Supporting information

(Carbene)→SO_2 Complexes: Ligand Stabilised Carbocyclic Carbenes (*ls*CCCs) are Better than *N*-Heterocyclic Carbenes

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Table S1. C→S bond length screening of (1,3-Dimethyl-imidazolidine-2-ylidene)→SO_2 (complex no. 7) in different quantum chemical levels.

Methodology	**C_1-S Bond length (Å)**	**C_1-S Bond* Dissociation Energy (BDE) (kcal/mol)**
Experimental	2.030	
HF/6-311++G(2d,p)	1.958	-5.65
M06-2x/6-311++G(2d,p)	2.010	3.71
M06-2x/6-311++G(2d,p) (SDD)	1.985	17.42
B3LYP/6-311++G(2d,p)	2.203	0.13
B3LYP/6-311++G(2d,p)+SDD	2.312	9.80
MPW1PW91/6-311++G(2d,p)	2.004	3.32
B3PW91/6-311++G(2d,p)	2.048	1.63
CAM-B3LYP/6-311++G(2d,p)	2.030	0.68
CAM-B3LYP-GD3BJ/6-311++G(2d,p)	**2.010**	**3.00**
Wb97xd/6-311++G(2d,p)	2.008	2.73

Table S2. Lists of energies (ΔG) (sum of electronic and thermal free energies) of optimized Carbene→SO_2 molecules (given in Hartrees) calculated at CAM-B3LYP-GD3BJ level of theory using 6-311++G(2d,p) basis set.

Str.	E (Hartrees)
1	-587.868310
2	-666.430578
3	-698.594552
4	-855.649796
5	-1112.405566
6	-853.303377
7	-854.484530
8	-869.354420
9	-1156.896909
10	-833.895172
11	-835.088080
12	-1088.968028
13	-1090.143156
14	-1006.870609
15	-1310.464762
16	-956.257112
17	-1072.901702
18	-1305.005663
19	-995.525011
20	-994.340747
21	-1069.569308
22	-1046.375722
23	-1120.428619
24	-1002.582587
25	-1233.482529
26	-892.575169
27	-853.262600
28	-1327.681490
29	-1006.850527
30	-1006.809543
31	-1006.841195
32	-1310.449343
33	-853.245484
34	-836.033162
35	-989.578615
36	-989.584040
37	-989.579045
38	-836.032528
39	-989.593489
40	-1143.143231
41	-742.556186
42	-931.774329
43	-781.838307

44	-856.836812
45	-819.954486
46	-875.262732
47	-1048.540727
48	-780.675325
49	-891.312290
50	-1119.777669
51	-962.703739
52	-1002.057213
53	-929.468066
54	-1197.210307
55	-1086.518059
56	-1040.192745
57	-1193.751841
58	-1351.955973
59	-1349.590720
60	-1956.771361
61	-1503.160258
62	-1656.726604
63	-2263.896729
64	-1579.283701
65	-2186.449399

Table S3. Lists of energies of second order delocalization ($n_O \rightarrow \sigma^*_{C(1)-S}$) in different Carbene→$SO_2$ molecules (given in kcal/mol) calculated at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory.

Structure	$E^{(2)}$ (kcal/mol)	Energy of Donor orbital E(i) (a.u.)	Energy of Acceptor Orbital E(j) (a.u.)	E(j)-E(i) (a.u.)	F(i,j) (a.u.)
6 (NHC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	36.97	-0.30494	0.08304	0.39	0.109
LP-3 of O (2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	37.13	-0.30669	0.08304	0.39	0.110
7 (NHC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	37.83	-0.30518	0.07588	0.38	0.109
LP-3 of O (2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	39.09	-0.30687	0.07588	0.38	0.112
17 (CAAC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	25.99	-0.30014	0.13479	0.43	0.096
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	23.28	-0.29695	0.13479	0.43	0.090
19 (CAAC→SO_2)					
LP-3 of O (1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	30.10	-0.30205	0.10642	0.41	0.100
LP-3 of O (2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	32.53	-0.30034	0.10642	0.41	0.101
26 (MIC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	22.83	-0.27990	0.16981	0.45	0.091
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	23.00	-0.28110	0.16981	0.45	0.092
28 (MIC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	22.31	-0.28680	0.16062	0.45	0.090

LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	24.87	-0.28227	0.16062	0.44	0.094
38 (*r*NHC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	18.64	-0.27871	0.17957	0.46	0.083
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	23.61	-0.28428	0.17957	0.46	0.094
39 (*r*NHC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	15.13	-0.28298	0.23457	0.512	0.080
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	23.34	-0.28110	0.23457	0.52	0.099
52 (CCC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	8.98	-0.31425	0.21935	0.53	0.062
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	10.14	-0.31406	0.21935	0.53	0.066
53 (CCC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	15.71	-0.25443	0.23662	0.49	0.079
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	16.51	-0.25592	0.23662	0.49	0.081
58 (Ligand Stabilized (CCC→SO_2)					
(LP-3 of O)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	10.00	-0.26282	0.26210	0.52	0.065
(LP-3 of O)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	12.58	-0.26385	0.26210	0.53	0.073
61 (Ligand Stabilized (CCC→SO_2)					
LP-3 of O(1)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	7.38	-0.26584	0.28120	0.54	0.056
LP-3 of O(2)					
$n_O \rightarrow \sigma^*_{C(1)-S}$	9.37	-0.26520	0.28065	0.54	0.064

Table S4. List of uncorrected, empirical dispersion corrected and BSSE corrected bond dissociation energy values obtained by CAM-B3LYP-GD3BJ/6-311++G(2d,p) quantum chemical method.

Complex NO.	Uncorrected BDE (kcal/mol)	BDE after Empirical Dispersion (kcal/mol)	BSSE correction values (kcal/mol)	BSSE corrected BDE (kcal/mol)
1	41.14	42.64	1.44	41.20
2	32.92	35.80	1.85	33.95
3	6.11	8.74	1.22	7.52
4	2.57	6.76	1.46	5.29
5	-4.57	0.84	1.93	-1.09
6	0.35	4.06	1.38	2.67
7	0.69	4.38	1.38	3.00
8	-1.20	1.50	1.23	0.27
9	-1.82	1.19	1.04	0.16
10	-1.56	0.95	0.92	0.02
11	-1.06	1.32	1.11	0.21
12	-4.39	0.60	1.47	-0.86
13	-6.05	-0.80	1.40	-2.21
14	-1.05	2.62	1.38	1.25
15	-2.04	0.89	1.02	-0.13
16	5.85	10.57	1.62	8.94
17	6.41	11.41	1.67	9.74
18	5.73	10.74	1.70	9.04
19	6.60	11.67	1.66	10.01
20	5.48	10.32	1.61	8.70
21	1.53	6.59	1.65	4.94
22	-1.75	2.55	1.35	1.19
23	-4.47	-0.03	1.16	-1.20
24	-4.19	-1.03	0.82	-1.85
25	-11.39	-5.97	2.43	-8.40
26	10.81	14.38	1.49	12.89
27	7.60	11.04	1.42	9.62
28	11.02	15.09	1.50	13.59
29	10.86	14.92	1.55	13.37
30	8.72	12.63	1.51	11.11
31	8.59	12.54	1.52	11.02
32	7.65	11.91	1.55	10.35
33	12.92	15.95	1.34	14.60
34	16.67	19.86	1.37	18.48
35	25.61	28.85	1.40	27.44
36	24.65	28.03	1.41	26.62
37	23.85	27.15	1.41	25.73
38	16.78	19.90	1.34	18.56
39	14.59	18.40	1.49	16.91
40	7.20	11.92	2.10	9.82

Complex NO.	Uncorrected BDE (kcal/mol)	BDE after Empirical Dispersion (kcal/mol)	BSSE correction values (kcal/mol)	BSSE corrected BDE (kcal/mol)
41	-0.46	1.08	0.76	0.32
42	1.58	4.73	1.13	3.60
43	31.17	15.01	2.00	13.01
44	27.08	30.24	2.01	28.22
45	27.65	31.67	2.19	29.48
46	16.27	20.28	2.14	18.14
47	28.17	32.40	2.23	30.17
48	21.70	24.91	2.00	22.91
49	17.65	21.58	2.08	19.50
50	-0.70	4.03	2.23	1.80
51	6.72	10.32	1.49	8.83
52	31.82	36.25	1.82	34.42
53	25.15	28.38	1.40	26.97
54	11.02	16.77	1.84	14.93
55	-1.65	4.10	1.72	2.38
56	33.45	38.28	2.14	36.14
57	24.15	29.33	2.13	27.19
58	31.58	38.74	2.34	36.40
59	35.09	41.71	2.49	39.21
60	19.25	26.01	2.31	23.70
61	34.67	41.19	2.34	38.85
62	35.80	43.17	2.52	40.64
63	19.23	27.02	2.54	24.48
64	37.01	45.89	2.69	43.19
65	24.21	31.58	2.62	28.96

Table S5. Singlet-Triplet gap in carbene (1-4) values obtained by CAM-B3LYP-GD3BJ/6-311++G(2d,p) quantum chemical method. (Positive values imply that the singlet state is stable over triplet state)

Carbene NO.	ΔE_{S-T} (kcal/mol)
1	-12.54
2	-0.70
3	51.07
4	40.70
45	-18.77
46	-3.03
47	-5.59
48	-7.03
50	20.98

Table S6. Lists of NMR chemical shift values (theoretical) calculated at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory by using GIAO Method through Implicit solvent (DMSO) effect (IEFPCM)

Structure NO.	^{13}C NMR shift of Carbene→SO_2 Complex (ppm)	^{13}C NMR shift of free Carbene (ppm)	Differences in NMR (ppm)
6	177.76	226.26	48.50
14	186.46	239.53	53.13
16	232.47	323.41	90.94
17	230.36	324.51	94.15
26	163.42	223.23	59.81
33	165.75	221.83	56.08
35	182.56	238.77	56.01
36	185.00	242.57	57.57
37	182.88	238.81	55.93
61	179.18	259.06	79.25
62	178.78	262.39	83.61

Table S7. Population of different Valance Basins (in electrons) in respective examples of (carbene)→SO_2 complexes

	Complex											
Type of basins	**6**	**7**	**17**	**19**	**26**	**28**	**38**	**39**	**52**	**53**	**58**	**61**
V(S)	2.40	2.42	2.37	2.38	2.37	2.37	2.38	2.35	2.33	2.35	2.34	2.34
$V(O_1)$	6.11	6.10	6.15	6.13	6.13	6.14	6.18	6.21	6.18	6.22	6.27	6.25
$V(O_2)$	6.10	6.08	6.15	6.14	6.14	6.15	6.17	6.17	6.15	6.22	6.25	6.25
V (S, O_1)	1.49	1.50	1.44	1.44	1.41	1.45	1.40	1.38	1.33	1.38	1.33	1.35
V (S, O_2)	1.49	1.49	1.43	1.44	1.43	1.40	1.44	1.42	1.34	1.38	1.34	1.33
V (C_c, S)	2.42	2.22	2.22	2.20	2.24	2.24	2.14	2.14	2.18	2.16	2.22	2.20
∑(S)	17.59	17.58	17.53	17.52	17.50	17.51	17.54	17.54	17.50	17.54	17.54	17.52
V (C_c)*	2.47	2.30	2.26	2.21	2.28	2.29	2.25	2.26	2.31	2.27	2.46	2.33

* V (C_c) value is calculated for the free carbenes of corresponding (carbene)→SO_2 complexes.

Table S8. Population of different Valance Basins (in electrons) of SO_2

Type of basins	**SO_2**
V(S)	2.98
$V(O_1)$	5.64
V(O2)	5.64
V (S, O_1)	1.71
V (S, O_2)	1.71
∑(S)	17.70

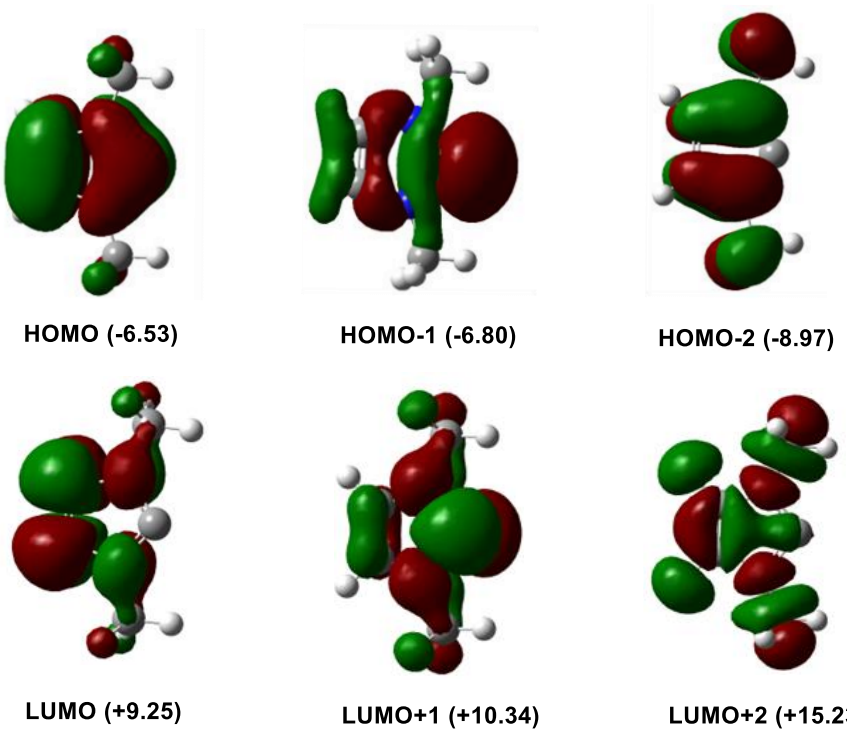


Figure S1. Plots of molecular orbitals of fragment **1** ((1,3-Dimethyl imidazol-2-ylidene) of complex **6** at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory. Isosurface value 0.03. Energies in eV are given in parenthesis.

