

Supplementary Materials

Halogen-bonded guanine base pairs, quartets and ribbons

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Section S1. Calculation of CP-corrected interaction energies

Section S2. Convergence problems

Table S1. Selected geometrical parameters (distances in Å; angles in degrees) and van der Waals ratios (vdW) for the (1,2X-G)₄ quartets (X = Br, I, At)

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Section S1. Calculation of CP-corrected interaction energies

The CP-corrected interaction energy for an n-mer G_n , consisting of n guanines G^1 to G^n , is calculated as follows:

$$\Delta E^{CP} = E^{CP} - \sum_{i=1}^n E_{G^i}^{\{G^i\}}(G^i) \quad (1)$$

With the CP-corrected n-mer energy calculated as:

$$E^{CP} = E_{G_n}^{\{G_n\}}(G_n) - BSSE \quad (2)$$

where

$$BSSE = \sum_{i=1}^n E_{G^i}^{\{G_n\}}(G_n) - \sum_{i=1}^n E_{G^i}^{\{G^i\}}(G_n) \quad (3)$$

In these equations the subscripts denote the molecular system (The n-mer G_n or individual monomers G^i), the superscripts in curly brackets denote the basis set employed (*i.e.* the monomer basis set $\{G^i\}$ or the n-mer basis set $\{G_n\}$) and the attribute in round brackets indicates the geometry (*i.e.* the optimised monomer geometry (G^i) or the n-mer geometry (G_n)). With this definition of BSSE [1], BSSE values are negative. This is in accordance with the notion that BSSE is an (artificial) attraction.

- [1] F.B. van Duijneveldt, J.G.C.M. van Duijneveldt-van de Rijdt, J.H. van Lenthe, State of the art in counterpoise theory, Chem. Rev. 94 (1994) 1873.

Section S2. Convergence problems

In some cases def2-TZVP the SCF did not converge, or converged to a clearly wrong energy, in single-point calculations. In most cases we could solve this by switching from the default DIIS to the second-order (SOSCF) or Newton Raphson (NRSCF) algorithm. In two cases we did not manage to solve the convergence problems. For the R-II I-doped trimer, one of the monomer+ghost CP calculations converged to a too high energy. Here, we calculated the BBSE using Gaussian 09 [2] with BLYP-D3/def2-TZVP and used this to calculate the CP-corrected interaction energy. The second problem case was the At-substituted quartet 6. Here the single-point def2-TZVP calculation of the quartet converged to a too high energy. We calculated the CP-corrected interaction energy of this quartet with Gaussian 09. The Gaussian calculations employed the “Ultrafine” integration grid.

- [2] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. A., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, Ö. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, D.J. Fox, Gaussian 09, Gaussian, Inc., Wallingford, CT, 2009.

Table S1. Selected geometrical parameters (distances in Å; angles in degrees) and van der Waals ratios (vdW) for the (1,2X-G)₄ quartets (X = Br, I, At)

Quartet	R(X•••N)				R(X•••O)			
(1,2BrG) ₄	2.43	2.46	2.43	2.46	3.64	3.09	3.64	3.09
(1,2IG) ₄	2.46	2.48	2.46	2.48	3.88	3.31	3.88	3.30
(1,2AtG) ₄	2.58	2.57	2.57	2.54	3.13	3.13	2.81	3.23
	∠(NX•••N)				∠(NX•••O)			
(1,2BrG) ₄	179	176	179	176	101	142	101	142
(1,2IG) ₄	179	177	179	177	100	133	100	134
(1,2AtG) ₄	175	175	176	175	151	159	148	169
	vdW(X•••N)				vdW(X•••O)			
(1,2BrG) ₄	0.71	0.72	0.71	0.72	1.08	0.92	1.08	0.92
(1,2IG) ₄	0.70	0.70	0.70	0.70	1.11	0.94	1.11	0.94
(1,2AtG) ₄	0.72	0.72	0.72	0.71	0.88	0.88	0.79	0.91

Table S2. Cartesian coordinates (in Å) of the undoped and halogenated reverse Hoogsteen base pairs, R-I and R-II ribbons and G-quartets, in xyz format. The title line provides the molecular system (rHS = reverse Hoogsteen, R1 and R2 refer to the R-I and R-II ribbons and G4 denotes a quartet)

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rHS-H-basepair
N  2.79021100  2.97027200 -3.81266300
C  2.05276600  3.66018600 -4.78301100
H  1.03572200  4.01705500 -4.57969800
N  2.71486200  3.81237500 -5.91387200
C  3.94262600  3.19637600 -5.69441500
C  5.09387700  3.03878400 -6.54562800
O  5.27716600  3.44438000 -7.71853700
N  6.12001400  2.31625700 -5.89122300
H  7.02178600  2.14592600 -6.41319700
C  6.09286000  1.86809700 -4.58492400
N  7.22374200  1.23127700 -4.15677100
H  8.07658900  1.28598200 -4.71960700
H  7.28200800  0.98913600 -3.17006500
N  5.04139900  2.01436900 -3.77818600
C  4.01426500  2.66199200 -4.37829600
H  2.50398600  2.72798400 -2.86346800
N  11.65718000  4.67293500 -9.25393900
C  12.34181800  3.76740500 -8.43435200
H  13.43858700  3.74529800 -8.39897400
N  11.52983700  2.98582400 -7.74857300
C  10.25079500  3.38057400 -8.12629700
C  8.95128000  2.91668800 -7.71412200
O  8.65204600  2.03094900 -6.87740900
N  7.92076500  3.61291700 -8.38812200
H  6.92178700  3.37461700 -8.14697800

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C	8.09067900	4.65990700	-9.27261000
N	6.93961000	5.20927400	-9.76649200
H	6.04903700	4.98659100	-9.31417400
H	7.02958000	6.07939300	-10.28787000
N	9.28463100	5.11420200	-9.65447500
C	10.30569500	4.44326400	-9.07010000
H	12.05470900	5.38103500	-9.87250900

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rHS-Cl-basepair

N	-0.00195000	1.51182200	-4.04583200
C	0.13143300	2.54476400	-3.11081500
H	-0.49133300	2.58570500	-2.20850800
N	1.06647900	3.41369500	-3.44776800
C	1.57917400	2.94433300	-4.65177900
C	2.63030900	3.47591100	-5.50123000
O	3.34287900	4.46558800	-5.38075700
N	2.77133300	2.62866600	-6.67191200
H	3.44625300	2.98487000	-7.35517200
C	2.03745700	1.49713800	-6.97934400
N	2.31094500	0.87689300	-8.17904100
H	2.54922200	1.52331700	-8.94148200
H	1.54771300	0.25502600	-8.46191800
N	1.10111200	1.00818100	-6.16941500
C	0.92267500	1.75330800	-5.04818100
H	-0.62805200	0.70682200	-4.00641200
N	-2.17669900	1.89292900	-7.57318900
C	-1.66089800	0.99595500	-8.50644700
H	-2.13318700	0.02416800	-8.69208500
N	-0.57435300	1.45394200	-9.10742400
C	-0.35877100	2.70529300	-8.54702400
C	0.73036600	3.63279900	-8.76063900
O	1.71139300	3.53633700	-9.48760200
N	0.53642500	4.82177500	-7.91300700
C	-0.47083300	4.98932100	-6.96487600
N	-0.56411000	6.19046500	-6.26076100
H	-1.39976700	6.11858100	-5.66487200
N	-1.41406600	4.07780800	-6.76873700
C	-1.34206800	2.99615200	-7.57704200
H	-2.99443600	1.76950000	-6.97455200
Cl	1.71480100	6.08065800	-8.17719800
Cl	0.78699000	6.52039300	-5.10177600

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rHS-Br-basepair

N	2.00781600	1.36855000	-2.62310100
C	1.04739500	2.35563300	-2.81617900
H	0.15013300	2.43893800	-2.19319100
N	1.35326200	3.14003400	-3.83685900
C	2.55149700	2.65947500	-4.34881600
C	3.36651300	3.11422600	-5.46316600
O	3.23458200	4.05234700	-6.23770600
N	4.52169500	2.23919900	-5.59257600
H	5.15252400	2.52237200	-6.34838500
C	4.83571100	1.15632500	-4.79367100
N	6.00984800	0.48775500	-5.05571400
H	6.40712200	0.51983800	-5.99464300
H	6.11647300	-0.39619000	-4.55621500
N	4.08069900	0.76798600	-3.77305400
C	2.97918400	1.53968500	-3.59737400

H	2.01174900	0.63865900	-1.90878400
N	-4.81764400	3.72537700	-9.54789300
C	-4.72756000	2.99460000	-10.73482200
H	-5.62345600	2.68642100	-11.28768400
N	-3.47802300	2.73655600	-11.08122200
C	-2.70570000	3.32029900	-10.08661000
C	-1.26087000	3.37391600	-9.94946100
O	-0.39179200	2.91294700	-10.66924500
N	-0.91165000	4.15192700	-8.73989000
C	-1.81436100	4.68801300	-7.82068500
N	-1.35323000	5.43755500	-6.75064600
H	-2.18439500	5.75937500	-6.23802100
N	-3.13413900	4.57579400	-7.98506400
C	-3.51959700	3.94401900	-9.11652800
H	-5.66146200	4.04475800	-9.07087400
Br	-0.23664100	4.49073400	-5.37188200
Br	0.97193700	4.45481000	-8.54669200

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rHS-I-basepair

N	3.98958500	1.85296100	-1.41140300
C	2.83760000	1.10422100	-1.66968000
H	2.39201300	0.45676300	-0.90424700
N	2.38300600	1.27641000	-2.89874800
C	3.26660600	2.17402200	-3.48210300
C	3.25225500	2.76734300	-4.80804100
O	2.44709200	2.59965100	-5.71447900
N	4.36962300	3.70316200	-4.95432500
I	4.24300700	4.82836000	-6.78146600
C	5.35528000	3.95420400	-3.99799300
N	6.34570600	4.87608700	-4.26550000
I	7.86809600	4.40423900	-5.82076300
H	6.89355400	4.96624900	-3.39920500
N	5.32922400	3.37027900	-2.79206900
C	4.27938300	2.55005500	-2.57346600
H	4.53085200	1.89270300	-0.54714500
N	11.44558000	3.08354900	-8.70625000
C	10.83595100	3.33208600	-7.48484300
H	11.30388400	3.10036500	-6.52271100
N	9.63461700	3.86675400	-7.64882700
C	9.43417000	3.97711500	-9.01810200
C	8.30608300	4.48291700	-9.78096800
O	7.23548200	4.95210700	-9.42366000
N	8.60437400	4.36124600	-11.20016700
H	7.82971800	4.66748400	-11.79640600
C	9.76415600	3.86031300	-11.76266400
N	9.83435000	3.79320900	-13.13140400
H	9.22190800	4.36399400	-13.71226700
H	10.74624000	3.54707200	-13.51653800
N	10.78593300	3.41472200	-11.03898900
C	10.56813800	3.48587700	-9.70321500
H	12.36844800	2.67579900	-8.86291500

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rHS-At-basepair

N	4.06003900	1.76936400	-1.34267500
C	2.99323600	0.89433000	-1.57018900
H	2.62752300	0.22130100	-0.78466800
N	2.51223200	0.98593000	-2.79785400
C	3.28801800	1.95845600	-3.41226800

C	3.19832500	2.52192600	-4.74974100
O	2.39905700	2.24633200	-5.63915500
N	4.20020600	3.55834100	-4.93133000
At	3.88182300	4.67564900	-6.88025600
C	5.16353500	3.93987900	-3.99989600
N	6.04713800	4.94648200	-4.31832500
At	7.69894500	4.50781400	-5.91443700
H	6.58984700	5.12596600	-3.46227700
N	5.21305500	3.38939700	-2.77514700
C	4.26267300	2.46538800	-2.52415500
H	4.59952800	1.89028500	-0.48497900
N	11.46295300	3.27070200	-8.64830200
C	10.78501600	3.50931200	-7.46233700
H	11.20830300	3.29853300	-6.47506300
N	9.57779500	4.00794700	-7.69258000
C	9.44615000	4.10265600	-9.07158900
C	8.34650200	4.57490900	-9.89410500
O	7.24955100	5.02083400	-9.59073600
N	8.72076200	4.45792300	-11.29454500
H	7.99649900	4.80373900	-11.93108900
C	9.91987500	3.98188400	-11.79319400
N	10.09527600	3.99254900	-13.15402000
H	9.29116000	4.03113700	-13.77910100
H	10.92624200	3.50895200	-13.49553300
N	10.90912200	3.55396600	-11.01540800
C	10.62727500	3.64039200	-9.69284800
H	12.40425000	2.88904500	-8.75276000

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R1-H-dimer

N	3.76615100	1.50541900	-3.47211600
C	2.48443900	1.75777100	-3.97612700
H	1.61420300	1.83397800	-3.31211100
N	2.47256600	1.88624900	-5.28963800
C	3.79660700	1.71298200	-5.68110500
C	4.41246200	1.73657700	-6.99434900
O	3.90766100	1.91753900	-8.11075800
N	5.82191100	1.50272400	-6.88058500
H	6.32389400	1.49322000	-7.80009300
C	6.53068100	1.27737200	-5.72146700
N	7.87643700	1.07274000	-5.84002200
H	8.38317000	1.07171400	-6.73325700
H	8.38680700	0.89069900	-4.97888300
N	5.96512800	1.25247100	-4.50993900
C	4.62816700	1.47181200	-4.55629600
H	4.04155800	1.36158300	-2.50023400
N	6.69008700	1.67604800	-11.69063100
C	6.06426100	1.71880000	-10.44514100
H	4.99524900	1.90784500	-10.27858600
N	6.92816600	1.49987200	-9.46717300
C	8.15506800	1.30656000	-10.07153900
C	9.44085600	1.03362200	-9.48259200
O	9.76214900	0.90625800	-8.29626400
N	10.43489600	0.91417700	-10.51812300
H	11.38343500	0.75721800	-10.16465200
C	10.20790600	1.03266400	-11.88343600
N	11.30153700	0.93360700	-12.71412700
H	12.12134300	0.40911800	-12.40861800

H	11.07632200	0.87366800	-13.70831400
N	9.01318700	1.27647400	-12.40550100
C	8.03435800	1.41333400	-11.47428900
H	6.25201200	1.81484500	-12.60247900

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R1-H-trimer

N	8.97992965102586	-1.40674503759260	-12.88613540271741
C	9.92542087749755	-1.68091159350519	-13.87357160431962
H	11.01052851997738	-1.72253445875164	-13.71101743524010
N	9.35228963453730	-1.85558408928782	-15.05296304399107
C	7.99258108041111	-1.68550200450966	-14.85174390869455
C	6.89591202541882	-1.71512238027551	-15.78303475813619
O	6.92250248224518	-1.91261711989019	-17.01775059909540
N	5.66698218202462	-1.46664045914674	-15.12146075881671
H	4.82609714445160	-1.46511528143306	-15.75447147008934
C	5.51147103841486	-1.20858573317374	-13.77087999196052
N	4.24142813340085	-1.00668858956083	-13.31892228845611
H	3.41663921751465	-0.92822326169988	-13.92998449244696
H	4.15004540721979	-0.74264965326799	-12.33995585212530
N	6.53314777800858	-1.16136132982729	-12.90599601522361
C	7.72838519089794	-1.40040540249810	-13.49092100762619
H	9.15968401470547	-1.21944002771172	-11.89910705320006
N	13.89754675477910	-1.42260862240406	-20.03441868447014
C	15.02837796960834	-1.30684973361750	-19.21749061618228
H	16.02846622018510	-1.15618694863684	-19.64321031803090
N	14.73679709322199	-1.39567475227793	-17.93316570953686
C	13.35793727364998	-1.57929102055794	-17.88749905974934
C	12.45237189250932	-1.72977406450677	-16.76241191449288
O	12.68526508065742	-1.72564311759988	-15.54674386554952
N	11.10851035712704	-1.89782460475894	-17.23058369530773
H	10.39364433736674	-1.97214584196225	-16.46214817933642
C	10.68626297219856	-1.89367995926530	-18.54030690720449
N	9.35020045974149	-2.07838772196133	-18.76971639495461
H	8.63118374872048	-2.02242134360418	-18.03080782405596
H	9.05426331970826	-1.94456337232173	-19.73487377650205
N	11.51642050786894	-1.74426317800111	-19.58020279140471
C	12.80790217981268	-1.59862885476478	-19.19525413683843
H	13.85267351346437	-1.38346277585346	-21.05306819731842
N	2.81379771112554	-1.83175689063406	-19.08317247708816
C	3.92846677206295	-1.82209092543375	-18.24747614456048
H	4.95418189783050	-2.04425173906278	-18.56673898524454
N	3.59623949502871	-1.50715167607575	-17.00574071944352
C	2.22929065876852	-1.30169727428349	-17.01349502338168
C	1.34248502508345	-0.93915738582951	-15.93822302148335
O	1.58482935384659	-0.72843444489069	-14.74431802462383
N	-0.00493052274832	-0.83672608041115	-16.42987062219629
H	-0.69413355755387	-0.61393640790663	-15.70567857429992
C	-0.41307586820748	-1.05136004484420	-17.74099645375307
N	-1.75771527501995	-0.95304288117735	-18.00482383777398
H	-2.36358744010858	-0.40379910654957	-17.39593659908676
H	-2.01123579648941	-0.98576361136005	-18.99281598847299
N	0.42168535643546	-1.38151946601976	-18.71866847644485
C	1.71013510949304	-1.50011402428196	-18.31135473083279
H	2.79559896208144	-2.05050426701336	-20.08057767824000

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R1-Cl-dimer

N	3.59006200	1.63176600	-2.78691900
C	2.31457900	1.19265600	-3.14265200

H	1.51201700	1.10090400	-2.40020600
N	2.21199400	0.91246500	-4.43160100
C	3.46861300	1.17508600	-4.95485900
C	3.94119600	1.06030400	-6.32646600
O	3.35146200	0.71263300	-7.33269300
N	5.35793800	1.48745400	-6.38656300
C	6.12438700	1.89116300	-5.30869700
N	7.42157900	2.38207100	-5.51997800
H	7.78206100	2.64263400	-4.59188400
N	5.65860600	1.94835100	-4.06493800
C	4.34787700	1.62655100	-3.94607200
H	3.92302300	1.90707700	-1.86199600
N	7.44295700	2.38102800	-12.47881300
C	6.58496900	2.34462400	-11.38601900
H	5.60810500	2.84123400	-11.38475800
N	7.09407700	1.65062900	-10.37980500
C	8.33101300	1.20992500	-10.81326100
C	9.30812100	0.37785700	-10.13095400
O	9.28823300	-0.13203900	-9.03133400
N	10.46122500	0.15499900	-11.05331000
C	10.60284500	0.68950700	-12.32790100
N	11.70442700	0.32174000	-13.10851600
H	11.58577400	0.78301700	-14.02122500
N	9.68161600	1.46451200	-12.88281600
C	8.57173200	1.65652600	-12.13050700
H	7.28931300	2.84695300	-13.37465000
Cl	6.04107100	1.53466800	-8.02710900
Cl	8.63316200	1.16814700	-6.13314200
Cl	11.63542600	-0.98797800	-10.45110800
Cl	13.30708000	0.95487000	-12.51099200

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R1-Cl-trimer

N	9.01110092436307	-1.19493661487754	-11.97482213887815
C	9.99656520922630	-1.06834168525486	-12.94535417335850
H	11.06443133890517	-1.02012773108670	-12.70325122829761
N	9.48406763635741	-1.02377714847434	-14.16548794573358
C	8.11207471559062	-1.12945796406664	-14.00685042093958
C	7.05533690655681	-1.17056980027687	-15.00569924334331
O	7.12135326917358	-1.12309211725527	-16.22041940888369
N	5.75503443716519	-1.33155999900442	-14.32193116815470
C	5.56667347637957	-1.40126014783827	-12.95436685333357
N	4.29423688272539	-1.68175433686264	-12.44091421144728
H	4.39251066255330	-1.72062783519301	-11.41726984645484
N	6.56401066522728	-1.33047500307985	-12.07626379070510
C	7.79255481742084	-1.23876025325447	-12.63656591049563
H	9.14040652385846	-1.25486419988840	-10.96354317913067
N	14.68440799922416	-1.83547791096885	-20.61946628030138
C	15.53474580499277	-2.78391686791876	-20.04982037524343
H	16.42111627547004	-3.15181050771784	-20.58104176734626
N	15.14577171124938	-3.15850328688709	-18.84225211930217
C	13.99021889388836	-2.43112190274324	-18.59791677849258
C	13.13245969735017	-2.42366571149070	-17.42229569583818
O	13.22541691443929	-3.04977435018776	-16.38181005252947
N	12.03610408515541	-1.45194430799501	-17.62737139294020
C	11.82982153097397	-0.70262895456850	-18.76928890264493
N	10.82546875417948	0.27576616969416	-18.79524097722526
H	10.87225492110752	0.70978766987928	-19.72688193706302
N	12.61876868961128	-0.76892149848291	-19.83884825267402

