28			
Dimer 81 of the z...z type			
C	2.166052	0.653868	1.077943
C	2.778707	0.440410	-0.341266
O	2.879134	0.333425	2.048207
O	1.014704	1.150759	1.066774
H	3.075973	1.420660	-0.718370
C	1.815639	-0.204333	-1.331924
N	4.035594	-0.372258	-0.175871
H	4.762481	-0.142175	-0.853027
H	2.274293	-0.294673	-2.317634
H	0.930797	0.424515	-1.419421
S	1.330012	-1.926485	-0.872326
H	4.364063	-0.207241	0.788202
H	3.817070	-1.372900	-0.251179
H	0.827877	-1.631701	0.344469
C	-1.578917	1.654225	-0.872555
C	-1.713719	0.362322	-0.010912
O	-1.912039	2.722136	-0.305649
O	-1.186730	1.464595	-2.043120
H	-0.894910	-0.309435	-0.244615
C	-3.047420	-0.319253	-0.292226
N	-1.577964	0.733889	1.432261
H	-0.563186	0.919203	1.606991
H	-3.116337	-0.518480	-1.360334
H	-3.880830	0.325652	-0.006570
S	-3.293669	-1.890974	0.646553
H	-2.097707	1.603481	1.589481
H	-1.914635	-0.005582	2.053197
H	-2.252438	-2.554130	0.102391
28			
Dimer 82 of the z...z type			
C	-2.369028	-1.926355	0.118193
C	-2.016891	-0.405918	0.071153
O	-2.877079	-2.405352	-0.926203
O	-2.128952	-2.486447	1.207419
H	-1.003368	-0.259581	0.436883
C	-2.993055	0.378433	0.944231
N	-2.045065	0.057048	-1.350569
H	-1.071365	-0.032266	-1.750584
H	-2.902453	0.009787	1.963930
H	-4.021807	0.227939	0.609914
S	-2.726121	2.209018	0.906184
H	-2.691196	-0.559078	-1.858337
H	-2.327122	1.037126	-1.422577
H	-1.377430	2.164559	0.949351
C	1.053456	0.684973	-1.063256
C	2.538734	0.466113	-0.679198
O	0.449187	1.608143	-0.478526
O	0.590609	-0.152295	-1.878598
H	3.142510	0.281298	-1.565345

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C	2.623064	-0.714044	0.292239
N	3.046986	1.720862	-0.024764
H	3.318503	2.421297	-0.715930
H	2.238548	-1.596519	-0.215064
H	2.002947	-0.527596	1.171630
S	4.312270	-1.041210	0.947972
H	2.276153	2.122499	0.526041
H	3.858242	1.526048	0.572891
H	4.878216	-1.357411	-0.234880
28			
Dimer 83 of the z...z type			
C	-1.211093	0.111643	0.356147
C	-2.276249	-0.806647	-0.303067
O	-0.821233	-0.227778	1.498072
O	-0.807153	1.066231	-0.346874
H	-1.724825	-1.524484	-0.914696
C	-3.290956	-0.074719	-1.170024
N	-2.941493	-1.589334	0.796255
H	-3.302454	-2.492933	0.489491
H	-4.001467	-0.772050	-1.615502
H	-2.751229	0.433473	-1.965497
S	-4.301605	1.152222	-0.234468
H	-2.238165	-1.711803	1.539688
H	-3.714905	-1.043657	1.193877
H	-3.268613	1.966134	0.066701
C	3.690139	0.690824	-0.269058
C	2.719802	0.258825	0.875912
O	3.587666	1.881474	-0.649482
O	4.483140	-0.194604	-0.654423
H	3.287330	0.334842	1.808019
C	2.194705	-1.168622	0.766441
N	1.607080	1.257929	0.984191
H	1.077101	1.147526	1.850903
H	1.429669	-1.354279	1.520390
H	3.029118	-1.847124	0.927550
S	1.401355	-1.590726	-0.843226
H	2.006378	2.196612	0.914382
H	0.882250	1.175451	0.235537
H	2.524860	-1.463064	-1.578059
28			
Dimer 84 of the z...z type			
C	1.716185	-0.828620	-0.772107
C	1.797324	-0.227052	0.664219
O	2.374965	-1.865553	-0.971829
O	0.977251	-0.201840	-1.575701
H	0.931695	-0.603353	1.215621
C	1.816223	1.295561	0.704216
N	3.014239	-0.811759	1.328669
H	2.927806	-0.879198	2.342903
H	1.859698	1.659767	1.731285
H	0.904071	1.665943	0.242850
S	3.266969	2.037425	-0.160511
H	3.156430	-1.743726	0.911627
H	3.842817	-0.248458	1.105145
H	2.923005	1.596289	-1.388369
C	-1.433346	-1.654633	0.392386
C	-1.808301	-0.182239	0.032085
O	-1.681228	-2.504332	-0.493212
O	-0.957372	-1.813079	1.537228
H	-1.099030	0.504795	0.488596
C	-3.221140	0.119476	0.522810
N	-1.694759	-0.013329	-1.449432
H	-0.673135	-0.022718	-1.686422
H	-3.260682	-0.051384	1.597392
H	-3.941691	-0.545303	0.042404
S	-3.802007	1.830216	0.146194
H	-2.133419	-0.820779	-1.902833
H	-2.131055	0.854767	-1.769197
H	-2.892863	2.470208	0.909875

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28		
Dimer 85 of the z...z type		
C	3.930235 -0.118931 0.357340	
C	2.865759 -0.270703 -0.772671	
O	3.880194 -0.960915 1.283836	
O	4.705927 0.849350 0.206769	
H	3.381476 -0.477903 -1.712220	
C	2.031520 0.994181 -0.955643	
N	1.978310 -1.447776 -0.488386	
H	1.094760 -1.420500 -1.047683	
H	1.289284 0.862991 -1.742218	
H	2.699497 1.810011 -1.220515	
S	1.066377 1.473435 0.542983	
H	2.475674 -2.324859 -0.631608	
H	1.688790 -1.434915 0.494025	
H	2.080584 2.027158 1.235242	
C	-1.058636 -0.979695 -0.184515	
C	-2.216218 -0.013834 0.178864	
O	-0.539090 -0.808310 -1.326583	
O	-0.759192 -1.823566 0.673275	
H	-2.085956 0.338351 1.200321	
C	-3.557183 -0.730290 0.021619	
N	-2.154958 1.190112 -0.722371	
H	-1.423330 1.839482 -0.420601	
H	-3.555152 -1.600930 0.674558	
H	-3.691244 -1.072567 -1.006536	
S	-5.022636 0.327142 0.382202	
H	-1.906227 0.878228 -1.668662	
H	-3.051319 1.689626 -0.732484	
H	-4.735738 0.543399 1.682386	
28		
Dimer 86 of the z...z type		
C	-4.040284 0.045178 -0.193865	
C	-2.665168 0.252080 0.539166	
O	-4.458508 -1.138721 -0.226202	
O	-4.577053 1.083355 -0.625829	
H	-2.890973 0.663983 1.523974	
C	-1.744823 1.189104 -0.228218	
N	-2.042663 -1.098270 0.742926	
H	-1.490600 -1.178222 1.597081	
H	-2.291769 2.105623 -0.429441	
H	-1.442278 0.738949 -1.173251	
S	-0.201578 1.625878 0.713964	
H	-2.820045 -1.772960 0.742872	
H	-1.380266 -1.338630 -0.042353	
H	-0.308169 2.965046 0.627565	
C	0.928229 -1.389755 -0.121841	
C	2.273516 -0.741694 -0.558755	
O	0.007889 -1.325006 -0.991850	
O	0.863491 -1.887972 1.011458	
H	2.835701 -1.486426 -1.125329	
C	3.102917 -0.227720 0.610519	
N	1.954540 0.372761 -1.520103	
H	1.387459 0.010397 -2.289829	
H	3.289916 -1.057083 1.287608	
H	2.555414 0.536906 1.162527	
S	4.695031 0.557677 0.112336	
H	1.383846 1.085337 -1.033826	
H	2.804918 0.812997 -1.881983	
H	5.275588 -0.560648 -0.368838	
28		
Dimer 87 of the z...z type		
C	2.036952 1.068770 0.614673	
C	1.971671 0.384631 -0.788573	
O	3.067844 1.732238 0.836325	
O	1.045426 0.908616 1.370575	
H	1.500041 1.103659 -1.460384	
C	1.210606 -0.929402 -0.868336	
N	3.394433 0.223241 -1.255513	

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H	3.489504 0.223385 -2.271303	
H	1.303310 -1.362801 -1.865730	
H	0.153025 -0.745138 -0.706807	
S	1.824619 -2.230700 0.282296	
H	3.924859 1.004955 -0.840698	
H	3.792805 -0.648068 -0.889981	
H	1.654167 -1.517991 1.414339	
C	-2.738252 -0.942146 -0.322943	
C	-2.450892 -0.036616 0.919498	
O	-1.994553 -1.948024 -0.443969	
O	-3.676625 -0.562715 -1.049742	
H	-3.270962 -0.190956 1.623577	
C	-2.377874 1.449228 0.581710	
N	-1.196070 -0.531702 1.580674	
H	-1.283147 -0.579707 2.594096	
H	-2.000184 2.021789 1.429948	
H	-3.381092 1.799750 0.350780	
S	-1.278880 1.866384 -0.842378	
H	-1.045834 -1.479870 1.198077	
H	-0.341062 0.053051 1.366482	
H	-2.065801 1.298511 -1.778894	
28		
Dimer 88 of the z...z type		
C	-0.952288 -1.099757 -0.517825	
C	-2.492617 -0.912663 -0.509088	
O	-0.473748 -1.632597 0.525303	
O	-0.353620 -0.643774 -1.502306	
H	-2.916421 -1.180519 -1.474769	
C	-2.803031 0.547249 -0.167986	
N	-3.089234 -1.829107 0.524537	
H	-3.164780 -2.786267 0.177496	
H	-2.362211 1.174848 -0.939690	
H	-2.357022 0.817325 0.791425	
S	-4.597060 0.927814 -0.004714	
H	-2.454754 -1.851992 1.333105	
H	-4.023644 -1.512030 0.807347	
H	-4.926590 0.662781 -1.285843	
C	4.003809 -0.302001 -0.325390	
C	2.508675 0.052820 -0.034473	
O	4.460609 -1.290729 0.305016	
O	4.570484 0.416657 -1.172694	
H	1.919400 -0.245792 -0.902997	
C	2.307607 1.537576 0.234376	
N	2.025847 -0.796010 1.104788	
H	1.068180 -1.195859 0.906430	
H	2.694845 2.092275 -0.616704	
H	2.860898 1.851061 1.123006	
S	0.551082 2.018911 0.551596	
H	2.737924 -1.536711 1.205194	
H	1.984698 -0.277200 1.981508	
H	0.056102 1.480511 -0.581120	
28		
Dimer 89 of the z...z type		
C	4.000602 -0.218283 0.411748	
C	2.791912 0.398686 -0.371105	
O	4.265232 -1.417189 0.148617	
O	4.586947 0.564887 1.186742	
H	3.210354 1.038540 -1.150460	
C	1.864761 1.204667 0.530220	
N	2.039718 -0.704469 -1.049127	
H	1.504351 -0.394222 -1.861094	
H	2.451537 1.955278 1.052717	
H	1.391728 0.554474 1.267091	
S	0.462711 2.013740 -0.357808	
H	2.710647 -1.434947 -1.304459	
H	1.317651 -1.116030 -0.401273	
H	1.198022 2.939858 -1.006035	
C	-1.002965 -1.233937 -0.503153	
C	-2.466304 -1.023889 -0.035186	

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O	-0.142745	-1.333040	0.421838		
O	-0.815094	-1.233099	-1.728527		
H	-3.128371	-1.688110	-0.587956		
C	-2.869504	0.435425	-0.245497		
N	-2.572573	-1.388328	1.422006		
H	-2.592297	-2.400612	1.553056		
H	-2.728874	0.677605	-1.296822		
H	-2.232828	1.098141	0.342121		
S	-4.592326	0.824171	0.276289		
H	-1.736187	-1.042661	1.907086		
H	-3.420336	-0.992032	1.842797		
H	-5.207318	0.019224	-0.614138		
28					
Dimer 90 of the z...z type					
C	4.021599	-0.186744	0.342523		
C	2.784457	0.394805	-0.423429		
O	4.296657	-1.387780	0.100951		
O	4.615780	0.622510	1.083999		
H	3.172978	1.020635	-1.229203		
C	1.872206	1.210898	0.484524		
N	2.030288	-0.735097	-1.053671		
H	1.468960	-0.450498	-1.857145		
H	2.461466	1.987844	0.963899		
H	1.436272	0.575001	1.255733		
S	0.424004	1.965956	-0.376378		
H	2.704672	-1.461010	-1.312443		
H	1.334182	-1.142256	-0.372801		
H	1.115048	2.880111	-1.087324		
C	-0.977114	-1.268206	-0.358356		
C	-2.407303	-0.985241	0.170422		
O	-0.071842	-1.330668	0.524981		
O	-0.858166	-1.385398	-1.586902		
H	-3.041815	-1.841716	-0.058806		
C	-2.986923	0.286635	-0.444322		
N	-2.362954	-0.870365	1.672268		
H	-2.074692	-1.753721	2.095917		
H	-2.957594	0.179353	-1.526108		
H	-2.383425	1.154514	-0.174673		
S	-4.697221	0.683538	0.114151		
H	-1.663804	-0.177416	1.953045		
H	-3.277901	-0.597832	2.047057		
H	-5.295185	-0.388873	-0.444101		
28					
Dimer 91 of the z...z type					
C	2.459066	-0.595852	-0.866579		
C	2.555789	0.886146	-0.376673		
O	1.745412	-0.782097	-1.882947		
O	3.121414	-1.420019	-0.205836		
H	3.510446	1.270200	-0.745731		
C	2.529704	1.053531	1.136237		
N	1.483574	1.685034	-1.055592		
H	1.747103	2.661479	-1.181844		
H	2.444251	2.105904	1.411494		
H	3.463321	0.669833	1.540888		
S	1.139604	0.188457	1.986515		
H	1.334444	1.245989	-1.972984		
H	0.540456	1.677755	-0.581498		
H	1.610115	-1.052003	1.743732		
C	-2.166148	1.504072	-0.253522		
C	-2.060615	0.054530	0.293067		
O	-3.309092	1.929095	-0.503180		
O	-1.064113	2.095194	-0.392395		
H	-1.494566	0.067266	1.221435		
C	-1.390492	-0.873546	-0.715069		
N	-3.444094	-0.442014	0.622639		
H	-3.828183	0.052118	1.429219		
H	-0.408507	-0.486521	-0.971727		
H	-1.979034	-0.938800	-1.632750		
S	-1.197349	-2.607223	-0.121833		

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H	-4.075148	-0.251302	-0.161514
H	-3.432841	-1.447218	0.826347
H	-0.297099	-2.326258	0.840789
28			
Dimer 92 of the z...z type			
C	1.325156	-0.351695	0.031191
C	2.424060	0.742008	0.082539
O	0.733126	-0.577803	1.127797
O	1.098440	-0.856848	-1.078727
H	1.954849	1.658389	-0.280779
C	3.652393	0.430113	-0.761235
N	2.781914	0.977194	1.525122
H	3.123986	1.921119	1.707157
H	4.373144	1.247801	-0.722674
H	3.328028	0.296603	-1.790547
S	4.562060	-1.074645	-0.204792
H	1.935356	0.783728	2.078750
H	3.498392	0.303860	1.820652
H	3.571181	-1.944260	-0.491349
C	-4.128645	-0.781728	0.165787
C	-2.727900	-0.082571	0.279761
O	-4.099512	-2.025976	-0.009729
O	-5.112929	-0.027514	0.292188
H	-2.596297	0.190248	1.328437
C	-2.634390	1.161348	-0.593584
N	-1.663917	-1.085781	-0.043772
H	-2.123295	-2.006332	0.024825
H	-3.471564	1.810513	-0.349695
H	-2.711280	0.895799	-1.650739
S	-1.052987	2.101793	-0.443816
H	-1.295563	-0.988480	-0.992345
H	-0.818520	-1.014243	0.574304
H	-1.156613	2.371274	0.873287
28			
Dimer 93 of the z...z type			
C	1.169202	-0.244595	-0.769128
C	2.251393	0.764785	-0.303130
O	0.660052	-0.948849	0.152170
O	0.935875	-0.269958	-1.983542
H	2.094837	1.714523	-0.814141
C	3.661241	0.257341	-0.606789
N	2.066786	1.022271	1.167947
H	2.760248	1.671717	1.543511
H	4.408911	1.005164	-0.336712
H	3.726318	0.081454	-1.679710
S	4.146907	-1.267012	0.311307
H	1.125037	1.410591	1.321159
H	2.123832	0.134886	1.677564
H	3.171053	-2.062248	-0.173133
C	-3.690962	-0.947514	-0.124804
C	-2.709605	0.097610	0.518166
O	-3.600746	-2.115982	0.329005
O	-4.466188	-0.493055	-0.986706
H	-3.306720	0.720078	1.186229
C	-2.031677	0.961195	-0.534943
N	-1.724350	-0.655395	1.362772
H	-2.170974	-1.570688	1.535889
H	-2.806426	1.433602	-1.133116
H	-1.404397	0.359875	-1.195374
S	-0.906688	2.269081	0.130294
H	-0.818154	-0.824051	0.855627
H	-1.511869	-0.187266	2.241017
H	-1.761725	2.800951	1.026881
28			
Dimer 94 of the z...z type			
C	-2.576560	-0.670209	0.990276
C	-2.782722	-0.577526	-0.555313
O	-3.592256	-0.477629	1.683673
O	-1.414544	-0.961711	1.367915