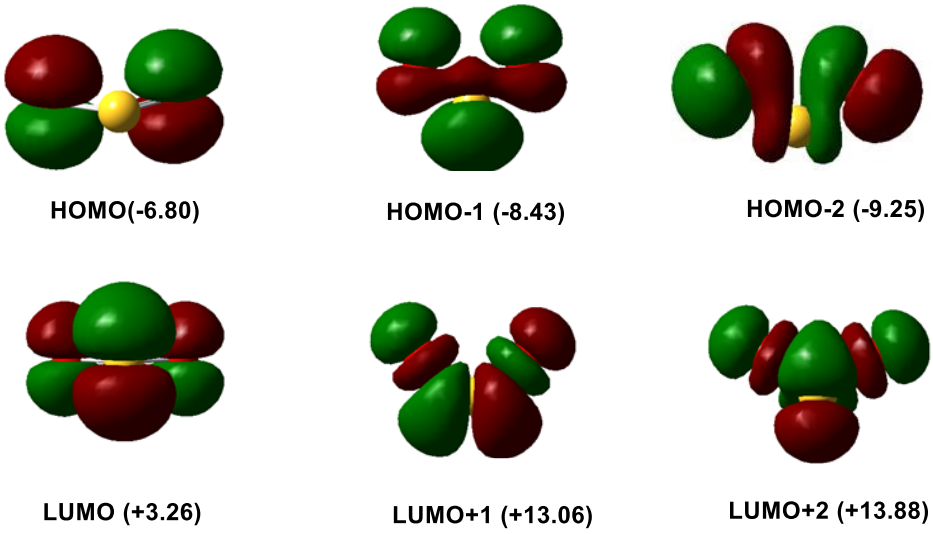


Figure S2. Plots of molecular orbitals of fragment **2**(SO_2) of complex **6** at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory. Isosurface value 0.03. Energies in eV are given in parenthesis.

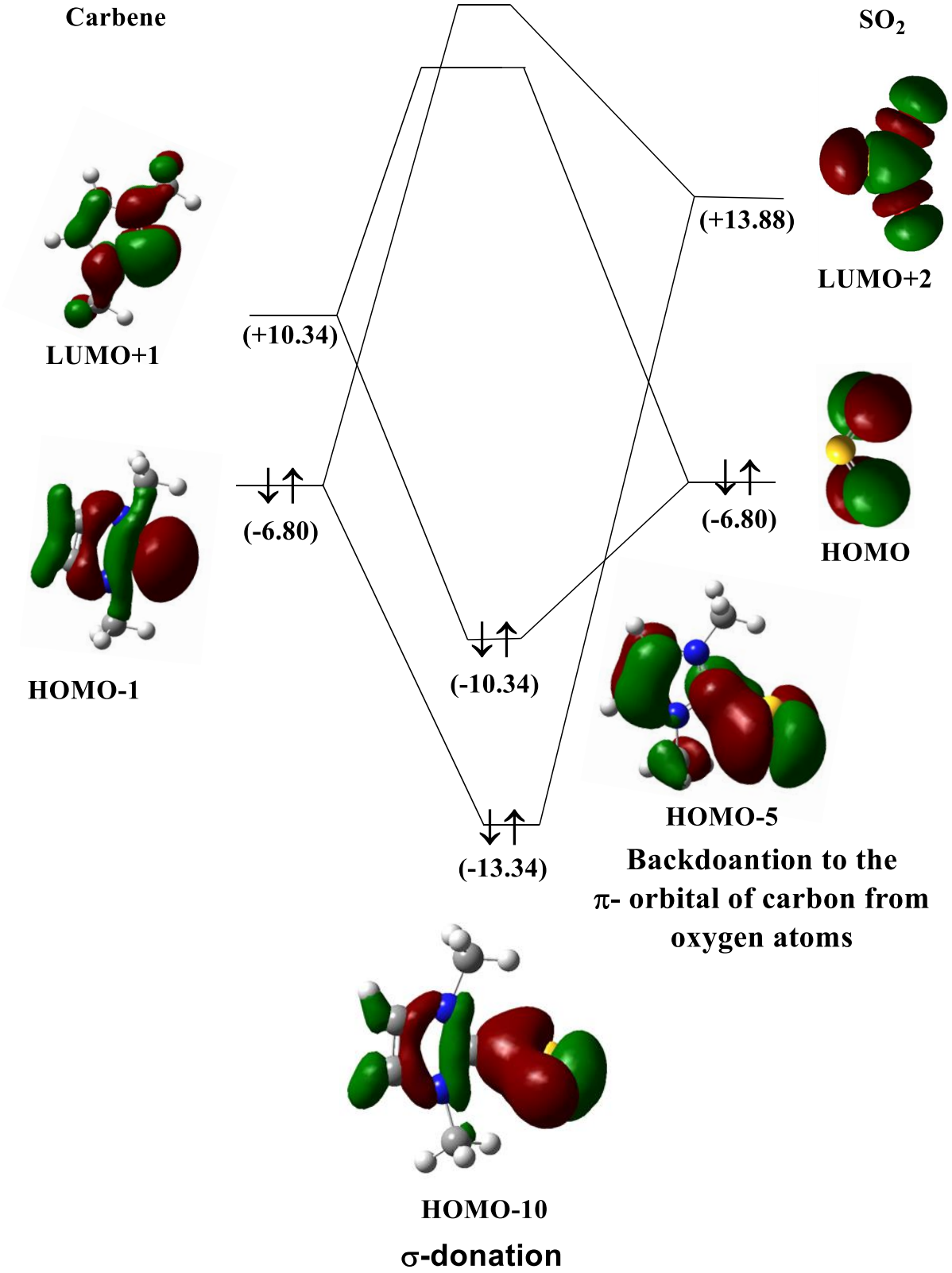


Figure S3. Frontier Molecular orbital interaction diagram of the representative NHC→SO_2 complex (**6**). Isosurface value 0.03. Energies in eV are given in parenthesis.

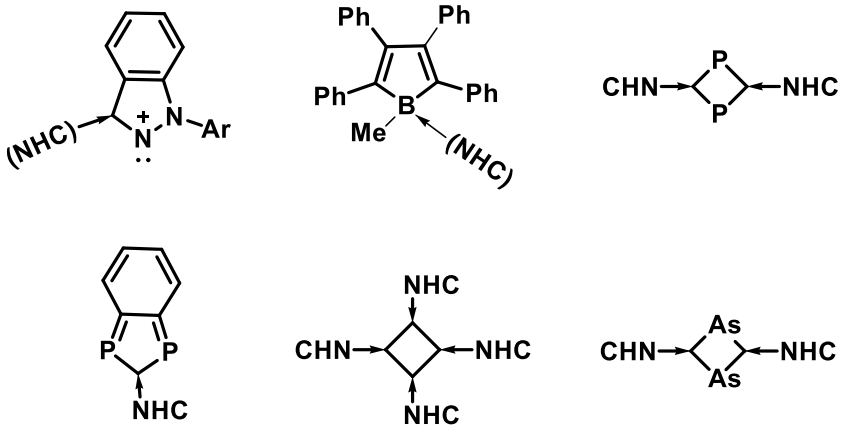


Figure S4. A few examples of ligand stabilized ring systems.

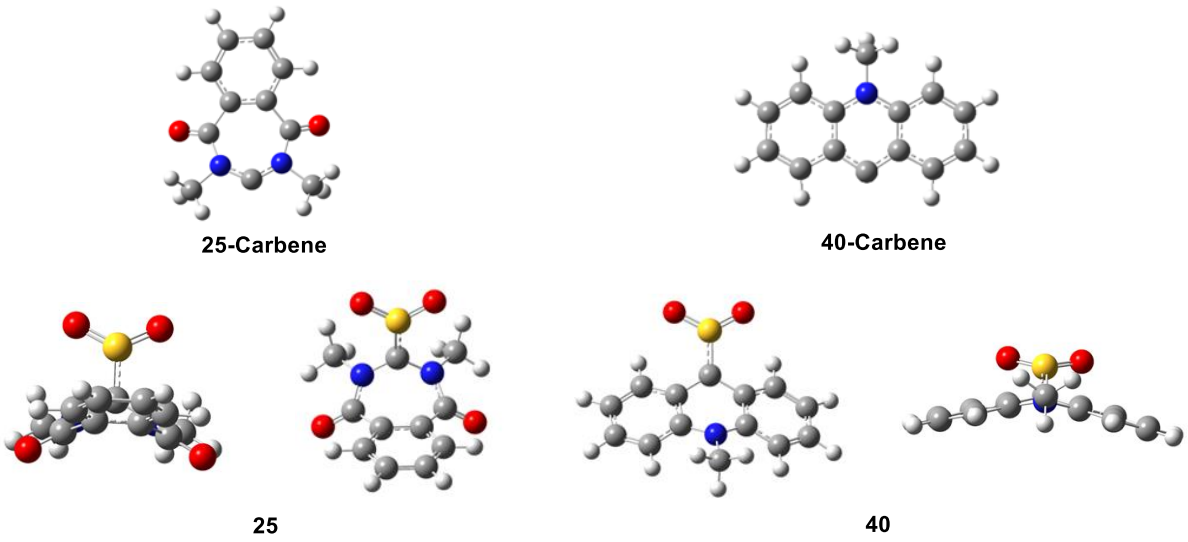


Figure S5. The 3D structures of the complex **25** and **40** (in two different poses each) to show the distortions from planarity of the carbenes upon coordination.

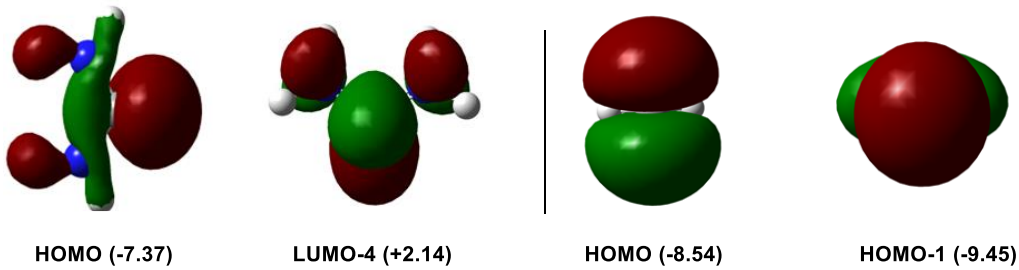


Figure S6. Plots of molecular orbitals of Carbene 3 (diamino carbene) in singlet state and carbene 1 (methylene carbene) at the triplet state obtained through CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory. Isosurface value 0.03. Energies in eV are given in parenthesis.

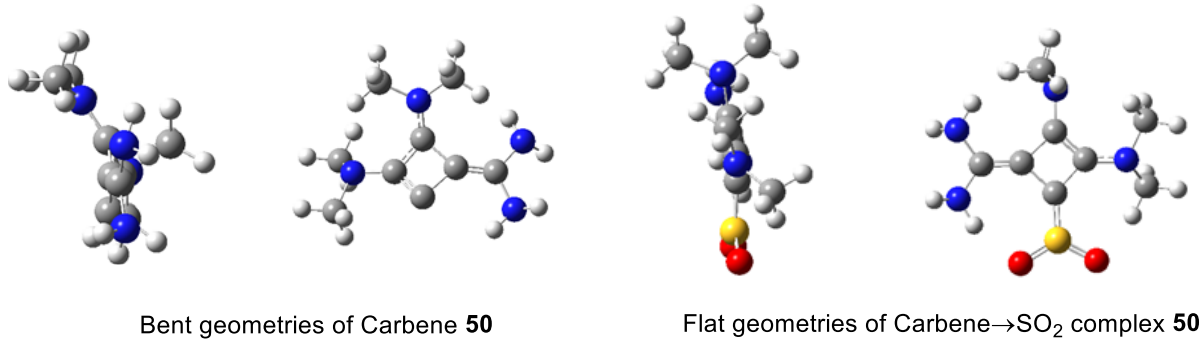


Figure S7. The 3D structures of the complex **50** and its corresponding carbene (in two different poses each) to show the change in the geometry of the carbene unit from bent (free carbene) to flat (complex) arrangement.