C	13.68164789234072	-1.59622040216674	-19.69404641951826
H	14.76109087682417	-1.39671155821218	-21.53781265993658
N	1.78709542509343	-2.50818548167166	-19.17916290416984
C	2.86782471088322	-2.45165507415253	-18.30887976853777
H	3.86693358482752	-2.81424500418134	-18.57587622521914
N	2.53687815565023	-1.90845148206971	-17.14673653711295
C	1.19527605203269	-1.58975942777160	-17.24490215103755
C	0.31479577367974	-0.98057413550332	-16.26269552370981
O	0.53002750176915	-0.59895094501257	-15.13230159400879
N	-1.05516128625362	-0.89551154810647	-16.85027826852870
C	-1.41470859579656	-1.26564216887960	-18.14069230048428
N	-2.75811121123868	-1.19886459926073	-18.52556408449283
H	-2.80876664238465	-1.56703061535055	-19.48579099663463
N	-0.54827353575250	-1.77787477446411	-19.00354586623153
C	0.70170280026770	-1.95938465494671	-18.51432331955286
H	1.77781898350899	-2.87177937512130	-20.13357614750128
Cl	-3.42884982474237	0.48850489449626	-18.67327999394389
Cl	-2.27797789214080	-0.37330004289552	-15.71913401216364
Cl	4.37935436093543	-1.56464757955223	-15.43151254183945
Cl	3.01657596526601	-0.42576524100280	-12.72134268344990
Cl	9.11537086186094	-0.32061961674374	-18.66395876990372
Cl	10.97588414022464	-1.23181309163002	-16.20553360126531

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R1-Br-dimer

N	3.33464700	1.42063600	-2.56125700
C	2.09475900	0.93960900	-2.98125100
H	1.26094900	0.81352200	-2.27939700
N	2.06417900	0.66579400	-4.27622100
C	3.33354300	0.97693200	-4.73620900
C	3.88008000	0.89299300	-6.08464200
O	3.33632700	0.52808800	-7.11411900
N	5.27000000	1.37004900	-6.08656400
C	5.96906700	1.78774400	-4.97009900
N	7.25606300	2.31980600	-5.11955700
H	7.54374200	2.61107900	-4.17432600
N	5.44776900	1.81615700	-3.74224200
C	4.14693300	1.45080600	-3.68350900
H	3.61290300	1.69961900	-1.61957900
N	7.35716700	2.37280200	-12.33035500
C	6.53785000	2.32634600	-11.21252500
H	5.53800900	2.77302800	-11.18596700
N	7.11624200	1.68263600	-10.20713000
C	8.35832300	1.28752900	-10.66867900
C	9.41795700	0.56004300	-9.98759700
O	9.45933000	0.11867100	-8.85745400
N	10.57714900	0.43351500	-10.90489500
C	10.61597200	0.86302200	-12.22658000
N	11.79944000	0.72697100	-12.95385900
H	11.63520500	1.19083100	-13.85894200
N	9.59413500	1.48524000	-12.80724800
C	8.53206700	1.71216600	-12.00243000
H	7.14649500	2.79788800	-13.23495300
Br	12.13312900	-0.29172100	-10.06402000
Br	12.22994600	-1.13611100	-13.51361400
Br	8.68222100	1.00476200	-5.59569700
Br	6.07147000	1.47840000	-7.87175900

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R1-Br-trimer

N	8.98237959638552	-0.73561332019891	-11.85424361237220
C	9.98135386704931	-1.12296731821383	-12.73347616210148
H	11.03908260748989	-1.17576942313072	-12.45333538024502
N	9.49010398829908	-1.41024268188015	-13.93185108316349
C	8.12196834097945	-1.20626523869234	-13.85161196530319
C	7.08204895772002	-1.36325328156834	-14.85948446523113
O	7.18477926076204	-1.73915344966753	-16.01502293152414
N	5.79039305542819	-0.95256625802473	-14.30092424022383
C	5.57957739669547	-0.56942524435039	-12.99233623197809
N	4.31643330433658	-0.11370766798917	-12.59846635140286
H	4.40932588187715	0.16220255341720	-11.61105138920689
N	6.54922492021119	-0.49944814346138	-12.07561799041506
C	7.78191559649120	-0.77771744103267	-12.55266559320327
H	9.09111567607981	-0.46401910505550	-10.87603221283424
N	14.61655897221527	-2.21547242583068	-20.66226945343976
C	15.44610760085449	-3.21771849865568	-20.15971731565737
H	16.31229294287404	-3.58244936115558	-20.72554981323658
N	15.06543851268042	-3.64622373354787	-18.96639462440726
C	13.93682840434781	-2.90041413926188	-18.66277179780106
C	13.09289785607950	-2.92932867176336	-17.47396211055272
O	13.19783390225844	-3.62441516549770	-16.47600050397824
N	12.02924357679420	-1.92575512752144	-17.59328637995728
C	11.82885527197099	-1.11248495449678	-18.68896328821031
N	10.84898187717299	-0.11070656107860	-18.64329332222451
H	10.92501873056066	0.38332331035362	-19.54388856064431
N	12.59510640919576	-1.13825658976677	-19.78310394173970
C	13.63567985074391	-1.99873452945227	-19.70669753043836
H	14.68914583212731	-1.73346453409311	-21.55896048597506
N	1.59409405576955	-0.24589382229917	-19.36219816602715
C	2.73434489293591	-0.17754434202558	-18.57817996358262
H	3.66684260018290	0.28823688883974	-18.91499518359854
N	2.54613397563215	-0.74559353672851	-17.39362478397909
C	1.24276337884762	-1.20819316894231	-17.38872992847827
C	0.50023715710703	-1.89775105031218	-16.34584035932331
O	0.85130237236736	-2.23663886758282	-15.23381376583071
N	-0.88459605332317	-2.13217560314494	-16.81987566309895
C	-1.37224435252525	-1.82089792523589	-18.08442533984679
N	-2.71783752422564	-2.05172493694170	-18.37249677461676
H	-2.88245302199227	-1.66602185844504	-19.31347821916468
N	-0.62846462123130	-1.22396323634627	-19.01117387770715
C	0.62435894040508	-0.90289272133807	-18.61860128116614
H	1.47774515213770	0.10539622664212	-20.31434176095484
Br	-3.21003341539400	-3.96396413630528	-18.60897215952515
Br	-2.04469846656008	-2.81365263745920	-15.46236008639991
Br	2.86948308770986	-1.46527810477919	-12.54435789936975
Br	4.34542501966186	-0.87811433621993	-15.63750228798535
Br	10.90956105718805	-1.74466311934765	-15.97514778356182
Br	8.95699763562566	-0.74489042041122	-18.67139494831530

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R1-At-dimer

N	3.25210500	1.40660000	-2.40048400
C	2.03188000	0.88189800	-2.82137900
H	1.19876800	0.73493900	-2.12259100
N	2.01503300	0.59463700	-4.11576300
C	3.27331900	0.94236300	-4.57430500
C	3.84255800	0.86870900	-5.91718900
O	3.30080000	0.46905800	-6.94432800
N	5.19145900	1.38275200	-5.93557700

C	5.87351600	1.82775200	-4.82344200
N	7.14220100	2.37242500	-4.99148300
H	7.41416100	2.71155700	-4.05504900
N	5.35376400	1.85455400	-3.58138200
C	4.06995300	1.45256600	-3.52096800
H	3.51752000	1.70048600	-1.45977300
N	7.43326900	2.43368900	-12.55035700
C	6.57450600	2.40014400	-11.46787800
H	5.58023600	2.85868000	-11.47059900
N	7.11432400	1.74731400	-10.44020600
C	8.36807700	1.33455300	-10.85756400
C	9.40620900	0.60495700	-10.14596700
O	9.37858200	0.17702400	-9.00166200
N	10.58177600	0.46833600	-10.98833500
C	10.67684700	0.88553900	-12.30874900
N	11.87676200	0.70490300	-12.97542500
H	11.77232500	1.18816300	-13.88101000
N	9.67905800	1.52147900	-12.94091400
C	8.59181500	1.75874300	-12.18340400
H	7.25781500	2.86336700	-13.46042400
At	12.34261000	-0.34367400	-9.82901700
At	12.29128500	-1.46732100	-13.72140300
At	8.88542200	0.83051700	-5.35085200
At	6.06511600	1.51214500	-8.07519500

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R1-I-trimer

N	8.98128939600825	-1.37819582076938	-11.64197166720651
C	9.99431068896057	-1.38196853561180	-12.58189791399040
H	11.05902696809227	-1.38457094318649	-12.32580990702053
N	9.50246949571611	-1.38420488707479	-13.81813772203626
C	8.12116090737992	-1.38220322427359	-13.69634870156753
C	7.07404530132383	-1.41438329044294	-14.70933965176772
O	7.21026568217897	-1.45180921458214	-15.92570502042169
N	5.76554547041489	-1.44472175168714	-14.08730900628585
C	5.55294614852719	-1.39361323076718	-12.72730850944786
N	4.24660590455298	-1.50194403536737	-12.24481285075548
H	4.33187551387065	-1.53578550118633	-11.21794413346928
N	6.53110289730054	-1.33996607567741	-11.80859614325548
C	7.77261382278255	-1.37810056330058	-12.33155272885290
H	9.08626494567055	-1.36920570879778	-10.62601677938365
N	14.81755011779957	-1.43514874367663	-20.77754782483242
C	15.60363245498065	-2.51488049875216	-20.37827098017447
H	16.47803682115306	-2.83347464352784	-20.95926628877894
N	15.17468481134044	-3.07442407291856	-19.25618281164340
C	14.05815575026660	-2.33860211208624	-18.89446647047511
C	13.17168308873714	-2.47780464850602	-17.74262865212643
O	13.23780083214900	-3.30183269346564	-16.83736427521078
N	12.14756378581223	-1.44901645318714	-17.75185667764550
C	11.99775370898544	-0.51337443910372	-18.75064759393501
N	11.02313411908342	0.47793516583754	-18.61144487923127
H	11.15402261373039	1.10083261694862	-19.42309371733239
N	12.79557249513632	-0.42049290899167	-19.82818491436637
C	13.81148129685961	-1.30748927117732	-19.83006719998408
H	14.92854953646071	-0.85265303616491	-21.60837258493497
N	1.40382571494039	-3.08112302157668	-19.12000608153331
C	2.53006090512069	-3.03737023998381	-18.32079816087364
H	3.45264553641020	-3.58479570205283	-18.54133865212184
N	2.34364619371628	-2.24303816323041	-17.26925206805452

C	1.05718287073546	-1.74293301954585	-17.37698273434176
C	0.32041598163435	-0.84271300583194	-16.50551529194582
O	0.68709228027333	-0.31974464858244	-15.46676130379762
N	-1.03236574782786	-0.64799285180344	-17.02968206028033
C	-1.51535273583621	-1.17551188533963	-18.22330482140557
N	-2.83354894476986	-0.92669503590406	-18.57928189465209
H	-3.01887657792831	-1.50455647759890	-19.41306357141546
N	-0.78408797926248	-1.97522819336539	-19.00587391004019
C	0.44698723253613	-2.25974796984503	-18.53694294987050
H	1.29147470781076	-3.59784381954158	-19.99432659316528
I	-3.25137405442099	1.10344064723258	-19.36972858007104
I	-2.28830814300850	0.42290386296485	-15.66715319330947
I	2.94641278835821	0.25385256346698	-12.51735783538035
I	4.13463431477152	-1.78383410562632	-15.54987939297532
I	10.89802956084752	-1.43662723945405	-15.91598046664313
I	8.91374564062547	-0.15517224288546	-18.91143395199051

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R1-At-dimer

N	3.25210500	1.40660000	-2.40048400
C	2.03188000	0.88189800	-2.82137900
H	1.19876800	0.73493900	-2.12259100
N	2.01503300	0.59463700	-4.11576300
C	3.27331900	0.94236300	-4.57430500
C	3.84255800	0.86870900	-5.91718900
O	3.30080000	0.46905800	-6.94432800
N	5.19145900	1.38275200	-5.93557700
C	5.87351600	1.82775200	-4.82344200
N	7.14220100	2.37242500	-4.99148300
H	7.41416100	2.71155700	-4.05504900
N	5.35376400	1.85455400	-3.58138200
C	4.06995300	1.45256600	-3.52096800
H	3.51752000	1.70048600	-1.45977300
N	7.43326900	2.43368900	-12.55035700
C	6.57450600	2.40014400	-11.46787800
H	5.58023600	2.85868000	-11.47059900
N	7.11432400	1.74731400	-10.44020600
C	8.36807700	1.33455300	-10.85756400
C	9.40620900	0.60495700	-10.14596700
O	9.37858200	0.17702400	-9.00166200
N	10.58177600	0.46833600	-10.98833500
C	10.67684700	0.88553900	-12.30874900
N	11.87676200	0.70490300	-12.97542500
H	11.77232500	1.18816300	-13.88101000
N	9.67905800	1.52147900	-12.94091400
C	8.59181500	1.75874300	-12.18340400
H	7.25781500	2.86336700	-13.46042400
At	12.34261000	-0.34367400	-9.82901700
At	12.29128500	-1.46732100	-13.72140300
At	8.88542200	0.83051700	-5.35085200
At	6.06511600	1.51214500	-8.07519500

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R1-at-trimer

N	9.02476540101266	-1.11624555344569	-10.81795310429990
C	10.03952354840287	-1.22021174487986	-11.75191762779536
H	11.10388278018933	-1.17117462303312	-11.50157148876364
N	9.54637637465330	-1.38639717032959	-12.97717142759182
C	8.16016593945885	-1.39774521383502	-12.85347495489046
C	7.07072650390868	-1.49513470930207	-13.77653126452481

O	7.25207959069095	-1.60722322456632	-15.06381635978255
N	5.83168195432337	-1.44515487474496	-13.26070376264757
C	5.60683683670828	-1.29092606688402	-11.92380745583049
N	4.30031854520429	-1.30153934317076	-11.51744898636700
H	4.11953440179847	-0.99100755646832	-10.55997101491102
N	6.57307032925945	-1.14949709233424	-10.97047709116533
C	7.80442161981392	-1.22229259029722	-11.48741974753343
H	9.13557117271330	-0.97322204231476	-9.81327480803372
N	13.94568258149883	-2.07672510962307	-21.05144307205037
C	14.99923676692969	-2.23807496281620	-20.15198273306673
H	16.02459959545987	-2.41946966311421	-20.49785728828546
N	14.61805576777331	-2.15216618106211	-18.88418460838568
C	13.25537741133849	-1.92110076088954	-18.93785150783302
C	12.23418182532392	-1.75349285852005	-17.92657832729796
O	12.55334908922758	-1.81876679168121	-16.66784210358217
N	10.96998201923535	-1.53768262998592	-18.34660557077640
C	10.67776958498328	-1.49089352986483	-19.67280959382963
N	9.39077699803548	-1.20463570295395	-20.03414746812064
H	9.19128665914841	-1.33822117295874	-21.03019436545957
N	11.54995998341314	-1.67617444130958	-20.71897037027408
C	12.79951232262276	-1.86815123033425	-20.29219538464738
H	13.98479970018239	-2.10104534073627	-22.07094005718482
N	2.54523660270546	-1.35291491643199	-20.02269071380578
C	3.68879086683228	-1.44553923920614	-19.26214281754850
H	4.70103476019198	-1.53898045674295	-19.67615730305049
N	3.40116031484441	-1.39584184241949	-17.96041152972897
C	2.01766434082179	-1.26837951376977	-17.85654109587605
C	1.13470046141784	-1.12600109362696	-16.71425946460995
O	1.45001846810834	-1.07474269410386	-15.52128837762713
N	-0.22660212525038	-1.00362153223815	-17.12919796524412
C	-0.68803844252460	-1.05102650172635	-18.44819569289533
N	-2.02541464301726	-0.91887724404894	-18.66633098901691
H	-2.16062697531530	-0.89748743305603	-19.68814300408919
N	0.16644751998443	-1.17106604031344	-19.48949195052861
C	1.46029838346445	-1.24254358786637	-19.15584807255217
H	2.48737665382838	-1.37702531104298	-21.04274107886281
At	-3.35481782274395	-2.93288719959880	-18.19933393907930
At	-1.61709987810006	-0.45522960762199	-15.41860989406567
At	2.71226435682807	-1.12763407613420	-13.05615884438627
At	5.25368259677959	-1.51993772806872	-16.25414814158055
At	10.94190645957145	-1.59525660824693	-15.02480830510218
At	7.67987691826292	-1.35646426228086	-18.56116839541863

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R2-H-dimer1

N	-4.27327511459580	-0.20310656842641	-0.64638240736868
C	-5.44115472637549	0.51122308500299	-0.94647157856487
H	-6.38316087738696	0.31281262673179	-0.42099711355402
N	-5.25426018729492	1.40645385252328	-1.89636552644994
C	-3.91628225999500	1.28535854886901	-2.24988181530080
C	-3.13996919254588	1.99266417094500	-3.25205720342201
O	-3.44374927977649	2.88044718095267	-4.03718487941998
N	-1.77647263398317	1.47403969627284	-3.25808257316964
C	-1.24712145325680	0.48323523242675	-2.45244045852748
N	0.04941331456448	0.11417615483132	-2.64023441383979
H	0.67634692813937	0.73962394722016	-3.14417812460693
N	-1.98556754760298	-0.13329603094805	-1.52072031908262
C	-3.28300693469523	0.28161563890553	-1.48116772265823

H	-4.16987463365043	-0.97487082730928	0.01380444558509
H	-1.19526916696378	1.89868886652349	-3.98652891207232
H	0.47096294863966	-0.60138725483497	-1.99980657255223
N	3.18931945298382	-2.52220536714282	-2.04845722357044
C	4.41543207858253	-3.09047064554965	-1.67667841002273
H	5.17051401622395	-3.36013004274909	-2.42518777129876
N	4.52379798068601	-3.24544989950167	-0.37167568589134
C	3.32785105842853	-2.76876040820970	0.15025998101675
C	2.86279988910034	-2.69706875304182	1.52345934330003
O	3.39126399505541	-3.02283612851773	2.57766930457797
N	1.51590967110239	-2.13781062776840	1.54598073199529
C	0.76091222257558	-1.71216706883435	0.46910094944831
N	-0.49865358452603	-1.25090057890536	0.69768903079120
H	-0.76193064009944	-0.96871493438320	1.64051533658855
N	1.22998517949285	-1.76992199753492	-0.78412149643129
C	2.47641817190320	-2.31204331639547	-0.88248785416633
H	2.85311405478210	-2.33382234172548	-2.99360502312210
H	-1.05942341752716	-0.88357499588916	-0.10856264546880
H	1.11328343801538	-2.11267981353732	2.48714969725813

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R2-H-dimer2

N	3.72750383517111	-2.01397403804558	-1.05290297930820
C	5.02013146519331	-2.54867190890244	-1.11291598010274
H	5.69553820492084	-2.31715501393742	-1.94603130014381
N	5.29872719758769	-3.32636314017796	-0.08431846704735
C	4.14601372321800	-3.31496809312091	0.69408114900617
C	3.83420759512411	-3.96263787339223	1.94222282636710
O	4.55309354400280	-4.70672737318286	2.65106731274216
N	2.51485851600869	-3.66638119522550	2.35833371517004
C	1.62525470208147	-2.83467536603131	1.70846961708077
N	0.40871807014937	-2.68400107853090	2.31169109493838
H	0.25966168492183	-3.04458677997011	3.25645157865203
N	1.89835506458518	-2.21733769663160	0.55834411751646
C	3.14401205065471	-2.49479658908975	0.10537628568951
H	3.27634234895405	-1.39070752775177	-1.72367394249679
H	-0.23427977769136	-2.00028401534378	1.91823208350185
H	2.17657185211354	-4.07859390173597	3.26927974766753
N	2.77536443086055	-5.83544414857424	9.00985121793376
C	1.43808435206538	-5.42105872316501	9.01845862114343
H	0.83912983519018	-5.44395030003874	9.93740020615626
N	1.01989076147220	-5.02211169561553	7.83249071593584
C	2.11995308108739	-5.17763682109722	6.99559452700959
C	2.29363472080278	-4.90644661612824	5.59157984167057
O	1.47002201590621	-4.44629506095872	4.76505361180583
N	3.60250476376467	-5.23114438303551	5.16414610559192
C	4.62270485914351	-5.70944554301577	5.96199376140829
N	5.81059161348035	-5.93831075737220	5.32675960408908
H	5.94907938920930	-5.60367937243375	4.37069080764865
N	4.48492512158769	-5.95886110727639	7.26469695843663
C	3.23693637347472	-5.68606476156467	7.71457421591580
H	3.32784484006569	-6.18236315227719	9.79473111370854
H	3.85155012522349	-5.06273851312498	4.15195466028410
H	6.61242506967052	-6.19186577325169	5.89950455202862

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R2-H-trimer

N	-2.98495765379756	0.30275086582331	1.11710219998094
C	-4.29145340839509	0.79296712351740	0.99864066429239
H	-4.89048854575628	1.04193349411095	1.88300701239595