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H	-2.969194	-1.593161	-0.910832
C	-1.605339	0.005147	-1.321733
N	-4.045562	0.205123	-0.793895
H	-4.524980	-0.051907	-1.657128
H	-1.817978	0.053775	-2.390261
H	-0.755410	-0.657854	-1.178004
S	-1.171448	1.728849	-0.827510
H	-4.651234	0.035931	0.023744
H	-3.839652	1.209896	-0.819273
H	-0.967691	1.459426	0.478172
C	2.294603	-1.754833	-0.599375
C	1.873005	-0.349851	-0.061669
O	2.370005	-2.665459	0.261635
O	2.538868	-1.794113	-1.821358
H	1.133424	0.088168	-0.725417
C	3.090041	0.569663	0.003777
N	1.249443	-0.518767	1.288830
H	1.696737	-1.341464	1.715702
H	3.525499	0.631607	-0.991372
H	3.842134	0.170709	0.687601
S	2.706370	2.264855	0.628788
H	1.381634	0.310127	1.874382
H	0.220777	-0.713948	1.232173
H	1.765265	2.551893	-0.295186
28			
Dimer 95 of the z...z type			
C	3.961758	0.498854	-0.556831
C	2.845650	-0.264734	0.239878
O	4.169789	1.682636	-0.195215
O	4.540802	-0.170848	-1.435381
H	3.357412	-0.932379	0.935597
C	1.924964	-1.061850	-0.674805
N	2.078148	0.728232	1.059030
H	2.732084	1.456501	1.361083
H	2.539117	-1.697928	-1.306252
H	1.340363	-0.393268	-1.308065
S	0.666249	-2.096571	0.194681
H	1.321053	1.180391	0.486703
H	1.599830	0.311460	1.858906
H	1.521326	-2.865004	0.898326
C	-0.939133	0.832806	0.583044
C	-2.152072	0.037416	0.039032
O	-0.811539	0.894667	1.822514
O	-0.194834	1.330555	-0.300767
H	-1.834628	-0.586928	-0.794075
C	-3.262035	0.991849	-0.394515
N	-2.633700	-0.879244	1.127899
H	-1.977658	-1.652425	1.260336
H	-2.858854	1.657971	-1.155109
H	-3.596997	1.597316	0.449996
S	-4.775416	0.152943	-1.029180
H	-2.656667	-0.357612	2.011790
H	-3.560932	-1.261552	0.914182
H	-4.198447	-0.403534	-2.113947
28			
Dimer 96 of the z...z type			
C	-1.160961	0.021164	0.065067
C	-2.624205	-0.243035	-0.375223
O	-0.711299	-0.764394	0.952528
O	-0.594843	0.987239	-0.463428
H	-2.686755	-0.241968	-1.462177
C	-3.540437	0.828497	0.217950
N	-3.043679	-1.609164	0.098982
H	-2.623292	-2.345755	-0.469155
H	-3.199313	1.798802	-0.137290
H	-3.479212	0.821849	1.308305
S	-5.326805	0.601410	-0.171587
H	-2.703121	-1.745364	1.057379
H	-4.064099	-1.713858	0.066813

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H	-5.220265	0.783763	-1.503792
C	2.736992	-1.705304	-0.360283
C	2.417413	-0.202073	-0.091912
O	2.805787	-2.445469	0.651509
O	2.923108	-1.992692	-1.561790
H	1.646114	0.138481	-0.780404
C	3.687475	0.627511	-0.262117
N	1.854499	-0.057133	1.284875
H	0.831186	-0.343312	1.267370
H	4.080978	0.457365	-1.262246
H	4.446497	0.325905	0.463159
S	3.450275	2.439080	0.011043
H	2.358422	-0.690859	1.911443
H	1.920856	0.907542	1.616624
H	2.561063	2.625605	-0.985765
28			
Dimer 97 of the z...z type			
C	-3.960701	-0.500594	-0.557090
C	-2.845758	0.265126	0.239170
O	-4.168364	-1.683840	-0.193553
O	-4.539369	0.167210	-1.437348
H	-3.358491	0.933840	0.933145
C	-1.924647	1.060980	-0.676246
N	-2.078378	-0.725778	1.060950
H	-2.732158	-1.453434	1.364738
H	-2.538571	1.695807	-1.309174
H	-1.339424	0.391517	-1.307999
S	-0.666843	2.097433	0.192446
H	-1.321153	-1.179258	0.489847
H	-1.600306	-0.307002	1.859948
H	-1.522609	2.866651	0.894410
C	0.939031	-0.831284	0.585317
C	2.151886	-0.037143	0.039236
O	0.811605	-0.890311	1.824937
O	0.194635	-1.331092	-0.297255
H	1.834285	0.585446	-0.795128
C	3.261531	-0.992750	-0.392636
N	2.634198	0.881581	1.126031
H	1.978626	1.655402	1.257033
H	2.857863	-1.660723	-1.151348
S	3.596909	-1.596116	0.453225
S	4.774514	-0.155403	-1.030233
H	2.657012	0.361651	2.010934
H	3.561600	1.262918	0.911329
H	4.196843	0.398441	-2.115984
28			
Dimer 98 of the z...z type			
C	-0.917107	-0.854015	0.635660
C	-2.163218	-0.033650	0.197020
O	-0.264463	-1.387111	-0.311057
O	-0.702473	-0.910457	1.851938
H	-2.225068	0.875921	0.791519
C	-3.428261	-0.872929	0.361376
N	-1.982056	0.384614	-1.235509
H	-1.262081	1.115416	-1.290414
H	-3.504893	-1.172179	1.405187
H	-3.373697	-1.775874	-0.250292
S	-4.974725	-0.015566	-0.160340
H	-1.634298	-0.418012	-1.771782
H	-2.856435	0.732969	-1.641436
H	-4.936184	0.952177	0.778251
C	3.952817	-0.547568	0.058252
C	2.807012	0.395856	-0.456111
O	4.095600	-1.615536	-0.588466
O	4.608932	-0.115115	1.024185
H	3.290343	1.206020	-1.005202
C	1.972753	0.960892	0.683271
N	1.979122	-0.378904	-1.438866
H	2.595210	-1.138025	-1.769541

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H	2.640430	1.480596	1.365342
H	1.464982	0.167524	1.234304
S	0.625477	2.115260	0.161900
H	1.141401	-0.818743	-0.981696
H	1.653354	0.188069	-2.219123
H	1.370695	2.903308	-0.639073
28			
Dimer 99 of the z...z type			
C	-0.917256	0.850804	-0.639009
C	-2.163721	0.032030	-0.198470
O	-0.265598	1.387241	0.306540
O	-0.701500	0.903274	-1.855247
H	-2.227198	-0.877963	-0.792132
C	-3.427906	0.872743	-0.362259
N	-1.981397	-0.385047	1.234262
H	-1.263666	-1.118158	1.288787
H	-3.505601	1.170628	-1.406387
H	-3.371328	1.776454	0.248088
S	-4.974768	0.018098	0.162747
H	-1.630077	0.417378	1.768624
H	-2.856146	-0.730005	1.642282
H	-4.938325	-0.951412	-0.774100
C	3.952134	0.549269	-0.057214
C	2.806476	-0.394016	0.457794
O	4.093174	1.618806	0.587333
O	4.609847	0.115318	-1.021379
H	3.289791	-1.202611	1.009181
C	1.974184	-0.961963	-0.681560
N	1.976803	0.382142	1.437996
H	1.650566	-0.183468	2.219037
H	2.643249	-1.482307	-1.361782
H	1.466378	-0.170139	-1.234766
S	0.627296	-2.116802	-0.160085
H	2.592009	1.142343	1.767867
H	1.139279	0.820546	0.979001
H	1.371924	-2.901988	0.644239
28			
Dimer 100 of the z...z type			
C	1.664923	-0.454802	-0.221998
C	3.109413	-0.910451	0.127429
O	1.289963	-0.628766	-1.399358
O	1.010274	0.030213	0.737320
H	3.035246	-1.900437	0.581955
C	3.845249	0.027244	1.077059
N	3.850435	-1.078956	-1.170912
H	4.587583	-1.782957	-1.127906
H	4.849919	-0.341453	1.287847
H	3.286089	0.074219	2.008358
S	4.060123	1.730286	0.403607
H	3.148133	-1.330491	-1.882631
H	4.263679	-0.183813	-1.457512
H	2.744541	2.029070	0.380470
C	-2.580291	-1.705614	0.431346
C	-2.555870	-0.143686	0.378282
O	-1.940039	-2.294557	-0.472221
O	-3.277103	-2.186040	1.349746
H	-2.427355	0.250515	1.385569
C	-3.874005	0.351082	-0.216738
N	-1.391920	0.305949	-0.438901
H	-0.482182	0.267130	0.107156
H	-4.693817	-0.028679	0.389848
H	-3.995592	-0.023931	-1.235421
S	-4.006439	2.187139	-0.359493
H	-1.253547	-0.349967	-1.215753
H	-1.522526	1.254821	-0.796820
H	-3.930002	2.448785	0.961535
28			
Dimer 101 of the z...z type			
C	-1.644954	1.257107	-0.992055

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C	-2.718737	0.134170	-1.006052
O	-0.464037	0.881929	-1.262487
O	-2.049470	2.382583	-0.677918
H	-3.428340	0.326446	-1.812610
C	-3.473614	0.051560	0.317160
N	-2.047458	-1.176863	-1.319323
H	-2.714345	-1.943514	-1.426228
H	-4.140313	-0.811507	0.336971
H	-4.074241	0.951870	0.422089
S	-2.384006	-0.101692	1.803023
H	-1.502399	-1.089471	-2.179525
H	-1.366686	-1.430142	-0.583820
H	-2.007928	1.193592	1.818554
C	3.446958	0.849363	0.097357
C	2.327653	-0.157205	0.543706
O	3.231768	2.052032	0.383543
O	4.437102	0.333397	-0.456881
H	2.687798	-0.643837	1.452513
C	2.020019	-1.196951	-0.522862
N	1.104540	0.625167	0.912055
H	1.417546	1.509632	1.326024
H	2.947851	-1.696964	-0.786721
H	1.606161	-0.722192	-1.414327
S	0.757366	-2.455343	-0.031010
H	0.540283	0.851646	0.052621
H	0.487990	0.121483	1.550504
H	1.186432	-2.670393	1.229044
28			
Dimer 102 of the z...z type			
C	3.585586	-0.407529	0.724469
C	2.691737	0.410244	-0.269492
O	3.520358	-1.657521	0.623934
O	4.244016	0.286561	1.525541
H	3.303934	1.174461	-0.744572
C	1.539150	1.054981	0.497301
N	2.183146	-0.521946	-1.331311
H	2.795052	-0.531865	-2.144948
H	1.944918	1.533600	1.385835
H	0.829169	0.290975	0.814696
S	0.576045	2.310203	-0.457225
H	2.210708	-1.459835	-0.902669
H	1.189609	-0.356222	-1.639498
H	1.461227	3.317039	-0.309461
C	-0.866806	-1.109789	-0.786114
C	-2.358100	-0.924450	-0.405383
O	-0.163619	-1.788664	-0.007888
O	-0.503784	-0.477183	-1.808619
H	-2.998004	-1.084550	-1.271080
C	-2.546901	0.488315	0.151938
N	-2.713951	-1.955101	0.630852
H	-2.917509	-2.859737	0.203982
H	-2.272517	1.196250	-0.626553
H	-1.887393	0.655196	1.006152
S	-4.244268	0.847531	0.769183
H	-1.894249	-2.088134	1.237691
H	-3.530583	-1.665854	1.180639
H	-4.870930	0.718101	-0.418374
28			
Dimer 103 of the z...z type			
C	3.587470	0.547315	0.402175
C	2.412040	-0.441094	0.679065
O	3.418383	1.725413	0.795363
O	4.562821	0.042532	-0.193143
H	2.746249	-1.180804	1.409684
C	1.954478	-1.181038	-0.575139
N	1.263044	0.294796	1.302840
H	1.011856	1.084677	0.704474
H	1.152512	-1.881599	-0.339744
H	2.805089	-1.728175	-0.974408

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S	1.270872	-0.078748	-1.890103
H	0.426175	-0.345758	1.420692
H	1.544144	0.696456	2.196318
H	2.389397	0.651631	-2.078632
C	-1.709509	-1.608867	0.646051
C	-2.035339	-0.305550	-0.136914
O	-2.480295	-2.568507	0.481693
O	-0.702598	-1.526930	1.400128
H	-1.129626	0.107932	-0.576774
C	-2.685112	0.714783	0.797450
N	-2.962720	-0.644141	-1.270613
H	-2.456382	-1.055857	-2.056134
H	-2.010839	0.897318	1.632040
H	-3.622779	0.325563	1.198868
S	-3.117442	2.306578	-0.023504
H	-3.631981	-1.350989	-0.940595
H	-3.456809	0.189357	-1.608260
H	-1.854831	2.657013	-0.343861
28			
Dimer 104 of the z...z type			
C	-1.161800	1.358526	0.133741
C	-2.648776	0.938704	0.266229
O	-0.769712	1.698338	-1.001579
O	-0.493515	1.255135	1.193727
H	-3.092397	1.393529	1.149936
C	-2.740130	-0.585737	0.339177
N	-3.396124	1.447574	-0.936539
H	-3.625127	2.438312	-0.845812
H	-2.160186	-0.919589	1.197011
H	-2.310638	-1.035309	-0.557382
S	-4.460189	-1.236037	0.437588
H	-2.780762	1.356097	-1.755153
H	-4.268416	0.926192	-1.078758
H	-4.774588	-0.662698	1.617476
C	4.230789	0.114679	0.288224
C	2.695447	-0.205915	0.310781
O	4.529459	1.332162	0.194417
O	4.984132	-0.873336	0.393156
H	2.448236	-0.504964	1.331220
C	2.330650	-1.324995	-0.655253
N	1.935109	1.052254	0.028619
H	1.080096	1.179529	0.634221
H	2.938513	-2.194621	-0.418309
H	2.549064	-1.030324	-1.684799
S	0.543183	-1.783693	-0.652951
H	2.614557	1.817952	0.150374
H	1.573919	1.096452	-0.926233
H	0.466925	-2.113637	0.652286
28			
Dimer 105 of the z...z type			
C	2.321528	-1.333753	-0.765052
C	2.061994	-0.280268	0.354447
O	3.509576	-1.610964	-1.000561
O	1.284346	-1.761806	-1.333821
H	1.293459	-0.647470	1.032080
C	1.650083	1.049456	-0.275240
N	3.324660	-0.119709	1.156003
H	3.408425	-0.848142	1.866759
O	0.790591	0.881748	-0.922224
H	2.454149	1.443041	-0.900498
S	1.279344	2.387563	0.936636
H	4.118778	-0.239350	0.511693
H	3.369263	0.789853	1.626602
H	0.362967	1.709006	1.657662
C	-2.294343	-1.439133	1.075055
C	-1.672278	-0.398461	0.084522
O	-2.638322	-2.533354	0.564363
O	-2.399271	-1.041165	2.250841
H	-0.760375	-0.009447	0.527655

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C	-2.656233	0.744013	-0.153864
N	-1.316438	-1.104283	-1.185680
H	-0.296496	-1.388144	-1.201185
H	-2.896356	1.197320	0.805565
H	-3.579565	0.364508	-0.596248
S	-2.053301	2.038173	-1.324827
H	-1.897662	-1.956745	-1.199313
H	-1.492467	-0.532903	-2.014261
H	-1.064100	2.520080	-0.541274
28			
Dimer 106 of the z...z type			
C	-1.027894	1.185569	1.115653
C	-2.373978	0.650102	0.568222
O	-0.525453	2.152656	0.508343
O	-0.531826	0.517341	2.057983
H	-2.993110	0.253086	1.369385
C	-2.068246	-0.421661	-0.479982
N	-3.114150	1.794648	-0.070275
H	-3.562034	2.390758	0.627613
H	-1.458243	-1.204806	-0.032118
H	-1.493361	0.012801	-1.301307
S	-3.564456	-1.151834	-1.267379
H	-2.427668	2.371886	-0.573793
H	-3.835434	1.456855	-0.717049
H	-4.062161	-1.721440	-0.149954
C	1.328456	-1.804468	0.512873
C	1.712124	-0.356654	0.074906
O	1.817844	-2.189442	1.601628
O	0.604629	-2.424349	-0.294834
H	0.860801	0.124171	-0.401529
C	2.891632	-0.405394	-0.890878
N	2.035520	0.443408	1.296893
H	1.126126	0.616120	1.804878
H	2.622132	-1.035061	-1.737254
H	3.769364	-0.837576	-0.405846
S	3.433499	1.251234	-1.500970
H	2.643115	-0.114131	1.903334
H	2.479437	1.333759	1.062620
H	2.282634	1.562178	-2.131460
28			
Dimer 107 of the z...z type			
C	2.215608	-1.357918	-0.355337
C	2.713096	-0.526580	0.863489
O	3.094768	-1.824207	-1.105218
O	0.970298	-1.491953	-0.443009
H	2.616121	-1.156906	1.750081
C	1.965253	0.782913	1.092194
N	4.185350	-0.276117	0.664676
H	4.697183	-0.147652	1.537835
H	2.362468	1.298406	1.967907
H	0.910499	0.580598	1.259905
S	2.108037	1.971489	-0.310391
H	4.559660	-1.072953	0.131039
H	4.316419	0.555943	0.077704
H	1.165849	1.401726	-1.090355
C	-1.410979	0.856805	-0.489754
C	-1.914703	-0.612291	-0.590935
O	-1.238431	1.288763	0.677375
O	-1.271724	1.451870	-1.577728
H	-1.448768	-1.088400	-1.452059
C	-3.434086	-0.672993	-0.741604
N	-1.438583	-1.350002	0.623109
H	-0.407302	-1.493718	0.486979
H	-3.763468	-1.701126	-0.904585
H	-3.709841	-0.084565	-1.616303
S	-4.389510	-0.097448	0.729651
H	-1.588579	-0.752317	1.441680
H	-1.906353	-2.245695	0.759526
H	-3.773570	1.096122	0.858553