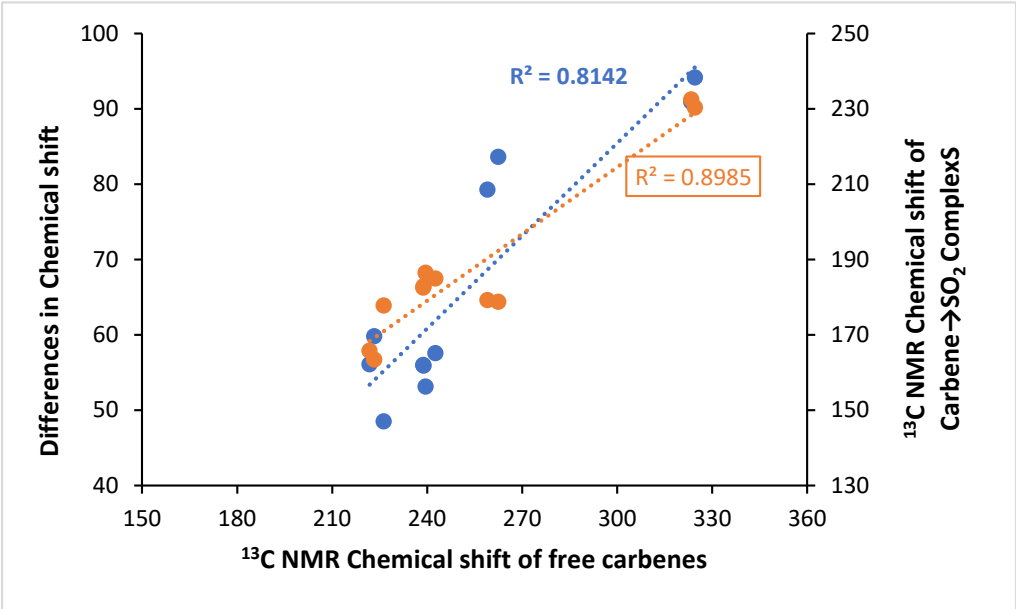


Figure S8. Correlation diagram – ^{13}C NMR chemical shift at the carbenic carbon (C_1) of free carbenes vs. the extent chemical shift at the carbon centre of corresponding carbene→SO_2 complexes (brown dotted lines) and ^{13}C NMR chemical shift at the carbenic carbon (C_1) of free carbenes vs. the extent of deviation in chemical shift (blue dotted lines).

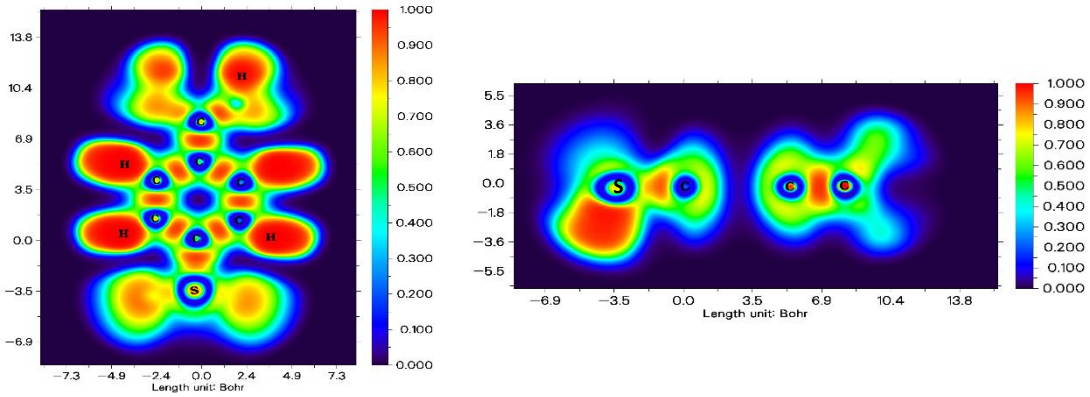
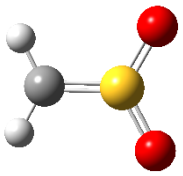


Figure S9. Colour-filled electron localization function diagram of complex **53** in plane and perpendicular to the plane.

2.1 Cartesian coordinates of the optimized geometries of Carbene→SO_2 complexes in singlet state at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory

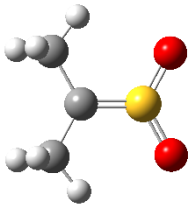
1



0 1

C	-1.51811000	-0.00014900	0.00005000
H	-2.01771700	-0.95336900	0.00018800
H	-2.01757200	0.95315700	-0.00014600
S	0.06219700	-0.00001100	-0.00007200
O	0.75944400	-1.25414400	0.00003500
O	0.75915600	1.25430400	0.00006600

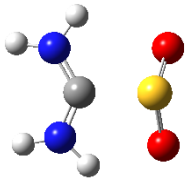
2



0 1

C	0.85151200	0.00000100	0.00005200
C	1.59283200	1.29812800	0.00004600
H	2.23551500	1.35963800	0.88167400
H	2.23598200	1.35932800	-0.88125500
H	0.92208200	2.15311200	-0.00025600
C	1.59285800	-1.29811400	-0.00002400
H	2.23585200	-1.35934700	-0.88143500
H	2.23568600	-1.35957100	0.88149800
H	0.92211900	-2.15310900	-0.00016700
S	-0.74027800	-0.00000300	-0.00001100
O	-1.44787800	1.25854800	-0.00002100
O	-1.44787100	-1.25855900	-0.00001900

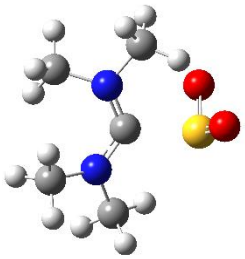
3



0 1

C	-0.98489000	0.02615300	-0.08430400
S	0.94469600	-0.09244600	-0.37519000
O	1.17482600	-1.25773900	0.50828800
O	1.24462600	1.24912500	0.19275400
N	-1.42066100	1.23191000	0.12025900
H	-0.66218500	1.91574100	0.21140100
H	-2.36555300	1.47511700	0.38165700
N	-1.68278800	-1.07907300	-0.08445000
H	-2.66615400	-1.13188400	0.14097000
H	-1.14338000	-1.93770900	-0.08416700

4



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C	-0.30238100	-0.02473400	0.00493700
S	1.57551500	-0.79007300	-0.08880700
O	2.04351100	-0.42441800	1.26409500
O	2.08524000	0.07899300	-1.16462000
N	-0.45461600	1.28385500	0.04157700
N	-1.33642600	-0.85452000	-0.02069300
C	0.66652600	2.16628400	0.38175800
H	1.41549300	1.61940400	0.94420600
H	1.11738600	2.57004200	-0.52356100

H	0.27161600	2.97818800	0.99411600
C	-1.61192400	1.99487700	-0.49287800
H	-2.21342300	1.33870300	-1.11346300
H	-2.23211900	2.42864000	0.29365200
H	-1.23769900	2.80402100	-1.11995000
C	-2.65937300	-0.54052900	0.50992900
H	-3.40170000	-0.40246000	-0.27813000
H	-2.97472900	-1.37703000	1.13417900
H	-2.61752800	0.34751600	1.13162900
C	-1.16503800	-2.26722600	-0.34951800
H	-1.20594000	-2.87897000	0.55388400
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H	-0.21624700	-2.43150300	-0.84585300

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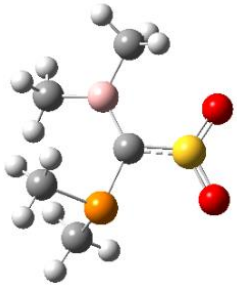

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C	-0.11536800	0.07181800	-0.08733200
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O	-1.28306500	-2.28933700	-0.06951800
B	-0.31121900	1.60619500	0.10121600
P	1.42831300	-0.88962000	-0.44072700
C	-1.58098200	2.37180800	-0.39684000
H	-2.29565200	2.41574400	0.43361600
H	-1.34244100	3.40701300	-0.65180400
H	-2.11168100	1.90680800	-1.22638800
C	0.79170500	2.44934400	0.83184100
H	1.31448200	3.07057300	0.09553600
H	0.30850700	3.15707800	1.51161600
H	1.53994400	1.89107300	1.38987500
C	2.11342300	-1.10921700	1.25606900
H	3.10585000	-1.55411700	1.16734500
H	2.18960500	-0.17989000	1.81861400
H	1.48289300	-1.81018700	1.80235800
C	2.53345500	0.42959900	-1.09645300
H	2.74789300	1.23607800	-0.40010600
H	3.47167500	-0.05482300	-1.37060400
H	2.10207500	0.84214500	-2.00883300

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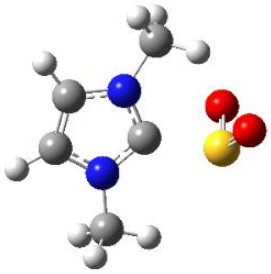

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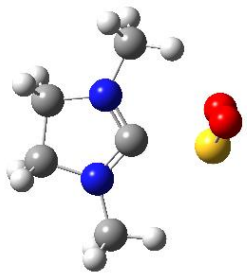
C	0.27416100	-0.08578200	-0.03969500
O	-1.99047400	-0.11912400	1.27176400
N	1.40611600	-0.79187000	-0.01783900
C	1.47914900	-2.24401600	-0.03097000
H	1.98415600	-2.59763000	0.86620400
H	0.46831100	-2.64042900	-0.05385600
H	2.01856500	-2.58078800	-0.91455700
C	-0.33145400	2.31002900	0.00492500
H	-1.20755000	2.02552400	-0.57167900
H	-0.62966600	2.51461900	1.03063700
H	0.14607100	3.18239000	-0.43497700
C	1.99198400	1.31493700	0.01916200
H	2.48837000	2.26904300	0.03833600
C	2.49131200	0.06269300	0.01879300
H	3.50645600	-0.29233500	0.03505500

7



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S	-1.69753700	-0.67249600	-0.00018700
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O	-2.21659100	0.09080800	-1.14791200
C	0.22577800	-0.09175800	-0.08111300
O	-1.98349500	-0.06390300	1.31145200
N	1.26538400	-0.90011700	0.01517300
C	2.04749200	1.29292800	0.11882100
H	2.22913900	1.69455900	1.11911100
H	2.49492300	1.96540000	-0.61194400
C	2.52756800	-0.15519200	-0.02326400
H	3.03465300	-0.33567600	-0.97478000
H	3.18683200	-0.46828800	0.78568600
C	1.23163500	-2.34148000	-0.07298300
H	1.76544700	-2.78110100	0.77060700
H	0.19825800	-2.67625600	-0.05152600
H	1.69712000	-2.67986800	-1.00178900
C	-0.27437200	2.31864900	-0.04282600
H	-1.27183500	2.01964500	-0.35043600
H	-0.30938800	2.71376500	0.97412500
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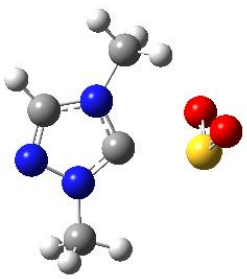
8



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S	-1.70366600	-0.76316600	0.00124000
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O	-2.08301000	-0.07521200	1.23769300
C	0.31385600	-0.12314900	-0.01045900
O	-2.10781600	-0.06977600	-1.22445900
N	0.63746500	1.18124300	-0.00642500
C	1.69010100	-2.18512200	-0.00494100
H	0.71914600	-2.67259000	-0.00854400
H	2.25136700	-2.46704100	-0.89300400
H	2.24606300	-2.46964700	0.88559400
C	-0.32021000	2.28405100	-0.00238200
H	0.23126300	3.21686100	-0.08871000
H	-1.00326600	2.16333000	-0.83891000
H	-0.89301900	2.26034200	0.92094000
N	2.54488600	0.09625100	0.00543800
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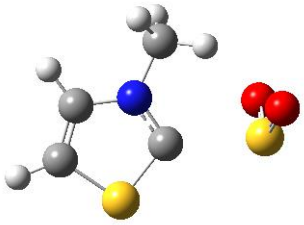
H	2.54150200	2.19922000	0.00854800

9



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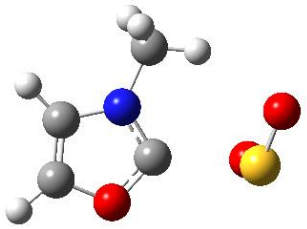
S	-1.95818100	-0.65868700	0.00339500
O	-2.35309800	0.14233400	-1.14859500
C	0.29413500	-0.28812400	-0.11073700
O	-2.14113600	-0.00002100	1.28974500
N	0.78744000	0.93789600	-0.04055600
C	2.16728400	1.03894500	0.05851500
H	2.62614800	2.01325200	0.11861400
C	2.77202300	-0.15613100	0.05980500
H	3.82776900	-0.35809300	0.11757200
C	-0.07133500	2.12762600	-0.02309900
H	0.44426900	2.93706100	-0.53483700
H	-1.00080100	1.89768200	-0.53467500

