Supporting Information

Unusual *para*-substituent effects on the intramolecular hydrogen bond in hydrazone-based switches: insights from chemical landscape analysis and DFT

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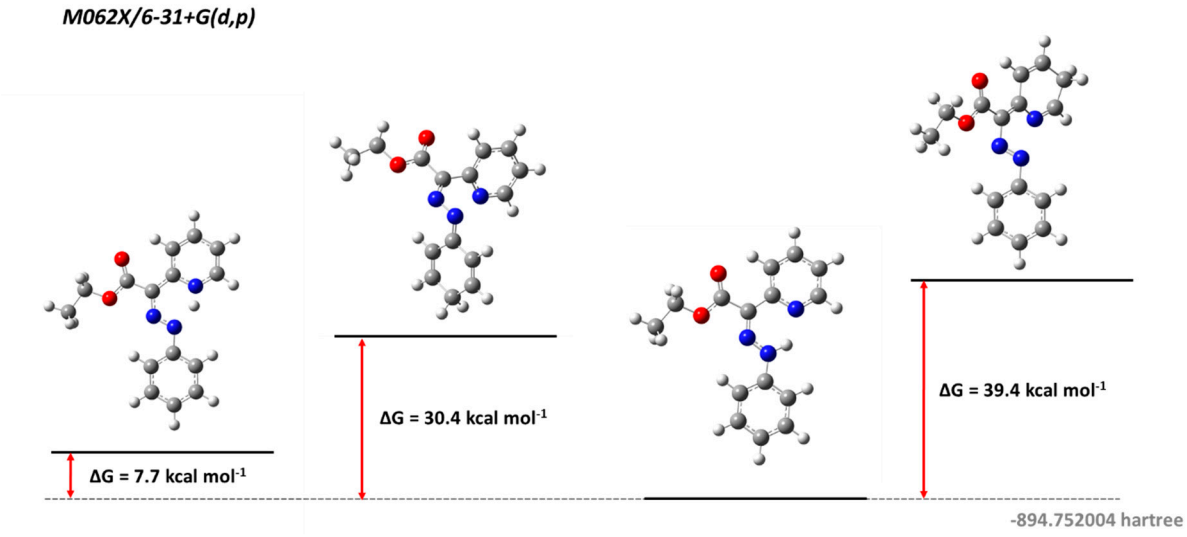


Figure S1. Relative energies of selected conventional and ring-chain tautomers of compound 1.