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28		
Dimer 108 of the z...z type		
C	-0.864260 -0.523016 -0.853705	
C	-2.032071 -0.114763 0.080512	
O	-0.687306 0.173188 -1.875067	
O	-0.189730 -1.510606 -0.464869	
H	-1.707134 -0.182234 1.117852	
C	-3.244850 -1.010202 -0.162714	
N	-2.365946 1.326024 -0.184808	
H	-1.586279 1.927120 0.119362	
H	-2.948481 -2.042191 0.016760	
H	-3.580901 -0.925367 -1.198202	
S	-4.713404 -0.589455 0.868011	
H	-2.467053 1.470187 -1.194697	
H	-3.226516 1.605337 0.296528	
H	-4.156828 -0.895991 2.057563	
C	3.650552 -0.857005 0.609258	
C	2.794062 0.229206 -0.131552	
O	3.846135 -1.919514 -0.026736	
O	4.068747 -0.521365 1.736157	
H	3.481840 0.996982 -0.490209	
C	1.741458 0.848595 0.778100	
N	2.162945 -0.399239 -1.340668	
H	2.865004 -0.957661 -1.829271	
H	2.237129 1.178353 1.686420	
H	0.991282 0.106683 1.049274	
S	0.865975 2.309612 0.029560	
H	1.380469 -1.039994 -1.057891	
H	1.745959 0.285865 -1.974296	
H	1.379260 3.252389 0.842722	
28		
Dimer 109 of the z...z type		
C	1.006495 -0.282250 -1.237942	
C	2.001051 -0.020499 -0.071354	
O	1.216006 -1.290450 -1.934411	
O	0.094709 0.580814 -1.344412	
H	1.466360 0.340230 0.804926	
C	3.056270 0.993551 -0.509335	
N	2.637576 -1.329890 0.301945	
H	1.995240 -1.884818 0.874844	
H	2.547748 1.916986 -0.780607	
H	3.596662 0.628773 -1.384846	
S	4.348720 1.333587 0.759607	
H	2.812952 -1.859381 -0.561509	
H	3.509358 -1.189772 0.823625	
H	3.521563 1.870388 1.679845	
C	-3.598168 1.122904 0.253171	
C	-2.844402 -0.248033 0.149818	
O	-3.922757 1.644253 -0.842513	
O	-3.819358 1.522854 1.413082	
H	-3.569911 -1.030595 0.377824	
C	-1.660176 -0.332088 1.102936	
N	-2.414536 -0.441933 -1.277814	
H	-2.387797 -1.423779 -1.547905	
H	-2.012804 -0.170124 2.117370	
H	-0.931917 0.440314 0.860753	
S	-0.750064 -1.942845 1.018458	
H	-3.089443 0.077941 -1.853636	
H	-1.458746 -0.028042 -1.446813	
H	-1.454255 -2.598512 1.960459	
28		
Dimer 110 of the z...z type		
C	-3.454662 -0.407566 -0.853472	
C	-2.638404 0.441037 0.176589	
O	-3.651881 -1.606368 -0.545585	
O	-3.834585 0.222595 -1.863281	
H	-3.319016 1.168215 0.622878	
C	-1.465105 1.157895 -0.484770	
N	-2.147300 -0.452584 1.274394	

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H	-2.919237 -0.994253 1.661181	
H	-1.840833 1.713661 -1.339779	
H	-0.735247 0.429918 -0.841579	
S	-0.537845 2.300865 0.632993	
H	-1.432054 -1.121962 0.889105	
H	-1.671064 0.068596 2.014672	
H	-1.485154 3.259100 0.683714	
C	0.902426 -1.128085 0.990595	
C	2.316702 -0.974702 0.373650	
O	0.041334 -1.678633 0.240205	
O	0.733448 -0.631005 2.112466	
H	3.079948 -1.221825 1.108235	
C	2.481979 0.466752 -0.112853	
N	2.452714 -1.936962 -0.775057	
H	2.670955 -2.880069 -0.450208	
H	2.359528 1.127845 0.742332	
H	1.711927 0.715730 -0.845353	
S	4.079685 0.807210 -0.961290	
H	1.545511 -1.986642 -1.256741	
H	3.190226 -1.641092 -1.424681	
H	4.873030 0.575695 0.104740	
28		
Dimer 111 of the z...z type		
C	-3.498927 -0.640056 -0.067935	
C	-2.088878 0.023448 0.107808	
O	-3.761258 -1.054187 -1.225391	
O	-4.202847 -0.659561 0.958975	
H	-1.570586 -0.474844 0.926519	
C	-2.252131 1.510416 0.403494	
N	-1.305091 -0.218334 -1.146162	
H	-0.587670 -0.982211 -0.980232	
H	-2.899922 1.622443 1.269964	
H	-2.719850 2.019479 -0.442065	
S	-0.670967 2.416395 0.700948	
H	-2.005702 -0.547538 -1.833332	
H	-0.837155 0.618258 -1.493760	
H	-0.355898 1.808791 1.863042	
C	1.446140 -2.046499 0.186183	
C	1.907346 -0.571971 0.362345	
O	2.176911 -2.926487 0.668893	
O	0.380839 -2.180281 -0.474857	
H	1.077980 0.042929 0.705816	
C	2.451817 -0.034610 -0.961541	
N	2.971011 -0.515700 1.423014	
H	2.567492 -0.561179 2.359748	
H	1.686364 -0.153552 -1.725434	
H	3.326354 -0.607465 -1.275898	
S	2.998168 1.723122 -0.888242	
H	3.577854 -1.338315 1.320112	
H	3.519989 0.348283 1.351358	
H	1.782732 2.230652 -0.590199	
28		
Dimer 112 of the z...z type		
C	-3.817958 0.746251 -0.364781	
C	-2.459251 0.005847 -0.113999	
O	-3.718718 1.928514 -0.780455	
O	-4.842534 0.069925 -0.150859	
H	-2.327694 -0.713254 -0.924654	
C	-2.430527 -0.717094 1.224220	
N	-1.338804 0.993367 -0.247941	
H	-0.542969 0.565176 -0.798507	
H	-3.264727 -1.413327 1.254366	
H	-2.548979 -0.009990 2.048846	
S	-0.851972 -1.610465 1.574490	
H	-1.751414 1.805801 -0.732626	
H	-0.997122 1.312264 0.658134	
H	-0.826626 -2.334671 0.436780	
C	1.470426 -0.940126 -1.385778	
C	2.136793 -0.302757 -0.134220	

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O	2.081289	-1.870605	-1.938295
O	0.381539	-0.404497	-1.724018
H	1.407928	-0.238056	0.671877
C	2.688539	1.079825	-0.479001
N	3.238194	-1.210401	0.339309
H	2.864000	-2.004702	0.860347
H	1.870183	1.690915	-0.854750
H	3.446282	1.009808	-1.262029
S	3.514196	1.930454	0.931445
H	3.721041	-1.595646	-0.481261
H	3.898347	-0.709843	0.944372
H	2.419692	2.016562	1.714934
28			
Dimer 113 of the z...z type			
C	1.058858	-0.936735	-0.097882
C	2.306231	-0.020261	-0.057100
O	0.597802	-1.274429	1.029734
O	0.636488	-1.243817	-1.226092
H	2.215410	0.748382	-0.822308
C	3.577813	-0.840044	-0.258935
N	2.326582	0.678905	1.273670
H	1.548725	1.342196	1.327911
H	3.505974	-1.347493	-1.219454
H	3.675710	-1.597471	0.521408
S	5.132305	0.148208	-0.185767
H	2.173641	-0.010300	2.017542
H	3.209936	1.175914	1.425701
H	4.892525	0.889765	-1.286459
C	-4.272903	-0.300133	0.072717
C	-2.750290	0.043789	0.276802
O	-4.542996	-1.526250	0.024646
O	-5.042593	0.678268	0.024718
H	-2.640554	0.338453	1.321775
C	-2.277696	1.164631	-0.638106
N	-1.960017	-1.214866	0.090576
H	-1.113187	-1.299092	0.697541
H	-3.039700	1.939774	-0.645785
H	-2.156304	0.805344	-1.662088
S	-0.666454	1.957149	-0.195298
H	-2.627621	-1.985361	0.242025
H	-1.585882	-1.305841	-0.858378
H	-1.119925	2.634073	0.878867
28			
Dimer 114 of the z...z type			
C	1.452346	-0.286140	-0.297351
C	2.757038	-0.067176	-1.118059
O	0.627899	0.671423	-0.336010
O	1.342039	-1.375720	0.289481
H	2.606491	-0.539003	-2.091351
C	4.003758	-0.647805	-0.462497
N	2.895905	1.410971	-1.367532
H	3.409205	1.632802	-2.221110
H	4.885582	-0.484734	-1.082966
H	3.853952	-1.717773	-0.339769
S	4.388312	0.108159	1.175376
H	1.940119	1.794825	-1.405351
H	3.369517	1.855346	-0.572387
H	3.280839	-0.351020	1.794084
C	-3.048264	-1.248412	-0.500083
C	-2.775934	-0.638366	0.914167
O	-2.106400	-1.907187	-0.998612
O	-4.190579	-1.032818	-0.959848
H	-3.184215	-1.343927	1.643555
C	-3.432502	0.716512	1.148594
N	-1.300719	-0.581245	1.150950
H	-1.067742	-0.393301	2.125982
H	-3.186413	1.105661	2.138309
H	-4.510284	0.585860	1.086820
S	-2.924690	2.026169	-0.046505

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H	-0.851607	-1.460197	0.870702
H	-0.799196	0.124048	0.557439
H	-3.457868	1.419753	-1.127160
28			
Dimer 115 of the z...z type			
C	1.147810	-1.889687	-0.218692
C	2.008204	-0.701464	0.299817
O	1.764609	-2.930304	-0.504932
O	-0.079316	-1.638580	-0.346955
H	1.487608	-0.153882	1.082545
C	2.340580	0.219825	-0.876532
N	3.275064	-1.257196	0.889900
H	3.126375	-1.609522	1.836457
H	1.411622	0.601468	-1.295705
H	2.856000	-0.340154	-1.659420
S	3.462376	1.618163	-0.457611
H	3.568519	-2.054243	0.309070
H	4.012580	-0.543734	0.921912
H	2.604437	2.259622	0.361597
C	-3.705676	-0.268760	-0.336853
C	-2.599135	0.481039	0.481457
O	-3.959176	-1.438142	0.042866
O	-4.233408	0.396948	-1.249907
H	-3.113839	1.164503	1.159488
C	-1.631996	1.250002	-0.408170
N	-1.866091	-0.520083	1.324750
H	-1.445549	-0.100355	2.152560
H	-2.196760	1.950077	-1.017524
H	-1.099358	0.562364	-1.066832
S	-0.312752	2.148662	0.520890
H	-2.540433	-1.247728	1.585720
H	-1.107791	-0.978759	0.752394
H	-1.120604	2.996993	1.187968
28			
Dimer 116 of the z...z type			
C	-1.073810	-1.103815	-0.163387
C	-2.626917	-1.219899	-0.203607
O	-0.520138	-1.427717	0.905578
O	-0.556235	-0.695739	-1.231926
H	-2.872725	-2.157527	-0.706191
C	-3.310427	-0.063826	-0.925130
N	-3.103058	-1.345917	1.218363
H	-3.970304	-1.874776	1.312372
H	-4.392426	-0.199561	-0.947211
H	-2.938209	-0.038280	-1.946374
S	-3.021170	1.571819	-0.122771
H	-2.339395	-1.794586	1.746062
H	-3.239288	-0.411678	1.622598
H	-1.680285	1.583555	-0.296819
C	3.032403	-0.874897	0.204970
C	2.874380	0.447443	-0.619650
O	2.919698	-1.925275	-0.472761
O	3.300692	-0.742838	1.416083
H	3.851236	0.632515	-1.076681
C	2.507368	1.687711	0.181631
N	1.922501	0.180635	-1.748056
H	1.832906	0.977997	-2.377458
H	2.567435	2.582836	-0.440602
H	3.236032	1.773507	0.985210
S	0.810436	1.708813	0.899225
H	2.273850	-0.623723	-2.271604
H	0.954646	-0.110117	-1.413125
H	0.782058	0.422958	1.309650
28			
Dimer 117 of the z...z type			
C	-2.691190	1.367294	-0.174132
C	-2.161575	-0.083924	-0.372664
O	-2.612073	1.835675	0.985540
O	-3.159310	1.892216	-1.208410

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H -1.341500	-0.068536	-1.092217	
C -3.246726	-1.023872	-0.890006	
N -1.571341	-0.578810	0.909706	
H -1.237970	-1.539434	0.818060	
H -2.855098	-2.031760	-1.039898	
H -3.600624	-0.642603	-1.845568	
S -4.683101	-1.223746	0.253809	
H -0.719601	-0.000713	1.122821	
H -2.251613	-0.501785	1.666788	
H -5.120462	0.049330	0.166160	
C 1.368978	-0.169854	0.031161	
C 2.819839	0.164189	-0.403212	
O 0.855423	0.623072	0.873391	
O 0.874401	-1.198301	-0.457912	
H 2.912983	0.075730	-1.483629	
C 3.791260	-0.785826	0.299093	
N 3.122576	1.592272	-0.035149	
H 2.722919	2.244962	-0.710739	
H 3.527822	-1.804069	0.020009	
H 3.700071	-0.692881	1.383163	
S 5.566778	-0.464948	-0.072634	
H 2.680443	1.791375	0.871036	
H 4.134555	1.756621	0.012405	
H 5.499566	-0.740712	-1.391404	
28			
Dimer 118 of the z...z type			
C -1.040408	2.089556	-0.023217	
C -1.571373	0.624733	0.047316	
O -1.231601	2.792339	1.000047	
O -0.481529	2.386671	-1.097707	
H -0.766028	-0.039258	-0.243750	
C -2.741317	0.398816	-0.900443	
N -1.922141	0.304092	1.470347	
H -1.145718	-0.266189	1.883934	
H -2.417158	0.667037	-1.903930	
H -3.597505	1.020257	-0.630769	
S -3.352233	-1.349021	-0.875224	
H -1.989516	1.212629	1.954300	
H -2.793325	-0.222765	1.553038	
H -2.130494	-1.928728	-0.864233	
C 0.727532	-1.555109	0.863173	
C 2.132805	-1.086912	0.396027	
O 0.079993	-2.277358	0.077961	
O 0.365904	-1.065534	1.963217	
H 2.866525	-1.259820	1.181102	
C 2.073041	0.401545	0.038774	
N 2.539928	-1.902835	-0.800777	
H 2.910664	-2.812956	-0.523909	
H 1.741353	0.943888	0.921834	
H 1.353458	0.596566	-0.759062	
S 3.663246	1.097287	-0.572773	
H 1.700613	-2.082615	-1.365924	
H 3.254066	-1.420374	-1.357090	
H 4.368528	0.886560	0.557498	
28			
Dimer 119 of the z...z type			
C -0.992744	0.076242	-0.153854	
C -2.410300	0.000469	0.470586	
O -0.585890	1.200172	-0.506594	
O -0.409978	-1.032552	-0.272753	
H -2.398230	-0.632278	1.355394	
C -3.392540	-0.544705	-0.567290	
N -2.806701	1.387122	0.898502	
H -2.424821	1.619661	1.816454	
H -3.054506	-1.535899	-0.863036	
H -3.405389	0.092436	-1.454211	
S -5.139862	-0.615260	0.011125	
H -2.398518	2.049454	0.224552	
H -3.826624	1.489692	0.939894	