H	-0.28536400	2.40757100	1.00625400
S	1.57425200	-1.39976000	-0.06121600

10



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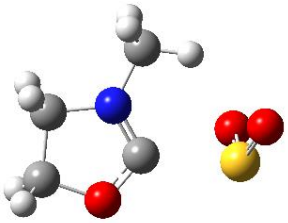
O	-1.98340700	-0.24563300	1.31641400
N	1.16115900	0.68404300	-0.00364200
C	2.51858700	0.40999700	0.14270000
H	3.25366700	1.17142200	0.33280200
C	2.63283500	-0.90795700	-0.00676800
C	0.55430000	2.00312200	0.10747600
H	1.07916400	2.69853600	-0.54505500
H	-0.48529200	1.93131900	-0.19886100
H	0.60952300	2.34840500	1.13838200
O	1.38328200	-1.42058400	-0.23380400
H	3.46079900	-1.59214500	0.01310000

11



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S	-1.85530700	-0.59174100	-0.06342100
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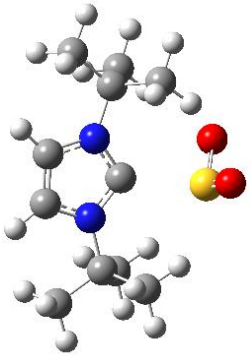
O	-1.90564500	-0.17090500	1.33371900
N	0.98870800	0.72854000	-0.04407700
C	2.42745600	0.53480700	0.16329300
H	2.70584000	0.85866500	1.16722700
C	2.54857200	-0.97285000	-0.03853200
C	0.36559900	2.03561100	0.05315300
H	0.85551100	2.72155000	-0.63827500
H	-0.68545300	1.94509300	-0.20678900
H	0.46101000	2.41602000	1.07061300
O	1.16838400	-1.41971900	-0.21207800
H	2.95676400	-1.50081100	0.81849300
H	2.99742900	1.11257800	-0.56406800
H	3.09381100	-1.24821600	-0.93787700

12



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S	-0.09604400	2.16574600	0.05488900
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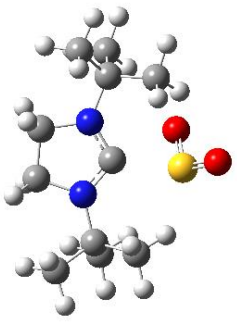
C	-0.04582500	-0.13691000	0.08156300
O	1.02266300	2.50855200	0.92401000
N	-1.16404600	-0.88830400	-0.01667400
C	0.50855400	-2.27718100	-0.25958300
C	-0.83215200	-2.21039100	-0.23243000
C	2.43427300	-0.64655100	0.04010900
C	3.27397500	-1.90240800	-0.17383200
H	3.08341600	-2.66117300	0.58625500
H	4.32314400	-1.62079300	-0.09949300
H	3.11917000	-2.33644700	-1.16264000
C	2.69459200	-0.10254900	1.44119800
H	2.12231600	0.80367500	1.62273400

H	3.75362100	0.13690500	1.54591600
H	2.43705700	-0.85125100	2.19277300
C	2.78272100	0.36882100	-1.04202700
H	2.24136700	1.30164400	-0.92476400
H	2.55963100	-0.03565900	-2.03049900
H	3.84985800	0.58903300	-0.99377500
C	-2.56361900	-0.38089300	0.09059400
C	-3.53226400	-1.56045000	0.10248800
H	-3.33926600	-2.23810200	0.93495500
H	-3.50684300	-2.12299600	-0.83112000
H	-4.54184200	-1.16943600	0.21986700
C	-2.87174500	0.49469100	-1.12155200
H	-2.20435800	1.34834000	-1.19886000
H	-3.89560600	0.86426800	-1.05318400
H	-2.77766700	-0.08601900	-2.04026800
C	-2.71356500	0.37846400	1.40642000
H	-2.06409600	1.24771700	1.45015800
H	-2.48077000	-0.27312800	2.24961200
H	-3.74360600	0.72085000	1.51108900
H	1.14286100	-3.13009200	-0.39910000
H	-1.55431100	-2.99464400	-0.34504000

13



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S	-0.12171800	2.16969300	0.28177800
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O	0.26878500	2.84277200	-0.94338400
C	-0.04952400	-0.14269300	-0.20730500
O	0.89318500	2.13992200	1.32613300
N	-1.16750200	-0.85417400	-0.02665100
C	0.62005400	-2.28691500	0.37505600
H	1.14436400	-2.60708700	1.27440700
H	0.85814700	-2.98486600	-0.42812100
C	-0.88059400	-2.16121200	0.58138200
H	-1.42681400	-2.96408400	0.09475800
H	-1.15380000	-2.15025400	1.64036900
C	2.43894200	-0.58281600	-0.18737000
C	3.13767100	-1.77800200	-0.84146200
H	3.13485300	-2.66488900	-0.20738500
H	4.17828100	-1.51528700	-1.02756900
H	2.67754300	-2.02867800	-1.79901900
C	3.06428800	-0.29869200	1.17806400
H	2.58287800	0.55976600	1.64153200
H	4.12809200	-0.08515600	1.06284900
H	2.96977500	-1.16107400	1.84164800
C	2.58907500	0.61845800	-1.11054900
H	2.23301500	1.53835200	-0.66193000
H	2.05286200	0.46103100	-2.04680300
H	3.64714800	0.75117600	-1.33936800
C	-2.55713900	-0.35720900	-0.13849400
C	-3.47563600	-1.54233700	-0.44471200
H	-3.53463700	-2.24757000	0.38457000
H	-3.14706500	-2.07529400	-1.33838300
H	-4.48268700	-1.16898800	-0.62709500
C	-2.66038500	0.62117600	-1.30493900
H	-2.04290600	1.50450900	-1.17813300
H	-3.69550900	0.94961900	-1.40497600
H	-2.36251600	0.13399900	-2.23400000
C	-2.99834300	0.28618800	1.17768700
H	-2.40322300	1.16682200	1.40725600
H	-2.90377200	-0.41910800	2.00540300
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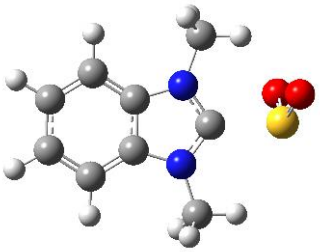
14



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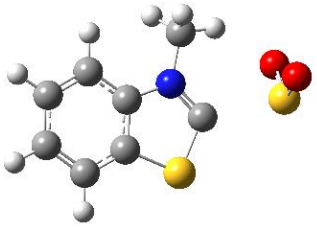
C	-1.27789000	-0.70357100	-0.01790500
C	-1.42569100	0.68000100	-0.02502400
C	-2.67293500	1.27941400	0.00312600
C	-3.76935000	0.43774900	0.04227300
C	-3.62207800	-0.95155000	0.05220200
C	-2.37475200	-1.54738900	0.02185900
C	0.75115200	0.20509900	-0.08304500
H	-2.78895300	2.35474100	-0.00352400
H	-4.76349600	0.86359300	0.06698400
H	-4.50549200	-1.57513700	0.08528600
H	-2.26366500	-2.62291100	0.03269900
N	-0.13759000	1.20326100	-0.06592200
N	0.08897800	-0.95120700	-0.06149400
C	0.18880000	2.61690600	-0.07683800
H	-0.24452500	3.09212500	-0.95622400
H	-0.19677700	3.09429600	0.82331900
H	1.26896200	2.72415100	-0.10520400
C	0.70470300	-2.27104900	-0.04222900
H	0.62381100	-2.70126700	0.95472100
H	0.19738000	-2.90654300	-0.76632000
H	1.75010800	-2.16844900	-0.31651200
S	2.75872600	0.36559600	0.01045700
O	2.91483000	-0.26825800	1.32987000
O	3.09911800	-0.51201500	-1.12201400

15



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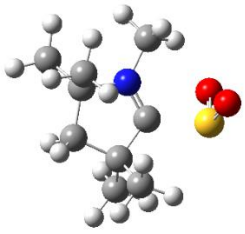
C	-1.67258500	-0.81746100	-0.04085200
C	-1.31799700	0.52576800	-0.04489400
C	-2.28187900	1.52095000	0.03829600
C	-3.60421500	1.13474400	0.12223700
C	-3.96269700	-0.21348000	0.12272100
C	-3.00254500	-1.20145100	0.04105000
C	0.78975400	-0.41158500	-0.19971000
H	-2.00776800	2.56658000	0.04113000
H	-4.37483800	1.89109100	0.18953900
H	-5.00696500	-0.48825900	0.18940900
H	-3.27954100	-2.24714300	0.04302400
N	0.07077900	0.69140200	-0.14062700
C	0.67645800	2.02232900	-0.15519500
H	0.20901300	2.61790000	-0.93785400
H	0.53042300	2.50023300	0.81234300
H	1.73677100	1.92361900	-0.36098100
S	3.09464400	-0.39328200	0.07004600
O	3.43568700	0.51579400	-1.01447900
O	3.05904800	0.22088500	1.38869000
S	-0.22003100	-1.78522700	-0.15053500

16

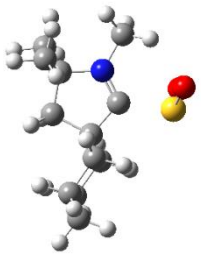


0 1

S	-2.28497300	-0.10994900	-0.00632000

O	-2.50597900	-1.06327000	-1.11935100
C	-0.37306200	0.15002200	-0.14412600
O	-2.23379300	-0.74554600	1.33566900
N	0.47424000	-0.80743300	-0.13521100
C	1.77866100	1.14845600	-0.21670500
H	2.38851000	1.69793000	0.49901400
H	2.12903400	1.40965600	-1.21541300
C	1.90567600	-0.37021300	-0.00562100
C	0.10951900	-2.22349300	-0.09463800
H	0.09411000	-2.55889900	0.94054300
H	-0.88214500	-2.33635700	-0.52368800
H	0.83806000	-2.79309300	-0.66501200
C	0.27915600	1.49306100	-0.08227000
C	-0.22286100	2.37598700	-1.22620300
H	-1.29310400	2.56006400	-1.13587000
H	0.29487500	3.33641900	-1.20233500
H	-0.03861600	1.91209000	-2.19617600
C	-0.06355200	2.14170400	1.26639300
H	-1.13828000	2.28864900	1.36640000
H	0.26538100	1.52972800	2.10590700
H	0.42767000	3.11386200	1.33162500
C	2.76532000	-1.02186100	-1.07830500
H	3.75515300	-0.56456500	-1.06458000
H	2.89626800	-2.09058800	-0.91071600
H	2.33544600	-0.87089800	-2.06928700
C	2.40108900	-0.73798700	1.38839800
H	2.40322100	-1.81798000	1.53733100
H	3.42340200	-0.38123600	1.51618000
H	1.77939300	-0.28709400	2.16159400

17



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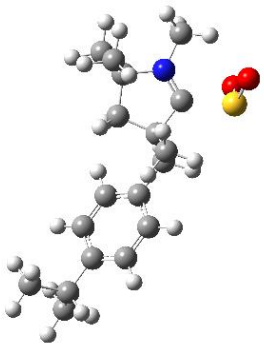
O	1.91427100	-2.22147600	1.26562200
N	1.42911300	0.59106700	0.01036200
C	-0.64811200	1.65583000	-0.31510400
H	-1.28298400	2.26086400	0.32919600
H	-0.90870700	1.89824500	-1.34535600
C	0.83844200	1.96749700	-0.06572200
C	2.87793700	0.39398800	0.05924500
H	3.32741700	1.21906900	0.60571000
H	3.08306800	-0.54894800	0.55814200
H	3.26814600	0.36138200	-0.95586500
C	1.47149700	2.73569000	-1.21577200
H	0.96504400	3.69457200	-1.32981700
H	2.52819300	2.93623800	-1.03751800
H	1.37444200	2.18457000	-2.15188100
C	1.06356300	2.68041900	1.26293400
H	2.12303500	2.82889800	1.47133400
H	0.59248100	3.66308800	1.22870700
H	0.62635000	2.11898600	2.08856700
C	-0.83236800	0.14064400	-0.06663600
C	-1.57622400	-0.56325400	-1.21549800
C	-1.53408900	-0.18056100	1.27106800
C	-3.05093500	-0.18071100	-1.24823100
H	-1.48528400	-1.64375200	-1.08269800
H	-1.08916900	-0.32504300	-2.16342000
C	-3.01661300	0.17492700	1.23937800
H	-1.42058600	-1.24907000	1.47168600
H	-1.03177300	0.34280900	2.08755700
C	-3.73180900	-0.50462600	0.07696100
H	-3.54263800	-0.70694700	-2.06830300
H	-3.15581000	0.88883400	-1.46046800
H	-3.47354500	-0.11073800	2.18870600
H	-3.13841000	1.25966800	1.15417300
H	-4.78053000	-0.20206300	0.05050500