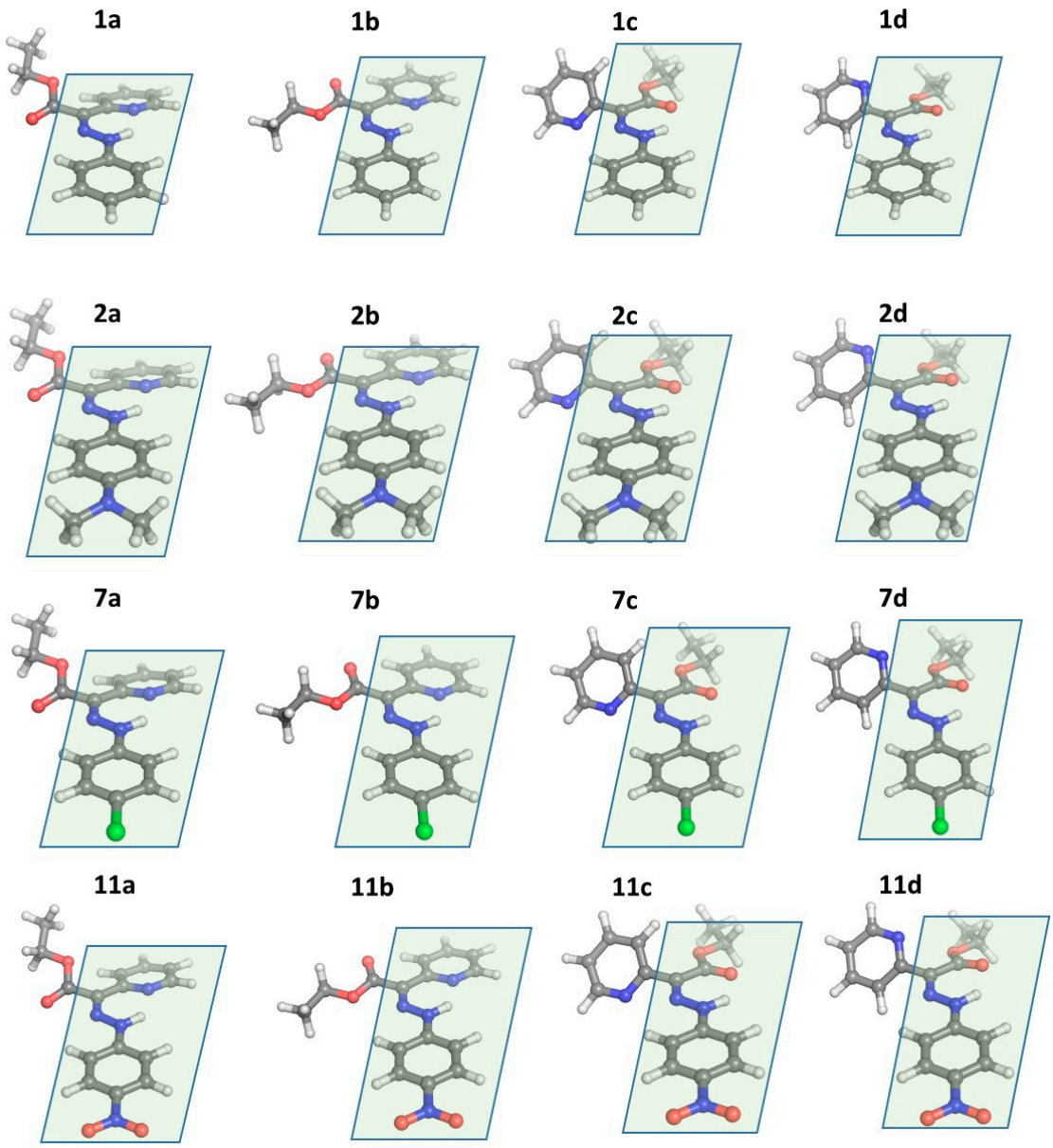


Figure S2. Optimized structures of compounds **1-11**.

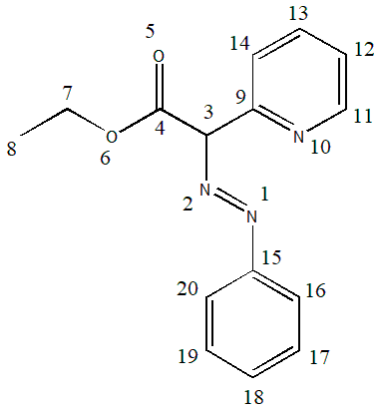
Table S1. Gibbs energy differences (kcal mol^{-1}) in the gas phase (ΔG^{1}) and in acetonitrile (ΔG^{36}) calculated for compounds **1-11**.

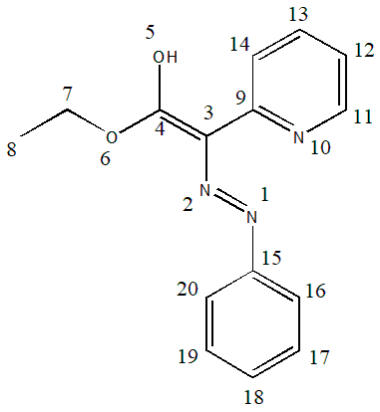
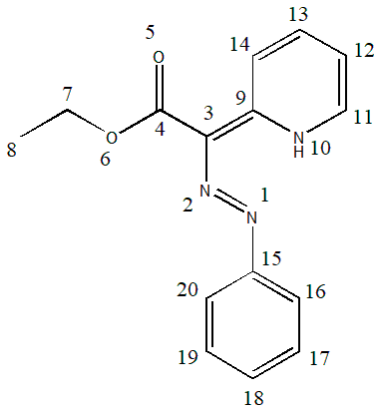
Compound	M062X/6-31+G(d,p)		MN12-SX/6-31+G(d,p)	
	ε=1	ε=36	ε=1	ε=36
1a	2.54	1.11*	2.51	1.32*
1b	0.00	0.00*	0.00	0.00*
1c	2.93	2.09*	2.82	2.35*
1d	1.09	1.49*	1.17	2.10*
2a	2.56	0.85	2.35	1.62
2b	0.00	0.00	0.00	0.00
2c	3.43	1.65	1.49	1.70
2d	1.99	1.01	0.62	1.79