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H -4.931931	-1.495433	1.011943	
C 3.201404	-1.621480	0.391692	
C 2.941478	-0.252844	-0.321169	
O 2.820103	-2.640399	-0.231708	
O 3.800497	-1.546590	1.485943	
H 3.886369	0.050907	-0.777329	
C 2.450180	0.836798	0.623943	
N 1.954235	-0.455357	-1.429556	
H 2.269489	-1.207289	-2.041713	
H 3.113090	0.873473	1.484145	
H 1.440600	0.618509	0.969152	
S 2.352445	2.511491	-0.152078	
H 1.012948	-0.739861	-1.021004	
H 1.818285	0.403134	-1.966251	
H 3.682432	2.739517	-0.167931	
28			
Dimer 120 of the z...z type			
C -3.197976	0.698192	0.532835	
C -3.062368	-0.368619	-0.606528	
O -3.165175	1.887469	0.140031	
O -3.358537	0.248985	1.686677	
H -4.068233	-0.506803	-1.014068	
C -2.566016	-1.739846	-0.174756	
N -2.242771	0.229860	-1.712307	
H -2.206059	-0.366217	-2.539270	
H -2.501146	-2.420226	-1.025777	
H -3.291307	-2.138982	0.530881	
S -0.908288	-1.800282	0.626178	
H -2.665469	1.127254	-1.962106	
H -1.259389	0.471421	-1.413704	
H -1.140684	-0.826349	1.529825	
C 0.829905	1.133022	-0.034603	
C 1.992810	0.109927	0.106774	
O 0.234040	1.118195	-1.153132	
O 0.632224	1.859808	0.945247	
H 1.874987	-0.432992	1.043760	
C 3.343848	0.818332	0.070080	
N 1.885002	-0.900318	-0.999331	
H 1.034444	-1.459141	-0.850256	
H 3.358286	1.560965	0.865351	
H 3.484677	1.333686	-0.882253	
S 4.790577	-0.313085	0.237661	
H 1.768580	-0.417803	-1.894855	
H 2.704471	-1.514234	-1.032489	
H 4.512977	-0.725209	1.491593	
28			
Dimer 121 of the z...z type			
C 1.062276	-0.183198	-0.115768	
C 2.496007	0.066602	0.419780	
O 0.530475	-1.273900	0.169889	
O 0.597276	0.746787	-0.824633	
H 2.572707	1.067670	0.839195	
C 3.500837	-0.116913	-0.719345	
N 2.761594	-0.918788	1.525304	
H 2.377872	-0.597290	2.415058	
H 3.268837	0.612416	-1.492891	
H 3.411923	-1.115464	-1.152369	
S 5.263414	0.038631	-0.207011	
H 2.276839	-1.794812	1.287617	
H 3.767555	-1.080123	1.648532	
H 5.193235	1.325588	0.190612	
C -3.435862	-1.416451	0.061783	
C -2.494607	-0.169287	-0.001177	
O -3.367684	-2.195771	-0.922263	
O -4.122753	-1.519648	1.098146	
H -1.643694	-0.389534	0.644944	
C -3.179558	1.111398	0.450897	
N -1.925831	-0.052275	-1.382917	
H -0.924124	0.282071	-1.331444	

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H	-3.481016	0.982220	1.487190
H	-4.076274	1.303114	-0.142416
S	-2.137217	2.633227	0.274890
H	-1.989316	-0.994861	-1.790777
H	-2.470762	0.580031	-1.968531
H	-0.946349	2.054036	0.536377
28			
Dimer 122 of the z...z type			
C	-0.993872	0.310360	-1.318638
C	-2.457646	0.315700	-0.809753
O	-0.494937	-0.833812	-1.536988
O	-0.433578	1.413003	-1.390986
H	-3.038862	1.061299	-1.349565
C	-2.464584	0.613386	0.691535
N	-3.081347	-1.028043	-1.079448
H	-3.345840	-1.126264	-2.060592
H	-1.992235	1.581419	0.845314
H	-1.889033	-0.138729	1.235229
S	-4.139298	0.593910	1.457990
H	-2.387346	-1.758937	-0.883586
H	-3.918548	-1.168019	-0.502135
H	-4.636012	1.639127	0.765089
C	3.019632	1.398747	0.412809
C	2.114560	0.147970	0.159051
O	3.390074	2.016034	-0.616733
O	3.241023	1.664050	1.611607
H	1.092859	0.460010	0.372343
C	2.491693	-1.039903	1.031188
N	2.136221	-0.190192	-1.300768
H	1.190694	-0.539653	-1.597105
H	2.367203	-0.744685	2.069861
H	3.537903	-1.314336	0.879400
S	1.525740	-2.581075	0.683391
H	2.371273	0.684046	-1.788435
H	2.852261	-0.881715	-1.521565
H	0.349146	-1.983034	0.402799
28			
Dimer 123 of the z...z type			
C	-0.978533	0.736557	-1.184279
C	-2.445883	0.632968	-0.694256
O	-0.510693	-0.318350	-1.710562
O	-0.386291	1.796321	-0.943337
H	-2.995728	1.537922	-0.943915
C	-2.438586	0.407613	0.820080
N	-3.114266	-0.519308	-1.395226
H	-3.433224	-0.254952	-2.328292
H	-1.938243	1.255245	1.284173
H	-1.880885	-0.496579	1.072994
S	-4.107407	0.169682	1.560037
H	-2.418325	-1.267192	-1.513888
H	-3.923350	-0.859306	-0.862692
H	-4.581479	1.397639	1.265724
C	3.174479	1.134206	0.651489
C	2.142099	0.060397	0.172575
O	3.642817	1.873516	-0.250563
O	3.390104	1.159000	1.879642
H	1.156011	0.438970	0.441963
C	2.372305	-1.301968	0.809452
N	2.158450	-0.000080	-1.325572
H	1.180921	-0.139169	-1.686992
H	2.258287	-1.191833	1.884847
H	3.386002	-1.656246	0.609840
S	1.255332	-2.639054	0.181701
H	2.551941	0.899863	-1.634297
H	2.761763	-0.745893	-1.671229
H	0.157430	-1.875348	0.007717
28			
Dimer 124 of the z...z type			
C	-1.802326	-1.533412	-0.267946

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C	-2.126218	-0.162707	-0.944075
O	-2.525348	-2.488228	-0.607069
O	-0.835458	-1.539862	0.534716
H	-1.465668	-0.067494	-1.808921
C	-1.958461	1.059065	-0.050697
N	-3.530457	-0.259538	-1.477217
H	-3.695708	0.325287	-2.296702
H	-2.258666	1.966037	-0.578010
H	-0.909945	1.171150	0.205661
S	-2.973366	1.006279	1.484962
H	-3.688458	-1.254994	-1.698447
H	-4.203648	-0.001988	-0.747098
H	-2.355301	-0.070768	2.012548
C	3.267079	-1.188430	0.039843
C	2.128436	-0.119860	-0.086887
O	3.421587	-1.683586	1.184899
O	3.901683	-1.407246	-1.009466
H	1.461495	-0.417591	-0.895125
C	2.731481	1.251261	-0.377013
N	1.335893	-0.130695	1.185334
H	0.422258	-0.628087	1.025173
H	3.323574	1.180828	-1.286638
H	3.389622	1.560615	0.438003
S	1.491940	2.609273	-0.536710
H	1.911936	-0.671919	1.852635
H	1.148370	0.803281	1.551179
H	0.845250	2.104308	-1.607107
28			
Dimer 125 of the z...z type			
C	2.596916	-1.727874	-0.374186
C	2.771213	-0.176025	-0.434442
O	1.877261	-2.163139	0.556003
O	3.236181	-2.358714	-1.242522
H	2.708631	0.155944	-1.470179
C	4.131453	0.193780	0.155206
N	1.661616	0.477507	0.316897
H	0.744799	0.445856	-0.218017
H	4.905713	-0.332316	-0.399792
H	4.188699	-0.113303	1.201881
S	4.495940	2.004093	0.161758
H	1.467865	-0.049537	1.174655
H	1.880588	1.448944	0.548648
H	4.486154	2.165887	-1.177311
C	-1.441379	-0.012326	0.271705
C	-2.932505	-0.365232	0.029016
O	-1.053559	0.044015	1.455601
O	-0.783040	0.218546	-0.776555
H	-3.012679	-1.149453	-0.722162
C	-3.692880	0.885168	-0.415018
N	-3.509865	-0.903566	1.310183
H	-3.234492	-1.874497	1.464236
H	-3.240211	1.245970	-1.336226
H	-3.608998	1.670883	0.338624
S	-5.501920	0.628248	-0.652383
H	-3.129553	-0.359693	2.094079
H	-4.534890	-0.854549	1.302537
H	-5.399840	-0.245784	-1.674450
28			
Dimer 126 of the z...z type			
C	-1.636072	-2.033373	0.111249
C	-2.062133	-0.645178	-0.457610
O	-2.503528	-2.925618	0.092403
O	-0.466422	-2.094395	0.567139
H	-1.316988	-0.276060	-1.159838
C	-2.246424	0.347347	0.695212
N	-3.349140	-0.837152	-1.211394
H	-3.180055	-1.106904	-2.180722
H	-1.272199	0.542701	1.137998
H	-2.899124	-0.072344	1.462917

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S	-3.034073	1.942811	0.222428
H	-3.848001	-1.619066	-0.761185
H	-3.916189	0.019134	-1.207615
H	-2.071179	2.356237	-0.624562
C	3.537442	-0.750009	-0.339455
C	2.178770	0.003430	-0.129951
O	3.917810	-1.461418	0.624910
O	4.090625	-0.543252	-1.436045
H	1.504120	-0.272262	-0.940053
C	2.409728	1.510247	-0.125064
N	1.573104	-0.475449	1.154627
H	0.727738	-1.078942	0.966788
H	2.917573	1.786570	-1.046150
H	3.045603	1.798630	0.715016
S	0.870640	2.513415	0.057746
H	2.317174	-1.045738	1.594430
H	1.302941	0.284108	1.778802
H	0.340003	2.175206	-1.134769
28			
Dimer 127 of the z...z type			
C	-2.510542	-1.710946	0.406458
C	-2.731486	-0.163478	0.416889
O	-1.841191	-2.162215	-0.553480
O	-3.068945	-2.324684	1.339940
H	-2.612466	0.212403	1.432432
C	-4.139658	0.138260	-0.094050
N	-1.694316	0.489601	-0.433249
H	-0.760328	0.551238	0.071012
H	-4.857220	-0.386492	0.533661
H	-4.255554	-0.215661	-1.120874
S	-4.563309	1.934388	-0.151757
H	-1.509025	-0.101451	-1.250847
H	-1.979125	1.425144	-0.731189
H	-4.460366	2.157371	1.174527
C	1.430583	0.040867	-0.312177
C	2.898482	-0.329651	0.024979
O	1.085144	-0.026404	-1.508112
O	0.746117	0.411488	0.677867
H	2.927219	-0.992997	0.887081
C	3.697813	0.944596	0.301178
N	3.479466	-1.076589	-1.145013
H	3.193295	-2.056495	-1.141092
H	3.232332	1.457715	1.140249
H	3.670843	1.609818	-0.564445
S	5.485241	0.659552	0.644308
H	3.107574	-0.660715	-2.008459
H	4.504772	-1.040588	-1.138143
H	5.310930	-0.056791	1.773733
28			
Dimer 128 of the z...z type			
C	3.714335	-1.031530	-0.424610
C	2.462504	-0.131547	-0.158361
O	4.184831	-1.624082	0.578491
O	4.116535	-1.033390	-1.604869
H	1.679484	-0.386082	-0.871613
C	2.842450	1.338956	-0.300129
N	1.930401	-0.445668	1.205793
H	1.121171	-1.095545	1.102034
H	3.274603	1.485008	-1.287876
H	3.587411	1.620026	0.447530
S	1.436467	2.508285	-0.049444
H	2.698623	-0.885295	1.730994
H	1.550897	0.372319	1.689458
H	0.637555	1.988421	-1.003646
C	-1.110678	-0.381104	0.776443
C	-2.322849	0.044103	-0.094426
O	-0.455775	-1.376334	0.347952
O	-0.916690	0.279532	1.807214
H	-2.337014	1.126928	-0.201921

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C	-3.615647	-0.453112	0.552665
N	-2.158169	-0.551964	-1.467155
H	-1.538047	0.011941	-2.049625
H	-3.686035	-0.015885	1.546749
H	-3.597818	-1.540129	0.656043
S	-5.139219	-0.079057	-0.413909
H	-1.711220	-1.471974	-1.355590
H	-3.059779	-0.638443	-1.949211
H	-5.033303	1.264081	-0.349929
28			
Dimer 129 of the z...z type			
C	2.177515	-1.235026	0.466668
C	2.587608	0.231791	0.827048
O	3.054249	-1.908847	-0.128331
O	1.037245	-1.571901	0.838044
H	2.767207	0.258435	1.902942
C	1.532946	1.273294	0.478069
N	3.904844	0.507145	0.148856
H	4.552750	1.058427	0.710268
H	1.831071	2.264502	0.823229
H	0.598331	1.001504	0.964138
S	1.250936	1.462331	-1.337152
H	4.291186	-0.430228	-0.067234
H	3.750622	0.983906	-0.746465
H	0.837022	0.197213	-1.560672
C	-2.199753	0.306890	1.406199
C	-2.930139	0.454173	0.028025
O	-1.471946	1.283448	1.724210
O	-2.451554	-0.731006	2.040815
H	-3.940659	0.805226	0.248514
C	-3.022384	-0.833884	-0.778737
N	-2.244086	1.559040	-0.727269
H	-2.866621	2.097969	-1.328199
H	-3.643389	-0.696718	-1.665295
H	-3.481291	-1.586121	-0.140910
S	-1.407709	-1.461235	-1.408415
H	-1.813264	2.154407	0.001025
H	-1.473598	1.188154	-1.296510
H	-0.745023	-1.534481	-0.228418
28			
Dimer 130 of the z...z type			
C	-1.862647	1.140563	0.848075
C	-2.883526	-0.032052	0.665706
O	-2.202097	2.231027	0.330285
O	-0.850915	0.868841	1.525218
H	-3.441596	-0.111970	1.600705
C	-2.248629	-1.379117	0.342217
N	-3.859038	0.391264	-0.398219
H	-4.813097	0.069291	-0.240689
H	-2.997946	-2.171976	0.344752
H	-1.508580	-1.599198	1.107723
S	-1.468094	-1.448169	-1.325363
H	-3.805590	1.425251	-0.413871
H	-3.534973	0.049009	-1.311960
H	-0.554566	-0.453264	-1.157958
C	1.861902	1.141876	-0.846832
C	2.883402	-0.030286	-0.665018
O	2.200692	2.232232	-0.328386
O	0.850386	0.869974	-1.524228
H	3.441566	-0.109431	-1.600027
C	2.249207	-1.377858	-0.342247
N	3.858626	0.393008	0.399180
H	4.812880	0.071682	0.241511
H	2.998946	-2.170316	-0.345161
H	1.509293	-1.597929	-1.107888
S	1.468633	-1.448152	1.325265
H	3.804575	1.426955	0.415394
H	3.534724	0.050067	1.312721
H	0.554584	-0.453654	1.158271

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28		
Dimer 131 of the z...z type		
C 1.861950	1.481505	-0.876693
C 1.850937	-0.025025	-0.482284
O 2.957096	1.940830	-1.269883
O 0.766037	2.066651	-0.719945
H 0.996541	-0.533889	-0.924427
C 1.811317	-0.163566	1.036897
N 3.096996	-0.672262	-1.028859
H 2.974089	-0.957954	-2.000785
H 0.988958	0.440507	1.412044
H 2.730634	0.217786	1.486219
S 1.638031	-1.908732	1.609988
H 3.839706	0.041309	-1.017438
H 3.367529	-1.498653	-0.486646
H 0.564968	-2.184061	0.824554
C -1.861924	-1.481539	-0.876678
C -1.850925	0.024980	-0.482256
O -2.956971	-1.940818	-1.270103
O -0.766065	-2.066722	-0.719741
H -0.996514	0.533839	-0.924382
C -1.811347	0.163572	1.036918
N -3.096928	0.672280	-1.028872
H -2.974165	0.957416	-2.000974
H -0.988982	-0.440465	1.412106
H -2.730662	-0.217786	1.486238
S -1.638119	1.908767	1.609948
H -3.839902	-0.040966	-1.016942
H -3.367038	1.499026	-0.487011
H -0.565050	2.184108	0.824542
28		
Dimer 132 of the z...z type		
C 1.643706	1.462882	0.048602
C 2.955146	0.615527	0.106324
O 1.150886	1.765301	1.166165
O 1.242752	1.762057	-1.090474
H 3.785138	1.305214	-0.059134
C 3.027191	-0.510241	-0.919518
N 3.085384	0.099946	1.514369
H 4.046190	0.049340	1.851184
H 4.013094	-0.976833	-0.911582
H 2.850998	-0.079535	-1.902567
S 1.825743	-1.877307	-0.619228
H 2.515001	0.748886	2.086440
H 2.653508	-0.829655	1.583650
H 0.684598	-1.240978	-1.011013
C -1.943276	-0.012641	-1.349688
C -1.677949	0.765857	-0.026894
O -2.903256	0.406873	-2.039758
O -1.158015	-0.954197	-1.595065
H -0.891692	1.491039	-0.239272
C -1.246743	-0.093826	1.150220
N -2.927792	1.544368	0.289270
H -2.748908	2.418427	0.783253
H -1.084306	0.519229	2.036176
H -0.304572	-0.571290	0.904919
S -2.480399	-1.383628	1.617912
H -3.384657	1.716927	-0.621173
H -3.570931	0.973642	0.848331
H -2.404420	-2.061961	0.453963
28		
Dimer 133 of the z...z type		
C 1.424365	-1.426893	-0.089091
C 2.685685	-0.808852	0.594896
O 1.604919	-1.950188	-1.203570
O 0.364574	-1.356965	0.582495
H 3.050982	-1.553734	1.304828
C 2.420292	0.494147	1.338329
N 3.743686	-0.652643	-0.462558