N	-4.67646268607799	0.90594208845717	-0.25793306443773
C	-3.58903291870225	0.47685444595363	-1.00877233977196
C	-3.41785442352105	0.37972098982080	-2.44663445073701
O	-4.17068664571765	0.64494281480280	-3.37445326968399
N	-2.07965842308239	-0.12142720781838	-2.73829094719139
C	-1.09423123191470	-0.47235527336549	-1.83383824379297
N	0.11247338611432	-0.88422577052245	-2.31535619772123
H	0.16931922335050	-1.22064703856852	-3.27547112840575
N	-1.29126651163286	-0.38681389986552	-0.51340706472068
C	-2.51785079424284	0.09547368809126	-0.16754389691319
H	-2.45871717334167	0.14241382489348	1.97706658735964
H	-1.88317756959506	-0.16332217044444	-3.74239120778841
H	0.84519614404339	-1.20472491589710	-1.63845379438454
N	4.17279857106912	-1.75944675943173	-1.75192152995316
C	5.46052588851598	-2.28029038593620	-1.55510226431464
H	6.25464053953234	-2.13123161062574	-2.29723555752605
N	5.57383177568077	-2.93411855776989	-0.41649779374100
C	4.31805841009369	-2.84735273728359	0.17512651950014
C	3.82133724884963	-3.35157338659429	1.43110570158478
O	4.42028210116889	-4.01627280901966	2.30704337543611
N	2.46690445717610	-2.99782094297425	1.62791881991722
C	1.66723905087215	-2.27384589933940	0.76615194370794
N	0.39506876124098	-2.04658874805317	1.16230763331148
H	0.09459300388321	-2.41239282635854	2.06800224150902
N	2.11755212800012	-1.81482252255906	-0.41742570967676
C	3.42170906083408	-2.11340500785404	-0.64579313889321
H	3.84605008428710	-1.19709609301645	-2.53841954079138
H	-0.22841227365154	-1.43199877756317	0.59056834147310
H	2.00632461636758	-3.29389566507104	2.53227932359977
N	1.41106971766885	-5.54070991003404	8.11836705769652
C	0.13123379718151	-5.00724921612588	7.92328281616326
H	-0.63814480733993	-5.07046708879283	8.70305315871998
N	-0.01376572786764	-4.45060117636841	6.73596596610461
C	1.21733083774074	-4.61845966692832	6.11064065461551
C	1.68356471865933	-4.22425354208590	4.80660926781045
O	1.07280440629549	-3.61404217857450	3.89682494146967
N	3.02788795760612	-4.61452910536382	4.60166176915844
C	3.82935597462249	-5.27775321322319	5.50985638419261
N	5.09749234963711	-5.55762279459911	5.08723219477335
H	5.43620883544769	-5.19414222654936	4.19506730116243
N	3.41803667494481	-5.64642338130350	6.72338327378506
C	2.13028951004698	-5.30074201999741	6.96156323614849
H	1.77022478465378	-6.01731866338937	8.94647997958744
H	3.47601371051160	-4.36650688590235	3.68007189593012
H	5.74594510853994	-5.96351555030061	5.75787424905865

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R2-Cl-dimer1

N	-4.24592457002011	0.51966590222210	-0.60125096602827
C	-5.44485021430843	1.22086432238014	-0.76452989634076
H	-6.20604248118425	1.24603574525531	0.02510740317386
N	-5.52940962494581	1.81630070299386	-1.94023829167702
C	-4.34121304765640	1.50176845566805	-2.58537735819071
C	-3.87372917476245	1.90015941335068	-3.89691826243131
O	-4.37495239242293	2.58538577486459	-4.76421452007342
N	-2.51086013791458	1.30971203027109	-4.10836548278094
C	-1.79943716030535	0.50021235991847	-3.21965639831831
N	-0.58770406247211	-0.00392321976499	-3.66215937860333
H	-0.10876928382333	0.53435358207049	-4.39106171106591

N	-2.29541613041399	0.18249291988016	-2.03429659155637
C	-3.52430896036957	0.69184248929255	-1.76617462701767
H	-3.92688254049949	-0.00494823142267	0.21596965951448
Cl	-1.79317675089925	1.72359751318444	-5.66281968958680
Cl	0.50740726160000	-0.64437606255845	-2.43979138765402
N	3.66838912845385	-1.97186622616223	-1.48738092827388
C	4.88140452644485	-2.64687253888872	-1.31756625865103
H	5.66235189784514	-2.62431853764802	-2.08774194143827
N	4.95288649993352	-3.28037572147654	-0.16107368541664
C	3.74119500065059	-3.01924627215046	0.46391406909321
C	3.25314542690196	-3.47385744203256	1.74945008806468
O	3.75095612936163	-4.17628466657043	2.60489534824885
N	1.87190099409548	-2.92325163833908	1.94811516118591
C	1.16180564890923	-2.10071639406050	1.07041847707377
N	-0.06905468578194	-1.63600616450938	1.50361930151417
H	-0.55459116405863	-2.21216913866852	2.19857328549556
N	1.67535962976047	-1.73402388799370	-0.09315828257064
C	2.92326493466745	-2.20265906221062	-0.34758347654992
H	3.35705050329689	-1.42541470354682	-2.29309529111462
Cl	-1.14842950327343	-0.96991639238360	0.28053611804286
Cl	1.13086645319098	-3.40267399096464	3.47243887393249

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R2-Cl-dimer2

N	3.52458184033346	-1.85661199650074	-2.07839314128143
C	4.81911304915472	-2.38508418971954	-2.07083858824166
H	5.47786294196953	-2.29812331510108	-2.94371577345675
N	5.12381598549490	-2.97063867468277	-0.92699162818625
C	3.98855430894392	-2.82543393745401	-0.14058972187625
C	3.73754011063342	-3.28388870217982	1.20870233556128
O	4.46148285018717	-3.90532684532443	1.97571210785059
N	2.36899342642417	-2.89260452801274	1.60472966214791
C	1.45934072594516	-2.18169845382569	0.81885021783531
N	0.26325941301776	-1.83823742367480	1.43153418825432
H	-0.02611966507172	-2.41324598684838	2.23067401658807
N	1.73368100879244	-1.79624747073820	-0.41369542280676
C	2.97493958741446	-2.13146675711387	-0.84038290315528
H	3.05370424624660	-1.36067506940868	-2.83659154647537
Cl	-1.09121404761197	-1.40004868512916	0.42149936453051
Cl	1.91116188217742	-3.41282203956223	3.22946103123554
N	2.77600409780919	-6.54420278801988	9.80751118974480
C	1.48134104850664	-6.01602441047763	9.80009629931481
H	0.82258375443921	-6.10346394922943	10.67292038102760
N	1.17656988725941	-5.43009497940808	8.65646893866556
C	2.31187522873032	-5.57480815626241	7.87002864221853
C	2.56288246644857	-5.11576977711708	6.52094707082883
O	1.83895304672462	-4.49407800461668	5.75412650769046
N	3.93143071265882	-5.50687606004515	6.12473900827880
C	4.84126839592516	-6.21776400737334	6.91043095564137
N	6.03746568118994	-6.56050259446959	6.29785848120849
H	6.32652927203618	-5.98612795179326	5.49818565045297
N	4.56699024211225	-6.60360165970443	8.14289958665305
C	3.32563258607873	-6.26880156671642	8.56961631023483
H	3.24695468496129	-7.04034346896620	10.56553013535982
Cl	4.38883167084122	-4.98678143698400	4.49985717509861
Cl	7.39179406022699	-6.99956256354029	7.30731529905766

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R2-Cl-trimer

N	-4.04076797374599	0.24679452654891	-0.29965371682740
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C	-5.29379456695060	0.86718403659792	-0.32545179599154
H	-5.97349544921716	0.82026459047281	0.53422831416200
N	-5.53285667094165	1.48307836901589	-1.46896698616777
C	-4.39551763693773	1.26651461854922	-2.23485158386766
C	-4.08704096388725	1.72646128742787	-3.57318857344084
O	-4.71706860555195	2.39574370031757	-4.36637476340907
N	-2.71734861227375	1.23661733112781	-3.93397669168326
C	-1.86924438578396	0.45752274130482	-3.14281917901637
N	-0.67784172150102	0.04686877438448	-3.71585547781643
H	-0.30833059515393	0.63198030792186	-4.47196919864456
N	-2.22222098042422	0.08012161783134	-1.92389905550187
C	-3.45011848251145	0.49598241703486	-1.52294569820795
H	-3.61033366441152	-0.27553583610269	0.46632657554182
C1	-2.18558178421876	1.73520884903164	-5.53834016478397
C1	0.57070247732614	-0.55068705111397	-2.62369155887884
N	3.85505989900713	-1.80617430821913	-2.13535464602551
C	5.10274058228909	-2.43837334962496	-2.11553175858385
H	5.77318456922038	-2.40820921208603	-2.98323304255414
N	5.34908479359625	-3.04270592363134	-0.96752195077637
C	4.22173083659588	-2.80611639168064	-0.19134148392577
C	3.91591111913609	-3.24731729419988	1.15229745326617
O	4.57597467455895	-3.92410569485585	1.92852938048612
N	2.57255157065995	-2.75410034783431	1.53001044230700
C	1.72571831547468	-1.97370642829052	0.74068684303307
N	0.54824490453722	-1.55371882910607	1.33088135180876
H	0.20624179409154	-2.10564359937243	2.12496260242460
N	2.05903844406609	-1.60422212786310	-0.48893195356870
C	3.27591179617206	-2.03529841261105	-0.90262494146979
H	3.41834257795137	-1.29087179493408	-2.90233390014704
C1	-0.72464115152459	-0.96570616086835	0.27258511573218
C1	2.05245220811649	-3.25083498968444	3.14184976711779
N	2.45212332000045	-6.42139381758707	9.71799251054816
C	1.20502423414165	-5.79093033342022	9.66746746771070
H	0.51420230614457	-5.81997381281347	10.51921953342833
N	0.98483383774229	-5.18871097030817	8.51296022431881
C	2.12934693094344	-5.42840048384501	7.76400897829377
C	2.45903125436003	-4.99832991358937	6.42267733958961
O	1.80959344833524	-4.32483869931743	5.63248148515664
N	3.80366939218253	-5.49827851622578	6.07120682575949
C	4.62932116209525	-6.27470701457532	6.88843039752100
N	5.81415858978783	-6.71245283706758	6.31617297484667
H	6.17268239888271	-6.16611999590290	5.52514330744459
N	4.28517786122653	-6.63150343403811	8.11181452502310
C	3.06137410000111	-6.19740962288540	8.49781196836527
H	2.85717314528119	-6.94935809096709	10.49249787926627
C1	4.35477598324958	-5.02270331581642	4.46224961580151
C1	7.09639667786185	-7.25251801712882	7.36919972233524

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R2-Br-dimer1

N	-4.29954255035416	0.62515528966259	-0.61816376593167
C	-5.55001495841015	1.21783988025453	-0.83396720715803
H	-6.32714093313839	1.21025977694729	-0.05977883525445
N	-5.65541664962247	1.75624936482297	-2.03374415266074
C	-4.43048670672588	1.51466346786502	-2.64132467213630
C	-3.97355412000474	1.87759322647958	-3.96545218705414
O	-4.53004607611872	2.47326201507072	-4.86908225009620
N	-2.57824376324774	1.39226434544251	-4.14525912615517
C	-1.80283603338392	0.69326162833139	-3.21051637021841

N	-0.53920342441010	0.33808837497833	-3.58584329390653
H	-0.19022126762588	0.59035479779549	-4.51224057856504
N	-2.29516410397538	0.39354763441815	-2.00597758472289
C	-3.56761140531442	0.80953723656592	-1.77517440179525
H	-3.97211327469360	0.14740927164514	0.22428143638793
Br	-1.85893929032901	1.81870830247353	-5.88116230794462
Br	0.61381853623612	-0.60694023680936	-2.40964034950042
N	3.68988856228927	-2.16141760490596	-1.50910445245233
C	4.94595691399647	-2.74018733009971	-1.28812434388814
H	5.72587046845810	-2.72459986409949	-2.05937107094109
N	5.05267378067222	-3.27662996121882	-0.08757447230049
C	3.82285449288866	-3.04807809193885	0.51518067738493
C	3.36517064661297	-3.41445322954310	1.83809320155044
O	3.92475892969563	-4.00327997987436	2.74428449885887
N	1.96418934250177	-2.94363559592184	2.01255676524477
C	1.18446766746812	-2.25454218502863	1.07405396237653
N	-0.08533352918556	-1.91536336341890	1.44332269945897
H	-0.43047431635206	-2.15901776518658	2.37346114638529
N	1.67782351716274	-1.95086698956816	-0.12907471741859
C	2.95564681612756	-2.35301247246319	-0.35475245161986
H	3.36050652821183	-1.68724561468060	-2.35281328091555
Br	-1.23658416781104	-0.96410663681241	0.27054912372599
Br	1.24363673838176	-3.37524644118321	3.74664394126218

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R2-Br-dimer2

N	3.52385713008190	-1.80775738310371	-2.15928085324724
C	4.83301322061192	-2.29773648439445	-2.10306879726949
H	5.52777353534887	-2.17050018249095	-2.94247067637578
N	5.10266620595155	-2.90232764802178	-0.96038734832190
C	3.92657356461310	-2.81466059392302	-0.22715667968546
C	3.63249224288818	-3.28626424389158	1.10799396963796
O	4.36921539740708	-3.87842401405058	1.89334940087146
N	2.24874144359242	-2.94456184766055	1.46340135953527
C	1.34001231458857	-2.28192684671863	0.63449910246182
N	0.04937573918594	-2.14845388334288	1.11918577938008
H	-0.05530216105229	-2.20675921021575	2.13958579166099
N	1.65717203955895	-1.85666313096109	-0.57768218635347
C	2.92557908381747	-2.13446419424782	-0.95700517908600
H	3.07223469340786	-1.31187215150781	-2.92914070424086
Br	-1.07521666433864	-0.79812376921795	0.38743196818197
Br	1.75361806642306	-3.49248649949938	3.24962298141182
N	2.78304351336720	-6.57919001566119	9.89499174177417
C	1.47162949570709	-6.09556171756398	9.83719616465429
H	0.77894240036274	-6.21912909108639	10.67885640666835
N	1.19717645966021	-5.50151317544265	8.69012343607653
C	2.37232941591839	-5.58987656876716	7.95547489036416
C	2.66192201332259	-5.12779697656428	6.61598010053989
O	1.92124067998550	-4.54542853789398	5.82706924872210
N	4.04659407062544	-5.46626940326988	6.26079467983641
C	4.95986214625059	-6.11751239142498	7.09360252150597
N	6.25035112116114	-6.24865372857641	6.60796042007323
H	6.35341193717804	-6.19548426128841	5.58709866931647
N	4.64682325732912	-6.53445254164200	8.30979383310402
C	3.37773293614369	-6.25964146526296	8.68899930950352
H	3.23830230690285	-7.06667744500917	10.66805627608115
Br	4.53686246756811	-4.92691230274611	4.47055665745632
Br	7.38161205643135	-7.58989294455255	7.34639146576219

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R2-Br-trimer

N	-4.08079563875857	0.67071122236680	-0.37134992021653
C	-5.39772329101106	1.13002072026490	-0.48743595988139
H	-6.09605440409780	1.08185480817110	0.35705068817076
N	-5.66645715550987	1.60323365975656	-1.69004981653200
C	-4.48471744320182	1.45432946436178	-2.40276929675781
C	-4.19272040445846	1.78831318722887	-3.78124802939572
O	-4.89135979594434	2.27680949314124	-4.64990377644572
N	-2.78072132827826	1.42622025875646	-4.07718853739194
C	-1.85427426626050	0.86636151872546	-3.18936459729189
N	-0.56746093133709	0.69650204648547	-3.64644805631835
H	-0.44196662887757	0.65657086354696	-4.66292249833545
N	-2.20060869524933	0.57135578993710	-1.93726307843483
C	-3.47994361296095	0.87468880457473	-1.59862012403631
H	-3.63238042921400	0.26033095416975	0.45064199982696
Br	-2.27294549775841	1.82326808143469	-5.89438047721839
Br	0.60991607748481	-0.45030508297950	-2.65180411475300
N	3.76533633984653	-1.96809778242761	-2.20192894947378
C	5.09070595711632	-2.40399751487076	-2.09070629941657
H	5.80486144381451	-2.27554567257847	-2.91330608151735
N	5.34715191055184	-2.95988659552020	-0.92115592239744
C	4.14706019605973	-2.89234514654902	-0.22490311194892
C	3.83213375105104	-3.32583830100287	1.11744082233734
O	4.56284895049056	-3.86258036963233	1.94511872069110
N	2.42673246685256	-3.02037277865183	1.42375578238167
C	1.50498119399660	-2.42746410800638	0.55525419677092
N	0.21200654614097	-2.32659359992870	1.01314721046991
H	0.07317022994040	-2.41587959613324	2.02580851236702
N	1.85263491717963	-2.03640544605754	-0.67302613764633
C	3.14579101219784	-2.27722700659322	-1.00713579000317
H	3.32088175467077	-1.50077892398236	-2.99560897146023
Br	-1.01247088008192	-1.15439167925796	0.13590684374482
Br	1.91171463321630	-3.53237431333062	3.21360594364461
N	2.57606816949611	-6.53227771199434	9.88604020739163
C	1.27849267736233	-6.02518222367617	9.75717832424559
H	0.53928366424999	-6.13524744790153	10.56030610179015
N	1.07701589837333	-5.42800321351828	8.59672397429914
C	2.28857159929045	-5.53825107346634	7.92707815628406
C	2.65848220057665	-5.08459951677764	6.60546002994029
O	1.96785010536703	-4.49097789710272	5.77888123053832
N	4.05410257214167	-5.44476293318841	6.32524362454859
C	4.90938889209416	-6.11400653992640	7.20566450407492
N	6.22067613065104	-6.27300184443636	6.79044447124602
H	6.38251305703489	-6.22526001591577	5.77734433982353
N	4.52254288545325	-6.52359985711714	8.40265736167790
C	3.24070282297947	-6.22488836780090	8.71409942420834
H	2.97935584757701	-7.02763483712547	10.68270614719049
Br	4.65407402779700	-4.91559044323331	4.56704352518524
Br	7.28468311194519	-7.62773109223850	7.59821298402384

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R2-I-dimer1

N	-4.64602014974521	1.06470099760255	-0.82303541599977
C	-5.80189327780655	1.82276639029206	-1.05262401333998
H	-6.54368479147047	1.98946021764155	-0.26162648432139
N	-5.87004998192988	2.28343801031525	-2.28785587899490
C	-4.71979062548823	1.81356909179300	-2.90710286541107
C	-4.24345921466166	2.00617842967181	-4.26266278950642
O	-4.74819057768425	2.63002457782188	-5.18804445994013

N	-2.96131824929812	1.32002814679930	-4.44692946055346
C	-2.27622421154959	0.57478090630876	-3.48109321031495
N	-1.11218387886343	-0.04746270420858	-3.83042215520346
H	-0.67013443119061	0.25400485841122	-4.70438681764248
N	-2.75743475579815	0.44001531208747	-2.24431068230976
C	-3.93794453405626	1.04945943510994	-2.01107176395998
H	-4.36130251385700	0.59739674460348	0.03863329684198
I	-2.19949145330730	1.58552746605061	-6.45070909506394
I	0.20531254407588	-0.77386738638881	-2.30056242083555
N	3.73537006903171	-1.59004274821943	-2.17622767318417
C	5.02609576471339	-2.12262709412875	-2.19874155737403
H	5.68674110457780	-1.98640512184905	-3.06350316857878
N	5.32674698811197	-2.78064399257268	-1.09052192108650
C	4.19296042623393	-2.68807903777067	-0.30416163706983
C	3.93921028899388	-3.20895708156624	1.02659886580380
O	4.66724100688408	-3.85156891869436	1.76603348222428
N	2.59016727114088	-2.82044114804086	1.46500711606037
C	1.64769159655081	-2.10880902613696	0.72181989024630
N	0.38109781171734	-1.91244497997949	1.23397002798004
H	0.28941927047505	-2.34032857392367	2.16664631143397
N	1.93978017846031	-1.67026178241887	-0.50874826057447
C	3.18749406281211	-1.94546886434606	-0.96229611518971
H	3.24705572664099	-1.06810823990773	-2.90916859505687
I	-0.30470938447364	0.13209550579867	1.53897801328965
I	2.21481450283548	-3.44707964653472	3.49610570041729