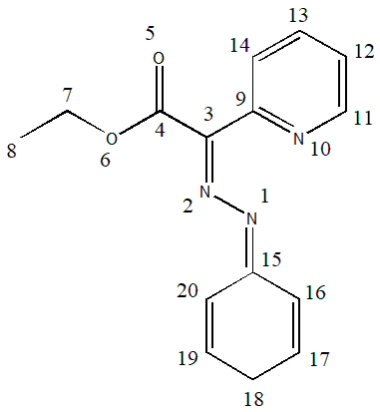
3a	2.46	0.75	2.77	1.32
3b	0.00	0.00	0.00	0.00
3c	2.97	1.41	2.74	2.12
3d	1.51	0.61	1.90	1.75
4a	1.99	1.09	3.11	1.88
4b	0.00	0.00	0.00	0.00
4c	2.71	1.12	2.64	1.01
4d	1.29	2.15	2.23	1.48
5a	1.99	0.69	2.33	1.84
5b	0.00	0.00	0.00	0.00
5c	2.78	1.98	1.24	1.58
5d	1.67	1.03	0.99	2.03
6a	2.45	2.04	2.32	0.80
6b	0.00	0.00	0.00	0.00
6c	2.79	1.58	2.52	2.12
6d	1.14	0.82	1.51	1.67
7a	2.32	0.83	2.46	1.06
7b	0.00	0.00	0.00	0.00
7c	2.61	2.20	2.39	1.97
7d	1.10	1.14	1.24	1.30
8a	2.31	1.76	2.35	1.03
8b	0.00	0.00	0.00	1.00
8c	2.76	3.03	2.33	2.12
8d	1.43	1.99	1.14	1.48
9a	2.76	1.11	2.29	0.64
9b	0.00	0.00	0.00	0.00
9c	2.97	1.93	2.95	2.07
9d	1.19	0.67	1.45	1.32
10a	1.90	0.94	-	-
10b	0.00	0.00	-	-
10c	2.51	2.21	-	-
10d	1.17	1.01	-	-
11a	1.92	1.05	2.67	1.93
11b	0.00	0.00	0.00	0.00
11c	2.69	2.06	3.23	3.13
11d	0.99	1.34	1.78	2.18

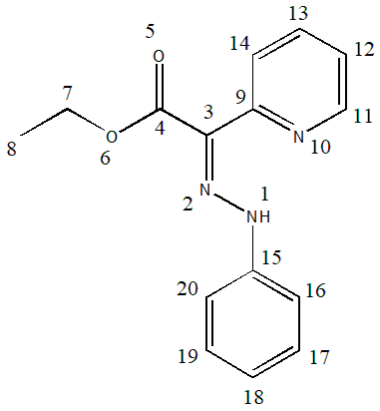
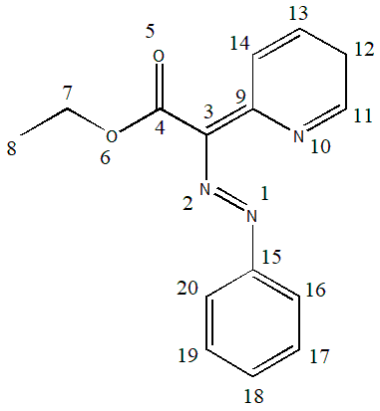
* S. Angelova, V. Paskaleva, N. Kochev, L. Antonov, DFT study of hydrazone-based molecular switches: the effect of different stators on the on/off state distribution, Mol. Phys. 117 (2019), https://doi.org/10.1080/00268976.2018.1548717.

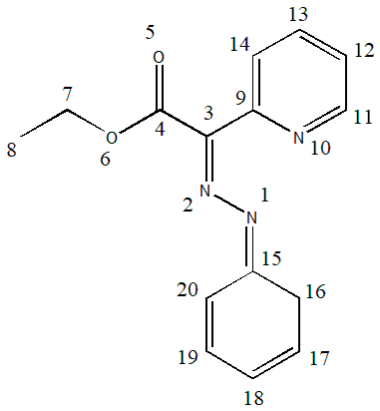
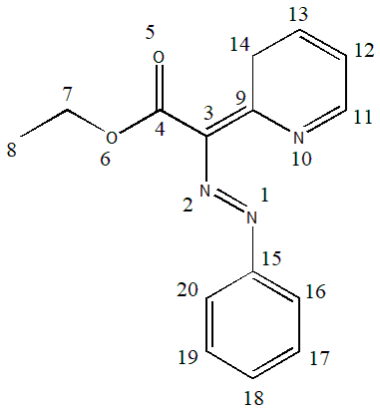
Table S2. List of generated tautomers for unsubstituted and substituted (substitutients H, $N(CH_3)_2$, NO_2) structures and their calculated rapid partial charges with Gasteiger Marsili and MMFF94 methods.

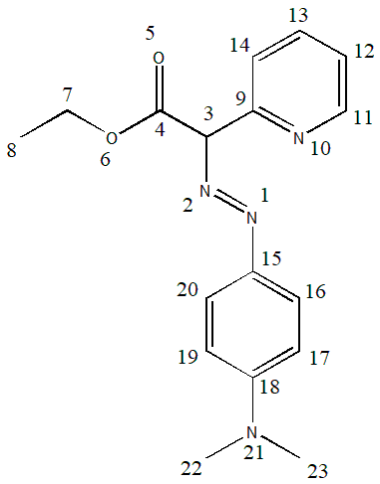
Structure	Substituent R	Tautomer №	Atom indices	Gasteiger Marsili Partial Charges	MMFF94 Partial Charges
	H	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	2	1 N	-0.15	-0.179
			2 N	-0.143	-0.171
			3 C	0.166	0.163
			4 C	0.211	0.153
			5 O	-0.339	-0.527