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H 4.693094	-0.783304	-0.113401
H 3.303628	0.821343	1.887897
H 1.624371	0.307894	2.056000
S 1.981122	1.912156	0.239182
H 3.522063	-1.348358	-1.192898
H 3.677267	0.278340	-0.891240
H 1.028142	1.278686	-0.497197
C -3.120283	-0.586553	0.538566
C -2.416354	0.813199	0.478550
O -2.962832	-1.195847	1.623559
O -3.785020	-0.914263	-0.464116
H -3.091877	1.515990	0.974487
C -2.143144	1.356581	-0.915827
N -1.181464	0.740538	1.334852
H -0.678210	1.628344	1.378545
H -1.802355	2.392790	-0.868538
H -3.086910	1.322287	-1.455723
S -0.854555	0.471996	-1.897839
H -1.464503	0.461755	2.276640
H -0.531060	-0.018504	1.003542
H -1.075774	-0.767903	-1.418038
28		
Dimer 134 of the z...z type		
C 1.935206	-0.136302	-1.334927
C 1.691059	-0.771991	0.066493
O 2.878527	-0.635254	-1.994132
O 1.154200	0.783154	-1.664104
H 0.920846	-1.533212	-0.063381
C 1.244477	0.195436	1.149938
N 2.959293	-1.485083	0.456720
H 2.801272	-2.294882	1.056219
H 1.111636	-0.324043	2.098527
H 0.284504	0.613715	0.869406
S 2.440702	1.565089	1.459658
H 3.407360	-1.761942	-0.431733
H 3.598375	-0.839340	0.932480
H 2.323316	2.112751	0.231954
C -1.637211	-1.456249	0.161313
C -2.949607	-0.607937	0.139793
O -1.153481	-1.666027	1.304208
O -1.227091	-1.847093	-0.945854
H -3.777601	-1.308492	0.015897
C -3.008129	0.438032	-0.968179
N -3.095784	0.010426	1.504364
H -4.058331	0.068212	1.834397
H -3.993080	0.905116	-1.004720
H -2.823093	-0.065768	-1.914155
S -1.806171	1.821310	-0.758752
H -2.515581	-0.585874	2.123450
H -2.680938	0.950049	1.506125
H -0.664407	1.152890	-1.092720
28		
Dimer 135 of the z...z type		
C -3.230873	0.677137	0.333952
C -3.041214	-0.595240	-0.558764
O -3.269963	1.756709	-0.304324
O -3.370497	0.478837	1.558068
H -4.035440	-0.841381	-0.943946
C -2.512377	-1.832242	0.152424
N -2.211498	-0.209105	-1.748799
H -2.103474	-0.976936	-2.411435
H -2.534565	-2.699367	-0.510638
H -3.173834	-2.024369	0.994743
S -0.775318	-1.726625	0.754143
H -2.674560	0.573761	-2.214865
H -1.250066	0.157951	-1.481986
H -0.882758	-0.510615	1.328885
C 0.792459	1.149616	-0.289974
C 2.331106	0.931082	-0.294363

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O	0.287562	1.524456	0.784969
O	0.232095	0.852621	-1.374606
H	2.773519	1.337644	-1.201254
C	2.613983	-0.566831	-0.173762
N	2.917393	1.668042	0.879176
H	3.055938	2.657609	0.671097
H	2.132864	-1.071418	-1.008545
H	2.187111	-0.962386	0.749527
S	4.402905	-1.002479	-0.109237
H	2.234432	1.614026	1.647740
H	3.819446	1.269906	1.161751
H	4.716658	-0.553447	-1.342155
28			
Dimer 136 of the z...z type			
C	2.070672	-1.205190	0.535712
C	2.620188	0.227284	0.838088
O	2.841669	-1.959197	-0.105658
O	0.932595	-1.437173	0.989382
H	2.865852	0.260515	1.900854
C	1.631441	1.342345	0.522332
N	3.911890	0.382825	0.077422
H	4.629970	0.901120	0.581885
H	2.021436	2.312765	0.833096
H	0.700144	1.146743	1.049981
S	1.273003	1.522856	-1.279736
H	4.217793	-0.584079	-0.131927
H	3.736739	0.844014	-0.822730
H	0.728793	0.298423	-1.451235
C	-2.182766	0.397856	1.343269
C	-2.926253	0.406221	-0.035401
O	-1.429153	1.386983	1.542972
O	-2.457214	-0.552437	2.094169
H	-3.948820	0.730763	0.166623
C	-2.968756	-0.946425	-0.736521
N	-2.282369	1.471011	-0.880561
H	-2.941861	2.033202	-1.416349
H	-3.630516	-0.915653	-1.603157
H	-3.354570	-1.672999	-0.024683
S	-1.343940	-1.522563	-1.390730
H	-1.754050	2.051548	-0.199378
H	-1.599071	1.055196	-1.522506
H	-0.646471	-1.539553	-0.223096
28			
Dimer 137 of the z...z type			
C	-2.053698	0.670475	1.178990
C	-2.395492	-0.800278	0.777038
O	-3.033779	1.422535	1.378280
O	-0.832758	0.921276	1.276068
H	-2.274803	-1.416095	1.670448
C	-1.528168	-1.364085	-0.340385
N	-3.856958	-0.835816	0.412990
H	-4.313012	-1.722413	0.627357
H	-1.811553	-2.392973	-0.568367
H	-0.486248	-1.367934	-0.026168
S	-1.703119	-0.452551	-1.935633
H	-4.295746	-0.055069	0.927218
H	-3.970408	-0.637550	-0.587761
H	-1.226855	0.729932	-1.492712
C	2.578249	-1.486054	0.290646
C	2.100404	-0.008243	0.423960
O	3.808727	-1.679650	0.454862
O	1.677645	-2.297345	-0.001318
H	1.212365	0.050983	1.048803
C	1.799679	0.559405	-0.959644
N	3.199780	0.782280	1.086089
H	3.126298	0.748251	2.102842
H	1.074094	-0.093626	-1.439169
H	2.699524	0.576094	-1.578401
S	1.167635	2.293770	-0.931531

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H	4.084175	0.317037	0.828450
H	3.193380	1.765724	0.799117
H	0.192252	2.051024	-0.017357
28			
Dimer 138 of the z...z type			
C	2.018568	-1.755235	0.403981
C	1.976145	-0.198783	0.267374
O	3.159412	-2.251977	0.575077
O	0.913830	-2.318559	0.287389
H	1.226918	0.224673	0.933467
C	1.660989	0.170976	-1.178499
N	3.325798	0.332442	0.675313
H	3.344391	0.599671	1.659424
H	0.719834	-0.306742	-1.443633
H	2.427176	-0.212653	-1.855146
S	1.574438	1.991301	-1.490254
H	3.974956	-0.466546	0.557010
H	3.615644	1.143932	0.122512
H	0.805499	2.266482	-0.406830
C	-1.485182	1.227097	1.491926
C	-2.357558	0.592035	0.366455
O	-0.473329	1.871097	1.108200
O	-1.864183	0.975718	2.647994
H	-3.413731	0.745729	0.580241
C	-2.042448	-0.901833	0.278334
N	-2.076339	1.274509	-0.947841
H	-2.538275	2.183276	-0.999155
H	-2.339652	-1.358712	1.220323
H	-0.974430	-1.088673	0.146459
S	-2.855923	-1.775297	-1.124882
H	-1.069883	1.449649	-1.045356
H	-2.401510	0.697517	-1.733333
H	-4.128319	-1.598096	-0.712825
28			
Dimer 139 of the z...z type			
C	-1.714411	1.120772	-0.948627
C	-1.574666	0.444891	0.450808
O	-2.111939	2.312593	-0.933868
O	-1.382670	0.410340	-1.918291
H	-0.519183	0.533357	0.716164
C	-2.013806	-1.009880	0.492341
N	-2.338298	1.289449	1.434738
H	-1.938938	1.286764	2.372642
H	-1.872420	-1.437747	1.485667
H	-1.405124	-1.570261	-0.211267
S	-3.797948	-1.254031	0.084375
H	-2.340627	2.240835	1.030190
H	-3.314915	0.979811	1.486223
H	-3.702826	-0.802881	-1.183750
C	2.534509	1.091682	0.466784
C	2.696197	0.141844	-0.769127
O	3.607839	1.414099	1.031059
O	1.366950	1.436091	0.734140
H	2.713102	0.775180	-1.658568
C	1.602902	-0.905263	-0.922257
N	4.060355	-0.487980	-0.656594
H	4.502487	-0.680577	-1.554998
H	1.803861	-1.554892	-1.776203
H	0.654767	-0.403200	-1.102934
S	1.459956	-2.034297	0.529646
H	4.619887	0.181016	-0.099101
H	4.002941	-1.360863	-0.121318
H	1.138567	-1.074201	1.420650
28			
Dimer 140 of the z...z type			
C	1.349234	1.408715	0.132048
C	2.845159	0.987516	-0.025309
O	0.965058	1.615174	1.307909
O	0.717391	1.536036	-0.936765

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H	3.390420	1.880008	-0.338178
C	3.090260	-0.131825	-1.034321
N	3.345794	0.619403	1.343562
H	4.319410	0.869444	1.511241
H	4.158348	-0.253445	-1.219685
H	2.601684	0.146938	-1.965429
S	2.487386	-1.783069	-0.480339
H	2.709969	1.101844	2.002661
H	3.226835	-0.393168	1.483711
H	1.139310	-1.558289	-0.605051
C	-1.349095	-1.408050	0.133637
C	-2.845137	-0.987136	-0.023375
O	-0.964287	-1.613258	1.309508
O	-0.717790	-1.536423	-0.935370
H	-3.390477	-1.879969	-0.335117
C	-3.090798	0.131205	-1.033358
N	-3.345109	-0.617758	1.345406
H	-4.318526	-0.867993	1.513947
H	-4.158981	0.252602	-1.218321
H	-2.602669	-0.148462	-1.964429
S	-2.487713	1.782998	-0.481280
H	-2.708698	-1.099310	2.004607
H	-3.226429	0.394994	1.484465
H	-1.139686	1.558030	-0.606143
28			
Dimer 141 of the z...z type			
C	-1.820197	1.193195	-0.689414
C	-2.687810	0.726271	0.526179
O	-2.400118	1.170174	-1.803201
O	-0.664785	1.560003	-0.407318
H	-2.979775	1.624021	1.073477
C	-1.964359	-0.223523	1.474338
N	-3.943515	0.113645	-0.031381
H	-4.784156	0.329658	0.502653
H	-2.564124	-0.418401	2.364547
H	-1.037238	0.256551	1.781396
S	-1.619979	-1.885202	0.751942
H	-4.003330	0.477886	-1.000573
H	-3.835295	-0.906314	-0.091939
H	-0.832768	-1.494269	-0.284937
C	1.773907	-1.560406	-0.838611
C	1.794321	-0.347982	0.138993
O	2.774357	-2.313666	-0.785514
O	0.777704	-1.617944	-1.591227
H	0.804120	-0.142256	0.531055
C	2.314144	0.889181	-0.587302
N	2.694174	-0.692595	1.296078
H	2.216660	-1.286304	1.975060
H	1.631022	1.097744	-1.406598
H	3.318173	0.718654	-0.981095
S	2.423676	2.381765	0.489953
H	3.484787	-1.233410	0.919901
H	3.021391	0.151929	1.778022
H	1.089457	2.483202	0.668813
28			
Dimer 142 of the z...z type			
C	1.230973	1.496156	0.079550
C	2.595125	0.983587	-0.473483
O	1.208126	1.833421	1.287276
O	0.323019	1.552299	-0.775560
H	2.919031	1.703822	-1.224846
C	2.519761	-0.410874	-1.115367
N	3.586415	1.029744	0.656946
H	4.494651	1.413041	0.400446
H	3.358291	-0.562345	-1.795158
H	1.581621	-0.478126	-1.665583
S	2.584911	-1.805012	0.087358
H	3.129011	1.596137	1.393336
H	3.705164	0.075760	1.032554

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H	1.290733	-1.667869	0.534915
C	-1.112588	-1.331653	-0.154608
C	-2.650569	-1.126224	0.020736
O	-0.460735	-1.402878	0.928143
O	-0.708931	-1.449780	-1.318370
H	-3.126391	-2.068105	-0.256757
C	-3.226981	0.002565	-0.833831
N	-2.919679	-0.900585	1.484035
H	-3.765615	-1.354129	1.826249
H	-4.316533	-0.043972	-0.849624
H	-2.854776	-0.127651	-1.848078
S	-2.810720	1.689529	-0.215155
H	-2.077055	-1.249242	1.972944
H	-2.980360	0.113157	1.658836
H	-1.445855	1.617516	-0.388640
28			
Dimer 143 of the z...z type			
C	-1.927777	-0.707858	-1.193308
C	-2.763098	-0.459158	0.108261
O	-1.242013	-1.764204	-1.186430
O	-2.065553	0.139099	-2.090170
H	-3.763854	-0.854358	-0.079270
C	-2.874972	1.000437	0.523026
N	-2.166863	-1.303107	1.201795
H	-2.828853	-1.550712	1.937676
H	-3.528817	1.114415	1.388656
H	-3.297982	1.553050	-0.312546
S	-1.271005	1.769386	1.004308
H	-1.798160	-2.147863	0.740971
H	-1.368286	-0.812643	1.624786
H	-0.647765	1.653015	-0.192319
C	1.927417	0.707500	-1.193636
C	2.763069	0.459320	0.107824
O	1.241443	1.763715	-1.186974
O	2.065161	-0.139712	-2.090245
H	3.763721	0.854593	-0.080106
C	2.875222	-1.000157	0.522950
N	2.167070	1.303452	1.201332
H	2.829113	1.550752	1.937279
H	3.529206	-1.113867	1.388512
H	3.298140	-1.552958	-0.312542
S	1.271363	-1.769152	1.004672
H	1.798596	2.148387	0.740743
H	1.368333	0.813187	1.624287
H	0.647969	-1.652856	-0.191835
28			
Dimer 144 of the z...z type			
C	1.241245	1.973967	0.658558
C	1.681383	0.761139	-0.217292
O	2.003879	2.970635	0.622489
O	0.203954	1.794201	1.328177
H	0.838756	0.331758	-0.752241
C	2.332824	-0.301473	0.667326
N	2.666588	1.256583	-1.243767
H	2.194972	1.657127	-2.054766
H	1.582751	-0.648448	1.374207
H	3.180203	0.119123	1.212293
S	2.975903	-1.751274	-0.273410
H	3.204097	2.014856	-0.799901
H	3.279334	0.498519	-1.565442
H	1.743385	-2.125061	-0.721137
C	-0.801096	-1.744851	-0.013871
C	-2.201559	-1.071156	-0.151027
O	-0.410173	-1.967136	1.153932
O	-0.204452	-1.932555	-1.097006
H	-2.814457	-1.616953	-0.865668
C	-2.020701	0.383736	-0.583235
N	-2.877962	-1.140796	1.192379
H	-3.395639	-2.011794	1.310311

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H	-1.526715	0.385894	-1.552957	
H	-1.387996	0.917408	0.131389	
S	-3.583603	1.353056	-0.675442	
H	-2.124133	-1.138554	1.897001	
H	-3.528189	-0.360818	1.333398	
H	-4.181804	0.608582	-1.628626	
28				
Dimer 145 of the z...z type				
C	0.687963	1.833525	-0.088389	
C	1.623990	0.611754	-0.306266	
O	-0.009653	2.133746	-1.098213	
O	0.643922	2.311209	1.057094	
H	1.005197	-0.270520	-0.117909	
C	2.847825	0.533454	0.583912	
N	1.987177	0.548085	-1.767820	
H	1.154871	0.850144	-2.291903	
H	2.523909	0.678192	1.611769	
H	3.580060	1.307924	0.346631	
S	3.729148	-1.085260	0.421130	
H	2.744719	1.193676	-2.000307	
H	2.275783	-0.389874	-2.052198	
H	2.648762	-1.849085	0.694967	
C	-1.036346	-2.118057	0.104577	
C	-1.721866	-0.779284	-0.323478	
O	-1.781608	-3.123821	0.125113	
O	0.168743	-2.017271	0.421548	
H	-1.110031	-0.225029	-1.032546	
C	-1.990074	0.079662	0.914062	
N	-3.016706	-1.115433	-1.012063	
H	-2.872535	-1.334645	-1.997992	
H	-1.036281	0.317621	1.381407	
H	-2.600181	-0.470087	1.633593	
S	-2.901981	1.640488	0.556439	
H	-3.385426	-1.966260	-0.563623	
H	-3.683823	-0.337631	-0.948012	
H	-1.913171	2.186142	-0.196637	
28				
Dimer 146 of the z...z type				
C	2.259487	-0.774060	1.090506	
C	2.875317	0.477481	0.377923	
O	2.835435	-1.864381	0.845837	
O	1.295095	-0.535945	1.839090	
H	3.446356	1.022859	1.131206	
C	1.839398	1.412159	-0.234977	
N	3.856029	-0.030544	-0.644128	
H	4.710884	0.520195	-0.711682	
H	2.305177	2.328661	-0.599670	
H	1.128172	1.674771	0.545125	
S	0.962685	0.706139	-1.695096	
H	4.052996	-1.005467	-0.346401	
H	3.409128	-0.073194	-1.567879	
H	0.428866	-0.403656	-1.107187	
C	-1.939962	-1.694645	-0.345130	
C	-2.280787	-0.173167	-0.372792	
O	-2.851950	-2.453035	0.055584	
O	-0.772189	-1.968671	-0.696315	
H	-1.934503	0.265221	-1.305445	
C	-1.640115	0.519515	0.824581	
N	-3.778539	-0.014230	-0.325046	
H	-4.198902	-0.136400	-1.247282	
H	-0.601078	0.208601	0.911462	
H	-2.141645	0.224088	1.749076	
S	-1.751013	2.358516	0.759548	
H	-4.143704	-0.768200	0.273348	
H	-4.057293	0.904823	0.030496	
H	-1.064791	2.489197	-0.396407	
28				
Dimer 147 of the z...z type				
C	-1.632765	-1.357942	-0.597534	