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R2-I-dimer2

N	3.90544664991342	-1.65766368631770	-2.09034892544013
C	5.15059289462392	-2.29510183931308	-2.03503302914226
H	5.86106173513787	-2.23413654036599	-2.86882713817627
N	5.34056055621745	-2.94597148189600	-0.90216941500203
C	4.17543860529407	-2.73839661420356	-0.17481884233432
C	3.81354363888229	-3.19105200279727	1.14910185061500
O	4.47997952810710	-3.87877129511624	1.92606764086870
N	2.48367934891145	-2.70883276959490	1.51323135729305
C	1.66254914394048	-1.93444608372839	0.69170650473999
N	0.39414141884356	-1.65512189642031	1.15865760733244
H	0.25670014205088	-1.74155187502726	2.17433437929955
N	2.03661872315328	-1.52252797522690	-0.51471413714005
C	3.26403227953512	-1.93567002665257	-0.89781049944427
H	3.52032305361153	-1.09952300091228	-2.85358625909801
I	-0.68966819624058	-0.03311187774105	0.34739205184693
I	1.88965316729233	-3.33040870105581	3.48633202264788
N	2.82208103052110	-6.93194711249857	10.07182881937347
C	1.58083951238379	-6.28670508183401	10.01917177225059
H	0.86841781124405	-6.34947944814285	10.85116351596021
N	1.39671423968575	-5.62632723085307	8.89082924364216
C	2.56177594841196	-5.83551802373416	8.16389547343383
C	2.92893441553101	-5.37499887518006	6.84413500430845
O	2.26856224684716	-4.67612657887642	6.07185837137213
N	4.25598040274965	-5.86316693539667	6.47834184764649
C	5.07118354140280	-6.64855587872919	7.29546665136121
N	6.33840082099823	-6.93242736843992	6.82827709957746
H	6.47787740337616	-6.83916911004723	5.81348937776127
N	4.69270591043464	-7.06663907522731	8.49835795556851
C	3.46715386751697	-6.64900607357861	8.88245832207514
H	3.20263865638735	-7.49769025645009	10.83175720145512
I	4.85539301501687	-5.23444222161075	4.50908652513988

I	7.41190959298925	-8.56580014449225	7.62997619798399
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R2-I-trimer			
N	-4.62373238970876	1.08034329536566	-0.81259036100336
C	-5.79053693401013	1.82155241635395	-1.04364923166723
H	-6.52855323477775	1.98938652425660	-0.24935130720767
N	-5.87249508669183	2.26616438440361	-2.28370164623427
C	-4.71979998488754	1.80293645752065	-2.90505829024276
C	-4.25485074541977	1.98239479304529	-4.26608279251505
O	-4.77389785170531	2.58782460096053	-5.19650485999602
N	-2.96665791764639	1.30847240133752	-4.45023567471190
C	-2.26375147126110	0.58503921551063	-3.47930451286208
N	-1.09290531362178	-0.02125522749303	-3.82392549688184
H	-0.66713195091662	0.25413794970184	-4.71365929473416
N	-2.73721303342042	0.46100110330064	-2.23761369574345
C	-3.92314359403666	1.05924140664178	-2.00501861991464
H	-4.32725619051100	0.62606936182246	0.05210185933087
N	3.73895321895566	-1.58306929246360	-2.17539788138984
C	5.03004236431936	-2.11522705579253	-2.18883904324719
H	5.69637050340443	-1.97725343230396	-3.04904783859956
N	5.32344207948427	-2.77423207979546	-1.07963035301778
C	4.18249185038739	-2.68238966164539	-0.29901311804058
C	3.91442409909333	-3.20995629673612	1.02341996775251
O	4.65426258763040	-3.86880505514499	1.74884269656237
N	2.57093797501670	-2.82261140587804	1.46435148113444
C	1.64318499374022	-2.10875798879285	0.71259527372722
N	0.37428486411540	-1.91042765451791	1.22321437990363
H	0.28615390492093	-2.33871471641424	2.15773883623817
N	1.93241073092297	-1.66467310494105	-0.51963878589772
C	3.18248126202934	-1.93951188062411	-0.96505493870740
H	3.25487679207651	-1.05972587707273	-2.91001027102896
N	2.63188945525958	-6.83410295988674	9.99136492923592
C	1.42572084586826	-6.13993310807371	9.83330962438112
H	0.64775082269273	-6.16259851931748	10.60662259655577
N	1.35817795672677	-5.48831918289931	8.68733293183041
C	2.56663137435764	-5.75521906021805	8.05812522527514
C	3.05710776112005	-5.32558350474680	6.77080644754039
O	2.47742610320638	-4.59610173048142	5.95779951317798
N	4.38123750563339	-5.87035592286143	6.50755038151689
C	5.09981103463325	-6.68264566076441	7.39378927563446
N	6.38017643104125	-7.03320531326433	7.02850803398049
H	6.61367198951954	-6.95735064376529	6.03074349515534
N	4.61045801182355	-7.06506708915623	8.56692021764681
C	3.37863923416068	-6.59452716765525	8.85441240118186
H	2.92640814313661	-7.40388510321513	10.78599475651604
I	-2.22192936718179	1.55679573802393	-6.46376618134994
I	0.22544164102598	-0.75666979929157	-2.29524980604269
I	-0.30639768756499	0.13345374910481	1.53623471010825
I	2.18386046831423	-3.48068312482173	3.48183105906469
I	5.18098488289096	-5.31901863481409	4.58444488941114
I	7.34734954585413	-8.64978860250093	7.97028765417411
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R2-At-dimer1			
N	-4.55457932966125	1.15586052140090	-1.06475401575313
C	-5.71761071703971	1.89934347373101	-1.28970474507083
H	-6.49232614567831	2.00001443149700	-0.51947359881722
N	-5.75490130138156	2.43816334013276	-2.49873027657188
C	-4.57573930180776	2.03991749285819	-3.10270230292446

C	-4.04726572684533	2.32346499081935	-4.42747253216768
O	-4.54733292422554	2.99026887661441	-5.32853487264915
N	-2.75045450214496	1.69099945631979	-4.60639575453785
C	-2.07351132848569	0.91268268599623	-3.66705719418899
N	-0.86577219316513	0.37820758772677	-3.95531032110435
H	-0.43707200808320	0.61280038254075	-4.85543789180274
N	-2.60820002737093	0.67763140038267	-2.45567103125929
C	-3.80409386660780	1.23578267828239	-2.22521755709501
H	-4.27546830205020	0.64754287174891	-0.22257596679512
At	-1.90440160008875	2.13248633598866	-6.67270278665084
At	0.24256632753580	-0.77465875375552	-2.34313386715063
N	3.69947382453033	-1.74542723187153	-1.55366380904762
C	4.97304960883489	-2.18867377162997	-1.19337584947535
H	5.84900798038463	-1.98490693569291	-1.82067211546242
N	4.97706706357058	-2.85419005079313	-0.04793255294138
C	3.66014539490145	-2.85533971312837	0.36807404199110
C	3.05929043426962	-3.42124405334025	1.56645180376526
O	3.59892292751766	-4.02900436697074	2.48079815618687
N	1.63170225396905	-3.14518190068727	1.59016777325126
C	0.88321424979968	-2.47854105504957	0.61630775532653
N	-0.46841875615556	-2.33634103725368	0.71084230974033
H	-0.82287232383573	-2.86573068340881	1.52165868572596
N	1.50405264030190	-1.98522159807468	-0.48546897037259
C	2.84384888424193	-2.16523135380005	-0.55664987798981
H	3.41787992178021	-1.21712418953517	-2.38453833840260
At	-1.25441521346644	-0.14897380842440	1.42585159365985
At	0.70429911445611	-3.89901136462373	3.51622498458379

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R2-At-dimer2

N	3.57538461786264	-1.79066567646080	-2.00011192679310
C	4.86061730147410	-2.34379367404472	-1.95872599885152
H	5.56922648713726	-2.20477900636524	-2.78469594745372
N	5.08988178814323	-3.02139238753543	-0.84858607021049
C	3.90970726018655	-2.92143513348115	-0.12306725528242
C	3.57090154480855	-3.43874408736269	1.18247119171840
O	4.29554150813855	-4.11256008545832	1.92936558627370
N	2.22545411900213	-3.05790421396246	1.56280254456078
C	1.35325950936218	-2.31991286051412	0.76434055958103
N	0.06544732877764	-2.15102182110940	1.22888835228037
H	-0.04967309057920	-2.27499032037332	2.24546346730659
N	1.69645588713933	-1.84231802107426	-0.43193048297518
C	2.94802977006543	-2.15549356923717	-0.82287702460918
H	3.15648638965549	-1.23359532251230	-2.74610955601659
At	-1.11537267604205	-0.38596994098550	0.52557583465710
At	1.67258787952830	-3.80553302890393	3.63351723469835
N	3.15304176364329	-6.89642987097540	10.27050534454393
C	1.84583516084153	-6.40175736303409	10.19342838252593
H	1.16487781993480	-6.45087925544246	11.05220439871633
N	1.55873205205635	-5.89876266013152	9.00657642838483
C	2.71800908334442	-6.06882695600465	8.26071486775693
C	3.01522651993336	-5.68892870778510	6.89906498210831
O	2.25061162214434	-5.13253185883061	6.09724971975228
N	4.37817765127776	-6.03024609709246	6.54544865092788
C	5.27917456259522	-6.67665051358333	7.39058920225680
N	6.49741605651816	-7.03658140482507	6.85421938244918
H	6.77468947121774	-6.51343701297840	6.01090651362977
N	4.98298829016057	-7.00542977494308	8.64802197484769
C	3.72965506541873	-6.68907888214284	9.03084031743837

H	3.61255771492962	-7.33076002721851	11.07196034920075
At	4.90815263003410	-5.39625301153464	4.43019522829744
At	8.24848939328989	-7.29742991209705	8.22036525827943
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R2-At-trimer			
N	-4.17350422402105	0.92468539051299	-0.44463082984765
C	-5.37390039390070	1.64410718066825	-0.45553537287098
H	-5.98532486344836	1.75280206580350	0.44868866131709
N	-5.65604240430191	2.14961408634507	-1.64505455215783
C	-4.60728810139918	1.75300992345155	-2.45885281219315
C	-4.35019532691338	2.01157963683715	-3.86544210565853
O	-5.02713852866318	2.64884543512939	-4.66773665274497
N	-3.09936317850105	1.39412825259168	-4.27799134871265
C	-2.23576096018314	0.65121809424021	-3.47141299556873
N	-1.09559281237451	0.12737770454392	-3.97772545811553
H	-0.83733350653018	0.37041677997517	-4.93794084096159
N	-2.52297141208852	0.44009448374645	-2.17554714147288
C	-3.66483286030544	0.98524194227316	-1.73052205149835
H	-3.72446753565796	0.44457110383147	0.33814168793209
At	-2.67432979323496	1.80900094923165	-6.47638615723182
At	0.35233606937345	-0.89703504403347	-2.55538784132022
N	3.92739512413902	-1.74465647944875	-2.36597584252686
C	5.25742428339362	-2.14528804058164	-2.22589238877123
H	5.99514932079759	-1.96551527993310	-3.01734251973688
N	5.49353792284366	-2.73988783432435	-1.06633504540372
C	4.27544997086147	-2.73669883847748	-0.40901993042528
C	3.92011156838438	-3.24171376612775	0.90472810181149
O	4.66555996284391	-3.79652997031635	1.71565240082716
N	2.52231626981372	-2.98712687826193	1.19689591035170
C	1.60276399263465	-2.39241136030764	0.33770450453755
N	0.28393364986043	-2.26969070444654	0.68495984035767
H	0.11484621899785	-2.75644852360297	1.58021465216542
N	1.97745595911500	-1.95619534220133	-0.89184530962785
C	3.28451201398943	-2.11658935484628	-1.20336250122712
H	3.48149661799208	-1.27136835350097	-3.15705685233842
At	-0.41983507445589	-0.08463607459452	1.37763988498917
At	1.99107240543796	-3.65767076867061	3.30413002695028
N	2.36820182147455	-6.71238140734376	9.89691769239127
C	1.10437230599961	-6.18206373261149	9.60820104672283
H	0.27095690011444	-6.27518021609768	10.31548548024709
N	1.05690637607074	-5.58531399642903	8.43146470225076
C	2.33942612279730	-5.71801219166728	7.91734243260279
C	2.88674586124418	-5.28209177985026	6.65618019365801
O	2.27436987038511	-4.65890213414717	5.77218131174966
N	4.27332815376526	-5.66430755889600	6.51894271140585
C	5.01057866859698	-6.33977304660560	7.49687632024761
N	6.35214513268952	-6.53074930484990	7.25980368461562
H	6.64277373114503	-6.47539835177360	6.27365408581954
N	4.47522401643462	-6.73868900542146	8.64918752730211
C	3.17681159068194	-6.42013094426866	8.81528673638916
H	2.65995453013948	-7.21137546264235	10.73863354939498
At	5.19387287068478	-5.05748074092965	4.53347600491030
At	7.42365935327771	-8.17223300197204	8.32060603546499

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N	-1.87124500	0.82698500	6.52368300
C	-3.06849700	0.48487600	5.89715600

H	-4.02923700	0.51572500	6.42378900
N	-2.88369400	0.13201600	4.63351200
C	-1.51480300	0.24729100	4.41417800
C	-0.72715500	0.00857200	3.22839600
O	-1.11612300	-0.36575500	2.10928200
N	0.64784500	0.26372300	3.45976600
H	1.25944900	0.21127700	2.60188600
C	1.19521200	0.67314200	4.66455800
N	2.53541600	0.87013600	4.71400600
H	3.21213600	0.53444300	3.99316400
H	2.89700000	1.12769500	5.63137600
N	0.46182300	0.89599500	5.77179000
C	-0.85452300	0.68049000	5.58610800
H	-1.74443400	1.13903100	7.48689400
N	6.53349600	-0.73275700	1.89369500
C	5.89801500	-0.37914000	3.08282000
H	6.42803200	-0.36157300	4.04204900
N	4.62187300	-0.07776600	2.89230200
C	4.40331500	-0.24063600	1.52810100
C	3.20705900	-0.06990600	0.73810900
O	2.07506400	0.27009700	1.12038200
N	3.44510600	-0.35368600	-0.63033700
H	2.58546200	-0.34464100	-1.24236500
C	4.66342000	-0.73200600	-1.16976800
N	4.71775700	-0.96271300	-2.50473900
H	3.99077700	-0.65382000	-3.18781300
H	5.64460400	-1.19316900	-2.86068300
N	5.77930600	-0.89500300	-0.43384900
C	5.58865300	-0.64984300	0.87661600
H	7.50674300	-1.01467400	1.77275200
N	1.89251700	0.65057600	-6.49425600
C	3.07882900	0.28295400	-5.86160800
H	4.03929500	0.27042100	-6.38952100
N	2.88441000	-0.03628200	-4.59042500
C	1.52046900	0.12870600	-4.37218500
C	0.72647500	-0.05856000	-3.18097900
O	1.10369500	-0.41932100	-2.05344800
N	-0.63977500	0.23501100	-3.41808600
H	-1.25293400	0.22500100	-2.55949800
C	-1.17502500	0.63437100	-4.63151300
N	-2.50895900	0.87182400	-4.68403000
H	-3.19329200	0.55213000	-3.96309600
H	-2.86428800	1.11401200	-5.60810900
N	-0.43606400	0.81045900	-5.74326900
C	0.87306400	0.55771900	-5.55289100
H	1.77446900	0.94635200	-7.46371900
N	-6.52059300	-0.69042100	-1.85303800
C	-5.88364000	-0.35804000	-3.04748800
H	-6.41046600	-0.36557500	-4.00860900
N	-4.61011300	-0.04433500	-2.85967900
C	-4.39481400	-0.17677100	-1.49168400
C	-3.20273400	0.01943800	-0.70163700
O	-2.07153700	0.35992600	-1.08685600
N	-3.44308600	-0.23759800	0.67137200
H	-2.58313700	-0.22178600	1.28239800
C	-4.66004700	-0.61369200	1.21540000
N	-4.71621300	-0.81706100	2.55450900
H	-3.99108200	-0.49419800	3.23280200

H	-5.64122500	-1.04896600	2.91412700
N	-5.77276700	-0.79871200	0.47974800
C	-5.57953100	-0.57977700	-0.83496800
H	-7.49233500	-0.97618600	-1.72911400

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C	2.16748100169149	5.35702377351588	-0.00000014932829
C	0.94617048696471	4.64646067603288	-0.00000020745789
N	-0.13291116039171	5.52391866232098	-0.00000023711723
C	0.39855795171286	6.73750484743802	-0.00000022622456
N	1.79123387086493	6.69599748443451	-0.00000016824586
N	3.41971907338246	4.86494905639116	-0.00000009373494
C	3.45920257329553	3.51821418418118	-0.00000010787798
N	2.32353242918178	2.72352872826395	-0.00000018074128
C	0.98672647166232	3.20298878637836	-0.00000022213282
O	0.03469450734825	2.40638428425714	-0.00000026551238
N	4.66653434674975	2.90735136551822	-0.00000005534022
H	-0.15578086278789	7.68301983455538	-0.00000024875820
H	2.41989403624943	1.67454494621311	-0.00000019490848
H	5.46830012052890	3.53567550278923	0.00000001655009
H	4.84565517961312	1.87876377665514	0.00000000312678
H	2.43360761245128	7.48884332509938	-0.00000014485080
C	-5.35702498286719	2.16748009641338	0.00000030975858
C	-4.64646179690869	0.94616962859401	0.00000006668860
N	-5.52391969479191	-0.13291209693251	0.00000014477458
C	-6.73750592188571	0.39855692293033	0.00000042471896
N	-6.69599866823882	1.79123285778429	0.00000054186386
N	-4.86495033536569	3.41971819300914	0.00000033091334
C	-3.51821543541858	3.45920177807397	0.00000009740595
N	-2.72352988370084	2.32353170390682	-0.00000013791756
C	-3.20298991171381	0.98672572623333	-0.00000016727035
O	-2.40638538873475	0.03469379048974	-0.00000035303857
N	-2.90735261161006	4.66653352868761	0.00000010098589
H	-7.68302086283256	-0.15578197249339	0.00000055793832
H	-1.67454594269943	2.41989339232100	-0.00000021475578
H	-3.53567674093649	5.46829931291280	0.00000032656963
H	-1.87876482976524	4.84565426829855	-0.00000004530093
H	-7.48884453708676	2.43360655935509	0.00000075975795
C	-2.16748194499488	-5.35702483973230	-0.00000017314949
C	-0.94617136247415	-4.64646184430977	-0.00000017744071
N	0.13291017439549	-5.52391996822163	-0.00000015274023
C	-0.39855904332996	-6.73750611275067	-0.00000013607806
N	-1.79123494799573	-6.69599860100893	-0.00000014148433
N	-3.41971995485878	-4.86495000460207	-0.00000018168175
C	-3.45920333670785	-3.51821511359047	-0.00000020710449
N	-2.32353312709102	-2.72352975325973	-0.00000022919646
C	-0.98672721065354	-3.20298992272895	-0.00000020763254
O	-0.03469525192983	-2.40638536616044	-0.00000021552216
N	-4.66653501882599	-2.90735213898110	-0.00000022220548
H	0.15577967894702	-7.68302114758326	-0.00000012043322
H	-2.41989464846978	-1.67454587697754	-0.00000028163873
H	-5.46830087577111	-3.53567617630763	-0.00000019146994
H	-4.84565566278696	-1.87876439996264	-0.00000009368376
H	-2.43360878699534	-7.48884436070121	-0.00000013175286
C	5.35702587392802	-2.16747860453696	0.00000026910381
C	4.64646204471476	-0.94616850936630	0.00000009068577
N	5.52391937379936	0.13291368954058	0.00000013776010
C	6.73750588262438	-0.39855468685896	0.00000032435554

N	6.69599936143477	-1.79123065359814	0.00000041676555
N	4.86495189219687	-3.41971695197287	0.00000029646325
C	3.51821699324517	-3.45920125220936	0.00000012877565
N	2.72353081975457	-2.32353161906436	-0.00000004435965
C	3.20299017633460	-0.98672538945110	-0.00000007206905
O	2.40638519645842	-0.03469382547361	-0.00000021676838
N	2.90735472932142	-4.66653324824638	0.00000012535343
H	7.68302053831065	0.15578470494884	0.00000040635834
H	1.67454674380477	-2.41989384680983	-0.00000012839650
H	3.53567921143831	-5.46829875583866	0.00000029294173
H	1.87876682125485	-4.84565441251857	0.00000000746498
H	7.48884556696079	-2.43360393529464	0.00000056824123

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C1-G4-1

H	-1.02626628581307	-3.11669730300382	6.73895462135718
C	-0.64584948115100	-1.42932951839222	5.46963559007455
N	0.24467610182841	-1.88653247757742	4.55821363107484
H	1.89365456900292	-2.32851086624168	3.01213735455191
C1	1.15590814713912	-1.41962511241202	1.03192474371980
N	1.67904295185756	-1.34403012037294	2.80003855752624
C	0.65743967144836	-0.97439698090235	3.68495699873582
C1	0.87298462825515	1.49044344919201	2.56721347203025
N	0.18663287057144	0.32804004458288	3.67681451487990
O	-1.31075663555059	1.98894326727211	4.39097914270330
C	-0.88163957128808	0.85892605852677	4.55087074435327
C	-1.24551820871194	-0.15114394267174	5.52667510749962
N	-2.16535604015130	-0.08511152659208	6.55813083699667
H	-2.72674339889799	-1.60022007704260	7.98672051662405
C	-2.13082439921746	-1.28198501111796	7.12249926656228
N	-1.22537310504833	-2.14337529814487	6.50358026629353
H	5.76101020982389	-1.72322845962741	2.81233514913330
C	4.67237747557493	-0.49479146489447	1.42932051850282
N	4.59997214957147	-1.23890119262223	0.30182890844909
H	4.47132425632558	-2.18324654836522	-1.80359362112508
C1	2.25752513893498	-1.96012317267880	-2.37105996730237
N	3.94520613272301	-1.30840791432833	-1.94430360688490
C	3.97489831634169	-0.64752560696831	-0.70847344069771
C1	2.66459106974918	1.34545929967371	-2.01737205817635
N	3.42113075560014	0.62068734910485	-0.61506783614818
O	2.74064960250461	2.49120373811257	0.62785630635210
C	3.35339235471815	1.43739222798942	0.61077348514863
C	4.09749754749594	0.77337006355959	1.66656037326364
N	4.31725093573103	1.17713360439790	2.97051807954424
H	5.37185244110135	0.16456207556165	4.55559767956633
C	5.00944238861873	0.19195393515946	3.52071888949891
N	5.25922215934157	-0.85274854297171	2.63161465068604
H	0.95260914214244	-3.29421976060285	-6.67700586003004
C	0.61770044327069	-1.56919522603202	-5.44601847799702
N	-0.28115523770600	-1.98314783732545	-4.52211269668742
H	-1.93516197047222	-2.34934140087558	-2.96215857390125
C1	-1.17170574027889	-1.41065700218163	-1.00585189457896
N	-1.69722958320893	-1.36533379463548	-2.77424680057205
C	-0.66943992053940	-1.04100343182407	-3.66957169266672
C1	-0.82292089664808	1.45423476050299	-2.61041123060601
N	-0.16745977358913	0.24946509143024	-3.69321965299093
O	1.36753812855449	1.85650081693417	-4.44957485513223
C	0.91136380315548	0.73350992059133	-4.58154981112041
C	1.24820878316103	-0.30771861924504	-5.53416236439165