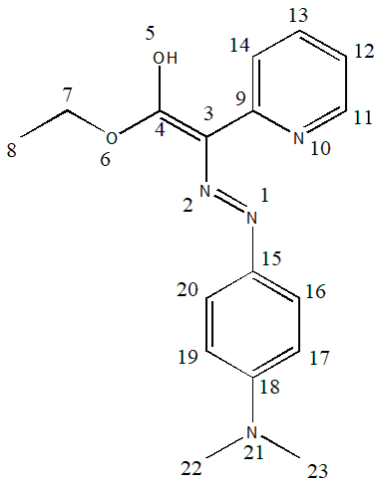
			6 O	-0.324	-0.357
			7 C	0.053	0.28
			8 C	-0.041	0
			9 C	0.095	0.318
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	3	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.176	0.185
			4 C	0.315	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.053	0.1
			10 N	-0.263	-0.6
			11 C	-0.018	-0.05
			12 C	-0.051	-0.15
			13 C	-0.059	-0.15
			14 C	-0.041	-0.15
			15 C	0.086	0.179
			16 C	-0.035	-0.15

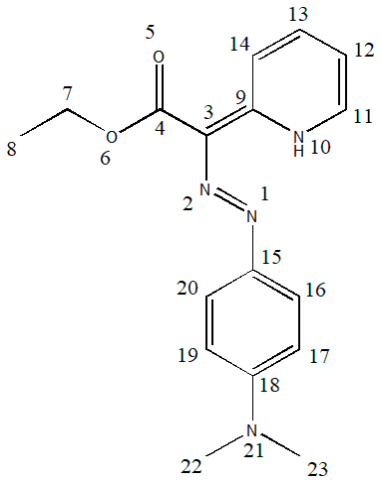
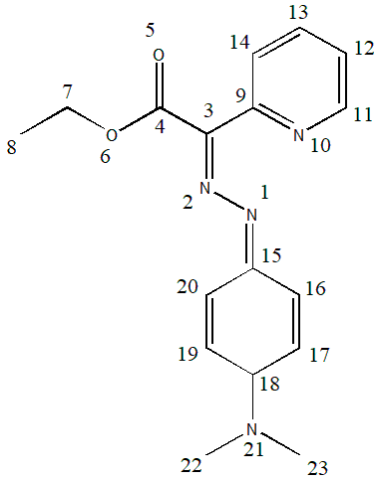
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	4	1 N	-0.15	-0.45
			2 N	-0.141	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.038	-0.136
			17 C	-0.078	-0.288
			18 C	-0.016	0.276
			19 C	-0.078	-0.288
			20 C	-0.038	-0.136
	H	5	1 N	-0.182	-0.458
			2 N	-0.188	-0.492
			3 C	0.175	0.482
			4 C	0.315	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28

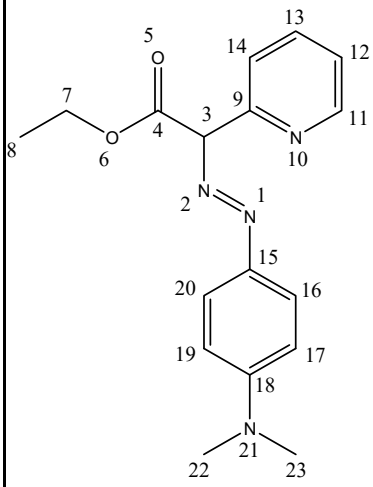
			8 C	-0.041	0
			9 C	0.096	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.036	0.1
			16 C	-0.042	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.042	-0.15
	H	6	1 N	-0.15	-0.179
			2 N	-0.141	-0.171
			3 C	0.183	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.171
			10 N	-0.258	-0.621
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15

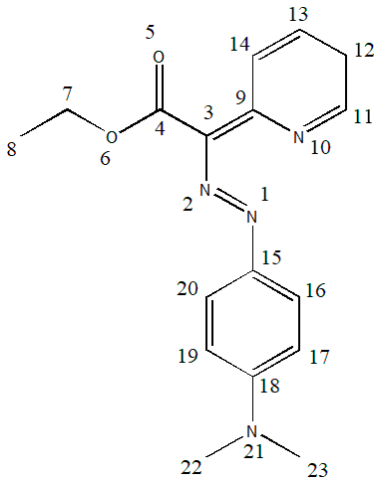
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	H	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	-0.038	-0.136
			17 C	-0.06	-0.15
			18 C	-0.066	-0.15
			19 C	-0.078	-0.288
			20 C	0.01	0.199
	H	8	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.179	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.078	0.033

			10 N	-0.258	-0.621
			11 C	0.027	0.376
			12 C	-0.047	-0.136
			13 C	-0.077	-0.288
			14 C	0.01	0.276
			15 C	0.086	0.179
			16 C	-0.035	-0.15
			17 C	-0.06	-0.15
			18 C	-0.062	-0.15
			19 C	-0.06	-0.15
			20 C	-0.035	-0.15
	$N(CH_3)_2$	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15