H	-3.71986900	-1.58852000	0.23057700

18



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O	4.34817900	-1.86724600	0.79187900
N	3.00767000	0.80575800	-0.11140900
C	0.76287100	1.45758500	0.17035500
H	0.20186300	1.94638800	0.96473900
H	0.21280300	1.61627600	-0.75495500
C	2.17729800	2.04738700	0.03482600
C	4.42279200	0.88401100	-0.47373300
H	4.85414900	1.77225600	-0.01910300
H	4.92371900	-0.00954200	-0.11193200
H	4.51076900	0.93944700	-1.55682700
C	0.93597600	-0.05470200	0.43120400
C	0.05379600	-0.93477500	-0.48864000
H	0.32888800	-0.73178000	-1.52548600
H	0.30684300	-1.97941700	-0.30330900
C	0.74495300	-0.42481300	1.90785200
H	0.96453800	-1.47938100	2.07676000
H	1.40426600	0.15954500	2.54990500
H	-0.28410000	-0.22997000	2.20648900
C	2.32482100	2.91347700	-1.20693400
H	1.63373900	3.75438000	-1.14177600
H	3.33282700	3.31725300	-1.30427400
H	2.08804000	2.34603100	-2.10775400
C	2.61981000	2.80112600	1.28386200
H	3.65088600	3.14597400	1.20596600
H	1.98680200	3.67872900	1.41707300
H	2.53239400	2.17841100	2.17369900
C	-1.42489600	-0.72669700	-0.30744000
C	-2.12559800	0.18449800	-1.09044500
C	-2.13979800	-1.44170000	0.64451300
C	-3.48092900	0.39226200	-0.91052000
H	-1.60664600	0.72919000	-1.87069900
C	-3.49743900	-1.23342100	0.82364900
H	-1.63153300	-2.18375600	1.24862200
C	-4.19248400	-0.30944100	0.05617100
H	-3.99208900	1.10716700	-1.54415600
H	-4.02957500	-1.80903500	1.57240300
C	-5.67553400	-0.09180700	0.25689300
H	-5.98677200	-0.75392400	1.06969500
C	-5.98260500	1.34357000	0.68429900
H	-7.04915000	1.46668300	0.88149200
H	-5.43487900	1.61208600	1.58863400
H	-5.70568200	2.05415200	-0.09723500
C	-6.47594300	-0.47694300	-0.98750900
H	-6.28002100	-1.50955100	-1.27872400
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H	-6.21827800	0.16258500	-1.83421900

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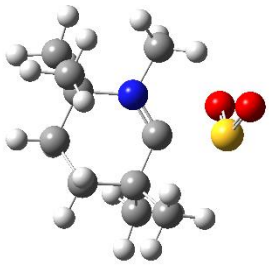

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C	-0.41427000	0.12280300	0.06766200
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C	1.32094200	1.93467800	0.20944000
C	2.18951900	0.93671400	-0.52306400
H	1.51014300	2.94784100	-0.14981800

N	0.50776200	-0.76881100	0.10002900
H	1.56262400	1.93426300	1.27422500
C	-0.15834000	1.59984500	0.01890400
C	-0.98064000	2.25229900	1.14118300
H	-0.77670500	3.32456000	1.14759200
H	-2.04916300	2.10533400	0.99829700
H	-0.70911500	1.84704400	2.11682300
C	-0.66056100	2.11398100	-1.34244800
H	-0.08323700	1.70253200	-2.17039800
H	-1.70480400	1.85398400	-1.50488300
H	-0.56875500	3.20098900	-1.36317000
H	3.24703300	1.18315000	-0.41954500
H	1.96560300	0.96328400	-1.59199100
C	2.62260800	-0.67653400	1.36245500
H	2.21355700	0.01943200	2.09331800
H	2.47331200	-1.68607500	1.74215400
H	3.69720500	-0.50674400	1.28911900
C	2.59591500	-1.45258700	-1.02685600
H	2.61357900	-2.48167000	-0.67467700
H	2.05378500	-1.41686000	-1.97229600
H	3.62600600	-1.14930000	-1.21581100
C	0.14509100	-2.19707100	0.22042700
H	0.93348500	-2.71035500	0.76064900
H	0.02175000	-2.62404000	-0.77081500
H	-0.79034300	-2.27961200	0.76335800
S	-2.32430900	-0.40242500	-0.07320400
O	-2.18872700	-1.26663300	-1.26858000
O	-2.49675600	-1.14462100	1.19732800
C	-1.00817000	1.41057800	1.27087100
C	-0.24904300	1.44652000	-0.07649700
C	-1.77478700	-0.63999200	0.03510300
C	-1.88681500	0.15553700	1.34428000
H	-0.28524600	1.42928200	2.08550900
H	-1.60427600	2.32205900	1.34285300
H	-1.58383000	-0.48631200	2.17232100
H	-2.93629700	0.40844900	1.49944500
C	0.45652100	0.13108900	-0.18312000
C	-2.20192600	0.25076700	-1.13777700
H	-2.15567300	-0.33049500	-2.05948900
H	-3.24553400	0.53019900	-0.98802900
C	-1.29353400	1.48429100	-1.21320400
H	-0.77825900	1.53373800	-2.17261900
H	-1.86513400	2.40810200	-1.11152000
N	-0.31167400	-0.90106700	-0.15275700
C	0.67802600	2.64934600	-0.15005100
H	1.39758600	2.65174900	0.66745500
H	1.23677600	2.66787000	-1.08578200
H	0.08669500	3.56473200	-0.08786600
C	-2.60007200	-1.90907900	0.09036900
H	-2.56079600	-2.46725400	-0.84441100
H	-2.29322900	-2.56489900	0.90407000
H	-3.63968300	-1.63060100	0.26342700
C	0.20398800	-2.27399500	-0.17499200
H	0.11148200	-2.70651000	0.81954600
H	-0.37041500	-2.85901700	-0.88806300
H	1.24778200	-2.25084500	-0.47063000
S	2.41201200	0.00843800	-0.01787800
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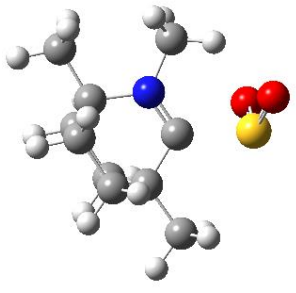
O	2.35373700	-0.54229400	1.36135200

20



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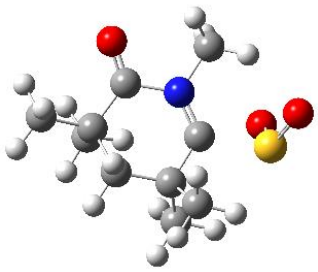

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C	0.62991000	0.08132300	-0.20764300
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C	-1.55766400	1.30179800	-0.51097500
C	-2.21032700	0.10275700	0.17838600
H	-2.03563900	2.21986700	-0.16309400
N	-0.01582700	-1.03967400	-0.28157000
H	-1.77809600	1.22615300	-1.57904200
C	-0.03973700	1.41080000	-0.32455100
C	0.58176600	2.04992300	-1.58519900
H	0.11640200	3.02375200	-1.74623700
H	1.65497400	2.19332400	-1.47083700
H	0.40776000	1.43661100	-2.47008600
C	0.32490600	2.29405900	0.88415000
H	-0.05000400	1.89415300	1.82249900
H	1.40184600	2.41131400	0.97666600
H	-0.11552200	3.27995400	0.73041900
C	-2.11462400	0.14778300	1.71396600
H	-2.53484300	1.08631200	2.07746500
H	-2.68932900	-0.67231300	2.14464800
H	-1.09297500	0.06529500	2.08148700
C	-3.67417700	0.00145000	-0.23574800
H	-4.14471300	-0.87830700	0.19890200
H	-4.20965600	0.88809400	0.10675100
H	-3.77651100	-0.06448700	-1.31923800
O	-1.97924000	-2.18197100	-0.53516200
C	0.67710900	-2.34698800	-0.29973100
H	0.65004500	-2.76744700	0.70272700
H	0.14057700	-2.99221400	-0.98635000
H	1.70310000	-2.19414100	-0.61306200
S	2.57452000	0.10621500	0.24556300
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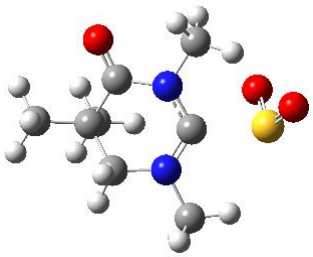

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N	-0.06409000	-0.92578100	-0.47489900
N	-0.08088200	1.36492500	-0.48312500
O	-1.96205800	-2.13828300	-0.22998100
C	-1.91928300	0.41212000	1.69768800
H	-2.41240600	1.32732700	2.03047000
H	-2.34681800	-0.42509600	2.24830900
H	-0.86089900	0.47607500	1.95267700
C	-3.63248800	0.11157500	-0.12022200
H	-3.80622200	-0.03507200	-1.18709100
H	-4.06738300	-0.73529500	0.40566200
H	-4.14820300	1.02078700	0.19368100
C	0.57795900	2.66301800	-0.53692100
H	0.28707500	3.26470400	0.32476000
H	1.65409200	2.53300200	-0.53703300
H	0.27763800	3.18006000	-1.44940600
C	0.69174300	-2.17749100	-0.63000600
H	1.69899600	-1.94051500	-0.95462600
H	0.72766200	-2.70862400	0.31790400
H	0.18440500	-2.79203300	-1.36838600

S	2.59829500	0.26932400	0.33745800
O	2.20892700	-0.49370300	1.52723300
O	3.35189700	-0.48308400	-0.66244400
H	-1.80702100	1.30225600	-1.65670100
H	-1.90731600	2.32188000	-0.21865300
H	0.93240200	-2.92720200	0.03084000
H	0.46041900	-2.84499500	-1.67198100
S	2.77578300	0.42942100	0.29805200
O	2.09643200	0.32065300	1.58090900
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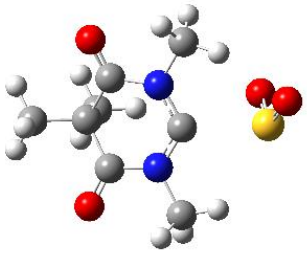

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C	-1.48667100	1.17358800	-0.25543900
C	-1.98801800	-0.12916800	0.32125900
C	-1.24223900	-1.32435100	-0.22495500
C	0.64943700	0.11067600	-0.71855600
N	0.10172100	-1.09657000	-0.57752300
N	-0.12950900	1.19403400	-0.62153500
O	-2.15094500	2.17057400	-0.32495200
O	-1.70792200	-2.42783200	-0.28332000
C	-1.64543000	-0.07652900	1.83441700
H	-2.16348200	0.76876800	2.28563500
H	-1.98853900	-0.99580500	2.30736300
H	-0.57384900	0.03109900	2.00963900
C	-3.48730400	-0.27813000	0.10887000
H	-3.73309200	-0.31766100	-0.95223700
H	-3.83275000	-1.19882500	0.57298800
H	-4.00525600	0.57125000	0.54791400
C	0.43549700	2.51107600	-0.92377800
H	0.40046700	3.14426300	-0.03918400
H	1.46030600	2.37332800	-1.24938800
H	-0.14614300	2.98155800	-1.71247500
C	0.90964900	-2.29121900	-0.85110500
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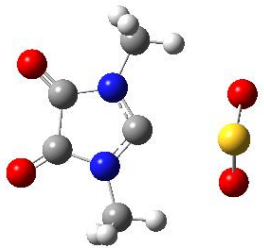
24



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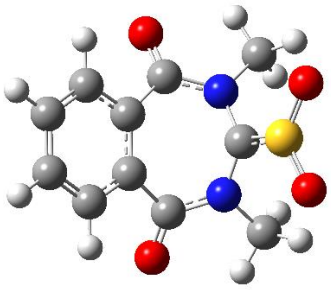
C	-0.04172000	-0.00002000	0.31077500
O	-2.77120300	-1.22927200	-0.49423400
N	0.73733600	-1.09380300	0.16353600
C	2.06971600	0.77073200	-0.07920100
C	2.06983300	-0.77059600	-0.07895700
C	0.26747100	-2.46872600	0.24635800
H	0.55063400	-2.90643600	1.20266400
H	-0.81208900	-2.47004400	0.13476900
H	0.72369600	-3.04635300	-0.55459600
N	0.73720900	1.09382600	0.16340100
C	0.26723000	2.46872600	0.24601300
H	-0.81250700	2.46972400	0.13618100
H	0.55189300	2.90712400	1.20155400
H	0.72199400	3.04592400	-0.55608500
O	2.98484500	-1.51308700	-0.24553400
O	2.98464900	1.51331200	-0.24579400

25



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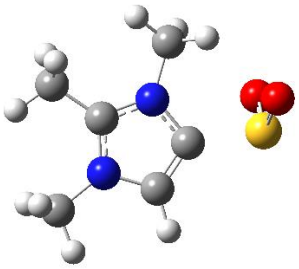
C	0.47961300	1.59785100	-0.82302800
C	0.47938400	-1.59769200	-0.82323200
C	-1.21468400	0.00018200	-0.21547200
S	-1.93985600	-0.00021800	1.24662900
O	-2.39809500	-1.26453000	1.75825400
O	-2.39811700	1.26380700	1.75894100
C	2.54657000	1.37653100	0.42849500
H	2.55012400	2.45642000	0.38124900
C	3.56995700	0.69240800	1.05135100
H	4.37438600	1.24019600	1.52467700
C	3.56982500	-0.69293300	1.05133200
H	4.37414600	-1.24088800	1.52464800
C	2.54631500	-1.37683800	0.42844100
H	2.54966500	-2.45672600	0.38114500
N	-0.84589900	1.21818300	-0.76573000
N	-0.84601700	-1.21751800	-0.76648400
O	0.81407200	-2.64136100	-1.33449100
O	0.81447800	2.64140700	-1.33440600
C	-1.87959600	2.09436200	-1.31049500
H	-2.39504300	1.60120100	-2.13449600
H	-2.59370500	2.35484000	-0.52965700
H	-1.39221000	2.99415600	-1.67183100
C	-1.87985400	-2.09342700	-1.31142300
H	-2.59236200	-2.35654200	-0.52999000
H	-2.39722600	-1.59869000	-2.13325200
H	-1.39221700	-2.99186200	-1.67579200