N	2.16638970810281	-0.28818833734687	-6.56904334609408
H	2.68658342617689	-1.84940920426183	-7.96317372810826
C	2.10102095434586	-1.49658475861480	-7.10534678729208
N	1.17658104902516	-2.32104158345898	-6.46444530658255
N	-5.26017966910687	-0.79628719342552	-2.62651198145854
C	-4.98654047812525	0.22209494207667	-3.53874178025970
H	-5.34832208391855	0.17909143231363	-4.57333732584525
N	-4.27383518229940	1.20438672663247	-3.00992924313775
C	-4.06460686585799	0.82578469797413	-1.69664883319444
C	-3.30744123160722	1.49730308686732	-0.65505731984871
O	-2.67201487403046	2.53684904761604	-0.69482019943268
N	-3.39388674721778	0.70990691141549	0.58889025877926
Cl	-2.62054042021718	1.44865686066748	1.97460263815137
C	-3.97639833039774	-0.54275826186942	0.71052397705726
N	-3.96424959247070	-1.17543934922461	1.96130986836561
Cl	-2.29336327725738	-1.85525884422878	2.40881122441317
H	-4.50991834942193	-2.04107939834525	1.83928137390990
N	-4.61311212609250	-1.14314276773374	-0.28717372251694
C	-4.66742720332719	-0.42376053914734	-1.43156025710012
H	-5.78044063257359	-1.65964136884738	-2.78834447392451

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N	-2.34960379570621	-0.18440001757676	7.89086574128327
C	-3.61205054045459	-0.34093684180513	7.32880931280079
H	-4.48809620110751	-0.63687722644980	7.91625780168803
N	-3.60282368601905	-0.08612087049968	6.03034101390742
C	-2.29643996372291	0.25440766892535	5.71326412765319
C	-1.71698272611758	0.64117790690539	4.43972386001219
O	-2.22981145915417	0.74683719156779	3.34310889864270
N	-0.28017132905673	0.96169832061418	4.64658147354801
C	0.42462420274819	0.83160813786231	5.84160404876096
N	1.74889209596305	1.22158165768114	5.91946453112957
H	2.07174728177068	1.04269898969360	6.87821599248234
N	-0.16412609999675	0.42558410435630	6.96954988094478
C	-1.49074113768833	0.19957740970823	6.86903159439659
H	-2.08050777989211	-0.33054232088637	8.86475128940239
Cl	2.96352950901133	0.40934995686270	4.80165044620625
Cl	0.50675676163107	1.62084476217862	3.23228292414656
N	5.93271187730829	-1.95884080907079	1.98956386478356
C	5.35076883164943	-1.65060435096102	3.21375935192403
H	5.56555936852243	-2.21471154852280	4.12805897651653
N	4.52824936443875	-0.61859623189488	3.11953524226052
C	4.55511904104295	-0.22561136839718	1.78909340842798
C	3.86572172226195	0.86399276514600	1.11930824758502
O	3.09704471330914	1.69975744784274	1.55435642352911
N	4.27921029767741	0.88269708318578	-0.30681065270516
C	5.13760046385633	-0.02114206028084	-0.92978304442793
N	5.47996182746203	0.16036360472268	-2.25863128293595
H	6.13556146589342	-0.59170050331829	-2.50599965024371
N	5.71668654479146	-1.01737953402652	-0.25844253617154
C	5.43516263720039	-1.05445381429587	1.06129179140496
H	6.59229254204940	-2.71101696381084	1.78533006670260
Cl	3.67462479350500	2.25989802661051	-1.19024853097338
Cl	4.09149377887339	0.00055035001225	-3.48363814312919
N	0.93937018983726	-0.29160522332910	-6.95738756585974
C	2.19877350294013	-0.46538058812012	-6.39357383363881
H	3.06846645608480	-0.78683738417890	-6.97704604759129
N	2.19539470935407	-0.19213304244681	-5.09883007999407

C	0.89623388984091	0.17867982018780	-4.78613193467680
C	0.32542720981721	0.59484007827726	-3.51799958218545
O	0.84095289838482	0.70581420942969	-2.42319470833479
N	-1.10505937423559	0.94027639466902	-3.72869728130318
C	-1.81287112869854	0.80807034701508	-4.92168568827655
N	-3.12904898553740	1.22365128676990	-5.00491682590691
H	-3.45549608604896	1.03793278482919	-5.96115216389469
N	-1.23292691198393	0.37489546072544	-6.04405645795686
C	0.08890910790526	0.12365883208875	-5.94074457153266
H	0.66695306593232	-0.44588463633128	-7.92907438932240
C1	-4.36000552475864	0.45129101007651	-3.87656410059583
C1	-1.87863574934781	1.63173561509669	-2.32243754337209
N	-7.38366185489673	-1.82130503352958	-1.04452504501686
C	-6.79430960913376	-1.53656462628467	-2.27093210639854
H	-7.02312366771528	-2.10174841279933	-3.18115646647899
N	-5.94645302211366	-0.52461238247410	-2.18410520836935
C	-5.96359175072344	-0.12124451173581	-0.85667182167113
C	-5.24847526203485	0.95684947592778	-0.19521832818186
O	-4.46050440211109	1.77105678074107	-0.63663242622820
N	-5.66127400964334	0.99635027366826	1.23057665499369
C	-6.54129557724420	0.11831272312880	1.86026676591314
N	-6.87902959299423	0.31825307884350	3.18761975281324
H	-7.55263924702450	-0.41567783201024	3.44093012023372
N	-7.14449214296642	-0.86866995642426	1.19647859533388
C	-6.86390045338713	-0.92265693832467	-0.12290470977219
H	-8.06297752034367	-2.55430657565922	-0.83519782252712
C1	-5.02483891399231	2.36610861683103	2.10312235670903
C1	-5.49471964521143	0.13531743326353	4.41399499353723

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C1-G4-3

N	-2.03144405404214	0.57419978462537	6.62777275547600
C	-2.71414416039446	-0.63805754521011	6.54311903148189
H	-3.57449711237742	-0.86264077184247	7.18479186831782
N	-2.21056447252456	-1.43693717344958	5.61495712935402
C	-1.15681704191303	-0.72509175603973	5.05804101924553
C	-0.28963918604767	-1.08115651658521	3.95113945276180
O	-0.19979475331891	-2.10818001681607	3.31130297568246
N	0.52260115239806	0.11548186022719	3.58038797044445
C1	1.14600156874043	0.03362447142690	1.93662969867952
C	0.58622319335039	1.30908078927586	4.28957708361865
N	1.34199518483065	2.36676250796658	3.80835294951578
C1	3.09790845072955	2.11896919927317	3.47687413907914
H	1.26516602067458	3.15485152645310	4.46259969359540
N	-0.14540307415461	1.52352586201026	5.37930740191122
C	-1.03650186113093	0.54282729971211	5.66345862306263
H	-2.22926555914870	1.36079470055830	7.24833053482837
N	6.64443174011593	-0.52132113680623	2.02053005252014
C	6.53828606039867	0.69915001126294	2.68544091200817
H	7.18376942709272	0.95223439895916	3.53497871810904
N	5.58635457420435	1.46809986181742	2.17970084944708
C	5.03520593951295	0.72696484190069	1.14326565296482
C	3.91245021199815	1.04373332778687	0.28106801993176
O	3.24941376064183	2.05480324269161	0.17946005115608
N	3.56014976731225	-0.17495571729630	-0.50610963934852
C1	1.90855974848190	-0.14059566755086	-1.11301133803724
C	4.29800099465513	-1.35140363837816	-0.56114085582017
N	3.83564167437823	-2.43061073805138	-1.29816126027699
C1	3.47797754150054	-2.21143276170467	-3.05341613343223

H	4.51136631687553	-3.20032145012033	-1.21977255713063
N	5.40026071596877	-1.52852026021074	0.16172216583666
C	5.66941725349440	-0.52811656792660	1.03557849695289
H	7.28586886254259	-1.28964694059454	2.22355651915520
N	2.03982065339235	0.39967520707326	-6.60372291147955
C	2.69989634606644	-0.82248926585945	-6.48828677741041
H	3.55394993908405	-1.08041729686809	-7.12579712744121
N	2.18411782015624	-1.58648585660655	-5.53773863307224
C	1.14566428763597	-0.84019945534365	-4.99734384936929
C	0.27481739247287	-1.14999271184387	-3.87953588392619
O	0.16735425272599	-2.15749563676854	-3.21198732754135
N	-0.51324709979851	0.07156513688212	-3.53867834821326
C1	-1.13346489295488	0.04440304152392	-1.89194661671666
C	-0.55678509155918	1.24661266126543	-4.27965140572151
N	-1.29105406599860	2.33114675224263	-3.82595371343306
C1	-3.04903163965283	2.12596965194138	-3.47736962067460
H	-1.20267724848124	3.09903045210719	-4.50246667674263
N	0.17538149829487	1.41753681273424	-5.37681182619293
C	1.04719910634060	0.41301877987775	-5.63650417878310
H	2.25032424644047	1.16515117979674	-7.24615456591738
N	-6.63075082264189	-0.42347446615374	-1.97954058927909
C	-6.50303642571370	0.78400437065559	-2.66392480833391
H	-7.14189225256462	1.03364550289371	-3.51943897825165
N	-5.54005488261156	1.54553744056759	-2.16789080181823
C	-5.00378462982194	0.81270042580689	-1.11789236959773
C	-3.87817765810560	1.12528210763146	-0.25780375494529
O	-3.19882545466447	2.12695684298036	-0.17154818766208
N	-3.54866705213598	-0.08516197523467	0.55129940867579
C1	-1.89816009350405	-0.06859714239328	1.16251323391333
C	-4.30556587459649	-1.24864403214053	0.62286171558175
N	-3.86276548210642	-2.32258393734821	1.37937074290000
C1	-3.51110572443349	-2.07929760202981	3.13254631483851
H	-4.54983281269423	-3.08315444856528	1.31053761041252
N	-5.40822154127721	-1.42005239046023	-0.10069314374560
C	-5.65863882853201	-0.42992309686568	-0.99168146800549
H	-7.28434685360607	-1.18435707886321	-2.17163144313808

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C1-G4-4

N	-11.20821850962558	-8.27054056945251	-1.07205399518447
C	-11.61156803294244	-6.94428154662673	-0.90745305933355
H	-12.63563321532312	-6.61737678893907	-1.12114428567239
N	-10.63164641897022	-6.16597847444064	-0.48361688788162
C	-9.52912884035602	-7.00067880450769	-0.35663951001877
C	-8.16384820350918	-6.82111836564827	0.01447573403327
O	-7.76924757209636	-5.59395260824990	0.37192299412547
N	-7.33099614993425	-7.85812088509610	0.00414714514570
C	-7.78292818997051	-9.08656740407278	-0.36260433759204
N	-6.91131082867852	-10.15269617401467	-0.27698428344865
H	-7.21703781135590	-10.99188077446881	-0.77696429519771
N	-9.04461231584879	-9.39381101820123	-0.76430748573802
C	-9.86445596727124	-8.33772756610331	-0.72544704994998
H	-11.77614121599413	-9.05670163663661	-1.38926504321611
C1	-5.91839046049432	-5.47071774842089	0.54361095146387
C1	-5.15440274013900	-9.92704901764218	-0.32670751929355
N	-0.41071048256369	-10.34709319186705	-1.07904680570716
C	-1.73612263164917	-10.75048905742813	-0.90825502535862
H	-2.06489472145044	-11.77332860836842	-1.12488485403162
N	-2.51125528240196	-9.77212036849546	-0.47510908354030

C	-1.67517425662723	-8.67061887533764	-0.34789209353282
C	-1.85198804199535	-7.30665095116891	0.02909455604066
O	-3.07703553865879	-6.91308627576617	0.39534218796808
N	-0.81484544679847	-6.47368571098587	0.01589054602117
C	0.41091950955053	-6.92506840278405	-0.36091401994964
N	1.47770922321782	-6.05415144097847	-0.27924796980981
H	2.31452858555451	-6.35844948524422	-0.78396052981140
N	0.71532666430494	-8.18529951144095	-0.76952682265975
C	-0.34063867204684	-9.00499045481714	-0.72660306081426
H	0.37317336198041	-10.91396538950363	-1.40369688626472
Cl	-3.20294039579842	-5.06193742680099	0.56052885591083
Cl	1.25292438154319	-4.29707503855828	-0.31808983717800
N	1.67256288940164	0.44155555935703	-1.08027695637839
C	2.07717913931931	-0.88187641111758	-0.89734696210652
H	3.10016855787592	-1.21183295604748	-1.11146705573127
N	1.09967877285527	-1.65386732748640	-0.45673361405842
C	-0.00268180261072	-0.81768520574929	-0.33709041914349
C	-1.36654522487947	-0.99265812103258	0.04125615152305
O	-1.75850229938613	-2.21454739619293	0.41938524553562
N	-2.20069141152627	0.04355257088336	0.01805069144070
C	-1.75064682613233	1.26585403126439	-0.37082236786401
N	-2.62239251171566	2.33299194644498	-0.29991959221866
H	-2.31765931094659	3.16469756213486	-0.81280409109865
N	-0.49052505848530	1.56796572645987	-0.78189967878590
C	0.33046780271047	0.51352643836334	-0.72816318381899
H	2.23865775706347	1.22294886014697	-1.41220013915923
Cl	-3.61087113695371	-2.34622584601304	0.56633771069071
Cl	-4.37948716309717	2.10772487447460	-0.34207831921431
N	-9.13029461887806	2.53499052828878	-1.06384020386533
C	-7.80398356686482	2.93854816970763	-0.90010288431190
H	-7.47774949653465	3.96322346095774	-1.11189874458943
N	-7.02468360116782	1.95791159347611	-0.47980538556695
C	-7.85873753106829	0.85468377318412	-0.35443082659399
C	-7.67777110741078	-0.51134653475181	0.01314010231619
O	-6.45009751101044	-0.90576685139259	0.36830297636250
N	-8.71428071645429	-1.34494524807335	0.00135910673002
C	-9.94343397508645	-0.89258742624558	-0.36221278240817
N	-11.00927118337569	-1.76476035133594	-0.27743362074155
H	-11.84935814450774	-1.45779185074462	-0.77511258334197
N	-10.25215959767455	0.37003568370403	-0.76003868234620
C	-9.19633399228596	1.19032707261804	-0.72047306853514
H	-9.91712079438018	3.10336100345637	-1.37857859401464
Cl	-6.32491026335122	-2.75726359701415	0.53486392274037
Cl	-10.78413284909321	-3.52150516765805	-0.33237638097011

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H	-1.97937798389673	-2.37025582824222	6.76048565019752
C	-1.05020435531232	-0.96302135517571	5.43240975131937
N	0.00756021644109	-1.62169054966599	4.91582256263819
H	1.93029821187705	-2.44308727407234	3.94516024979933
Br	1.68823124050034	-1.94227110299225	1.54532104002685
N	1.89044770178561	-1.49892188228543	3.53250675453586
C	0.74776668392487	-0.90566741400168	4.06849765257382
Br	1.64509968262466	1.41741808644452	2.59464904534617
N	0.45194258573032	0.40883834145452	3.73105515396056
O	-0.99996897550234	2.24034792190433	3.69428163143618
C	-0.73975735126829	1.12614787537033	4.14987068328712
C	-1.49609974195997	0.33900354330146	5.10218225250395

N	-2.66938318110072	0.64221130332350	5.76887361490024
H	-3.79896901122217	-0.55833360107097	7.15906870137513
C	-2.93626054879666	-0.43392815754766	6.49263209802509
N	-1.98752358292805	-1.44405518247688	6.33092055035150
H	6.71822772692554	-2.32562502578008	2.03564728831801
C	5.39746261017987	-0.93182842082568	1.07610985128366
N	4.90232511521349	-1.59964165556946	0.01381733652784
H	3.95923607413131	-2.44088785349930	-1.91463897370031
Br	1.55419666818779	-1.94822869925231	-1.69840699000630
N	3.54212156824949	-1.49817613460287	-1.88762282193496
C	4.06173163525129	-0.89350363965273	-0.74322126642372
Br	2.58760044834049	1.41504126538788	-1.67821471012179
N	3.71239802067987	0.42102072951874	-0.46132836574873
O	3.63745682560259	2.25855391052639	0.98113515160174
C	4.10570272262607	1.14681005840000	0.73349451454871
C	5.05067428182714	0.36998977587789	1.50982852273381
N	5.69436277535931	0.68332350258224	2.69313405993876
H	7.07267265460461	-0.50221261223491	3.85277717097656
C	6.42076285476335	-0.38650708834591	2.97786393053356
N	6.28274884980847	-1.40215790993633	2.03133060558885
H	1.97766186109835	-2.37326716427821	-6.75955890027076
C	1.04954097371571	-0.96482271993213	-5.43204338274175
N	-0.00873367286068	-1.62248005358567	-4.91520153232624
H	-1.93202579839184	-2.44206926410171	-3.94411542485336
Br	-1.68886397669377	-1.94083445021658	-1.54453574473692
N	-1.89144378468930	-1.49781042143402	-3.53173172793025
C	-0.74839241586820	-0.90557923616159	-4.06815644209225
Br	-1.64380990359320	1.41873748159010	-2.59504251719638
N	-0.45166477650065	0.40884955785726	-3.73126280010159
O	1.00130664271017	2.23949266973731	-3.69563053627198
C	0.74049611408755	1.12517051643477	-4.15054071472208
C	1.49636763385878	0.33702415757912	-5.10235565443554
N	2.66990895449119	0.63908326857605	-5.76913066781885
H	3.79866960574299	-0.56288513468525	-7.15875781302107
C	2.93602480918100	-0.43755680122742	-6.49241200864569
N	1.98651355057995	-1.44690996834886	-6.33034826491367
N	-6.28227827616744	-1.40168095227611	-2.03178293667760
C	-6.41974746760747	-0.38617492015420	-2.97854044293151
H	-7.07135809346434	-0.50189068059355	-3.85367504784957
N	-5.69319075177452	0.68353490186612	-2.69375918953379
C	-5.04992238622498	0.37024772934223	-1.51020834971559
C	-4.10515015320061	1.14710859419177	-0.73371631454928
O	-3.63680351225321	2.25883635087410	-0.98098011842246
N	-3.71214906650065	0.42116645414661	0.46126173126391
Br	-2.58704983018996	1.41480868175056	1.67811440354048
C	-4.06194965317032	-0.89320174125431	0.74330380706271
N	-3.54269592422533	-1.49786798302128	1.88789734235774
Br	-1.55485852727959	-1.94888184729054	1.69870579874705
H	-3.96007749165174	-2.44046604990114	1.91496158160774
N	-4.90261585501579	-1.59919252326921	-0.01379781152329
C	-5.39717243020516	-0.93141227387328	-1.07635333472614
H	-6.71801882058433	-2.32502510520202	-2.03605068296463

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Br-G4-2

N	-2.40151100	-0.62653500	7.80141300
C	-3.65846900	-0.58349800	7.21615200
H	-4.56689100	-0.93299900	7.71689800
N	-3.59825200	-0.07165800	5.99439200