			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	$N(CH_3)_2$	2	1 N	-0.15	-0.179
			2 N	-0.143	-0.171
			3 C	0.166	0.163
			4 C	0.211	0.153
			5 O	-0.339	-0.527
			6 O	-0.324	-0.357
			7 C	0.053	0.28
			8 C	-0.041	0
			9 C	0.095	0.318
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15
			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	$N(CH_3)_2$	3	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.176	0.185
			4 C	0.315	0.706
			5 O	-0.258	-0.57

			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.053	0.1
			10 N	-0.263	-0.6
			11 C	-0.018	-0.05
			12 C	-0.051	-0.15
			13 C	-0.059	-0.15
			14 C	-0.041	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15
			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	$N(CH_3)_2$	4	1 N	-0.15	-0.45
			2 N	-0.141	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15

			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.037	-0.136
			17 C	-0.061	-0.288
			18 C	0.047	0.546
			19 C	-0.061	-0.288
			20 C	-0.037	-0.136
			21 N	-0.299	-0.81
			22 C	-0.013	0.27
			23 C	-0.013	0.27
	$N(CH_3)_2$	5	1 N	-0.182	-0.458
			2 N	-0.188	-0.492
			3 C	0.175	0.482
			4 C	0.315	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.036	0.1
			16 C	-0.041	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.041	-0.15
			21 N	-0.281	-0.838

			22 C	-0.009	0.369
			23 C	-0.009	0.369
	$N(CH_3)_2$	6	1 N	-0.15	-0.179
			2 N	-0.141	-0.171
			3 C	0.183	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
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			10 N	-0.258	-0.621
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15
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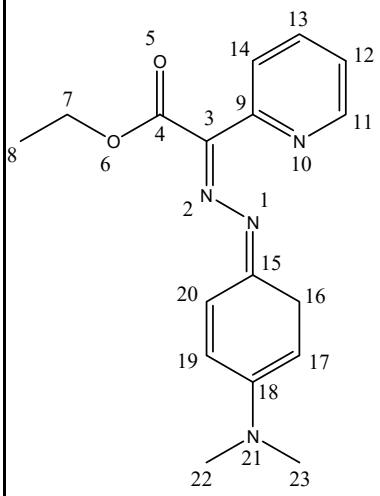
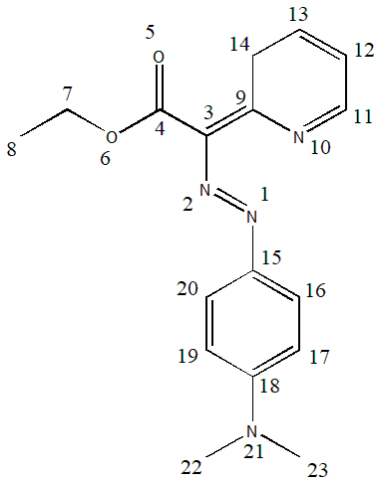
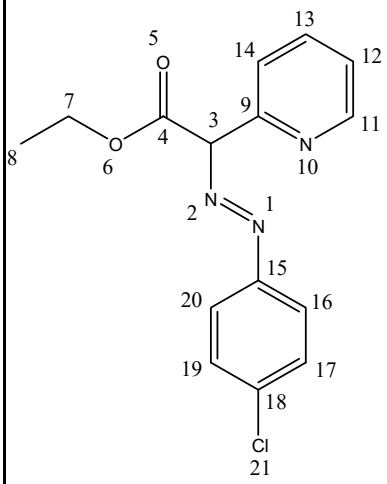
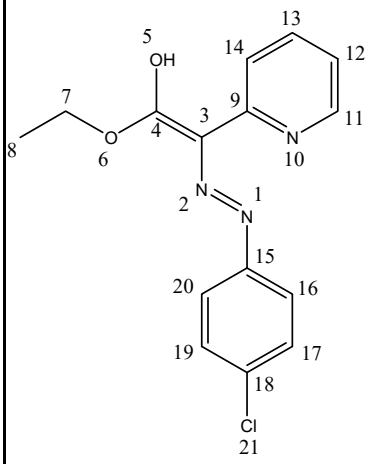
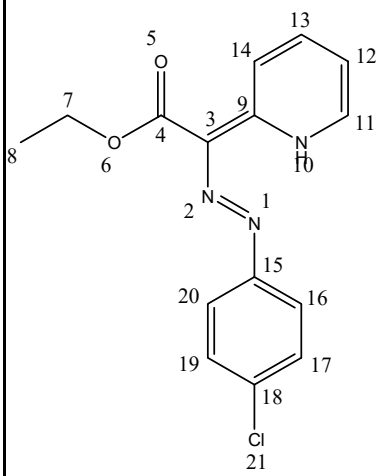
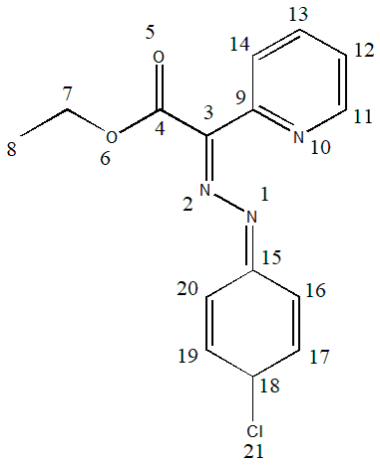
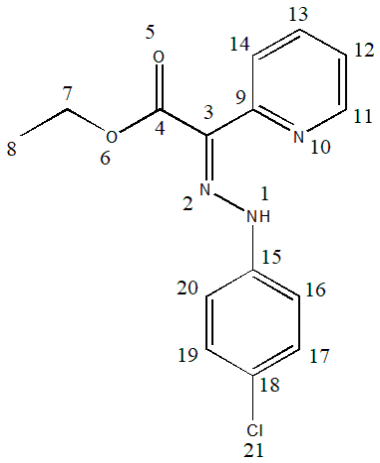
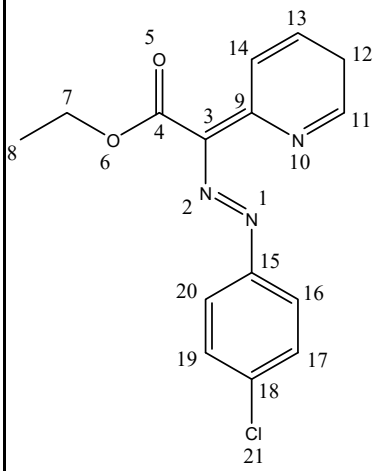
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	$N(CH_3)_2$	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43