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C	-3.045317	-0.977172	-0.037351	
O	-0.893854	-1.977415	0.209830	
O	-1.405663	-1.014148	-1.770730	
H	-3.738609	-1.757230	-0.359300	
C	-3.566944	0.376764	-0.498434	
N	-2.960092	-1.065941	1.463396	
H	-3.823829	-1.372310	1.910526	
H	-4.551369	0.582165	-0.075785	
H	-3.648528	0.357979	-1.582473	
S	-2.495043	1.794565	-0.000126	
H	-2.185325	-1.729744	1.644492	
H	-2.686503	-0.160617	1.859109	
H	-1.474030	1.481503	-0.820108	
C	3.194735	-0.612346	-0.588992	
C	1.983121	-0.603308	0.397248	
O	4.304498	-0.891951	-0.065420	
O	2.924716	-0.364046	-1.778967	
H	1.480106	-1.570207	0.331065	
C	0.947165	0.470422	0.120215	
N	2.546613	-0.486860	1.789410	
H	1.988782	-0.960265	2.499396	
H	0.138439	0.416813	0.846653	
H	0.533148	0.283046	-0.866549	
S	1.592346	2.193400	0.209409	
H	3.498466	-0.887450	1.728571	
H	2.645440	0.500239	2.049001	
H	2.439180	2.069937	-0.833666	
28				
Dimer 148 of the z...z type				
C	-2.178932	1.367349	0.383334	
C	-3.067688	0.180804	0.888907	
O	-2.730775	2.131212	-0.446353	
O	-1.040936	1.428280	0.884215	
H	-3.451383	0.463568	1.871004	
C	-2.321792	-1.141943	1.004852	
N	-4.251055	0.081425	-0.035162	
H	-5.115820	-0.195470	0.428313	
H	-2.955678	-1.916896	1.437849	
H	-1.467485	-0.984594	1.659411	
S	-1.766078	-1.820309	-0.618005	
H	-4.334127	1.020955	-0.463209	
H	-4.050579	-0.582787	-0.792062	
H	-0.985906	-0.781437	-0.999668	
C	1.494646	0.533544	-1.071805	
C	1.606063	-0.167898	0.321939	
O	0.907345	-0.154887	-1.948978	
O	1.956234	1.684490	-1.156063	
H	0.653939	0.027632	0.820481	
C	2.748999	0.311213	1.201618	
N	1.689478	-1.652938	0.075832	
H	1.326687	-2.215410	0.845716	
H	2.739453	-0.191496	2.169932	
H	2.627778	1.379994	1.360513	
S	4.419252	-0.008912	0.482440	
H	1.149388	-1.839827	-0.780634	
H	2.664598	-1.921994	-0.099440	
H	4.241026	0.786264	-0.592739	
28				
Dimer 149 of the z...z type				
C	1.896816	0.826594	1.133758	
C	2.207978	0.790221	-0.396406	
O	2.875457	1.048185	1.884540	
O	0.696576	0.661412	1.437018	
H	1.826317	1.718327	-0.827290	
C	1.599152	-0.390253	-1.144834	
N	3.707065	0.817073	-0.543578	
H	4.030694	1.289244	-1.387586	
H	1.824017	-0.327513	-2.210413	
H	0.522979	-0.385351	-1.006150	

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S	2.204330	-2.030624	-0.561547
H	4.065186	1.276890	0.309056
H	4.076490	-0.139570	-0.532389
H	1.327119	-2.115142	0.459649
C	-2.044385	-1.243539	0.495735
C	-2.973268	-0.406046	-0.449761
O	-2.390905	-1.256634	1.704828
O	-1.105107	-1.832449	-0.065970
H	-3.589112	-1.122190	-0.996452
C	-2.230030	0.476180	-1.448065
N	-3.893459	0.394671	0.430519
H	-4.852227	0.452495	0.090532
H	-2.918112	0.898298	-2.181926
H	-1.509317	-0.149989	-1.970353
S	-1.386916	1.926281	-0.681545
H	-3.842539	-0.083065	1.351182
H	-3.516682	1.344307	0.547709
H	-0.579895	1.245165	0.191152
28			
Dimer 150 of the z...z type			
C	2.289261	1.566833	-0.450178
C	1.978796	0.059452	-0.198093
O	3.497050	1.853031	-0.635717
O	1.291004	2.313615	-0.401841
H	1.148495	-0.251784	-0.826872
C	1.672396	-0.163935	1.279517
N	3.178972	-0.753281	-0.607772
H	3.162920	-0.962532	-1.606286
H	0.875601	0.516583	1.568381
H	2.545716	0.071863	1.891942
S	1.228035	-1.902047	1.710141
H	4.009932	-0.169478	-0.433172
H	3.229992	-1.640569	-0.097177
H	0.218397	-2.051873	0.815261
C	-1.257219	-1.222319	-1.277855
C	-2.287504	-0.154085	-0.804359
O	-1.273930	-2.297905	-0.623564
O	-0.481033	-0.860988	-2.179672
H	-2.652201	0.440452	-1.638473
C	-1.607810	0.722372	0.245918
N	-3.460496	-0.873233	-0.191733
H	-4.110353	-1.210001	-0.903142
H	-0.731557	1.202480	-0.191069
H	-1.282254	0.103202	1.084943
S	-2.696081	2.006525	0.994066
H	-3.083516	-1.697384	0.298532
H	-3.977318	-0.269979	0.457073
H	-2.886702	2.721024	-0.134047
28			
Dimer 151 of the z...z type			
C	-1.276740	1.408517	-0.442374
C	-1.662812	0.396471	0.684123
O	-1.511166	2.614002	-0.176876
O	-0.749059	0.913479	-1.457546
H	-0.772606	0.220638	1.290319
C	-2.172739	-0.948518	0.193202
N	-2.668573	1.084189	1.569405
H	-2.646730	0.766527	2.538026
H	-2.427899	-1.595570	1.033337
H	-1.381144	-1.428209	-0.375177
S	-3.700276	-0.823069	-0.836198
H	-2.453455	2.092149	1.502222
H	-3.614562	0.947554	1.196620
H	-3.122670	-0.121799	-1.833771
C	1.183188	-1.742844	0.590485
C	2.464631	-0.881483	0.342702
O	0.802093	-2.437006	-0.383553
O	0.661557	-1.595877	1.712083
H	3.181825	-1.030292	1.147806

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C	2.069417	0.589143	0.230358
N	3.095555	-1.355372	-0.940321
H	3.746270	-2.124519	-0.780376
H	1.598773	0.883831	1.166021
H	1.346188	0.727427	-0.575271
S	3.461995	1.731535	-0.155700
H	2.322188	-1.729064	-1.513892
H	3.599433	-0.604794	-1.423020
H	4.190932	1.474452	0.950085
28			
Dimer 152 of the z...z type			
C	1.462349	-1.330986	1.412270
C	2.356512	-0.658734	0.326060
O	0.452158	-1.950581	0.984964
O	1.823841	-1.131510	2.583566
H	3.407746	-0.837674	0.544180
C	2.062694	0.841626	0.296331
N	2.073120	-1.282498	-1.016769
H	2.560657	-2.172544	-1.123940
H	2.331330	1.251116	1.268256
H	1.003450	1.052248	0.128757
S	2.937730	1.763861	-1.036685
H	1.069098	-1.483903	-1.089422
H	2.363288	-0.658716	-1.779445
H	4.193486	1.526056	-0.603938
C	-1.913907	1.829232	0.377680
C	-1.927689	0.270337	0.276821
O	-3.020664	2.365400	0.631590
O	-0.807186	2.355433	0.152937
H	-1.131028	-0.163478	0.877031
C	-1.770336	-0.145293	-1.183300
N	-3.242756	-0.215396	0.827669
H	-3.179589	-0.425589	1.823743
H	-0.837789	0.277682	-1.551689
H	-2.582072	0.259017	-1.791869
S	-1.801756	-1.973107	-1.452964
H	-3.896971	0.578754	0.720094
H	-3.579481	-1.055107	0.347173
H	-0.913195	-2.261699	-0.470480
28			
Dimer 153 of the z...z type			
C	-1.217929	-1.201124	0.126869
C	-2.761980	-1.255039	0.381665
O	-0.517297	-1.000394	1.155022
O	-0.859669	-1.368309	-1.049975
H	-3.043027	-2.308264	0.442502
C	-3.591918	-0.573624	-0.698767
N	-3.005444	-0.656279	1.740736
H	-3.786963	-1.074574	2.244322
H	-4.659279	-0.678404	-0.500228
H	-3.360437	-1.048379	-1.649339
S	-3.281912	1.240308	-0.825079
H	-2.114481	-0.783225	2.252169
H	-3.165596	0.354087	1.655157
H	-1.975157	1.144798	-1.149162
C	3.456803	-0.899310	-0.379081
C	2.454348	0.042938	0.359987
O	4.639730	-0.474237	-0.448172
O	2.963911	-1.940209	-0.851758
H	1.799810	-0.517073	1.023990
C	1.606732	0.786571	-0.669552
N	3.266357	1.012333	1.180309
H	3.483159	0.635399	2.102777
H	0.996830	0.049064	-1.187054
H	2.237109	1.313556	-1.388745
S	0.501562	2.074047	0.057103
H	4.160280	1.127260	0.675593
H	2.779349	1.906565	1.302753
H	-0.182128	1.219861	0.847897

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28		
Dimer 154 of the z...z type		
C	-1.204440 -0.065443 0.281099	
C	-2.400847 -0.980825 0.694972	
O	-0.769078 0.685363 1.197451	
O	-0.795145 -0.190630 -0.882916	
H	-1.980561 -1.943158 0.994917	
C	-3.426640 -1.200206 -0.408540	
N	-3.026173 -0.377432 1.924334	
H	-3.469203 -1.062128 2.537102	
H	-4.233537 -1.852359 -0.071908	
H	-2.922983 -1.669229 -1.250355	
S	-4.234923 0.358819 -0.973455	
H	-2.266482 0.121416 2.413653	
H	-3.724536 0.323701 1.651379	
H	-3.109147 0.913540 -1.468986	
C	3.126856 -1.455508 -0.327847	
C	2.397694 -0.187236 0.216751	
O	4.353806 -1.525991 -0.054707	
O	2.424798 -2.228966 -1.005568	
H	1.434217 -0.437192 0.651913	
C	2.201383 0.819870 -0.917401	
N	3.261920 0.404445 1.299916	
H	3.048383 0.007910 2.214639	
H	1.492516 0.382652 -1.615342	
H	3.146102 1.023268 -1.425885	
S	1.560541 2.454262 -0.349055	
H	4.231374 0.138605 1.062146	
H	3.144441 1.423553 1.350161	
H	0.470208 1.928914 0.278691	
28		
Dimer 155 of the z...z type		
C	3.655915 -0.954043 -0.178932	
C	2.631634 0.093930 0.379159	
O	4.849680 -0.555571 -0.222802	
O	3.169700 -2.036382 -0.546961	
H	1.974701 -0.359072 1.120228	
C	1.799295 0.647169 -0.772994	
N	3.441876 1.181727 1.038083	
H	3.534050 1.030630 2.042217	
H	1.219087 -0.177193 -1.181064	
H	2.435647 1.063848 -1.556083	
S	0.666824 2.028852 -0.281501	
H	4.385755 1.087468 0.613119	
H	3.048880 2.115571 0.892175	
H	0.199518 1.432284 0.836800	
C	-0.945349 -0.899115 0.407926	
C	-2.200880 -0.008294 0.133292	
O	-0.618243 -1.640936 -0.547361	
O	-0.425245 -0.776610 1.535259	
H	-2.160320 0.913236 0.709731	
C	-3.465927 -0.797320 0.457443	
N	-2.175806 0.366395 -1.322462	
H	-1.465965 1.091207 -1.484090	
H	-3.441852 -1.073964 1.510407	
H	-3.501542 -1.711906 -0.137399	
S	-5.036029 0.096287 0.084411	
H	-1.892423 -0.469604 -1.850440	
H	-3.087350 0.705947 -1.645865	
H	-4.858654 1.094508 0.973922	
28		
Dimer 156 of the z...z type		
C	-3.594891 -0.337852 -0.847114	
C	-2.188812 -0.079392 -0.202496	
O	-4.360117 0.661240 -0.872002	
O	-3.794031 -1.502325 -1.230892	
H	-1.415657 -0.407275 -0.893367	
C	-2.079580 -0.820282 1.127272	
N	-2.067725 1.410387 -0.006232	

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H	-1.452713 1.858377 -0.687309	
H	-2.237563 -1.879558 0.935880	
H	-2.858434 -0.479513 1.813114	
S	-0.481955 -0.580953 2.019681	
H	-3.043771 1.748344 -0.155999	
H	-1.722585 1.667341 0.920422	
O	0.298623 -1.304530 1.165315	
C	2.593824 -1.497069 -0.432562	
C	2.578849 -0.016956 0.065928	
O	3.569675 -1.828716 -1.138483	
O	1.591553 -2.162110 -0.087980	
H	2.374654 0.008108 1.134303	
C	1.521554 0.765443 -0.704384	
N	3.942060 0.584117 -0.148765	
H	4.578144 0.345292 0.613188	
H	0.602211 0.190490 -0.669870	
H	1.804119 0.880724 -1.752226	
S	1.219548 2.465268 -0.063037	
H	4.332767 0.161502 -1.002696	
H	3.911803 1.604833 -0.225501	
H	0.864269 2.067227 1.178400	
28		
Dimer 157 of the z...z type		
C	1.652040 -1.236903 0.215878	
C	3.150833 -0.900694 0.508138	
O	1.425749 -1.793877 -0.883736	
O	0.855139 -0.921053 1.123432	
H	3.508210 -1.617269 1.249512	
C	3.366484 0.514761 1.034259	
N	3.919474 -1.150520 -0.761431	
H	4.845782 -1.549452 -0.614500	
H	4.408187 0.674189 1.315776	
H	2.738892 0.643775 1.913114	
S	2.985001 1.832372 -0.199745	
H	3.317772 -1.784063 -1.317744	
H	4.010493 -0.277237 -1.294081	
H	1.661004 1.580906 -0.303168	
C	-3.088479 -1.151034 0.026657	
C	-3.426139 0.238999 -0.610058	
O	-3.598906 -1.358750 1.158450	
O	-2.384303 -1.897688 -0.673896	
H	-4.157867 0.060009 -1.399597	
C	-2.218226 0.961825 -1.199115	
N	-4.108304 1.059641 0.451287	
H	-4.875190 1.634695 0.105532	
H	-2.525821 1.855496 -1.743586	
H	-1.723744 0.280627 -1.888085	
S	-1.014803 1.542718 0.071116	
H	-4.433544 0.361272 1.146348	
H	-3.421344 1.659702 0.923543	
H	-0.543231 0.326837 0.460075	
28		
Dimer 158 of the z...z type		
C	-3.619665 0.392675 0.771487	
C	-2.177343 0.118125 0.226891	
O	-4.343543 -0.627468 0.892858	
O	-3.886725 1.590374 0.973017	
H	-1.444598 0.689788 0.792865	
C	-2.125319 0.484459 -1.254636	
N	-1.895710 -1.349650 0.418702	
H	-1.513750 -1.549383 1.343696	
H	-2.393760 1.535018 -1.348160	
H	-2.852932 -0.105188 -1.815839	
S	-0.497123 0.188608 -2.069246	
H	-2.820833 -1.811333 0.368771	
H	-1.246794 -1.730827 -0.276673	
H	0.208737 1.089726 -1.324406	
C	2.382376 1.634347 0.331050	
C	2.556353 0.135084 -0.072253	