C	-2.26596400	0.23543300	5.75581800
C	-1.63045400	0.83234900	4.59709900
O	-2.13284800	1.20242400	3.55048900
N	-0.18726700	0.98660000	4.85393800
C	0.48757700	0.57697200	6.00777900
N	1.82572200	0.83240100	6.17322500
H	2.09789900	0.46736600	7.09350500
N	-0.16278800	0.00509500	7.03579400
C	-1.49384200	-0.10624100	6.88317100
H	-2.16599900	-0.97546600	8.73128800
Br	3.20994500	0.15845800	4.86838400
Br	0.73216500	1.89733000	3.44209700
N	6.27651500	-1.79246500	1.96141400
C	5.70201900	-1.57648900	3.20541100
H	5.94600900	-2.17451900	4.08955200
N	4.83310900	-0.57652400	3.16687100
C	4.82008100	-0.11352700	1.85699500
C	4.09218500	0.98513200	1.24704700
O	3.32301300	1.78420600	1.75688000
N	4.44626100	1.07373300	-0.17678200
C	5.31817000	0.22431600	-0.86660600
N	5.56980200	0.44302700	-2.19783000
H	6.27002800	-0.25060200	-2.48946800
N	5.97054900	-0.76471800	-0.23752500
C	5.72285100	-0.86935400	1.08073500
H	6.96769600	-2.50222500	1.71409500
Br	3.68604400	2.60044200	-1.04139700
Br	4.01828400	0.16644800	-3.50381100
N	0.98072600	-0.72618600	-6.86812300
C	2.23838300	-0.70733900	-6.28296900
H	3.13871100	-1.08079400	-6.78105300
N	2.18970500	-0.18583000	-5.06481800
C	0.86465000	0.15292100	-4.82862800
C	0.24287700	0.77225700	-3.67432200
O	0.75315200	1.13801200	-2.63004700
N	-1.19648200	0.95784100	-3.93295000
C	-1.88052500	0.55455700	-5.08343700
N	-3.21272900	0.83811500	-5.25072200
H	-3.49331100	0.47207400	-6.16806200
N	-1.24322900	-0.03931600	-6.10727100
C	0.08499300	-0.17923600	-5.95368100
H	0.73742500	-1.07564300	-7.79578900
Br	-4.61061800	0.20554100	-3.93950800
Br	-2.09493700	1.89951600	-2.52791200
N	-7.72195100	-1.64996400	-1.01675800
C	-7.14111200	-1.45937100	-2.26198400
H	-7.39915400	-2.05890500	-3.14108800
N	-6.24812500	-0.48053000	-2.23132300
C	-6.22527400	-0.00603600	-0.92572600
C	-5.47250800	1.08095100	-0.32520800
O	-4.68384700	1.85685000	-0.84091600
N	-5.82665900	1.19161800	1.09713900
C	-6.71845600	0.36904600	1.79393800
N	-6.96510500	0.60544600	3.12303200
H	-7.68111500	-0.06910400	3.42103400
N	-7.39347700	-0.61012500	1.17323900
C	-7.14702500	-0.73262400	-0.14376700
H	-8.43179300	-2.33919700	-0.76424500

Br -5.03225500 2.70863400 1.94804500
Br -5.41945900 0.30606700 4.43125600

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Br-G4-3

H	-1.87997609354591	-0.37412939615394	8.47812980927515
C	-0.85681794837346	0.05271425400987	6.63925391266126
N	0.45023935492721	-0.16076679266337	6.90290822770171
H	2.69491124734985	-0.65680624152903	6.98818045171527
Br	3.84965305969159	1.21684705790380	5.96603210899281
N	2.60122459370365	-0.33770987573829	6.01335771157721
C	1.25441061955203	-0.00240546825118	5.84867743361327
Br	1.99751255826027	0.32772239716453	3.02084775382560
N	0.81423346803210	0.38434022715427	4.59479921263154
O	-0.84649582928493	1.11683101942122	3.15249951608949
C	-0.54850992815302	0.72556656721299	4.29092815889694
C	-1.41898744871977	0.51191376106017	5.42606330273663
N	-2.78749534561392	0.67479195250370	5.54518373364081
H	-4.06357267951101	0.32132070100288	7.24391483063204
C	-3.06537262886469	0.32178385992392	6.78925632824530
N	-1.93091414906879	-0.06538874216739	7.50625586087653
H	8.47837004321961	1.72193576016768	1.87983635113709
C	6.63916734872773	1.29678471291452	0.85656315117772
N	6.90316242264918	1.50981515572851	-0.45049766613819
H	6.98911950818965	2.00546593900207	-2.69525197034285
Br	5.96540323842512	0.13248744714346	-3.84971182155524
N	6.01398831325501	1.68729851289053	-2.60161012075792
C	5.84884972793082	1.35240465710225	-1.25474644602084
Br	3.02083983823939	1.02469369447871	-1.99819453949342
N	4.59453625739398	0.96700818685019	-0.81463625877558
O	3.15123631391282	0.23651082114955	0.84609683527747
C	4.29014036497497	0.62641664162164	0.54815130798717
C	5.42543966581115	0.83895450349963	1.41869087747969
N	5.54426566363695	0.67615623228618	2.78723280280597
H	7.24325056852076	1.02799705746240	4.06341391756248
C	6.78868553757593	1.02788975991095	3.06517132177034
N	7.50619319352451	1.41413827805816	1.93072242140627
H	1.88023176984726	-0.37410916821154	-8.47800796336986
C	0.85696109501597	0.05263598778438	-6.63917101463563
N	-0.45005158238387	-0.16110477973949	-6.90283760331283
H	-2.69463457343643	-0.65757932129274	-6.98809255044033
Br	-3.84970831109630	1.21584190388163	-5.96600867788352
N	-2.60100884353003	-0.33843757184755	-6.01327942804107
C	-1.25426595747147	-0.00284207178303	-5.84862367209767
Br	-1.99751847281310	0.32741631040666	-3.02088337859980
N	-0.81418741492960	0.38407365688641	-4.59476844550543
O	0.84637128128817	1.11698989625749	-3.15248102193664
C	0.54848364965193	0.72557335322333	-4.29088600383330
C	1.41902114995869	0.51201280994448	-5.42599537815814
N	2.78749560548670	0.67516471843986	-5.54510908151889
H	4.06367133450994	0.32185313558974	-7.24379821793432
C	3.06546299425793	0.32214032087558	-6.78915766719436
N	1.93109459192196	-0.06530840426818	-7.50614921686072
N	-7.50628714828136	1.41379653382621	-1.93081845582195
C	-6.78875774576233	1.02750407857662	-3.06523861220324
H	-7.24331640602821	1.02752974775757	-4.06348403957154
N	-5.54432565202265	0.67583464917107	-2.78727107348443
C	-5.42551845220715	0.83871180197885	-1.41873728792198
C	-4.29022513118362	0.62625151248700	-0.54817028027339

O	-3.15129995600455	0.23637756583592	-0.84607783636885
N	-4.59464243968377	0.96690519739714	0.81459059972023
Br	-3.02099528196613	1.02459946500326	1.99816098017137
C	-5.84896105343260	1.35231639644426	1.25466614544459
N	-6.01408779896711	1.68734948674531	2.60149397976186
Br	-5.96543980426507	0.13270899155714	3.84970602860453
H	-6.98923443090542	2.00547330418468	2.69511283439732
N	-6.90327744279296	1.50963766322402	0.45040106746791
C	-6.63926591888493	1.29653492122246	-0.85664535782839
H	-8.47847451025873	1.72156526732088	-1.87995788740309

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Br-G4-4

N	-1.96205500	0.25376400	7.36866800
C	-2.96937800	-0.58810700	6.90684800
H	-3.87672100	-0.79034900	7.48671200
N	-2.69561200	-1.07498300	5.70502100
C	-1.46540600	-0.52796300	5.35043200
C	-0.66948400	-0.68382000	4.15360100
O	-0.82921700	-1.45398000	3.21200700
N	0.40607600	0.30450600	4.13287000
Br	1.15482900	0.57861300	2.37852400
C	0.81296100	1.07293600	5.22165100
N	1.84159200	1.97958200	5.12677400
Br	3.60667300	1.66013100	4.28668800
H	1.98530300	2.42147800	6.04102800
N	0.14356300	1.04507200	6.38700000
C	-0.99499000	0.32434900	6.37205300
H	-1.93321200	0.75269500	8.25885300
N	7.33269700	-0.24411300	1.99825600
C	6.88046200	0.62205700	2.98910700
H	7.46317200	0.83574200	3.89200700
N	5.68347100	1.11584000	2.70723100
C	5.32172400	0.54851400	1.48795900
C	4.12712000	0.70128200	0.68827300
O	3.19233300	1.48332100	0.83321900
N	4.09706600	-0.30386600	-0.37103600
Br	2.33951000	-0.57149500	-1.11552800
C	5.17680100	-1.09382100	-0.76073700
N	5.07328600	-2.02054800	-1.76998400
Br	4.24270800	-1.73365000	-3.54452200
H	5.98226400	-2.47710100	-1.90067400
N	6.34172800	-1.06600700	-0.09036900
C	6.33447000	-0.32327200	1.03364200
H	8.21789500	-0.75226900	1.97806600
N	1.97926500	0.09262700	-7.32388700
C	2.96962300	-0.76316600	-6.85122100
H	3.87381400	-0.98890800	-7.42730300
N	2.68514500	-1.23142400	-5.64454000
C	1.46499800	-0.65708000	-5.29785100
C	0.66483100	-0.78381200	-4.10046900
O	0.80964000	-1.54517800	-3.14927000
N	-0.39319000	0.22368500	-4.09295700
Br	-1.13428100	0.53489900	-2.34110000
C	-0.78278200	0.98849700	-5.19072400
N	-1.79346800	1.91579400	-5.10793000
Br	-3.56738700	1.63917600	-4.27241500
H	-1.92500200	2.35208800	-6.02667800
N	-0.11178200	0.93505900	-6.35423300

C	1.01250900	0.19284800	-6.32953000
H	1.96134000	0.58244800	-8.21938700
N	-7.32529600	-0.17282900	-1.96717400
C	-6.86330200	0.66774700	-2.97551000
H	-7.44195100	0.86669000	-3.88436600
N	-5.66295900	1.15766900	-2.70088300
C	-5.30950200	0.61420100	-1.46854200
C	-4.11441900	0.77351900	-0.67091100
O	-3.17214200	1.54255600	-0.83311800
N	-4.09495500	-0.20864800	0.41061900
Br	-2.33957300	-0.47736600	1.16063400
C	-5.18147100	-0.98279900	0.81337100
N	-5.08730300	-1.89155600	1.83955100
Br	-4.25479200	-1.58501200	3.60945200
H	-6.00006500	-2.33848500	1.97667400
N	-6.34524000	-0.95867600	0.14074000
C	-6.33018500	-0.23923700	-0.99832100
H	-8.21432700	-0.67384000	-1.93889500

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Br-G4-5

N	-11.28754854958778	-8.32723813982566	-1.11720745836102
C	-11.71029220481986	-7.01258477223934	-0.93173904858666
H	-12.72867257982669	-6.68402996271717	-1.16563556228053
N	-10.74274778438720	-6.23955488071758	-0.46364021756719
C	-9.63436023258948	-7.06638645635805	-0.32989172714916
C	-8.28180148225127	-6.87080890939443	0.08073482607447
O	-7.89588237029793	-5.67839590692513	0.49354826533390
N	-7.43556793244620	-7.90577778503453	0.04079832275271
C	-7.85636183680624	-9.13496455834271	-0.37372563587754
N	-6.96857301016557	-10.17671075339312	-0.32706575756425
H	-7.28535776924866	-11.02018527246366	-0.81169352956761
N	-9.11741214261246	-9.43795519522269	-0.79857606428580
C	-9.94810083376258	-8.39299968395341	-0.74338851964450
H	-11.84168700926421	-9.10868269797835	-1.46867558280126
Br	-5.84156952947095	-5.59790591462025	0.65959285556068
Br	-5.03708100537818	-9.96506669729124	-0.33702996014529
N	-0.35150624533670	-10.42737880851342	-1.12288848706335
C	-1.66591200185972	-10.84998042185840	-0.93556644746420
H	-1.99578224510971	-11.86729708014573	-1.17217788173754
N	-2.43713211097786	-9.88356351885729	-0.46206091210826
C	-1.60929606326972	-8.77618226674882	-0.32648359579066
C	-1.80309942586450	-7.42481808031657	0.08886845522156
O	-2.99488235368353	-7.03913832011377	0.50420272460094
N	-0.76780400011286	-6.57899226721037	0.04931581522937
C	0.45991733969251	-6.99909045375750	-0.37041113811953
N	1.50221567828058	-6.11173770302042	-0.32365201574397
H	2.34365365353780	-6.42757308939443	-0.81252064156600
N	0.76104811445400	-8.25878547983403	-0.80029487304074
C	-0.28396963701319	-9.08932281532194	-0.74450169345567
H	0.42868065801174	-10.98065430912763	-1.47850135178858
Br	-3.07762583562699	-4.98493419482353	0.66539536451511
Br	1.28963326769591	-4.18002194306381	-0.33392825789947
N	1.75088522997527	0.50438416838769	-1.12565742345151
C	2.17373316707388	-0.80960999097712	-0.93624722815148
H	3.19103600131019	-1.13973761665416	-1.17255276837126
N	1.20757766190377	-1.58015244806486	-0.46108465000417
C	0.10013404534298	-0.75225223401343	-0.32648749900146
C	-1.25112118031427	-0.94564000850884	0.08952657570865

O	-1.63639688438825	-2.13700738703960	0.50635354661645
N	-2.09714579818189	0.08953205869657	0.04861387950631
C	-1.67730694669453	1.31642957647375	-0.37374217816333
N	-2.56471082706172	2.35879687539642	-0.32874070363425
H	-2.24890091516723	3.19949765777754	-0.81886864192950
N	-0.41783198039323	1.61709272127209	-0.80459809550472
C	0.41291751961853	0.57237812432522	-0.74693231573675
H	2.30393511406435	1.28406519809592	-1.48273154854336
Br	-3.69090464403923	-2.22141899866209	0.66366919362638
Br	-4.49630433547267	2.14770456007833	-0.33722686657309
N	-9.18356399430771	2.61147830718279	-1.11860987378599
C	-7.86925389293020	3.03438292000937	-0.93104598486657
H	-7.54042799384679	4.05280849463474	-1.16435622168381
N	-7.09685556188817	2.06689976530773	-0.46171393254083
C	-7.92378254803613	0.95846018698474	-0.32927938205724
C	-7.72867588924936	-0.39410820102378	0.08146153777610
O	-6.53651875370862	-0.77998310582903	0.49540320178988
N	-8.76352476137818	-1.24038989780090	0.04043591173531
C	-9.99196746300285	-0.81982777967626	-0.37654002300647
N	-11.03373522205873	-1.70766702830529	-0.33170457928405
H	-11.87653566671208	-1.39074184977724	-0.81739332000200
N	-10.29443462713657	0.44112450408161	-0.80205313870779
C	-9.24975886922179	1.27202841425475	-0.74487148656096
H	-9.96449805832245	3.16548704258955	-1.47141595393269
Br	-6.45425828424064	-2.83418333170040	0.65788737606700
Br	-10.82312315343814	-3.63908336693077	-0.34050967701271

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I-G4-1

N	-11.41268981214231	-8.40795733332876	-1.15740488312835
C	-11.84376232302640	-7.10319106000543	-0.95343962442400
H	-12.85208533626069	-6.76139808951955	-1.20758807067021
N	-10.88036247496396	-6.34466502680613	-0.44295576709675
C	-9.77262139088292	-7.17464419552022	-0.30147983332722
C	-8.43457760283443	-6.98124473305850	0.15357661338691
O	-8.04009064567051	-5.82888868951839	0.62765727384227
N	-7.58175997175047	-8.01677580191950	0.07457597415345
C	-7.97656721105347	-9.24052514249588	-0.40141881696769
N	-7.06508584575992	-10.24540168978502	-0.42953585373955
H	-7.40980174180996	-11.09550505922086	-0.88298692737230
N	-9.24644143955067	-9.52744743229336	-0.83557554624445
C	-10.07610719507258	-8.48547065059800	-0.76126857944736
H	-11.95928885487065	-9.17866191828805	-1.54293132952368
I	-5.77004996999388	-5.84007828726405	0.80751191990037
I	-4.89938504925808	-10.05666245122950	-0.35512593568451
N	-0.26763913464292	-10.55505672599497	-1.15687285835193
C	-1.57253961012582	-10.98612779698233	-0.95365193318976
H	-1.91421238458255	-11.99440987745855	-1.20812732473472
N	-2.33127016658593	-10.02281631607066	-0.44330761677303
C	-1.50130291835092	-8.91517890281690	-0.30115858525308
C	-1.69504311422766	-7.57717450235408	0.15383815880834
O	-2.84796180819143	-7.18300684755108	0.62681256591681
N	-0.65948962949627	-6.72432302753166	0.07578207878887
C	0.56450010248872	-7.11903049490023	-0.39982411285242
N	1.56943305122764	-6.20756877595331	-0.42711940772979
H	2.41971425192352	-6.55226768078147	-0.88025966023724
N	0.85163302239117	-8.38877064832606	-0.83416966660544
C	-0.19030434849875	-9.21855521573899	-0.76039806221226
H	0.50322056071060	-11.10160138480316	-1.54216459272896

I	-2.83678261700468	-4.91277229499589	0.80693675755442
I	1.38055892823686	-4.04181198886841	-0.35323826184004
N	1.87894222178919	0.58967999212006	-1.15612904918983
C	2.30996802198334	-0.71516607451270	-0.95242724500298
H	3.31832510759474	-1.05691569887683	-1.20649685678728
N	1.34649151123407	-1.47376385497598	-0.44218910288773
C	0.23882829516696	-0.64375820057768	-0.30056298842438
C	-1.09933986766764	-0.83743038877456	0.15395561336062
O	-1.49380576546866	-1.99027749861242	0.62684666198366
N	-1.95212429924668	0.19813721512507	0.07556890285132
C	-1.55729154871122	1.42203537988096	-0.40019962410462
N	-2.46872927776307	2.42694942491886	-0.42767781109494
H	-2.12405699331000	3.27717935675563	-0.88093312657528
N	-0.28744992738766	1.70903316383420	-0.83435271317403
C	0.54232983083125	0.66712303920704	-0.76005526233673
H	2.42559570205295	1.36044706094972	-1.54145288804134
I	-3.76410120843501	-1.97907298040624	0.80588450569905
I	-4.63451907549761	2.23796614205732	-0.35349106555360
N	-9.26589112355954	2.73644841243434	-1.15599403346127
C	-7.96096926861551	3.16725084074876	-0.95243339741729
H	-7.61907757090403	4.17556543400176	-1.20648016229967
N	-7.20248663255331	2.20365930090788	-0.44225675384675
C	-8.03263508395198	1.09610564192767	-0.30049962339182
C	-7.83931556607090	-0.24208780430236	0.15409831043633
O	-6.68664311442961	-0.63682263212644	0.62731978577890
N	-8.87501706315682	-1.09466946403070	0.07562736266648
C	-10.09886772437965	-0.69956489429874	-0.39993667182173
N	-11.10386956223638	-1.61091238683634	-0.42757143923758
H	-11.95414593367216	-1.26612919652257	-0.88065265728438
N	-10.38567626215226	0.57036278822675	-0.83397075961053
C	-9.34352973428296	1.39985307243520	-0.75988055472527
H	-10.03662750736536	3.28324175226766	-1.54118137396191
I	-6.69757884154207	-2.90678377784542	0.80690272834043
I	-10.91476605066303	-3.77666413112085	-0.35387880310253

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N	-2.21203700	-1.59462400	7.78016600
C	-3.44699900	-1.44292000	7.17289700
H	-4.32519000	-2.04417600	7.42769600
N	-3.40577300	-0.49196100	6.24588100
C	-2.10361600	0.00003100	6.23074300
C	-1.49854200	1.08117100	5.47590800
O	-2.03614800	1.84364300	4.67926800
N	-0.09527900	1.21332400	5.82269300
C	0.60731900	0.40611500	6.72960700
N	1.93835800	0.61364700	6.92454600
H	2.23472800	-0.01861500	7.67922300
N	-0.02473500	-0.54844500	7.44630600
C	-1.33308900	-0.68883400	7.18938700
H	-1.96757200	-2.25670500	8.51806100
I	3.39217400	0.23297800	5.23051500
I	0.78779100	2.94502200	4.91603400
N	6.72185300	-0.92599500	2.20837600
C	6.14775000	-0.83534800	3.46512000
H	6.61343400	-1.22513800	4.37511400
N	4.96962200	-0.22252000	3.40142600
C	4.75329900	0.10123200	2.06617700
C	3.66289600	0.80476900	1.42357200