26



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S	-2.24270100	-0.66973800	0.00738000
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C	-0.35038700	-0.53348400	-0.01388500
O	-2.48982600	0.11260600	1.24903700
C	1.60061100	0.53393800	-0.00127900
N	1.84699000	-0.77913200	-0.00049000
C	2.61477000	1.61444600	0.00415700
H	2.57014900	2.19566100	-0.91825900
H	2.44947000	2.29489000	0.83968600
H	3.61628600	1.20169400	0.09582700
C	0.63635100	-1.45408600	-0.00800500
H	0.58971500	-2.52851400	-0.00710600
C	3.15640100	-1.40752900	0.00245300
H	3.72100700	-1.12922600	-0.88582800
H	3.71513100	-1.13251900	0.89554800
H	3.01331500	-2.48415900	0.00036100
C	-0.43212700	1.97439800	-0.00802200
H	-0.87524000	2.13060100	0.97227900
H	0.26366200	2.76973200	-0.26073100
H	-1.23697100	1.90786500	-0.73661500

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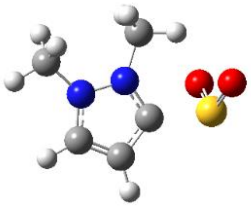

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S	2.07230100	0.37470800	-0.03243000
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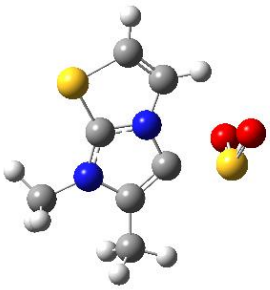
O	2.20246300	-0.60587200	-1.14019100
C	0.15587000	0.65006300	-0.09557700
O	2.12341100	-0.25833900	1.30716900
C	-0.35643500	-1.79473700	0.02868900
H	0.68334900	-1.88435600	-0.27987200
H	-0.47416900	-2.15419000	1.04953500
H	-0.99027700	-2.35273200	-0.65746100
N	-1.96643200	0.07524700	0.01635900
C	-0.61295200	1.81369800	-0.09039500
H	-0.24036200	2.82256700	-0.12314100
C	-1.92600400	1.41468000	-0.02139600
H	-2.84079800	1.98361800	0.00197900
C	-3.11308900	-0.80473600	0.04716600
H	-3.19634300	-1.36838300	-0.88137200
H	-3.04481600	-1.49094600	0.88942800
H	-3.99733900	-0.18524100	0.16738500

28



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C	-1.40528100	-0.05558600	0.00594900
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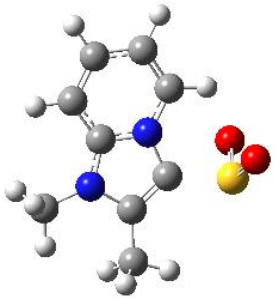
N	-1.32760000	1.27360700	0.00175600
C	-2.45100600	2.18800900	0.00117600
H	-2.69075800	2.50878400	-1.01274400
H	-3.31774600	1.69531100	0.43704300
H	-2.20887400	3.05820200	0.60600100
S	2.60481500	-0.00295600	-0.06177300
O	2.65749900	-0.52057800	1.32855200
O	2.53556000	-1.09410300	-1.07486900
N	-0.16683700	-0.55760100	-0.04931400
C	0.76191200	0.47078000	-0.09172700
C	0.49989400	3.02389000	-0.07641900
H	0.09427500	3.58066400	-0.92359200
H	0.22476400	3.54694500	0.84202200
H	1.58513200	3.03432100	-0.15343400
C	-1.32877700	-2.48242100	0.02194400
H	-1.58868500	-3.52633700	0.03965000
C	-0.10731500	-1.94619100	-0.03865000
H	0.86270800	-2.41531400	-0.10060000
S	-2.61142400	-1.27522200	0.06394800

29



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C	-1.09709200	-2.74199600	0.00010900
C	-0.03293100	-1.89820400	0.00006100
C	-0.05989100	1.62517500	-0.00003300
H	-3.64349800	-0.47634600	0.00009400
H	-3.24679500	-2.92206800	0.00015600
H	-0.91902600	-3.80692900	0.00014800
H	1.00879400	-2.18319400	0.00004200
N	-1.41980000	1.29362800	0.00000700
C	-2.54588800	2.20320600	-0.00008500
H	-3.15812600	2.05591200	-0.88999200
H	-3.15796300	2.05632100	0.89000300
H	-2.17400100	3.22282100	-0.00035700
S	2.50687700	0.08827600	-0.00005300

O	2.54673200	-0.74037700	1.23638900
O	2.54671900	-0.74044900	-1.23645400
N	-0.26923500	-0.55578300	0.00002400
C	0.65696400	0.48279500	-0.00001300
C	0.42652400	3.02593100	-0.00006400
H	0.09346500	3.57074400	-0.88575100
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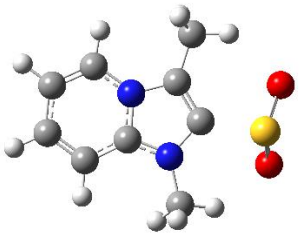

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C	1.29234000	-0.69950000	-0.05087700
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C	3.65795000	-0.70977400	0.08179000
C	3.64045100	0.70122800	0.12730800
C	2.46205900	1.36909400	0.08027100
C	-0.81061200	0.02475900	-0.14006700
H	2.47783300	-2.49380400	-0.04819000
H	4.60320400	-1.23366500	0.11755600
H	4.56107900	1.26124900	0.19949700
H	2.36985000	2.44350400	0.11058800
N	0.01350100	-1.08711800	-0.12644700
C	-0.42329400	-2.47787000	-0.17613600
H	-0.35879200	-2.85585100	-1.19630200
H	0.20544900	-3.07560400	0.48067600
H	-1.45212900	-2.50995200	0.17559900
C	-0.33924000	2.57399200	-0.03898600
H	0.00977700	3.03627900	0.88795800
H	0.11628400	3.10329100	-0.88031300
H	-1.42084800	2.67856200	-0.08574500
S	-2.72625400	-0.10142700	-0.28858400
O	-2.96563900	-1.12532200	0.76358700
O	-3.08202000	1.27998900	0.11051300
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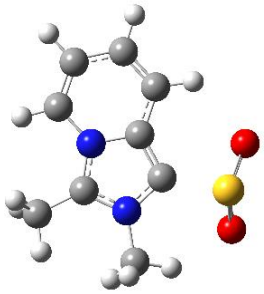
31



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C	-2.86455900	-0.03146600	0.08855100
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C	-2.16859700	-2.34698000	0.01466300
C	-0.86337700	-2.00409800	-0.06748100
H	-3.58296100	0.77057300	0.15239800
H	-4.22013000	-1.61756400	0.16290500
H	-2.46103400	-3.38745700	0.02774300
H	-0.05002000	-2.71476200	-0.11046300
C	-1.73071500	2.82354400	0.05575700
H	-2.49713300	2.86526700	-0.72090900
H	-2.22349900	2.94140700	1.02397100
H	-1.06410000	3.66897000	-0.08994300
S	2.44153000	-0.67317200	-0.31543000
O	3.14957000	0.16963300	0.68562400
O	2.13850500	-2.05170300	0.14039100
C	0.67807100	0.04938300	-0.13969400
C	1.32973600	2.46265100	-0.11704900
H	1.37062500	2.90552800	-1.11117800
H	1.05540700	3.21576400	0.61709800
H	2.29216900	2.02949600	0.14862800
C	-0.50970900	-0.63256800	-0.07883500
N	-1.52934000	0.32902500	0.00125100
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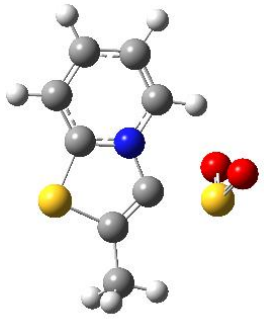

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C	1.62168200	0.52744800	0.00019100
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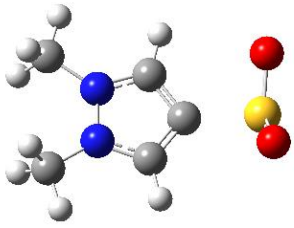
C	1.95365200	-2.18619500	-0.00009100
C	0.69878300	-1.65873600	-0.00034700
C	-0.56624700	1.67536700	-0.00023800
H	3.75491400	0.69097900	0.00076100
H	4.06769400	-1.76993900	0.00054100
H	2.06484800	-3.26038100	-0.00023400
H	-0.21813600	-2.22927200	-0.00068600
S	-2.30766600	-0.70799600	-0.00014400
O	-2.05150900	-1.49544500	-1.23398300
O	-2.05155200	-1.49430800	1.23444900
N	0.54484000	-0.30520900	-0.00018400
C	-0.69743100	0.34612700	-0.00039800
C	-1.64824600	2.69711400	-0.00036200
H	-1.59165100	3.33430900	0.88342900
H	-1.59118700	3.33455000	-0.88394800
H	-2.61375600	2.19493900	-0.00067900
S	1.12388400	2.16640000	0.00021400

33



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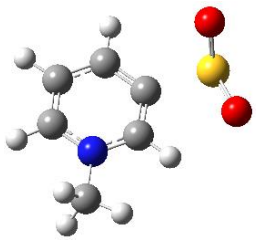
C	-0.41292400	-1.12324500	-0.23734700
C	-0.34356800	1.05814300	-0.16846000
H	-0.20476400	-2.18136000	-0.25645700
H	-0.04869000	2.09489000	-0.12207600
C	0.45193600	-0.05565400	-0.31198300
N	-1.62445900	0.68062500	-0.02416900
N	-1.66887000	-0.67321700	-0.06827900
C	-2.80206500	1.49563300	0.18227100
H	-3.26733700	1.27024500	1.14101600
H	-2.47631900	2.53156500	0.18532800
H	-3.52028500	1.35339400	-0.62422600
C	-2.89410000	-1.42179100	0.11053200
H	-3.61854600	-1.17264500	-0.66366700
H	-2.64060200	-2.47460800	0.02891300
H	-3.32191300	-1.23812200	1.09540400
S	2.35110500	-0.04478200	-0.31014200
O	2.55463300	-1.20084100	0.60287600
O	2.51266700	1.29618800	0.31901100

34



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C	-1.53994000	1.85670300	-0.05880800
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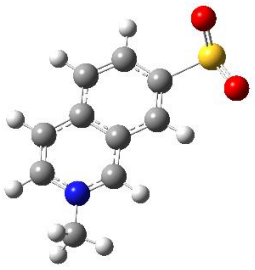
C	-0.58998400	-0.69645400	-0.12018800
H	-1.94928500	2.85666200	-0.01907900
H	0.51938900	2.45990800	-0.28339100
H	-0.22057900	-1.71717400	-0.10405100
S	2.15137000	-0.12915100	-0.30725000
O	1.97841300	-1.59019300	-0.05028000
O	2.58932300	0.66476400	0.86879000
C	-2.38566200	0.78674900	0.06778000

H	-3.45304500	0.88858600	0.20043800
N	-1.90383600	-0.47140900	0.03978600
C	-2.83429200	-1.59706300	0.18543400
H	-2.26170500	-2.51710500	0.24298500
H	-3.41345600	-1.47389500	1.09777700
H	-3.49995900	-1.63545500	-0.67460300

35



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C	1.51594100	0.23601000	-0.23616500
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C	-0.83283700	-0.19699100	-0.10472900
C	-1.10563600	1.20338100	-0.06323600
C	-0.03041200	2.09998700	-0.11167800
C	1.25050000	1.61564600	-0.19170000
H	-1.74648000	-2.14819600	-0.05209700
H	0.74382700	-1.71771700	-0.20502900
C	-1.90471700	-1.07837700	-0.03310900
C	-2.45740800	1.60153900	0.03833600
H	-0.22296800	3.16486800	-0.06736100
H	2.09459600	2.29636900	-0.19152100
C	-3.44756000	0.68296900	0.10039600
H	-2.71249900	2.65212900	0.07227500
H	-4.49359600	0.93623800	0.18171100
N	-3.15851300	-0.65718400	0.06617100
C	-4.26766700	-1.61038200	0.14771700
H	-3.87503600	-2.62138100	0.10191700
H	-4.79854200	-1.47191200	1.08761800
H	-4.94839300	-1.44925100	-0.68594600
S	3.28200600	-0.39804700	-0.25581500
O	3.78417200	0.34380900	0.93918600
O	2.99990800	-1.84822300	-0.02471300

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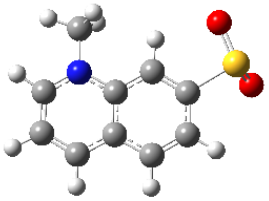