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O	3.293392	2.124209	1.030804
O	1.315867	2.150739	-0.071849
H	2.376571	0.017770	-1.138512
C	1.588853	-0.721609	0.736265
N	3.977896	-0.281153	0.191872
H	4.594641	-0.003655	-0.573035
H	0.611276	-0.255532	0.666136
H	1.872340	-0.744317	1.790269
S	1.488639	-2.477167	0.190731
H	4.297796	0.225572	1.028783
H	4.069969	-1.293034	0.319685
H	1.138320	-2.193352	-1.082849
28			
Dimer 159 of the z...z type			
C	4.094242	0.219888	0.072639
C	2.759785	-0.543143	0.404953
O	4.250800	1.304594	0.690354
O	4.842016	-0.344782	-0.742844
H	3.023971	-1.428286	0.982986
C	2.011069	-0.942039	-0.857126
N	1.950178	0.357094	1.299860
H	1.597648	-0.109023	2.134195
H	2.679446	-1.544504	-1.467176
H	1.722856	-0.064436	-1.438098
S	0.443472	-1.876258	-0.575783
H	2.626302	1.108769	1.553498
H	1.154202	0.792712	0.807302
H	0.952175	-2.823156	0.238318
C	-4.094344	-0.219598	0.072595
C	-2.759709	0.543067	0.404998
O	-4.251103	-1.304424	0.690013
O	-4.842032	0.345474	-0.742700
H	-3.023664	1.428191	0.983154
C	-2.010935	0.941926	-0.857059
N	-1.950323	-0.357522	1.299773
H	-1.597964	0.108380	2.134306
H	-2.679279	1.544439	-1.467100
H	-1.722770	0.064307	-1.438040
S	-0.443303	1.876096	-0.575738
H	-2.626567	-1.109184	1.553158
H	-1.154232	-0.793070	0.807355
H	-0.951908	2.822959	0.238464
28			
Dimer 160 of the z...z type			
C	-3.195143	-0.919512	0.478269
C	-2.722234	-0.131514	-0.792712
O	-4.406533	-0.758477	0.774307
O	-2.331327	-1.623439	1.030944
H	-2.805373	-0.812662	-1.642168
C	-1.300586	0.401608	-0.721327
N	-3.726929	0.968441	-1.021936
H	-3.858649	1.210006	-2.003762
H	-1.052020	0.975070	-1.616357
H	-0.617402	-0.443700	-0.649412
S	-1.026487	1.549461	0.697881
H	-4.604365	0.618932	-0.597769
H	-3.453634	1.811212	-0.506162
H	-1.222015	0.618275	1.654692
C	2.017757	-1.845112	-0.423611
C	2.185834	-0.461592	0.286733
O	3.023617	-2.595331	-0.380998
O	0.920905	-2.016072	-0.987670
H	1.321561	-0.236268	0.907562
C	2.377795	0.624160	-0.772715
N	3.393244	-0.548682	1.180547
H	3.152354	-0.909822	2.103681
H	1.480620	0.660458	-1.386324
H	3.222161	0.380207	-1.420477
S	2.745078	2.298279	-0.095679

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H	4.024076	-1.237319	0.738719
H	3.848676	0.362264	1.300638
H	1.568514	2.439508	0.551159
28			
Dimer 161 of the z...z type			
C	3.403334	1.408311	0.166684
C	2.998792	0.047134	-0.494408
O	3.730357	1.337436	1.376936
O	3.307886	2.399470	-0.579340
H	3.467858	-0.054781	-1.470616
C	1.478942	-0.014074	-0.601785
N	3.505071	-1.062177	0.390301
H	4.472995	-1.302291	0.174378
H	1.144793	0.838230	-1.189988
H	1.020964	0.037408	0.388756
S	0.828593	-1.575477	-1.344834
H	3.494911	-0.683359	1.351236
H	2.943739	-1.915411	0.316041
H	1.311304	-1.378516	-2.588484
C	-1.425317	-1.089990	1.188389
C	-2.012852	-0.108256	0.123037
O	-1.892098	-2.252680	1.155221
O	-0.587157	-0.586432	1.962417
H	-1.240221	0.562487	-0.245532
C	-3.158469	0.688752	0.739868
N	-2.496798	-0.920402	-1.043224
H	-1.689348	-1.230403	-1.597214
H	-2.770831	1.236013	1.597346
H	-3.947611	0.019280	1.087694
S	-3.981754	1.856382	-0.427154
H	-2.951004	-1.763269	-0.668693
H	-3.139864	-0.392334	-1.641010
H	-2.903501	2.636901	-0.644229
28			
Dimer 162 of the z...z type			
C	-1.165369	-1.515033	0.072451
C	-2.709241	-1.274368	0.186691
O	-0.542717	-1.479666	1.167389
O	-0.744513	-1.764837	-1.069345
H	-3.181456	-2.252589	0.079931
C	-3.288359	-0.324886	-0.861332
N	-2.975872	-0.800487	1.588083
H	-3.810063	-1.199526	2.014975
H	-4.376397	-0.397287	-0.885955
H	-2.894614	-0.624048	-1.830681
S	-2.928490	1.456530	-0.553480
H	-2.113751	-1.062967	2.106752
H	-3.047196	0.226345	1.592645
H	-1.574281	1.440001	-0.766730
C	0.943059	1.647984	-0.073922
C	2.338250	0.966888	-0.217215
O	0.651417	2.066400	1.069445
O	0.259240	1.658764	-1.120505
H	2.840254	1.319737	-1.115949
C	2.155677	-0.546862	-0.245641
N	3.173427	1.369999	0.970558
H	3.640415	2.264829	0.821518
H	1.496900	-0.807595	-1.070170
H	1.654939	-0.893453	0.659351
S	3.729662	-1.500161	-0.349672
H	2.518174	1.495139	1.756936
H	3.888452	0.668060	1.186985
H	4.125466	-1.032754	-1.551732
28			
Dimer 163 of the z...z type			
C	4.130553	-0.215325	-0.137490
C	2.758551	0.497367	-0.428764
O	4.264866	-1.345318	-0.674491
O	4.921713	0.424158	0.575111

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H	2.964164	1.371861	-1.044684
C	2.067183	0.911163	0.861685
N	1.934977	-0.460149	-1.248572
H	1.600815	-0.062358	-2.124550
H	2.762969	1.521433	1.432311
H	1.806356	0.040241	1.465591
S	0.489139	1.844475	0.648181
H	2.603782	-1.239744	-1.435304
H	1.123924	-0.838122	-0.732812
H	0.966304	2.802113	-0.172688
C	-4.130780	0.214793	-0.137627
C	-2.758399	-0.497427	-0.428677
O	-4.264932	1.345137	-0.673953
O	-4.922048	-0.425255	0.574242
H	-2.963475	-1.371953	-1.044707
C	-2.067265	-0.911029	0.861904
N	-1.934918	0.460642	-1.247981
H	-1.601030	0.063550	-2.124363
H	-2.762867	-1.521478	1.432577
H	-1.806565	-0.040042	1.465774
S	-0.488924	-1.844013	0.648286
H	-2.604153	1.240276	-1.433934
H	-1.123769	0.838533	-0.732340
H	-0.966147	-2.802177	-0.171942
28			
Dimer 164 of the z...z type			
C	-3.589972	-0.335213	-0.869154
C	-2.221298	-0.064802	-0.147521
O	-4.245208	0.696235	-1.170013
O	-3.853458	-1.531233	-1.080581
H	-1.436533	-0.284731	-0.870009
C	-2.048980	-0.905375	1.108801
N	-2.160049	1.412677	0.144888
H	-1.262473	1.851684	-0.098651
H	-2.163599	-1.951186	0.834371
H	-2.829607	-0.663541	1.833527
S	-0.445653	-0.669837	1.994942
H	-2.941605	1.803529	-0.421054
H	-2.344046	1.618823	1.127714
H	0.338442	-1.365654	1.124760
C	2.676754	-1.441139	-0.486633
C	2.595347	0.024727	0.050200
O	3.660961	-1.704428	-1.210732
O	1.714123	-2.163139	-0.147940
H	2.401894	0.009112	1.120527
C	1.491972	0.771626	-0.688509
N	3.927525	0.692995	-0.163548
H	4.571620	0.492893	0.602683
H	0.609197	0.141565	-0.678365
H	1.764296	0.948931	-1.730404
S	1.087397	2.422115	0.027054
H	4.337549	0.276623	-1.012910
H	3.852270	1.709905	-0.252267
H	0.828077	1.957488	1.269786
28			
Dimer 165 of the z...z type			
C	2.182088	-1.376693	-0.301908
C	1.912100	-0.306268	0.811170
O	3.124544	-2.169239	-0.055674
O	1.418382	-1.330653	-1.283808
H	1.103113	-0.691216	1.436199
N	1.534251	1.069761	0.282209
C	3.140019	-0.256047	1.679127
H	2.949097	-0.041326	2.657253
H	1.342560	1.765433	1.101073
H	0.636022	0.984342	-0.325041
S	2.859013	1.847460	-0.738700
H	3.581070	-1.186734	1.575163
H	3.800546	0.436477	1.308556

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H	2.808063	0.934057	-1.730606
C	-2.181966	1.376588	-0.301826
C	-1.911779	0.306392	0.811424
O	-3.124379	2.169186	-0.055588
O	-1.418435	1.330345	-1.283852
H	-1.102676	0.691467	1.436226
C	-1.534034	-1.069745	0.282671
N	-3.139539	0.256355	1.679618
H	-2.948440	0.041827	2.657751
H	-1.342195	-1.765255	1.101637
H	-0.635916	-0.984453	-0.324762
S	-2.858991	-1.847646	-0.737832
H	-3.580604	1.187024	1.575550
H	-3.800139	-0.436238	1.309309
H	-2.808225	-0.934438	-1.729928
28			
Dimer 166 of the z...z type			
C	2.140337	-0.708250	-1.101971
C	1.910038	-0.613099	0.444388
O	3.158647	-1.356206	-1.448934
O	1.274431	-0.154787	-1.804581
H	1.191015	-1.392626	0.701387
C	1.398260	0.736320	0.929677
N	3.207886	-0.989978	1.106740
H	3.094449	-1.460767	2.003994
H	1.254593	0.732282	2.011569
H	0.448382	0.963884	0.450006
S	2.562181	2.123283	0.577532
H	3.693952	-1.594047	0.421280
H	3.788022	-0.154118	1.238960
H	2.453059	2.041237	-0.764820
C	-2.439899	1.529028	-0.316613
C	-2.364202	0.154274	0.427082
O	-3.559541	1.806009	-0.812730
O	-1.368551	2.160974	-0.357389
H	-1.816642	0.263578	1.361572
C	-1.698431	-0.876317	-0.477418
N	-3.772060	-0.269004	0.755707
H	-4.091197	0.129000	1.639254
H	-0.721512	-0.506978	-0.786062
H	-2.292523	-1.030770	-1.380949
S	-1.536781	-2.551460	0.283823
H	-4.364769	0.129451	0.009004
H	-3.868420	-1.287614	0.808753
H	-0.942109	-2.148457	1.425460
28			
Dimer 167 of the z...z type			
C	1.397182	-0.625424	0.629007
C	2.053760	0.256421	-0.486451
O	0.993325	0.010334	1.637189
O	1.320940	-1.840001	0.377931
H	1.300009	0.410817	-1.259875
C	3.295241	-0.360996	-1.114879
N	2.330290	1.601291	0.126639
H	2.132932	2.383186	-0.496160
H	3.698499	0.278272	-1.901367
H	3.011882	-1.317210	-1.548456
S	4.676140	-0.616763	0.081184
H	1.708744	1.629837	0.957906
H	3.298681	1.657528	0.457158
H	4.016480	-1.497818	0.861501
C	-3.507468	-1.275614	-0.299247
C	-3.123636	0.239517	-0.395357
O	-3.992602	-1.634064	0.802642
O	-3.244361	-1.947487	-1.312681
H	-3.470764	0.660081	-1.336749
C	-1.611211	0.378072	-0.256082
N	-3.820035	0.961133	0.728402
H	-4.758779	1.257874	0.461331

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H	-1.142991	-0.200379	-1.050044	
H	-1.268354	-0.018824	0.700320	
S	-0.994388	2.114896	-0.289201	
H	-3.923341	0.264685	1.485099	
H	-3.302103	1.787431	1.042359	
H	-1.422334	2.415311	-1.532638	
28				
Dimer 168 of the z...z type				
C	-1.618238	-1.218034	-0.179970	
C	-3.133266	-0.951703	-0.458094	
O	-1.342420	-1.655208	0.961656	
O	-0.857538	-0.966024	-1.137348	
H	-3.481723	-1.719483	-1.150418	
C	-3.400007	0.425576	-1.058738	
N	-3.869458	-1.149402	0.839761	
H	-4.773927	-1.607852	0.738026	
H	-4.450056	0.539134	-1.331069	
H	-2.789594	0.522838	-1.953633	
S	-3.040804	1.820838	0.094708	
H	-3.225724	-1.707036	1.429382	
H	-4.000515	-0.246859	1.311795	
H	-1.714958	1.591083	0.223182	
C	3.138542	-1.119000	-0.102910	
C	3.408143	0.238741	0.629450	
O	3.678176	-1.232104	-1.234409	
O	2.452376	-1.937363	0.532648	
H	4.133058	0.038345	1.420280	
C	2.161557	0.874952	1.239409	
N	4.071923	1.154805	-0.362893	
H	4.798926	1.747133	0.035449	
H	2.425426	1.737461	1.853077	
H	1.674932	0.129693	1.864818	
S	0.969266	1.503769	-0.018724	
H	4.449279	0.520113	-1.091094	
H	3.362181	1.745069	-0.814377	
H	0.534915	0.301220	-0.484506	
28				
Dimer 169 of the z...z type				
C	-3.369971	-0.586170	0.994684	
C	-2.003201	-0.347691	0.263256	
O	-4.042673	-1.550645	0.551974	
O	-3.617306	0.188732	1.936359	
H	-1.235922	-0.850062	0.857536	
C	-1.628827	1.119054	0.099957	
N	-2.063952	-1.065781	-1.053174	
H	-1.151542	-1.460447	-1.319576	
H	-0.665203	1.232193	-0.396127	
H	-1.566669	1.564910	1.089672	
S	-2.826798	2.072973	-0.926940	
H	-2.772400	-1.808249	-0.922736	
H	-2.401811	-0.439400	-1.790208	
H	-3.870330	1.914596	-0.086439	
C	3.644976	1.216452	0.210821	
C	3.274604	-0.246548	-0.215200	
O	3.971418	1.353235	1.415220	
O	3.525987	2.066279	-0.689104	
H	3.758022	-0.500621	-1.155922	
C	1.757673	-0.352014	-0.339087	
N	3.792002	-1.178977	0.847807	
H	4.761501	-1.443591	0.670644	
H	1.436293	0.372003	-1.084691	
H	1.280890	-0.110250	0.613086	
S	1.133427	-2.029265	-0.789470	
H	3.783351	-0.635297	1.727044	
H	3.241604	-2.038288	0.930853	
H	1.648874	-2.062817	-2.035189	
28				
Dimer 170 of the z...z type				
C	-3.133648	-0.474732	-1.054847	

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C	-2.775052	0.395311	0.196603		
O	-3.342986	-1.690199	-0.818199		
O	-3.122438	0.137952	-2.137979		
H	-3.336050	1.327445	0.187849		
C	-1.272006	0.653993	0.196956		
N	-3.171201	-0.381349	1.424626		
H	-4.150255	-0.227262	1.666727		
H	-1.022028	1.175191	-0.725532		
H	-0.724686	-0.292472	0.231149		
S	-0.653236	1.620897	1.638837		
H	-3.075007	-1.377897	1.169891		
H	-2.599652	-0.143458	2.240691		
H	-1.298197	2.770668	1.354599		
C	1.845709	-1.889474	0.234110		
C	2.231401	-0.375736	0.266377		
O	2.806966	-2.691195	0.161392		
O	0.618438	-2.108529	0.247567		
H	1.671826	0.131534	1.047449		
C	1.956566	0.253789	-1.096165		
N	3.693789	-0.265510	0.608161		
H	3.845135	-0.277079	1.617676		
H	0.937681	0.014079	-1.387778		
H	2.624409	-0.164995	-1.851835		
S	2.219637	2.077850	-1.148750		
H	4.146025	-1.110129	0.225415		
H	4.118823	0.588027	0.234491		
H	1.343788	2.371241	-0.162122		
28					
Dimer 171 of the z...z type					
C	3.009093	-0.861231	1.208613		
C	1.893268	-0.022438	0.496774		
O	3.606444	-0.264659	2.137114		
O	3.153424	-2.025012	0.788708		
H	0.953921	-0.255306	1.002728		
C	1.746087	-0.295557	-0.993415		
N	2.162341	1.431466	0.760139		
H	1.304007	1.990593	0.685892		
H	0.960068	0.321167	-1.431127		
H	1.489297	-1.343752	-1.125453		
S	3.268621	0.088522	-1.959593		
H	2.581143	1.492918	1.697929		
H	2.853214	1.787628	0.091144		
H	4.033444	-0.849150	-1.362629		
C	-3.536905	-1.363219	-0.184225		
C	-3.121689	0.133249	-0.403535		
O	-4.372222	-1.554199	0.733126		
O	-2.952166	-2.178484	-0.918903		
H	-3.137174	0.378110	-1.463276		
C	-1.728413	0.344085	0.181544		
N	-4.137910	0.997876	0.294552		
H	-4.935293	1.196838	-0.310529		
H	-1.054732	-0.339071	-0.331380		
H	-1.716292	0.105388	1.246808		
S	-1.097332	2.074547	0.068488		
H	-4.491278	0.432607	1.084632		
H	-3.751512	1.891181	0.612996		
H	-1.052925	2.145843	-1.277776		
28					
Dimer 172 of the z...z type					
C	-3.568928	-0.933322	0.117241		
C	-2.843155	0.355250	-0.396366		
O	-4.402291	-0.739630	1.038546		
O	-3.202709	-1.996246	-0.414435		
H	-2.770796	0.349900	-1.481843		
C	-1.455721	0.428880	0.236399		
N	-3.677908	1.540729	0.012040		
H	-4.402447	1.748135	-0.675671		
H	-0.873381	-0.426287	-0.106877		
H	-1.528710	0.399706	1.325935		