O	2.66598500	1.28568000	1.94875000
N	3.90475200	0.92178600	-0.00681800
C	5.01020100	0.39743000	-0.69183500
N	5.15967400	0.57489500	-2.03236500
H	6.06302400	0.16243600	-2.29419900
N	6.00343900	-0.24339700	-0.03088800
C	5.84792700	-0.33560000	1.29574700
H	7.62160800	-1.34759800	1.97503500
I	2.39039100	2.10899600	-0.96408400
I	3.69363800	-0.01614200	-3.61727000
N	0.76643300	-1.68357200	-6.84355900
C	2.00489200	-1.55820500	-6.23742300
H	2.86823200	-2.18201800	-6.48896400
N	1.98710900	-0.60099400	-5.31607300
C	0.69714100	-0.07766400	-5.30351000
C	0.11864100	1.02240100	-4.55530300
O	0.67460600	1.77664900	-3.76336000
N	-1.28133000	1.18574100	-4.90179800
C	-2.00363700	0.39001900	-5.80343900
N	-3.32961900	0.62809000	-5.99830200
H	-3.64176100	-0.00115200	-6.74916300
N	-1.39499200	-0.58340600	-6.51487800
C	-0.09019400	-0.75348500	-6.25778500
H	0.50575200	-2.34409000	-7.57728900
I	-4.78959400	0.29070100	-4.30048100
I	-2.12215000	2.94347500	-4.00534600
N	-8.14302700	-0.77229400	-1.26940600
C	-7.56676500	-0.70487000	-2.52662100
H	-8.03944300	-1.09450900	-3.43307300
N	-6.37709400	-0.11421100	-2.46817700
C	-6.15513200	0.21819200	-1.13599600
C	-5.05129400	0.90620300	-0.49949800
O	-4.04496800	1.36245600	-1.02866800
N	-5.29118000	1.04109900	0.92967300
C	-6.40708700	0.54538800	1.61898300
N	-6.55314000	0.73877700	2.95770900
H	-7.46455000	0.34652800	3.22278300
N	-7.41244300	-0.08202500	0.96360700
C	-7.25825600	-0.19003000	-0.36199000
H	-9.05061900	-1.17465700	-1.03255800
I	-3.75272500	2.20480000	1.87704800
I	-5.09957300	0.12568500	4.54646600

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N	-1.69998400	0.55782300	7.58585300
C	-2.67347600	-0.41167300	7.30332200
H	-3.49386600	-0.61662500	8.00262900
N	-2.48082800	-1.01313000	6.14489600
C	-1.33294100	-0.42229300	5.62858000
C	-0.63217900	-0.62740700	4.39962500
O	-0.94084400	-1.46664900	3.49584000
N	0.47387900	0.22507400	4.20630500
I	1.21138600	0.07973200	2.05013300
C	0.90627400	1.14630100	5.15693300
N	1.93174800	2.01802300	4.90300800
I	3.93122800	1.57275100	4.14516600
H	2.03612300	2.62039100	5.72726900
N	0.27477600	1.30955900	6.34290500

C	-0.82590700	0.56537200	6.51133300
H	-1.62503100	1.14490700	8.41752000
N	7.46586000	-0.80648800	2.17551100
C	7.15515700	0.15180700	3.13302500
H	7.69770200	0.23974400	4.08026800
N	6.11928800	0.89484900	2.76190700
C	5.72713500	0.40549800	1.51808000
C	4.61124300	0.77388200	0.66896700
O	3.85729200	1.73299200	0.76502800
N	4.38988300	-0.25810800	-0.33691600
I	2.29490400	-0.30659700	-0.94274500
C	5.31846300	-1.24490900	-0.68963800
N	5.08781000	-2.06345300	-1.75132100
I	4.23976300	-1.43269900	-3.68293300
H	5.86481200	-2.72499600	-1.85568800
N	6.44069600	-1.43606500	0.03295000
C	6.53954600	-0.68204900	1.14407800
H	8.21011100	-1.50402900	2.22180500
N	2.32767000	0.73123100	-7.41174500
C	3.33704100	0.00067100	-6.81349500
H	4.33789300	-0.10583900	-7.24430800
N	2.93179500	-0.52884500	-5.66189500
C	1.60958700	-0.13148600	-5.48632400
C	0.65812000	-0.38848800	-4.41392200
O	0.83775400	-1.09266500	-3.41773400
N	-0.56556200	0.33159400	-4.61162100
I	-1.87294400	0.31396800	-2.78299700
C	-0.85041900	1.04403700	-5.75247400
N	-2.07619400	1.70469000	-5.83956300
I	-3.83547400	0.42097100	-6.12385200
H	-2.05362200	2.23047700	-6.72606400
N	0.00455800	1.22103600	-6.77775800
C	1.21421400	0.66832400	-6.57684300
H	2.37361200	1.22593900	-8.30396100
N	-7.47904000	-0.26024500	-2.02597300
C	-6.68870900	0.22789000	-3.06840400
H	-7.11019700	0.45532400	-4.05510400
N	-5.42130700	0.38075500	-2.72206600
C	-5.36149100	-0.02410000	-1.39893800
C	-4.25834200	-0.09344400	-0.47525500
O	-3.05303000	0.21901600	-0.68903100
N	-4.61110200	-0.59925500	0.78949200
I	-2.85653700	-1.04806700	2.13672600
C	-5.91071600	-0.90815400	1.14014200
N	-6.14327300	-1.43374200	2.40908500
I	-6.00041000	-0.02189200	4.10017000
H	-7.14393800	-1.67971000	2.43457600
N	-6.96214500	-0.82186900	0.30835100
C	-6.63930000	-0.42737100	-0.93627300
H	-8.48110000	-0.45626400	-2.03917400

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H	-1.87862595694565	-1.02364894990668	8.64159971410346
C	-0.88882095534368	-0.56407342176532	6.79169962401758
N	0.41499583739163	-0.81091325960145	7.01089962811194
H	2.70545791532290	-0.89457495996010	7.13896535721571
I	3.52202220516864	-2.49161350804380	5.25603161649239
N	2.58314312033609	-0.68098873694713	6.13715409586660

C	1.20505776761667	-0.56098369431933	5.95287873554912
I	2.09758512115827	0.27469098943261	2.97855468474348
N	0.74669683220829	-0.11643943117280	4.72769628179259
O	-0.93778700373878	0.55590117847012	3.31919543578329
C	-0.61596629042146	0.12593773109798	4.45990767213694
C	-1.48338588596686	-0.13031329858718	5.58017719116633
N	-2.85646571583807	-0.01478110774962	5.71559395672875
H	-4.09606858984537	-0.40641944470245	7.43344687050940
C	-3.10436383837666	-0.36746002925771	6.96646542916223
N	-1.94877071278964	-0.70764101972847	7.67327932992904
H	8.64120144070808	-1.02616159563354	1.87838416881520
C	6.79141899076179	-0.56577210776500	0.88873564643037
N	7.01035888650487	-0.81285320055609	-0.41507866963259
H	7.13811944394640	-0.89680056113038	-2.70563856271425
I	5.25425436576463	-2.49318953788556	-3.52161698826753
N	6.13640562454749	-0.68279010092099	-2.58315025380606
C	5.95237753928099	-0.56249393874391	-1.20505025324711
I	2.97835618329075	0.27438701885462	-2.09737469689988
N	4.72746871812211	-0.11727690654450	-0.74660781551421
O	3.31949623560765	0.55599467940619	0.93794186163667
C	4.45994886684020	0.12538837444828	0.61605588088816
C	5.58017359747426	-0.13135454333144	1.48339056368486
N	5.71581371935557	-0.01570747301979	2.85644007066107
H	7.43360822589037	-0.40806613877647	4.09589238121115
C	6.96653818032026	-0.36898449227956	3.10423464309844
N	7.67303817220851	-0.70969007102970	1.94860447677884
H	1.87857742127368	-1.02367499097358	-8.64159724383506
C	0.88878607912649	-0.56407855535649	-6.79169533794804
N	-0.41503085991785	-0.81093068018206	-7.01087957159729
H	-2.70549133227198	-0.89461387130137	-7.13891866243969
I	-3.52201631457332	-2.49162236876032	-5.25595449857928
N	-2.58317090920634	-0.68100687977556	-6.13711367915094
C	-1.20508475935865	-0.56098940059501	-5.95285544703434
I	-2.09758925427164	0.27470883449707	-2.97853188802882
N	-0.74671578117322	-0.11642307074250	-4.72768411581943
O	0.93777640609993	0.55594960283565	-3.31920828689357
C	0.61594788683899	0.12596827337893	-4.45991165668378
C	1.48335901006617	-0.13029403397331	-5.58018530366334
N	2.85643722804652	-0.01475567787021	-5.71561549475454
H	4.09602775590811	-0.40642086593893	-7.43347133632592
C	3.10432665709427	-0.36745758844176	-6.96648256813634
N	1.94872893670003	-0.70765266384200	-7.67328202577083
N	-7.67301188435365	-0.70965986916922	-1.94862106873765
C	-6.96650631980305	-0.36895505454689	-3.10424823601806
H	-7.43357496839863	-0.40802870588678	-4.09590695836350
N	-5.71578001203982	-0.01568769742942	-2.85644919551073
C	-5.58014472964345	-0.13134138436541	-1.48339982780775
C	-4.45991977195745	0.12539013295756	-0.61606249207569
O	-3.31946711707954	0.55599648221325	-0.93794711826246
N	-4.72744112664866	-0.11728665121123	0.74659915082241
I	-2.97832850090705	0.27436191717725	2.09737250029242
C	-5.95235300372613	-0.56250079651782	1.20503635589521
N	-6.13638348658804	-0.68280814591746	2.58313663269393
I	-5.25422631272304	-2.49321714440829	3.52161694877654
H	-7.13810684147248	-0.89679141990674	2.70564421376767
N	-7.01033558008770	-0.81284521229947	0.41506268087395
C	-6.79139295936433	-0.56575674634986	-0.88875010874043
H	-8.64117759614844	-1.02612461764882	-1.87840443737664

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H	-8.56427012839218	-0.39621712191788	-2.40530849754328
C	-6.79191432764999	-0.08362994397106	-1.23431837513663
N	-7.14518591628649	-0.35881597706659	0.03427262818930
H	-7.37248634488698	-0.96447154011116	2.24196212787136
I	-6.42304670765401	0.98389133609596	3.71035850778601
N	-6.38978802745226	-0.65349552732475	2.22573766703391
C	-6.13283245762159	-0.26806276672918	0.91226608617443
I	-3.11328813355076	-0.14731150973653	2.00730959214977
N	-4.84261921353149	0.09933000148056	0.58294422780672
O	-3.28348893403850	0.87576719955435	-0.91441365157078
C	-4.46979481933859	0.49369419307608	-0.71639811041221
C	-5.52813924225361	0.37218344978184	-1.68606299244295
N	-5.54984255177077	0.61770029356833	-3.04844404171205
H	-7.16317790437624	0.38794533634068	-4.45464917119767
C	-6.78011105782379	0.31688819386368	-3.42931838868911
N	-7.58355295349023	-0.11443384434052	-2.37142911260282
H	-2.02097109489746	1.98001832531380	8.28196050388220
C	-1.04447310920491	1.10270684500142	6.58310345407237
N	0.26718039614096	1.11062396631316	6.88138909233314
H	2.55170221359258	1.21879354625461	6.98607789928632
I	3.53988193128639	-1.13448299339506	6.43625733434178
N	2.42816519607062	0.74023083740372	6.08131229785385
C	1.05087244582737	0.62459573053182	5.90407868398950
I	1.94991209605841	-0.37968192548576	2.99146075359007
N	0.58204145820607	0.11579195786008	4.70864155280273
O	-1.12700837617252	-0.50079996459240	3.30360756548876
C	-0.78975867687989	0.01791874617740	4.40380843106449
C	-1.65087792394564	0.57017025125068	5.41775230284133
N	-3.02959165516183	0.68545163624080	5.48264275347757
H	-4.25925733508677	1.52613918700110	7.03793404366364
C	-3.26793326067160	1.27197854432339	6.64378908480510
N	-2.10126637057930	1.55196829812318	7.35863857489247
H	8.47376272563811	0.90572766761647	2.35066798324746
C	6.70696650136313	0.41504789206818	1.23291468724584
N	7.02037740118409	0.64318727227443	-0.05537464845353
H	7.16726017460267	1.16929220666368	-2.28356357428182
I	6.33144214159439	-0.86488142907673	-3.69689770738726
N	6.20938362206758	0.79094908607362	-2.23994723254820
C	6.00371683129036	0.43444794443826	-0.90928375135179
I	2.98585232479960	-0.00842306097049	-1.93286706396895
N	4.75114101933143	-0.01135850089874	-0.53592777792932
O	3.26543149489091	-0.78556042266225	1.03634453439691
C	4.42264683918676	-0.34292270220434	0.79246817322753
C	5.48280149664462	-0.09462717084674	1.73409896301659
N	5.54119026048094	-0.26009344381218	3.10802223935324
H	7.15918882969444	0.15432046100776	4.46652555148353
C	6.75505156900759	0.14053107611700	3.44684867243213
N	7.51244600333279	0.56215478950629	2.35103850495842
N	2.32767881390797	1.36975299425798	-7.43711628587994
C	3.41247539757367	0.93876233985580	-6.66977235064136
H	4.43519402053846	0.93605386584912	-7.06628127890320
N	3.05926385253650	0.54992447128031	-5.45597733780481
C	1.68752560448293	0.73221421224074	-5.40885239535564
C	0.73492253183145	0.50362243318765	-4.35328150248773
O	0.95915183853928	0.06352636358103	-3.19245693688847
N	-0.58596779933698	0.85341570469113	-4.69284643453003

I	-2.00294782486374	0.86620180609331	-2.94094825286155
C	-0.94518294450536	1.28537297760907	-5.95409245090154
N	-2.27827462456042	1.62445061539230	-6.17666388311020
I	-3.68035196717470	-0.07988314899880	-6.33310802505039
H	-2.31559307774007	2.00048843319158	-7.13590045656698
N	-0.08181858975173	1.48013904449603	-6.96477523324462
C	1.20173820567594	1.24112003069157	-6.63936549073073
H	2.33844811327234	1.70712143040121	-8.40059206257294

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I-G4-6

H	-1.89099702153744	-0.77353490105246	8.55978522939568
C	-0.86417306580201	-0.21425731777259	6.75866317315160
N	0.44547414556169	-0.36077172528732	7.03086656111835
H	2.71490197433151	-0.72317724214975	7.10674171717440
I	3.90620662032815	1.43808581364065	6.23721266865071
N	2.61045173945878	-0.35146828501435	6.15076937274839
C	1.24969137131191	-0.10223840955674	5.98616804519270
I	2.14506450482356	0.35681627674305	2.93088511096904
N	0.80918555485989	0.31007987423169	4.74434239031243
O	-0.84724475908385	1.01440694391855	3.32057295826576
C	-0.54531262443100	0.57480172835686	4.46387354092732
C	-1.43517286638798	0.26551949611571	5.55332215341240
N	-2.81358448012718	0.34317819409690	5.65614989934922
H	-4.09164929302510	-0.15657816531659	7.31534601900842
C	-3.08828168146131	-0.07887702900739	6.87918444238985
N	-1.94444895923251	-0.43188677798560	7.59920433239963
H	8.55969607681678	2.12333915238852	1.89112423320161
C	6.75865499516134	1.56394721002563	0.86422024808963
N	7.03092562840960	1.71036291054643	-0.44542403955313
H	7.10695710973376	2.07264684254494	-2.71482972128510
I	6.23763698880838	-0.08870955104645	-3.90609480888926
N	6.15096633717668	1.70095122022991	-2.61045656034554
C	5.98627286488532	1.45177820621506	-1.24969193876859
I	2.93099698428443	0.99282464146745	-2.14517344893700
N	4.74442396591731	1.03948361911176	-0.80923143118641
O	3.32057460271473	0.33532460278429	0.84717304767528
C	4.46390453314927	0.77487296379455	0.54526570310312
C	5.55328266306553	1.08419361835143	1.43517071913960
N	5.65599704196142	1.00667526261767	2.81360393185342
H	7.31510143214781	1.50654814381257	4.09174211432683
C	6.87901296012495	1.42875518289648	3.08834926488172
N	7.59911931196254	1.78167367815515	1.94453621285223
H	1.89088051106290	-0.77367800972797	-8.55980769448981
C	0.86410734622104	-0.21425737726401	-6.75870309234518
N	-0.44554852696644	-0.36066915384082	-7.03089935580032
H	-2.71499663712982	-0.72290960187925	-7.10676530385582
I	-3.90610144502794	1.43856091042642	-6.23746917672496
N	-2.61053699710601	-0.35113173097298	-6.15081917056869
C	-1.24975707455997	-0.10201711218456	-5.98621961826515
I	-2.14511337362769	0.35718593712102	-2.93093050850423
N	-0.80921694306561	0.31030160034489	-4.74440744117354
O	0.84726653268178	1.01452115993575	-3.32066940631278
C	0.54531009329561	0.57490786754635	-4.46396109834837
C	1.43514326252168	0.26553450505719	-5.55338453418056
N	2.81356456608185	0.34307497287732	-5.65621382756251
H	4.09159015513345	-0.15686703009550	-7.31538357485741
C	3.08822722507140	-0.07905764132167	-6.87923037110782
N	1.94436259204349	-0.43200349157441	-7.59923807421930

N	-7.59913066162917	1.78226581566199	-1.94442418002516
C	-6.87910506374770	1.42926608923124	-3.08825903295988
H	-7.31524932568399	1.50701461826525	-4.09163081310218
N	-5.65609595076739	1.00714095553697	-2.81355451918871
C	-5.55328136047215	1.08474899098562	-1.43513762175926
C	-4.46386490761521	0.77540920623758	-0.54526775250270
O	-3.32056985691075	0.33579416653828	-0.84719221711416
N	-4.74435742013273	1.04004252506353	0.80924904645725
I	-2.93097247365059	0.99308677628452	2.14521244749546
C	-5.98617269708887	1.45241010967742	1.24973197604142
N	-6.15078989888644	1.70162868534797	2.61049047886179
I	-6.23731473400513	-0.08794557786976	3.90622994746398
H	-7.10676361295715	2.07334906544259	2.71490865038125
N	-7.03083309491840	1.71102530942086	0.44549375152402
C	-6.75861492740877	1.56455568256349	-0.86414691124489
H	-8.55969895666223	2.12394859930869	-1.89097514263613

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At-G4-1

N	-11.50133465428265	-8.48573508691773	-1.13318923824309
C	-11.94050211011281	-7.18173247093625	-0.94922364589096
H	-12.95268467009173	-6.84999433607173	-1.20015889675437
N	-10.97471076200776	-6.40938841861214	-0.45929812342785
C	-9.86083184446275	-7.23110804811118	-0.31225483528600
C	-8.52193875685576	-7.01063550600761	0.12910384909959
O	-8.12620022385501	-5.85785384186696	0.57562046273079
N	-7.66001347303213	-8.04667037166559	0.05617778809805
C	-8.04795648144740	-9.28786249335892	-0.39133254834270
N	-7.13453393587708	-10.28441318746735	-0.40942305671925
H	-7.49744524384133	-11.14392239115585	-0.83057250114581
N	-9.32476557928542	-9.58671449322882	-0.80808984632163
C	-10.15928561521255	-8.54929667617099	-0.74711621118834
H	-12.04709356720893	-9.26564311820823	-1.50093781539853
At	-5.72205201826370	-5.95662736752035	0.73566195151380
At	-4.84881457457701	-10.11857880319941	-0.35164359282435
N	-0.19051421050139	-10.64425632142002	-1.13280063994211
C	-1.49469039204972	-11.08306411756227	-0.94923858087038
H	-1.82664352456261	-12.09515716158843	-1.20024395525954
N	-2.26690613153315	-10.11704777864115	-0.45952833296175
C	-1.44492101408967	-9.00344692536299	-0.31210739272032
C	-1.66504629177346	-7.66439604587098	0.12896503309960
O	-2.81800705635247	-7.26847051163106	0.57510868814548
N	-0.62888582710127	-6.80272320614794	0.05632682784913
C	0.61229081829403	-7.19103775751382	-0.39095464110799
N	1.60898972698149	-6.27774693144995	-0.40892327553415
H	2.46834834658129	-6.64069130602165	-0.83037477336802
N	0.91092223520179	-8.46793798723516	-0.80752672281143
C	-0.12669199195935	-9.30223366477009	-0.74667476869249
H	0.58940844614556	-11.19027847163951	-1.50012911676057
At	-2.71962972487207	-4.86468336352003	0.73548262865616
At	1.44259895177837	-3.99183879954893	-0.35154085976768
N	1.96785154983707	0.66687609679238	-1.13321395429257
C	2.40663283208721	-0.63731983301836	-0.94961038915687
H	3.41861521297906	-0.96938949035101	-1.20090321974565
N	1.44064105753348	-1.40944242619340	-0.45970766881685
C	0.32712564025900	-0.58738530891503	-0.31213549877257
C	-1.01191568528677	-0.80748776256253	0.12895219071814
O	-1.40764189329259	-1.96039458321499	0.57541943817267
N	-1.87362708925822	0.22862968355771	0.05621743294884

C	-1.48535311066534	1.46977160522204	-0.39117261456361
N	-2.39860983870380	2.46651461583992	-0.40934439428564
H	-2.03567736961467	3.32553502642766	-0.83152090800394
N	-0.20839589953172	1.76841246959057	-0.80764940744389
C	0.62588243559777	0.73079112699763	-0.74689976334236
H	2.51375533598345	1.44666521931331	-1.50100147359820
At	-3.81157088389390	-1.86237282211675	0.73587487552615
At	-4.68477181730567	2.30035742571495	-0.35147811331504
N	-9.34404487742623	2.82554145396821	-1.13278892239210
C	-8.03993517336426	3.26446638195166	-0.94891996844671
H	-7.70804830367111	4.27667117338709	-1.19955129618148
N	-7.26769055524222	2.29831716423366	-0.45948064964770
C	-8.08955784562973	1.18460374055302	-0.31257840394216
C	-7.86924034999502	-0.15445557074423	0.12840575009552
O	-6.71621885697661	-0.55019321910662	0.57443140386548
N	-8.90538900352543	-1.01612986181685	0.05585393283643
C	-10.14644977443928	-0.62798653550776	-0.39186146741759
N	-11.14302384699752	-1.54142506354900	-0.41020445490416
H	-12.00235205142642	-1.17858711692632	-0.83179700129045
N	-10.44524434931769	0.64890991681827	-0.80835913217310
C	-9.40775545651548	1.48336205465600	-0.74719256808145
H	-10.12393533631829	3.37150473184139	-1.50027522453243
At	-6.81389038761296	-2.95394182855805	0.73531540705747
At	-10.97682015003948	-3.82720251186143	-0.35179979472745