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C	-1.26510800	-0.43911300	-0.23792100
C	-0.31601500	0.53848200	-0.17053300
C	1.02589600	0.18325400	-0.06698600
C	1.40810500	-1.18876300	-0.06346200
C	0.39237200	-2.17247400	-0.15437000
C	-0.91393200	-1.80267000	-0.23367500
H	-0.68623900	1.55861400	-0.17032600
C	2.75924300	-1.51069300	0.04066000
H	0.68347200	-3.21581100	-0.14325500
H	-1.70163500	-2.54557400	-0.27219500
C	3.71128800	-0.52047600	0.14102300
H	3.05306700	-2.55330600	0.04632300
H	4.76371900	-0.74608600	0.22487800
S	-3.06244600	0.10663100	-0.24126100
O	-3.44071900	-0.47123500	1.08254500
O	-2.85301500	1.58738600	-0.23261100
C	3.30218000	0.79639200	0.14083000
H	4.00498400	1.61258600	0.22398600
N	2.01879400	1.13457700	0.04076700
C	1.63965100	2.55175200	0.05370500
H	1.12827100	2.80215200	-0.87292500
H	0.97143800	2.74385700	0.89019600
H	2.53829600	3.15207200	0.15303700

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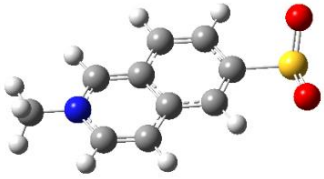

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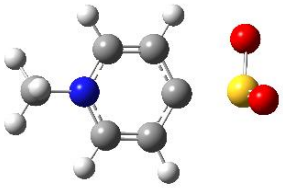
C	1.53408700	0.22049900	-0.19025200
C	0.66311700	-0.83384600	-0.13789900
C	-0.71004700	-0.59812900	-0.07590000
C	-1.18638800	0.74924700	-0.08864900
C	-0.26401800	1.82222800	-0.15816000
C	1.06808700	1.55162400	-0.20785300
H	-1.36124400	-2.66133300	0.03163200
H	1.08023200	-1.83580700	-0.10786000
C	-1.67851500	-1.62765300	0.01447600
C	-2.55124400	0.96747600	-0.01385300
H	-0.63283200	2.84113100	-0.15249400
H	1.80158900	2.34884600	-0.22760300
H	-2.96188500	1.96812200	-0.01417500
S	3.36915600	-0.11102300	-0.25994400
O	3.81205900	0.78111900	0.85243800
O	3.36966000	-1.57030900	0.05328800
C	-2.99474000	-1.33536400	0.08313000
H	-3.76985300	-2.08362600	0.15355800
N	-3.42419500	-0.03263400	0.06754800
C	-4.86196200	0.22719700	0.14959600
H	-5.25465700	-0.17769600	1.08053200
H	-5.03553100	1.29860000	0.12316400
H	-5.36695400	-0.23960000	-0.69411700

38



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C	-1.53802700	1.15804600	0.15091200
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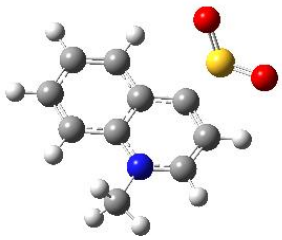
C	0.40200500	-0.15423800	-0.26019700
C	-0.41164700	-1.26833300	-0.40873300
C	-1.76504400	-1.13629100	-0.26745500
N	-2.31617900	0.06175000	0.01124500
H	-2.05920300	2.08025700	0.36862200
H	0.46394500	1.93956000	0.10835300
H	0.01265800	-2.24211400	-0.61961600
H	-2.45445800	-1.96321000	-0.36513100
S	2.29223000	-0.24608400	-0.21493800
O	2.33917300	-0.69062100	1.20939700
O	2.59709700	1.19444300	-0.41047600
C	-3.76186500	0.17087800	0.21895800
H	-4.26529300	-0.61610600	-0.33531000
H	-3.99345600	0.07607600	1.27882100
H	-4.10556500	1.13554700	-0.14455100

39



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C	-1.17984300	2.70424300	-0.06714900
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C	-0.24921900	0.47862200	-0.04946200
C	-1.56015400	-0.05119600	-0.01211300
C	-2.67182000	0.80633700	-0.01906300
C	-2.47252100	2.15982200	-0.05053200
H	-1.05050400	3.77817200	-0.07501600
H	0.91989000	2.27207200	-0.03834200
C	0.85582400	-0.40149400	-0.06078800
H	-3.67769300	0.41618400	0.00121200
H	-3.33123000	2.81901200	-0.05511800
C	-0.65459500	-2.23279100	0.05565900
C	0.63163800	-1.75710700	-0.00760900
H	-0.87347900	-3.28988000	0.12156900
H	1.48539500	-2.42476400	0.00423200
N	-1.71759400	-1.42171900	0.04125800
C	-3.05845800	-2.00026700	0.09436000
H	-3.58469400	-1.64668100	0.97913700

H	-3.62086200	-1.72790200	-0.79695100
H	-2.96974700	-3.08077100	0.14151200
S	2.65292300	0.15908600	-0.32095000
O	2.77599800	1.21263200	0.72292200
O	3.34556600	-1.11900800	-0.01771800

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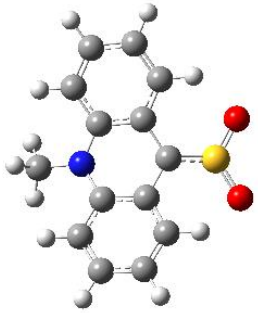

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C	-3.58579600	-0.07035400	-0.77792900
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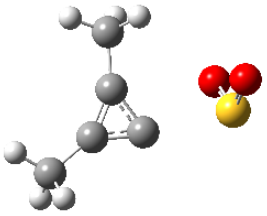
C	-1.20189400	-1.22930000	0.10508700
C	-2.36719200	-1.99054800	0.00060800
C	-3.54341000	-1.41200500	-0.42992200
C	-0.00004800	0.88832800	-0.10834800
C	1.20192900	-1.22922500	0.10508700
C	1.24522900	0.13490400	-0.22846800
C	2.44124200	0.69074500	-0.67855100
H	2.46784400	1.74055200	-0.92835300
C	3.58571400	-0.07022000	-0.77810400
C	3.54346300	-1.41179600	-0.42981000
C	2.36729800	-1.99037900	0.00083600
H	-4.50711500	0.37961200	-1.12173700
H	-2.46805200	1.74050800	-0.92798300
H	-2.35311900	-3.04463700	0.23164000
H	-4.43442600	-2.02206400	-0.50698000
H	4.50697800	0.37975200	-1.12205100
H	4.43454800	-2.02177800	-0.50669600
H	2.35335000	-3.04439900	0.23219300

N	0.00003900	-1.79740400	0.51753400
C	0.00019500	-3.12661300	1.09072500
H	0.00073800	-3.91750300	0.33328800
H	0.87693800	-3.24420700	1.72224400
H	-0.87694900	-3.24473900	1.72155400
S	-0.00004000	2.41625900	0.46811100
O	1.25851400	3.13540000	0.49828900
O	-1.25860200	3.13537500	0.49835200

41



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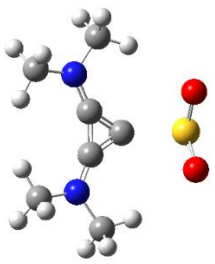
C	1.99640900	-0.35726200	0.00014000
S	-1.84393800	-0.67010300	-0.00095400
O	-1.93114800	0.09874900	-1.22429000
O	-1.93443800	0.09554200	1.22409600
C	3.36693500	-0.89057600	-0.00079200
H	4.11986500	-0.10481600	-0.01670300
H	3.51024700	-1.51083200	0.88551900
H	3.49991400	-1.53838400	-0.86866400
C	0.76630800	2.07822700	0.00077400
H	0.13550700	2.27737400	-0.86689500
H	0.14977000	2.28041600	0.87801600
H	1.63406100	2.73465500	-0.00691200

42



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C	-0.43590700	-0.00000800	-0.59615700
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C	0.70832300	-0.68956800	-0.29053900
S	-2.46816000	0.00000200	-0.24660500
O	-2.47814500	1.23887500	0.54878800
O	-2.47816300	-1.23892200	0.54870900
N	1.25195900	-1.86992500	-0.08144700
N	1.25192800	1.86993400	-0.08142400
C	2.63934600	-2.04731300	0.28789100
H	3.11883000	-2.76218800	-0.38412200
H	3.16705900	-1.10029800	0.21662500
H	2.72370000	-2.42286100	1.31073800
C	0.40706800	-3.05668500	-0.13152900
H	-0.63482100	-2.75231000	-0.20596700
H	0.68068000	-3.68779400	-0.98009100
H	0.53106000	-3.62907700	0.78941300
C	2.63932100	2.04733900	0.28788200
H	3.11883000	2.76210200	-0.38423400
H	2.72367900	2.42303400	1.31067300
H	3.16700700	1.10029700	0.21676400
C	0.40703500	3.05669100	-0.13155300
H	0.68064200	3.68776500	-0.98014200
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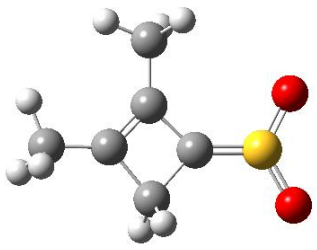
43



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C	0.11845000	-0.26970600	-0.00000400
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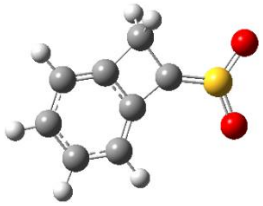
C	-1.04090400	0.62304500	0.00007900
S	1.68843600	-0.08671200	-0.00009200
O	2.53286200	-1.25902100	-0.00004500
O	2.23279900	1.25261800	-0.00007000
C	-1.15615300	2.09956900	0.00012300
H	-0.66809100	2.52765300	0.87743300
H	-0.66781400	2.52772300	-0.87699700
H	-2.20163300	2.40659900	-0.00002800
C	-3.36808300	-0.55523900	-0.00002500
H	-3.70791500	-1.11022400	-0.87845900
H	-3.70800000	-1.10983200	0.87862500
H	-3.85930500	0.41775100	-0.00025800
H	-0.73827400	-2.10562300	0.89287100
H	-0.73829100	-2.10574200	-0.89257700

44



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C	-0.66663900	-0.36797000	0.00007600
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C	-0.04430900	-1.77148400	-0.00000900
C	0.65694500	0.25059900	-0.00014300
S	-2.15299500	0.17358400	0.00019200
O	-3.23991400	-0.77360900	0.00028200
O	-2.36448400	1.59995400	0.00007100
H	-0.25127900	-2.36143000	-0.89177100
H	-0.25106600	-2.36140200	0.89182300
C	2.64176500	-1.12768900	-0.00011300
C	3.36709300	0.06527700	-0.00016700
C	1.35525500	1.43763100	-0.00018200
C	2.74167400	1.30948200	-0.00021100
H	3.14484200	-2.08607600	-0.00008000
H	4.44896200	0.02590200	-0.00016600
H	3.35500400	2.20147100	-0.00024900

H	0.87184700	2.40505700	-0.00020900

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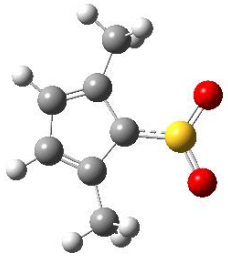

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O	-2.12272000	1.25512300	-0.00025500
C	2.28645600	0.72790100	-0.00013200
C	2.28644000	-0.72795400	0.00006700
C	1.02349900	1.19973500	0.00006800
C	1.02346300	-1.19974800	0.00004000
H	3.17269400	-1.34625700	0.00003600
H	3.17273600	1.34617100	-0.00018600
C	0.57419000	-2.61999100	0.00002300
H	-0.03306700	-2.85494900	0.87568100
H	-0.03297800	-2.85497500	-0.87569400
H	1.44385900	-3.27592000	0.00007600
C	0.57425200	2.61997700	0.00023400
H	-0.03316800	2.85499700	-0.87529300
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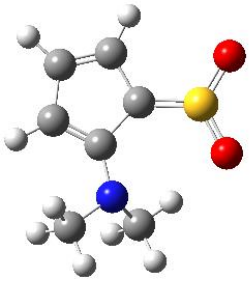
H	1.44393400	3.27589000	0.00005900

46



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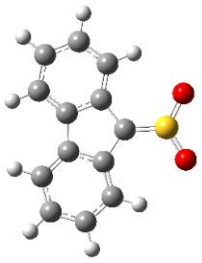
O	-1.26309600	-1.93183200	-0.30170600
C	1.38776300	1.72001900	-0.02463200
C	0.27920500	2.64788800	0.11693800
C	0.92337400	0.44439100	-0.00235800
C	-0.88356100	1.97695600	0.21845500
H	0.38303700	3.72234000	0.15129900
H	2.42271500	2.00650000	-0.12012300
N	1.62023600	-0.74321400	-0.15740800
C	2.97665400	-0.58948200	-0.64008700
H	3.63852800	-0.12045000	0.10276900
H	3.37886500	-1.57340100	-0.87883000
H	2.98112100	0.01778800	-1.54392900
C	1.53661900	-1.69288600	0.94386200
H	1.88509800	-2.66790900	0.60456300
H	2.15399100	-1.37123400	1.79398500
H	0.51198500	-1.80781800	1.28058000
H	-1.88112300	2.36273200	0.33968300