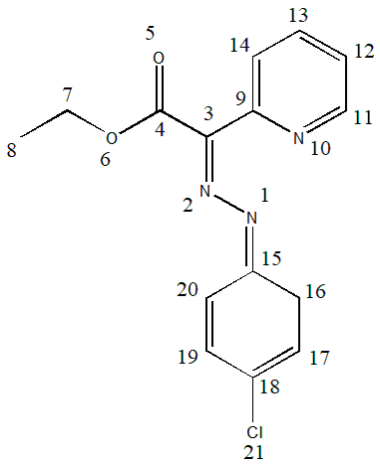
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	-0.037	-0.136
			17 C	-0.042	-0.15
			18 C	0.014	0.1
			19 C	-0.06	-0.288
			20 C	0.011	0.199
			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	$N(CH_3)_2$	8	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.179	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.078	0.033
			10 N	-0.258	-0.621
			11 C	0.027	0.376
			12 C	-0.047	-0.136
			13 C	-0.077	-0.288
			14 C	0.01	0.276

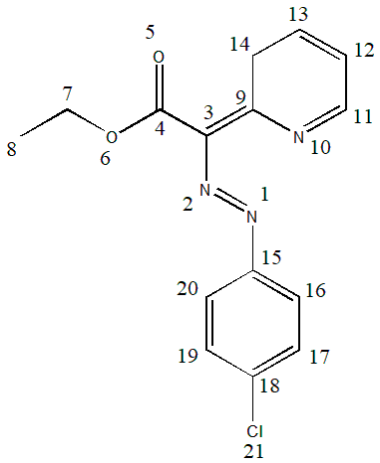
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.042	-0.15
			18 C	0.017	0.1
			19 C	-0.042	-0.15
			20 C	-0.033	-0.15
			21 N	-0.281	-0.838
			22 C	-0.009	0.369
			23 C	-0.009	0.369
	Cl	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
			1 N	-0.15	-0.179

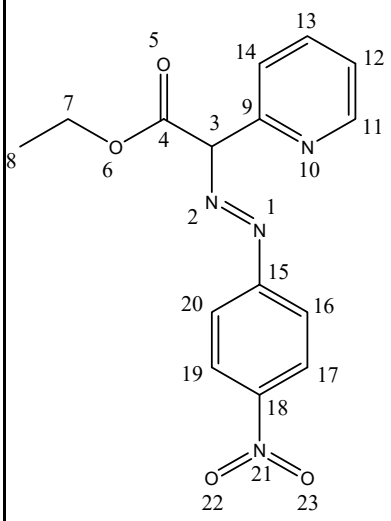
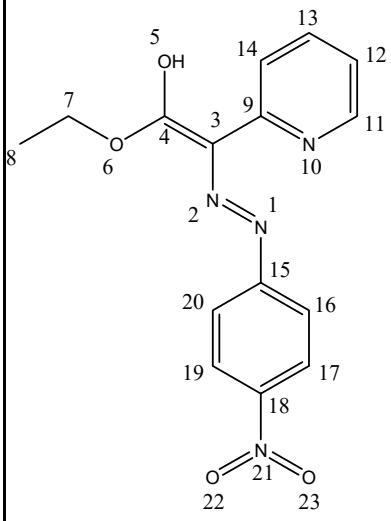
	Cl	2	2 N	-0.143	-0.171
			3 C	0.166	0.163
			4 C	0.211	0.153
			5 O	-0.339	-0.527
			6 O	-0.324	-0.357
			7 C	0.053	0.28
			8 C	-0.041	0
			9 C	0.095	0.318
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	Cl	3	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.176	0.185
			4 C	0.315	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.053	0.1
			10 N	-0.263	-0.6
			11 C	-0.018	-0.05