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At-G4-2

N	-2.48512700	0.76369600	8.51628800
C	-3.68096300	0.55242800	7.84702300
H	-4.65450600	0.84800200	8.24949700
N	-3.47336200	-0.01843700	6.66079100
C	-2.09668100	-0.19258400	6.54711800
C	-1.24841100	-0.68636100	5.50954100
O	-1.75289200	-1.20415300	4.42763000
N	0.08054600	-0.56923600	5.67473000
C	0.61740700	-0.04231200	6.82590600
N	1.96292100	0.02886100	6.92520100
H	2.27862200	0.50942300	7.77220000
N	-0.12697600	0.41163700	7.89516700
C	-1.44029500	0.31971500	7.69579400
H	-2.37250300	1.19157700	9.43583300
At	3.47879000	-0.08336200	5.20628100
At	-0.11823200	-1.12515600	2.68515100
N	7.22715900	0.46452000	2.34682500
C	6.57758000	0.29969000	3.56258000
H	7.06747800	0.45181600	4.52931300
N	5.30412400	-0.04149500	3.38846400
C	5.10410800	-0.10534900	2.01174700
C	3.97049200	-0.38634800	1.18730700
O	2.82048100	-0.71026200	1.68520200
N	4.13476400	-0.28930800	-0.15066000
C	5.34510300	0.03782700	-0.71538200
N	5.43213400	0.09063800	-2.06174200
H	6.34728400	0.39945600	-2.39895500
N	6.48358200	0.30617600	0.00813100
C	6.30347600	0.22249100	1.32623600
H	8.20034200	0.73855900	2.20889200
At	1.21999300	-0.74634200	-0.15636500
At	3.73941300	0.01808500	-3.59347500

N	1.09314800	0.32427000	-7.51013200
C	2.25722100	0.27075000	-6.75757300
H	3.25432500	0.42147600	-7.18287300
N	1.99521100	0.02796300	-5.47678800
C	0.61078500	-0.08333300	-5.37647900
C	-0.29766600	-0.32136600	-4.29970900
O	0.13817900	-0.52012200	-3.08491000
N	-1.61261900	-0.33199300	-4.57350200
C	-2.09161700	-0.13219200	-5.85177600
N	-3.42370900	-0.17107500	-6.05464100
H	-3.69463500	0.04292900	-7.01776300
N	-1.28601400	0.09670600	-6.94286300
C	0.01246300	0.10681500	-6.65155300
H	1.02244200	0.50986300	-8.51112900
At	-5.05240900	-0.18382200	-4.45591700
At	-1.67873600	-0.76877100	-1.58912300
N	-8.52131600	0.82400000	-1.39396900
C	-8.05374700	0.55298700	-2.67366200
H	-8.60246400	0.82330600	-3.58107800
N	-6.86271000	-0.03644000	-2.63569100
C	-6.53280500	-0.15887400	-1.28910500
C	-5.36601300	-0.68660700	-0.64080500
O	-4.42553800	-1.26421800	-1.23516200
N	-5.35803700	-0.48665900	0.75332900
C	-6.42352300	0.05192200	1.46668500
N	-6.42856500	0.13661100	2.81538600
H	-7.30361000	0.57618600	3.11534600
N	-7.55959800	0.50048700	0.84419500
C	-7.55226000	0.39303400	-0.48473900
H	-9.40548400	1.27127500	-1.15012900
At	-3.06006100	-0.93880500	1.48356800
At	-4.99337300	-0.03603600	4.62468900

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At-G4-3

N	-2.08204229971972	0.83882846612981	7.80707168859758
C	-3.30807044987693	0.41766057509325	7.30543951624764
H	-4.23763135702590	0.46525923250715	7.88137127948541
N	-3.19299493809763	-0.01829343353050	6.05449247784913
C	-1.84942956503560	0.11980063157020	5.72188481450574
C	-1.14659210250149	-0.14286470555106	4.49484727151655
O	-1.65279752474277	-0.66596378876821	3.48000336813778
N	0.18921685432584	0.29992135306360	4.51714311012182
At	0.90568248921391	0.40279886558484	2.15979531669055
C	0.82378852995082	0.80974543804727	5.63925503767431
N	2.11796553969430	1.21248269966573	5.57960799326532
At	3.93329341030287	0.47700708253801	4.33214328196507
H	2.41501034861637	1.55008863731218	6.50058385810519
N	0.17516534215114	0.97696839492203	6.83027283086141
C	-1.12897000290677	0.67482820101681	6.79995810914023
H	-1.90381527114334	1.22370376026567	8.73533703709160
N	7.84870652709880	-1.06556688591270	2.08802103773118
C	7.11486276367011	-0.71067526700002	3.21055749232484
H	7.48519765224101	-0.83554165485726	4.23276742631592
N	5.92410728323643	-0.22065813903655	2.87268862560940
C	5.87081985324405	-0.24945574854160	1.48032354792104
C	4.86875589068613	0.08066401942700	0.51585719981752
O	3.72676066904324	0.58171749051735	0.89668300385832
N	5.13224084023829	-0.15364466308072	-0.77819724388017

At	2.09803900056327	0.41419159106042	-0.82463427837043
C	6.34235296239061	-0.66881168272651	-1.18451008219467
N	6.54554275768617	-0.84313573668718	-2.50726428792640
At	4.98984292593122	-0.57882679376408	-4.15796590116177
H	7.44276399003263	-1.27588208677696	-2.73949420218219
N	7.36326544646246	-1.01603135460556	-0.32535431142873
C	7.07376426119039	-0.79133162202678	0.95481886116430
H	8.78611923898532	-1.46848617768860	2.07804351622601
N	2.10754854135172	0.65821863282739	-7.78228617828709
C	3.32530449909502	0.22291457654145	-7.27236412952924
H	4.25568331637531	0.24226483665286	-7.84862740155557
N	3.20145590009580	-0.18826007231949	-6.01387399245422
C	1.86069193243562	-0.01875210794390	-5.68470613246452
C	1.15252630680687	-0.24587115286898	-4.45364159958231
O	1.64831050104221	-0.75932346505356	-3.42882427332603
N	-0.17463073516299	0.22166416545276	-4.48483270244301
At	-0.88763965799406	0.38170199720411	-2.12852612236438
C	-0.79916009473486	0.72273503400458	-5.61636819786099
N	-2.08591131119346	1.14975032251906	-5.56509037380686
At	-3.91310088590814	0.47170070105762	-4.30351133792133
H	-2.37632147812454	1.47688513667972	-6.49194939319604
N	-0.14697250587114	0.85656716052174	-6.80972066794070
C	1.15124179563154	0.53042242539349	-6.77304191214126
H	1.93730320571813	1.03085268269072	-8.71703551269338
N	-7.85597868005912	-0.95517553972948	-2.03113527906710
C	-7.11549050924292	-0.63551139762298	-3.15986619963487
H	-7.48738233961658	-0.77377101983243	-4.17975762650190
N	-5.91604727415945	-0.16099380457799	-2.83069194970502
C	-5.86370950104969	-0.16379076679922	-1.43805785948396
C	-4.85612612659067	0.16601549753523	-0.47931611479806
O	-3.70392907380862	0.63700378652805	-0.86825409536577
N	-5.12462448344988	-0.03802896647001	0.81877393925664
At	-2.07906918631458	0.46692331194050	0.85557800670699
C	-6.34413308953033	-0.52291822968917	1.23411459782324
N	-6.55135030179386	-0.66675847177390	2.55989394265841
At	-4.98966383373138	-0.40550216410505	4.20558035654173
H	-7.45494496845341	-1.08197488394528	2.79945281483630
N	-7.37066689275360	-0.86827405828172	0.38097507754810
C	-7.07658344332005	-0.67338664251224	-0.90294858051089
H	-8.80013269159415	-1.34179922219090	-2.01402249781643

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At-G4-4

H	-1.91042811414333	-0.89353241724736	8.62726786088039
C	-0.86932964575626	-0.30897795920159	6.84140694828157
N	0.43700987312540	-0.44595451324972	7.12301995359203
H	2.71333490847310	-0.78477260860597	7.19962804891453
At	3.95289097151506	1.49203340505326	6.38635252668402
N	2.60598913957057	-0.41130126179329	6.24382829480359
C	1.24896770169752	-0.17042177371808	6.08199111464756
At	2.21580983348614	0.36312607429527	2.93868134748776
N	0.81300294077937	0.25319390815853	4.84261592049134
O	-0.83232889194442	0.95457731795363	3.41456640538158
C	-0.53451769463042	0.50325160454101	4.56020801916330
C	-1.43522084301787	0.17384412310868	5.63308602560486
N	-2.81530537875117	0.23264218073466	5.72149661787593
H	-4.10443304673269	-0.29457973780503	7.36375591598670
C	-3.09736567622110	-0.20189094884640	6.93928155733757
N	-1.95732717161121	-0.54575967494022	7.66857795194958

H	8.61882428980426	2.28603186947007	1.90980920608426
C	6.83644007970417	1.68957805428146	0.86951027882155
N	7.11672086015381	1.82811095233765	-0.43693602421522
H	7.19010730089698	2.16735436012438	-2.71337881123555
At	6.39081759050345	-0.11411222210169	-3.95369001736009
N	6.23699205678641	1.78726710246189	-2.60552189564772
C	6.07730238299181	1.54534168590916	-1.24852542754076
At	2.93736742975470	0.98994390027526	-2.21382074508064
N	4.84104283940214	1.11334586665380	-0.81193481278146
O	3.41854274570330	0.40187446905221	0.83379001554207
C	4.56087825627456	0.86140111546930	0.53570364812504
C	5.63164117415918	1.19863186766081	1.43593269007790
N	5.72086634486535	1.14090719230866	2.81601177699887
H	7.35984844788233	1.67992918929501	4.10447703875566
C	6.93571636836751	1.58391268609227	3.09757460128616
N	7.66229395408765	1.93243238281074	1.95718620129402
H	1.91536710192436	-0.92460718109534	-8.62161424690165
C	0.87265889357032	-0.33705439905786	-6.83770326242930
N	-0.43325389002013	-0.47924031229879	-7.11862164509147
H	-2.70842621383747	-0.82634838176865	-7.19330448767233
At	-3.95566362658514	1.44955506936047	-6.38959454061108
N	-2.60219915391210	-0.44845984148569	-6.23913105195434
C	-1.24597808642895	-0.20249084103473	-6.07847343348598
At	-2.21412322820850	0.34187859105788	-2.93723354033182
N	-0.81117706386585	0.22724566390054	-4.84079136639113
O	0.83222573124888	0.93866447481404	-3.41545264029283
C	0.53564295707767	0.48243121772044	-4.55942631175150
C	1.43713985719421	0.15183690574744	-5.63121214692594
N	2.81705624729296	0.21445152273787	-5.71984986478855
H	4.10767625996411	-0.31468080274476	-7.36037472305205
C	3.10037446789915	-0.22356472340160	-6.93610968258304
N	1.96134037642363	-0.57350765025666	-7.66410072985864
N	-7.66754439583512	1.89370751442572	-1.96197619048360
C	-6.93959832482557	1.54321327513293	-3.10087380845742
H	-7.36432655679131	1.63248982440258	-4.10814401979673
N	-5.72263557576319	1.10715477044526	-2.81753859886902
C	-5.63341129979381	1.17179631716387	-1.43776137750850
C	-4.56093867571748	0.84365643569192	-0.53619963625945
O	-3.41655543303967	0.38819934523428	-0.83258664540831
N	-4.84197643288255	1.10034840527575	0.81035014427010
At	-2.93766499274089	0.99116147818413	2.21270540179119
C	-6.08002128030040	1.52892785818159	1.24510485405009
N	-6.24043945062277	1.77633852974338	2.60113993270143
At	-6.38784604472269	-0.12037953096894	3.95657374594590
H	-7.19512438380342	2.15301875520026	2.70721247693105
N	-7.12091758291790	1.80325504413469	0.43249380880811
C	-6.84035135572060	1.65984713937671	-0.87337010386267
H	-8.62545987143639	2.24372733564302	-1.91608854193663

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N	-2.27167509618561	-0.94347885612501	8.37652090471248
C	-3.53374061270900	-0.90770154870713	7.80903318815026
H	-4.39594061686004	-1.44167936115658	8.21999248920629
N	-3.54001765890255	-0.16783904342753	6.70454971013496
C	-2.23600540790556	0.29861251867837	6.52873728346562
C	-1.65249650520859	1.19574333822418	5.55333753031498
O	-2.23730478150440	1.82913419685868	4.66754196961176
N	-0.23726018409182	1.32983334106809	5.74941365839091

C	0.50960104221502	0.72995525347472	6.77427359235483
N	1.84535142296943	0.93661806042091	6.85884731272231
H	2.16355883465343	0.47421027669159	7.71991693009687
N	-0.10179981984758	-0.02182211978283	7.72508464492898
C	-1.41853919606585	-0.19165879651848	7.56910339244691
H	-1.99518033624090	-1.43839082485605	9.22539048999007
At	3.37952957248328	0.25221084104211	5.18617441212507
At	0.64432957640029	2.78081834237613	4.24842538657949
N	6.70241602826550	-1.27921792727523	2.24837449368290
C	6.13578213306088	-1.09711997156724	3.49869696987801
H	6.58434796883367	-1.46087186443542	4.42759023698032
N	4.98731530602189	-0.43202643667598	3.40158592239297
C	4.78542924135191	-0.16716892017621	2.04967060547806
C	3.72454472681481	0.53028316216808	1.35806093043826
O	2.74118341824854	1.07766972761628	1.86059455483281
N	3.94105543765379	0.53958748510265	-0.06303475580348
C	5.04090995650819	-0.02609065902538	-0.72181007659983
N	5.23934597225997	0.09578925658153	-2.05723426759508
H	6.12910689480072	-0.36826637853994	-2.27209261381499
N	6.01807815242069	-0.66968308713630	-0.02233734409013
C	5.85676575478050	-0.69550157519893	1.30267383117606
H	7.58361582594080	-1.74992835381077	2.04012374962748
At	2.22742241791363	1.61369590339264	-1.11395979320055
At	3.84662459711551	-0.14467139491669	-3.91855889064166
N	0.84503613083605	-1.03756367263207	-7.44484994630995
C	2.10847397498486	-1.02545817027574	-6.87935574592738
H	2.95819345561391	-1.58088136785519	-7.28796602038895
N	2.13279601780418	-0.27837625209850	-5.78000667918183
C	0.83942013930841	0.21746891569681	-5.60558845087956
C	0.27684378858387	1.13287987423057	-4.63510073745525
O	0.87687044377588	1.75908362076183	-3.75419414427222
N	-1.13554345700931	1.29555307208583	-4.82889630952445
C	-1.89693754238801	0.70581724340709	-5.84894103958065
N	-3.22800060926600	0.94060597492443	-5.93373922938761
H	-3.55674292964982	0.47917258851115	-6.79135068140108
N	-1.30331803826755	-0.06470275882658	-6.79616223359737
C	0.00968580993902	-0.26196041238961	-6.64131419264722
H	0.55645987810325	-1.53252481094597	-8.28967043006603
At	-4.77909874762033	0.30724098069678	-4.25679694516788
At	-1.98302150331524	2.76958591754955	-3.33045606604033
N	-8.13530041763964	-1.12356680651628	-1.30577526823809
C	-7.56459933135876	-0.96620348338602	-2.55755134085206
H	-8.01977797951498	-1.33118580026671	-3.48275496273830
N	-6.40304100859636	-0.32330423318387	-2.46689027950051
C	-6.19644376698066	-0.04814083989119	-1.11769825957640
C	-5.12182493537418	0.63481055244281	-0.43272033516381
O	-4.12747179802942	1.15711039983615	-0.94028745356618
N	-5.33836001940904	0.66256504610067	0.98803674305780
C	-6.44955059447303	0.12596435147103	1.65208212886757
N	-6.64478075994892	0.26622800662686	2.98630064323447
H	-7.54407882361444	-0.17703639712592	3.20565865788185
N	-7.43945408772824	-0.50446853036987	0.95887124526331
C	-7.27839250501117	-0.54711171192291	-0.36580286362344
H	-9.02504545422866	-1.57576478346545	-1.09293574072207
At	-3.60279755164364	1.70968672146630	2.02969628126980
At	-5.25343584307262	-0.00240881902030	4.84587120826084

H	-1.87857813151413	0.56241861580915	8.56086608867644
C	-0.86911900600843	-0.13530644754964	6.79749795120376
N	0.44209870253984	0.00738240598833	7.05052376449020
H	2.70782942374901	0.36193721964630	7.06779702673531
At	3.99207456426672	-1.93693926226870	6.43945273866062
N	2.59646847683425	-0.09012729446949	6.14721197013079
C	1.23885982826505	-0.35143385270940	6.02263634606737
At	2.17707354264497	-1.22936368282046	2.94620897518043
N	0.78165897360395	-0.86269023154076	4.82392365790245
O	-0.90079507236589	-1.56948821176854	3.43913305823846
C	-0.57528987376693	-1.07959218127902	4.56290993252394
C	-1.45703645505556	-0.68089568627340	5.62704213995852
N	-2.83670093607216	-0.72163077300423	5.73826862784959
H	-4.09566624630099	-0.08567437031182	7.36539218199806
C	-3.09625089654452	-0.21386333993003	6.93215661476165
N	-1.94252116736194	0.16187461913760	7.62402975586229
H	8.55379953279841	0.59274657084802	1.87481196532967
C	6.79293546231726	-0.11374177495150	0.86709287751960
N	7.04580577105994	0.02583784190833	-0.44448016102425
H	7.06238955653823	0.37397811586915	-2.71108411405659
At	6.44253245685067	-1.93039236702696	-3.98944309904171
N	6.14336845501639	-0.08100203678394	-2.59870986470002
C	6.01938206491083	-0.33900050191941	-1.24040762288445
At	2.94656813019656	-1.23200625274230	-2.17675271709361
N	4.82241120958067	-0.85323545786522	-0.78198372810892
O	3.43938041818341	-1.55906605289707	0.90229278143399
C	4.56166079411864	-1.06652590397779	0.57560773516687
C	5.62412770786332	-0.66137958343995	1.45640290205411
N	5.73506027979893	-0.69729948948166	2.83621671816695
H	7.35971175066714	-0.05211259685728	4.09363728992030
C	6.92721276932305	-0.18485311848629	3.09450364622130
N	7.61820122289254	0.18948306364866	1.93978184860638
H	1.87738426672052	0.56434592310922	-8.55969379210985
C	0.86942869554822	-0.13570337395660	-6.79639275774677
N	-0.44204011422136	0.00578699551733	-7.04874816387909
H	-2.70831841397819	0.35729371218122	-7.06498145225475
At	-3.98868252110178	-1.94434985494457	-6.43919239173851
N	-2.59604485302209	-0.09551525066207	-6.14486698570763
C	-1.23801323502201	-0.35503853916571	-6.02096568329793
At	-2.17431335215706	-1.23784774116165	-2.94533238368690
N	-0.77976720486791	-0.86675196193043	-4.82283011101550
O	0.90422555320659	-1.57226037168838	-3.43909377882945
C	0.57755849220761	-1.08209955082216	-4.56243249362975
C	1.45840327988425	-0.68175855565706	-5.62667233137974
N	2.83803807975412	-0.72127616525754	-5.73867061433346
H	4.09567687766561	-0.08276944658858	-7.36577763566803
C	3.09656289872343	-0.21220457439648	-6.93222365583041
N	1.94215563045622	0.16313743711081	-7.62319793684194
N	-7.62169193290191	0.15890121317269	-1.94147515190712
C	-6.92931266069479	-0.21439513597917	-3.09569229128392
H	-7.36236170119022	-0.08469175139208	-4.09499087572363
N	-5.73521358571575	-0.72195479437315	-2.83672876237066
C	-5.62433391875325	-0.68357824674780	-1.45697413673134
C	-4.56020943201777	-1.08322883909893	-0.57566450210452
O	-3.43599508849816	-1.57175482866024	-0.90166560250872
N	-4.82184839066924	-0.86909405807896	0.78164443412750
At	-2.94471846437119	-1.23819110683594	2.17718139376151
C	-6.02094771322151	-0.35932937160795	1.23941804765778

N	-6.14613059277464	-0.10071226216057	2.59750228305733
At	-6.43842295600302	-1.95070596659382	3.98903802629341
H	-7.06700059107298	0.35064719365964	2.70940491197340
N	-7.04876791825043	0.00051198296538	0.44299783097980
C	-6.79525814772079	-0.13967378855852	-0.86838279183722
H	-8.55869429496978	0.55898268810135	-1.87707793318348