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S	-0.531397	1.981294	-0.141304		
H	-4.153680	1.259813	0.885220		
H	-3.109682	2.383960	0.143294		
H	-0.411400	1.771686	-1.467998		
C	1.663352	-1.908270	-0.355426		
C	2.145091	-0.600144	0.352313		
O	2.427760	-2.896225	-0.233481		
O	0.600162	-1.797043	-0.994996		
H	1.328390	-0.126243	0.891041		
C	2.713147	0.354310	-0.695886		
N	3.203579	-0.978446	1.353149		
H	2.792492	-1.258169	2.244104		
H	1.920495	0.580424	-1.405583		
H	3.536849	-0.115915	-1.236800		
S	3.401078	1.918286	-0.006618		
C	3.682800	-1.806747	0.966924		
H	3.859018	-0.210159	1.529593		
H	2.229365	2.373576	0.484358		
28					
Dimer 173 of the z...z type					
C	1.786943	0.648263	1.156060		
C	2.184423	0.788341	-0.353650		
O	2.371224	1.444413	1.930446		
O	0.925568	-0.215319	1.404734		
H	1.461774	1.464065	-0.814641		
C	2.208263	-0.526648	-1.120379		
N	3.514716	1.488950	-0.395944		
H	3.653743	2.063736	-1.226802		
H	2.463360	-0.370304	-2.169300		
H	1.218869	-0.972232	-1.062408		
S	3.441219	-1.732310	-0.468284		
H	3.547753	2.060620	0.465600		
H	4.274305	0.801327	-0.336814		
H	2.844089	-1.882562	0.732492		
C	-2.887348	-0.509234	1.098349		
C	-1.806332	-0.673015	-0.021291		
O	-3.717376	-1.452543	1.168367		
O	-2.793808	0.513850	1.800869		
H	-0.927139	-1.126196	0.438960		
C	-1.376367	0.625830	-0.682606		
N	-2.358685	-1.656778	-1.018690		
H	-1.648548	-2.230410	-1.472520		
H	-0.644068	0.440211	-1.469036		
H	-0.924190	1.251124	0.082066		
S	-2.752731	1.537183	-1.505167		
H	-3.019455	-2.239205	-0.474110		
H	-2.901737	-1.168981	-1.738692		
H	-3.449137	1.761187	-0.371366		
28					
Dimer 174 of the z...z type					
C	3.417557	0.810934	0.366146		
C	3.564341	-0.430082	-0.578208		
O	3.873921	0.652695	1.527890		
O	2.895962	1.814091	-0.150608		
H	4.407182	-0.229836	-1.242399		
C	2.325889	-0.726988	-1.415455		
N	3.950376	-1.602729	0.283568		
H	4.596683	-2.252034	-0.163446		
H	2.509127	-1.551077	-2.106307		
H	2.085123	0.166119	-1.987632		
S	0.861881	-1.229102	-0.414933		
H	4.362686	-1.178768	1.134449		
H	3.108837	-2.113028	0.576073		
H	0.678958	-0.047858	0.219570		
C	-1.440059	1.501691	0.179337		
C	-2.822073	0.792121	0.351753		
O	-1.242956	2.034470	-0.937684		
O	-0.674488	1.397386	1.158623		
H	-3.272721	1.062055	1.304647		

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C	-2.620839	-0.719334	0.256554		
N	-3.729135	1.272913	-0.748993		
H	-4.213646	2.132572	-0.489982		
H	-1.941817	-1.020122	1.051772		
H	-2.162873	-0.984224	-0.698114		
S	-4.173826	-1.707683	0.344728		
H	-3.114069	1.498617	-1.547064		
H	-4.433968	0.572449	-1.000838		
H	-4.535481	-1.316799	1.583999		
28					
Dimer 175 of the z...z type					
C	3.271864	0.908336	-0.519620		
C	3.169477	-0.604949	-0.916903		
O	4.359358	1.239795	0.016399		
O	2.279750	1.602082	-0.801807		
H	3.422951	-0.677082	-1.976457		
C	1.796674	-1.222498	-0.692803		
N	4.251164	-1.333440	-0.163359		
H	4.640378	-2.130647	-0.666347		
H	1.782148	-2.274342	-0.980564		
H	1.078286	-0.678867	-1.301390		
S	1.255614	-1.168928	1.071134		
H	4.972613	-0.613437	0.021775		
H	3.906726	-1.653522	0.747081		
H	1.082205	0.169745	1.132322		
C	-1.462053	1.454684	0.461842		
C	-2.227565	0.181054	-0.024114		
O	-0.977477	1.396773	1.617402		
O	-1.443024	2.386744	-0.364853		
H	-1.791221	-0.159980	-0.962837		
C	-3.710919	0.486756	-0.211489		
N	-2.035652	-0.925981	0.972966		
H	-1.050828	-1.244546	0.965012		
H	-3.798679	1.310119	-0.916791		
H	-4.163814	0.796374	0.733144		
S	-4.717396	-0.948540	-0.789262		
H	-2.208664	-0.568238	1.916455		
H	-2.655227	-1.718356	0.778895		
H	-4.110658	-1.085251	-1.986096		
28					
Dimer 176 of the z...z type					
C	-1.105759	1.346810	-0.046979		
C	-2.026904	0.116603	0.223655		
O	-1.125035	2.248542	0.819235		
O	-0.468658	1.289673	-1.121352		
H	-1.477050	-0.809273	0.063973		
C	-3.243513	0.180972	-0.698072		
N	-2.450332	0.161162	1.667636		
H	-1.765487	-0.290625	2.274076		
H	-2.886999	0.173601	-1.726012		
H	-3.799112	1.106710	-0.534180		
S	-4.467117	-1.173169	-0.440479		
H	-2.480446	1.156926	1.935011		
H	-3.356493	-0.295187	1.816106		
H	-3.636923	-2.188684	-0.754718		
C	2.432153	-2.036607	-0.125520		
C	2.030494	-0.545474	0.093788		
O	3.102562	-2.556955	0.801679		
O	2.073454	-2.521737	-1.215457		
H	0.991453	-0.382877	-0.178013		
C	2.929499	0.362519	-0.745719		
N	2.190783	-0.225356	1.556624		
H	1.357992	-0.472060	2.090763		
H	2.766224	0.114643	-1.792714		
H	3.981442	0.188246	-0.510145		
S	2.636476	2.163682	-0.468807		
H	2.962135	-0.816638	1.901961		
H	2.383194	0.772899	1.700538		
H	1.312766	2.118347	-0.787665		

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28		
Dimer 177 of the z...z type		
C	-1.539509	1.392492
C	-3.007704	0.905162
O	-0.894113	1.670633
O	-1.183731	1.459508
H	-3.658074	1.776593
C	-3.473574	-0.183175
N	-3.087325	0.461946
H	-3.998837	0.612483
H	-4.511654	-0.459497
H	-3.390518	0.201569
S	-2.505621	-1.747232
H	-2.346942	0.996075
H	-2.846161	-0.533336
H	-1.315826	-1.208827
C	2.882113	1.018823
C	3.242342	-0.484369
O	2.632326	1.304423
O	2.921533	1.757785
H	4.330825	-0.542397
C	2.636802	-1.068446
N	2.828089	-1.254605
H	3.445666	-2.031431
H	3.014846	-2.074501
H	2.918427	-0.425021
S	0.801840	-1.234599
H	2.802526	-0.546744
H	1.871389	-1.608971
H	0.501638	0.083484
28		
Dimer 178 of the z...z type		
C	3.382664	0.851496
C	2.756595	-0.317091
O	4.061717	0.489589
O	3.095196	1.994067
H	2.888380	-0.137573
C	1.276504	-0.436665
N	3.494555	-1.580260
H	4.327620	-1.704137
H	0.786277	0.500677
H	1.150483	-0.615486
S	0.405170	-1.839844
H	3.813263	-1.449953
H	2.910420	-2.416185
H	0.644221	-1.443307
C	-1.727045	2.019185
C	-2.668214	0.767879
O	-0.808047	1.969528
O	-1.967413	2.885545
H	-3.710751	1.075863
C	-2.323154	-0.078708
N	-2.436579	0.007981
H	-3.139836	0.224139
H	-2.556894	0.506184
H	-1.259674	-0.310665
S	-3.163491	-1.714938
H	-1.518066	0.352098
H	-2.419851	-1.006495
H	-4.423998	-1.239099
28		
Dimer 179 of the z...z type		
C	-3.639934	-0.141305
C	-3.125558	0.242903
O	-3.338905	-1.299954
O	-4.243806	0.765078
H	-3.904296	0.752156
C	-1.893515	1.134093
N	-2.780236	-1.030512

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H	-3.593418	-1.425840
H	-2.186626	2.032138
H	-1.125657	0.622221
S	-1.077824	1.592039
H	-2.488445	-1.699214
H	-2.034388	-0.898510
H	-2.120965	2.269527
C	3.714423	0.704557
C	3.010999	-0.590302
O	4.491471	1.262161
O	3.383286	1.043631
H	3.062134	-1.383381
C	1.560334	-0.261744
N	3.758040	-1.042052
H	4.526045	-1.670259
H	1.081282	0.104745
H	1.514762	0.524330
S	0.600267	-1.671180
H	4.177880	-0.183776
H	3.156968	-1.519337
H	0.634130	-2.447128
28		
Dimer 180 of the z...z type		
C	-3.916124	-0.726405
C	-2.459798	-0.269782
O	-4.393050	-1.628137
O	-4.427939	-0.131398
H	-1.819663	-0.376286
C	-2.475181	1.173299
N	-1.973811	-1.216921
H	-1.274752	-1.874514
H	-2.950652	1.781250
H	-3.063052	1.263916
S	-0.823987	1.895570
H	-2.842101	-1.745584
H	-1.587011	-0.748948
H	-0.322811	1.866338
C	2.295163	1.518774
C	2.094390	0.036870
O	2.828410	2.268064
O	1.907532	1.772851
H	1.160449	-0.346841
C	3.266906	-0.820956
N	1.984293	0.017270
H	1.076689	0.406729
H	3.343241	-0.744615
H	4.200700	-0.461642
S	3.138549	-2.594759
H	2.707925	0.640243
H	2.083107	-0.928589
H	2.029816	-2.868736
28		
Dimer 181 of the z...z type		
C	-3.214008	0.328946
C	-1.919114	0.437628
O	-3.681734	1.429464
O	-3.611477	-0.827534
H	-1.070867	0.301592
C	-1.832511	-0.584521
N	-1.851274	1.849592
H	-0.902899	2.200403
H	-0.909459	-0.472827
H	-1.849550	-1.575866
S	-3.197699	-0.436923
H	-2.368469	2.414060
H	-2.358921	1.923108
H	-4.184315	-0.744855
C	3.801701	1.114857
C	3.282180	-0.256885

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O	4.205813	1.092748	1.340958
O	3.705884	2.067124	-0.642794
H	3.675368	-0.444186	-1.394070
C	1.755404	-0.235350	-0.413330
N	3.784213	-1.338247	0.521562
H	4.704250	-1.676658	0.239012
H	1.438512	0.571526	-1.071807
H	1.372089	-0.028844	0.588132
S	0.962432	-1.819514	-0.924323
H	3.893753	-0.887033	1.445605
H	3.148589	-2.141213	0.563372
H	1.455820	-1.838080	-2.179168
28			
Dimer 182 of the z...z type			
C	-4.147917	-0.491119	-0.202813
C	-3.164799	0.507028	0.502780
O	-4.571886	-1.418002	0.531633
O	-4.408243	-0.237390	-1.392655
H	-3.764343	1.346537	0.861323
C	-2.052941	1.039978	-0.387931
N	-2.629878	-0.192168	1.723981
H	-2.395553	0.435817	2.492770
H	-1.398493	1.717215	0.161201
H	-2.511084	1.580643	-1.212534
S	-0.948004	-0.266293	-1.074040
H	-3.371371	-0.860335	1.996284
H	-1.801411	-0.745403	1.485243
H	-1.910766	-0.927664	-1.748518
C	3.947675	-1.086312	-0.226179
C	2.623299	-0.251598	-0.157522
O	4.135909	-1.867349	0.741367
O	4.668185	-0.849525	-1.211044
H	2.088903	-0.322367	-1.101936
C	2.954808	1.202210	0.166958
N	1.767256	-0.863790	0.919560
H	1.075642	-1.508600	0.534982
H	3.621492	1.576939	-0.606792
H	3.470621	1.272670	1.127106
S	1.487949	2.310481	0.320957
H	2.435569	-1.407948	1.499167
H	1.263090	-0.166583	1.472847
H	1.044468	2.150772	-0.942767
28			
Dimer 183 of the z...z type			
C	-2.711161	1.654096	-0.377218
C	-1.956700	0.294161	-0.188249
O	-2.535548	2.487119	0.546181
O	-3.371670	1.760559	-1.427262
H	-1.006094	0.384758	-0.718946
C	-2.697604	-0.926739	-0.713515
N	-1.625224	0.153263	1.269710
H	-0.790066	-0.423533	1.420832
H	-2.108332	-1.833749	-0.571387
H	-2.874159	-0.785151	-1.776903
S	-4.307117	-1.228590	0.135445
H	-1.498024	1.110462	1.630182
H	-2.417908	-0.261929	1.770624
H	-4.887687	-0.085121	-0.284138
C	4.473189	0.417580	-0.322554
C	3.215441	-0.211214	0.382842
O	4.694636	1.619258	-0.024182
O	5.112509	-0.349763	-1.060490
H	3.585180	-0.848022	1.187112
C	2.346412	-1.010580	-0.571851
N	2.469312	0.924399	1.035760
H	2.106253	0.699089	1.960989
H	2.975239	-1.755470	-1.052946
H	1.928265	-0.369274	-1.350446
S	0.895402	-1.848766	0.203705

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H	3.178956	1.685504	1.077049
H	1.694644	1.261144	0.462173
H	1.575681	-2.525845	1.150404
28			
Dimer 184 of the z...z type			
C	-1.680719	0.460984	1.046062
C	-3.200336	0.368008	0.724996
O	-1.109243	1.527289	0.735942
O	-1.181722	-0.552939	1.596035
H	-3.743561	0.578196	1.648793
C	-3.641033	-0.986075	0.178554
N	-3.512160	1.484670	-0.233042
H	-4.450567	1.869671	-0.123816
H	-4.718567	-1.008256	0.012270
H	-3.386121	-1.749232	0.909618
S	-2.881588	-1.410352	-1.446386
H	-2.793498	2.208796	-0.068771
H	-3.397826	1.155813	-1.199551
H	-1.616056	-1.523696	-0.994541
C	3.387291	-1.080180	0.054652
C	1.887860	-0.635111	0.032075
O	3.860175	-1.314255	1.195095
O	3.938511	-1.183974	-1.059943
H	1.297316	-1.530308	-0.182607
C	1.552765	0.421311	-1.014515
N	1.496139	-0.187481	1.405329
H	0.467388	-0.346494	1.594989
H	0.493527	0.676011	-0.981733
H	1.801547	0.030473	-1.997823
S	2.430926	2.022683	-0.758573
H	2.104990	-0.695862	2.058984
H	1.695484	0.811185	1.512793
H	3.671956	1.543500	-0.983241
28			
Dimer 185 of the z...z type			
C	-1.616033	-1.360679	-0.120821
C	-3.074608	-0.824198	-0.150539
O	-1.139754	-1.632405	1.000255
O	-1.070414	-1.478294	-1.247575
H	-3.708666	-1.623831	-0.537880
C	-3.259304	0.425613	-1.013227
N	-3.482620	-0.574561	1.274843
H	-4.453713	-0.812455	1.475113
H	-4.319079	0.652030	-1.135509
H	-2.831200	0.224853	-1.992455
S	-2.514804	1.952072	-0.298249
H	-2.832769	-1.131681	1.855096
H	-3.322302	0.417484	1.500917
H	-1.197556	1.595974	-0.384949
C	1.216444	0.728784	0.570527
C	1.866341	-0.669618	0.364543
O	0.709347	1.262352	-0.451397
O	1.282281	1.176274	1.731873
H	1.365025	-1.367142	1.036566
C	3.362964	-0.664973	0.666291
N	1.583676	-1.145850	-1.027833
H	0.539997	-1.333263	-1.142997
H	3.787665	-1.664218	0.553591
H	3.504772	-0.349284	1.697800
S	4.372397	0.411632	-0.442578
H	1.838979	-0.412843	-1.692834
H	2.100154	-1.995784	-1.255791
H	3.873310	1.590790	-0.018400
28			
Dimer 186 of the z...z type			
C	-3.086130	-1.169035	-0.083952
C	-3.399415	0.262415	-0.638541
O	-3.667055	-1.457999	0.995698
O	-2.333495	-1.864015	-0.786446

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H	-4.088688	0.136212	-1.475676
C	-2.175167	1.038333	-1.117505
N	-4.145986	0.993139	0.444725
H	-4.924135	1.559418	0.109490
H	-2.472048	1.950829	-1.635762
H	-1.625397	0.406209	-1.810994
S	-1.055888	1.589701	0.238118
H	-4.466794	0.231458	1.076930
H	-3.500000	1.586424	0.979270
H	-0.534753	0.377408	0.570913
C	1.696026	-1.286490	0.297515
C	3.174552	-0.838487	0.550012
O	1.518280	-1.991617	-0.724669
O	0.869245	-0.914710	1.154705
H	3.574327	-1.479382	1.338457
C	3.331310	0.620106	0.970654
N	3.941646	-1.150807	-0.705291
H	4.886569	-1.496876	-0.543363
H	4.360333	0.833113	1.263161
H	2.682147	0.797338	1.824950
S	2.946127	1.836081	-0.360574
H	3.356014	-1.855477	-1.193650
H	3.985735	-0.318189	-1.305445
H	1.610389	1.628352	-0.398419