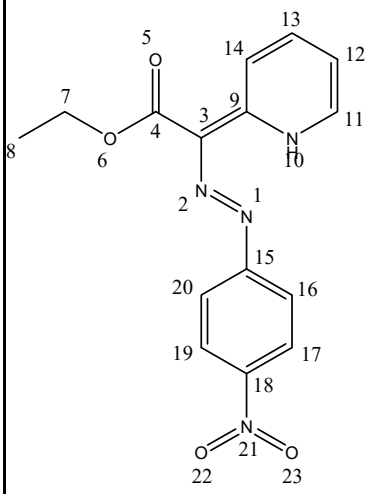
			12 C	-0.051	-0.15
			13 C	-0.059	-0.15
			14 C	-0.041	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	Cl	4	1 N	-0.15	-0.45
			2 N	-0.141	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.036	-0.136
			17 C	-0.055	-0.288
			18 C	0.097	0.566
			19 C	-0.055	-0.288
			20 C	-0.036	-0.136
			21 Cl	-0.161	-0.29

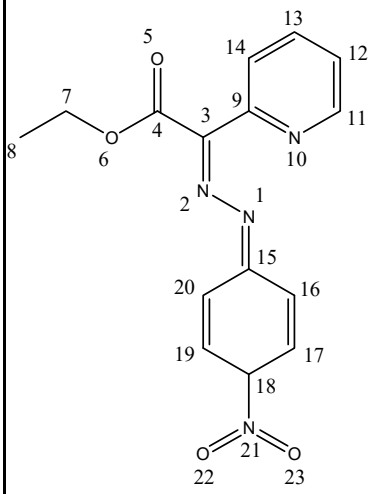
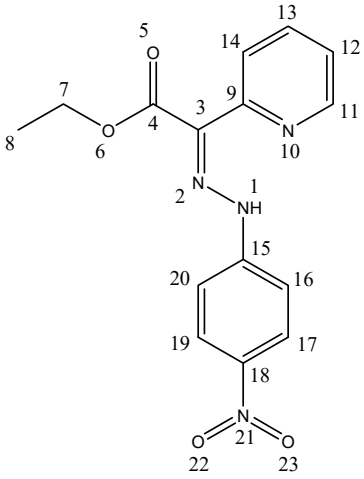
	Cl	5	1 N	-0.182	-0.458
			2 N	-0.188	-0.492
			3 C	0.175	0.482
			4 C	0.315	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.036	0.1
			16 C	-0.04	-0.15
			17 C	-0.036	-0.15
			18 C	0.073	0.177
			19 C	-0.036	-0.15
			20 C	-0.04	-0.15
			21 Cl	-0.13	-0.177
	Cl	6	1 N	-0.15	-0.179
			2 N	-0.141	-0.171
			3 C	0.183	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.171
			10 N	-0.258	-0.621

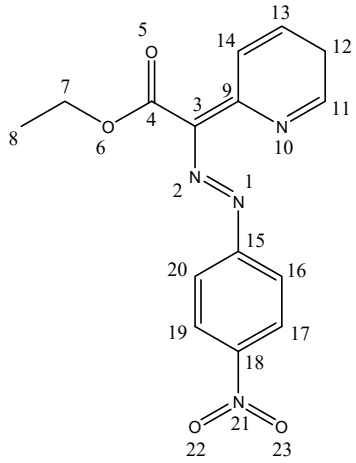
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	Cl	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	-0.036	-0.136
			17 C	-0.036	-0.15
			18 C	0.069	0.14
			19 C	-0.054	-0.288
			20 C	0.012	0.199

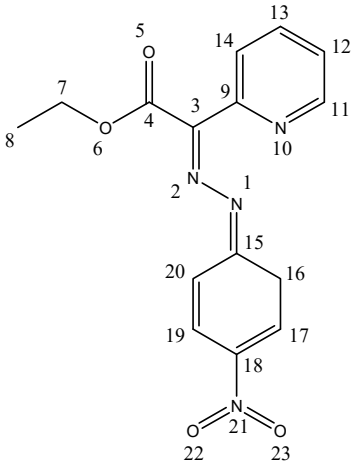
			21 Cl	-0.131	-0.14
	Cl	8	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.179	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.078	0.033
			10 N	-0.258	-0.621
			11 C	0.027	0.376
			12 C	-0.047	-0.136
			13 C	-0.077	-0.288
			14 C	0.01	0.276
			15 C	0.086	0.179
			16 C	-0.033	-0.15
			17 C	-0.035	-0.15
			18 C	0.073	0.177
			19 C	-0.035	-0.15
			20 C	-0.033	-0.15
			21 Cl	-0.13	-0.177
	NO_2	1	1 N	-0.154	-0.179
			2 N	-0.168	-0.246
			3 C	0.198	0.451
			4 C	0.294	0.659
			5 O	-0.263	-0.57
			6 O	-0.314	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.077	0.167

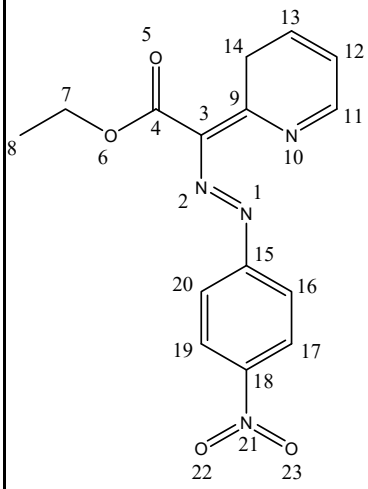
			10 N	-0.258	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.059	-0.15
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.032	-0.15
			17 C	-0.029	-0.15
			18 C	0.127	0.133
			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO_2	2	1 N	-0.15	-0.179
			2 N	-0.143	-0.171
			3 C	0.166	0.163
			4 C	0.211	0.153
			5 O	-0.339	-0.527
			6 O	-0.324	-0.357
			7 C	0.053	0.28
			8 C	-0.041	0
			9 C	0.095	0.318
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.086	0.179
			16 C	-0.032	-0.15
			17 C	-0.029	-0.15

			18 C	0.127	0.133
			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO_2	3	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.176	0.185
			4 C	0.315	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.053	0.1
			10 N	-0.263	-0.6
			11 C	-0.018	-0.05
			12 C	-0.051	-0.15
			13 C	-0.059	-0.15
			14 C	-0.041	-0.15
			15 C	0.086	0.179
			16 C	-0.032	-0.15
			17 C	-0.029	-0.15
			18 C	0.127	0.133
			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO_2	4	1 N	-0.15	-0.45
			2 N	-0.141	-0.45

			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.085	0.421
			16 C	-0.036	-0.136
			17 C	-0.049	-0.288
			18 C	0.147	0.517
			19 C	-0.049	-0.288
			20 C	-0.036	-0.136
			21 N	0.033	0.8
			22 O	-0.131	-0.52
			23 O	-0.131	-0.52
	NO_2	5	1 N	-0.182	-0.458
			2 N	-0.188	-0.492
			3 C	0.175	0.482
			4 C	0.315	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.278
			10 N	-0.254	-0.62

			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.036	0.1
			16 C	-0.04	-0.15
			17 C	-0.03	-0.15
			18 C	0.127	0.133
			19 C	-0.03	-0.15
			20 C	-0.04	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO_2	6	1 N	-0.15	-0.179
			2 N	-0.141	-0.171
			3 C	0.183	0.185
			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.096	0.171
			10 N	-0.258	-0.621
			11 C	0.009	0.329
			12 C	0.001	0.199
			13 C	-0.077	-0.288
			14 C	-0.038	-0.15
			15 C	0.086	0.179
			16 C	-0.032	-0.15
			17 C	-0.029	-0.15
			18 C	0.127	0.133

			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO_2	7	1 N	-0.154	-0.45
			2 N	-0.142	-0.45
			3 C	0.183	0.482
			4 C	0.316	0.72
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.097	0.278
			10 N	-0.254	-0.62
			11 C	0.028	0.16
			12 C	-0.044	-0.15
			13 C	-0.058	-0.15
			14 C	-0.034	-0.15
			15 C	0.067	0.375
			16 C	0.012	0.199
			17 C	-0.048	-0.288
			18 C	0.123	0.204
			19 C	-0.03	-0.15
			20 C	-0.036	-0.136
			21 N	0.056	0.836
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52
	NO_2	8	1 N	-0.15	-0.179
			2 N	-0.142	-0.171
			3 C	0.179	0.185

			4 C	0.316	0.706
			5 O	-0.258	-0.57
			6 O	-0.311	-0.43
			7 C	0.054	0.28
			8 C	-0.041	0
			9 C	0.078	0.033
			10 N	-0.258	-0.621
			11 C	0.027	0.376
			12 C	-0.047	-0.136
			13 C	-0.077	-0.288
			14 C	0.01	0.276
			15 C	0.086	0.179
			16 C	-0.032	-0.15
			17 C	-0.029	-0.15
			18 C	0.127	0.133
			19 C	-0.029	-0.15
			20 C	-0.032	-0.15
			21 N	0.056	0.907
			22 O	-0.127	-0.52
			23 O	-0.127	-0.52