47



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S	-2.38233200	0.00003600	0.00000000
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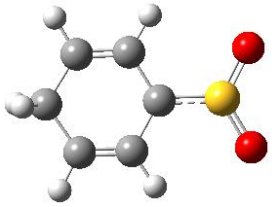
O	-3.07439300	0.00020500	-1.26309100
C	1.40164700	-0.00015000	-0.73246400
C	1.40164700	-0.00015000	0.73246400
C	0.07244100	-0.00000900	-1.18899100
C	0.07244100	-0.00000900	1.18899100
C	-0.21752100	0.00009700	2.54181200
C	2.44535100	-0.00021100	1.63862200

C	2.44535100	-0.00021100	-1.63862200
C	-0.21752100	0.00009700	-2.54181200
C	0.83954400	0.00004900	3.43975200
C	2.15544900	-0.00010300	2.99484000
C	0.83954400	0.00004900	-3.43975200
C	2.15544900	-0.00010300	-2.99484000
H	-1.24070500	0.00020800	-2.88995700
H	0.63370000	0.00013400	-4.50220400
H	2.96326500	-0.00014000	-3.71529100
H	3.47334700	-0.00033700	-1.29858100
H	3.47334700	-0.00033700	1.29858100
H	2.96326500	-0.00014000	3.71529100
H	0.63370000	0.00013400	4.50220400
H	-1.24070500	0.00020800	2.88995700

48



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C	-2.04739500	-1.25003300	-0.00007000
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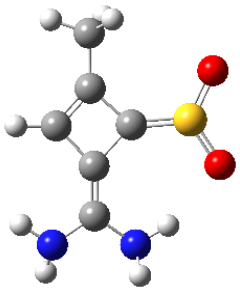
C	0.01270600	0.00000000	-0.00005000
C	-0.71868500	1.25591900	-0.00000100
C	-2.04739500	1.25003200	-0.00005000
H	-2.57836000	-2.19435000	-0.00009200
H	-0.15677900	-2.17923900	0.00002000
H	-0.15678000	2.17924000	0.00006800
H	-2.57836000	2.19435000	-0.00004100
C	-2.86837000	0.00000000	-0.00004100
S	1.61786900	0.00000000	0.00005300
O	2.31204800	1.26661000	0.00003300
O	2.31204700	-1.26661100	0.00003400
H	-3.54061700	0.00000000	0.86727900
H	-3.54081900	0.00000000	-0.86718200

49



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C	-0.44064600	0.24463600	-0.00372900
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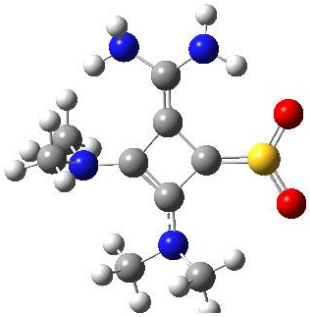
C	-0.75890100	1.69292800	0.01441100
C	2.16564400	-0.08545800	0.00486500
N	3.39385000	0.55081500	-0.15529000
H	3.34008300	1.55685700	-0.20214900
H	4.09282700	0.24148300	0.50741900
N	2.28873400	-1.45360100	0.15964600
H	1.41668300	-1.96737400	0.17453700
H	2.97109500	-1.86890500	-0.45959000
S	-1.32189700	-1.06823600	-0.01758000
O	-0.65701400	-2.35850300	-0.01912300
O	-2.76292800	-0.95939800	-0.02131200
C	-2.03814400	2.43289100	0.01686000
H	-2.62978100	2.20188500	-0.87150300
H	-2.64740300	2.16460500	0.88251200
H	-1.85472800	3.50677800	0.04126900
H	1.08501600	2.93941300	0.05284400

50



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C	-0.89100100	-0.07588800	0.03793000
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C	0.25813300	-1.01705600	0.04076400
C	0.05883300	1.07034100	-0.00417000
C	0.40673100	-2.34301900	0.13844200
N	1.64195300	-2.98165500	-0.00559900
H	2.42614800	-2.35500100	-0.08913800
H	1.80271900	-3.67593900	0.71333700
N	-0.61207500	-3.25008100	0.39889500
H	-1.54557200	-2.86095000	0.35758800
H	-0.53913600	-4.08424700	-0.16901100
N	-0.14901300	2.41789500	-0.10958200
C	-1.08511400	3.02093200	0.82753900
H	-0.64326800	3.12557100	1.82778400
H	-1.35992800	4.01081800	0.46407100
H	-1.99097800	2.42681500	0.89519000
C	1.03444000	3.22387400	-0.34220500
H	1.62926700	2.78867100	-1.14093700
H	0.71955100	4.22454600	-0.63826300
H	1.66857900	3.30430400	0.54972300
N	2.49996000	0.45086800	-0.07338400
C	3.23930600	0.10102900	1.12606500
H	3.35106000	-0.98356700	1.27846300
H	4.23899700	0.53570000	1.07170500
H	2.73227700	0.51036800	1.99808700
C	3.14861900	0.03702600	-1.30529100
H	4.14787900	0.47356000	-1.34903700
H	3.25441500	-1.05307300	-1.41453200
H	2.57684200	0.39935900	-2.15830100
S	-2.45190500	-0.22930700	-0.20141700
O	-3.02771400	-1.56311100	-0.18957100
O	-3.30281100	0.94048600	-0.24542700

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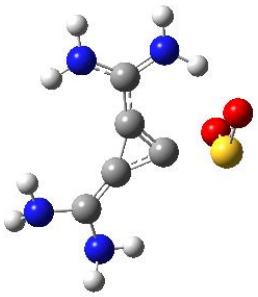

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C	-0.09721600	-0.51210300	-0.24858100
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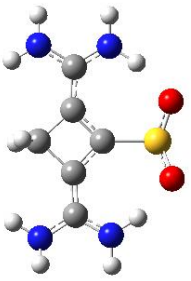
C	-0.63846200	1.97248800	0.04112900
C	2.54608200	-0.42384600	-0.07090500
N	-1.95252200	1.90348400	-0.07510400
H	-2.52882200	2.72223600	0.02941400
H	-2.37320200	0.96168900	-0.28741000
N	-0.02058800	3.14967400	0.27054800
H	0.95116100	3.13997000	0.52502100
H	-0.55177100	3.96865800	0.51391000
N	3.59734200	0.49789600	-0.10531400
H	3.30632300	1.46123900	-0.16254700
H	4.28081400	0.34858300	0.62658700
N	2.99905800	-1.74231300	0.03338800
H	3.66700800	-1.99173700	-0.68607800
H	2.25266600	-2.41956700	0.09844300
S	-1.63457000	-1.63680500	-0.18735300
O	-2.60361000	-0.61058600	-0.71054000
O	-1.67872600	-1.77040200	1.28340400

52



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C	-0.00149200	0.08183900	0.12447400
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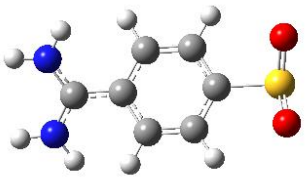
H	-0.00435900	-2.59035800	-0.93567500
H	-0.01033400	-2.68384100	0.85562700
C	-1.02526400	-0.87272000	0.05533700
C	1.01357800	-0.87603200	0.06207100
C	-2.40543200	-0.81886600	-0.02094200
C	2.39818000	-0.83011600	-0.01662500
N	-3.14238200	-1.96590000	0.07820700
H	-4.02521600	-1.99524700	-0.40692400
H	-2.63049800	-2.83246500	0.07875300
N	-3.06759000	0.32616000	-0.18952300
H	-4.04639600	0.37068400	0.03992800
H	-2.50670900	1.19943100	-0.24956600
N	3.07044000	0.31943100	-0.02621200
H	4.05267900	0.32038700	-0.24368000
H	2.51545400	1.19299600	-0.14800700
N	3.10222900	-1.99289700	-0.11688300
H	4.08704300	-1.98017400	0.09085300
H	2.62158700	-2.84431900	0.11954100
S	0.01797100	1.89106100	0.41255900
O	-1.24622500	2.31262500	-0.29227800
O	1.25663900	2.28037500	-0.35756100

53



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C	-0.97507400	1.19806300	-0.24624700
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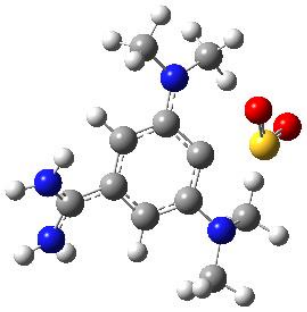
C	1.09054500	-0.01089600	-0.17064300
C	0.40547400	-1.20187600	0.03118200
C	-0.96761800	-1.20447100	0.09486900
H	-1.50944700	2.13059000	-0.38878900
H	0.96747100	2.09527500	-0.45139500
H	0.98956700	-2.10079500	0.19070500
H	-1.49133400	-2.12501600	0.32779900
C	-1.67620300	-0.00077100	-0.04349600
C	-3.10915600	0.00631400	0.04969400
N	-3.81561400	-1.06739000	-0.28623800
H	-3.35064200	-1.84438200	-0.72578100
H	-4.79928300	-1.14999000	-0.08738100
N	-3.75666700	1.08507500	0.47587300
H	-3.23293700	1.85272800	0.86285100
H	-4.75865600	1.16902700	0.42337400
S	2.94694600	-0.02463000	-0.29917200
O	3.24947700	-1.23511300	0.52122600
O	3.25649400	1.28758900	0.34244000

54



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C	1.51516900	1.14361400	-0.06023700
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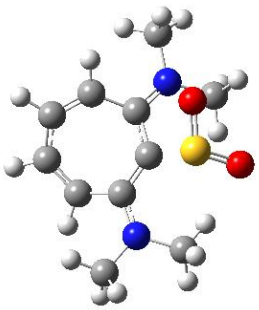
C	-0.67863100	0.10905100	-0.10261400
C	-0.08073900	-1.16632600	-0.25688100
C	1.31213600	-1.27635300	-0.14595000
H	2.13109500	2.02265000	0.05492700
H	1.79098400	-2.23778800	-0.26177100
C	2.08967200	-0.12637700	-0.02490900
C	3.51140300	-0.25269000	0.12137900
N	4.03397300	-1.32934200	0.69886300
H	3.41074500	-1.99023600	1.13424400
H	5.02098500	-1.52637300	0.68647500
N	4.33164700	0.69806000	-0.31710400

H	3.94554900	1.46212500	-0.84672600
H	5.30737400	0.72443600	-0.07146900
S	-2.37116400	0.29657600	0.85767500
O	-2.42166800	-1.01988400	1.54069000
O	-3.42056600	0.45020300	-0.18784200
N	-0.47950300	2.51372200	-0.06877000
N	-0.83083300	-2.27754400	-0.47462400
C	0.33033500	3.66005400	0.25342500
H	1.01580800	3.95258800	-0.55972000
H	-0.32734100	4.50673800	0.44683500
H	0.91346600	3.47970800	1.15664800
C	-1.50682300	2.80851100	-1.05827000
H	-2.15360700	3.60047500	-0.68010000
H	-1.05350900	3.14628700	-2.00235000
H	-2.13167800	1.94023100	-1.23888600
C	-0.26465600	-3.58892200	-0.30838400
H	-1.07558100	-4.31147700	-0.24004700
H	0.38409600	-3.88753200	-1.14489400
H	0.30839900	-3.65171300	0.61889400
C	-2.14286100	-2.23551800	-1.09295300
H	-2.12372700	-2.82155100	-2.01936400
H	-2.89834600	-2.63314000	-0.41719300
H	-2.43092000	-1.21374100	-1.31984800

55



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C	-0.21389900	2.92535000	-0.72709500
C	1.01374600	2.94601000	-0.00059100
C	1.69782500	1.87737800	0.45228300
C	-1.14237200	1.95407700	-0.69400500
C	1.38949200	0.47486000	0.23827900
C	-1.06168000	0.76773400	0.13686800
C	0.11432100	-0.01499600	0.12408700
H	-0.43156100	3.79807400	-1.33238400
H	1.46507400	3.92040100	0.14932000
H	2.63921800	2.08127600	0.94760500
H	-2.02553800	2.06379000	-1.31116500
S	-0.27415700	-1.75992800	-0.92480400
O	-1.61606600	-1.40412100	-1.43563300
O	-0.31997900	-2.84360300	0.07537300
N	2.48230500	-0.35519300	0.22117600
N	-2.17353700	0.31279700	0.68658200
C	3.80443000	0.13238700	-0.10339300
H	4.39458700	0.37915600	0.78829800
H	4.33938100	-0.64653900	-0.64963000
H	3.75138100	1.00851600	-0.74537800
C	2.45758200	-1.71773700	0.71560500
H	1.50450000	-1.93801300	1.18125200
H	2.60689500	-2.44383800	-0.08601400
H	3.25929500	-1.84161500	1.45093600
C	-3.46338000	0.94000100	0.45247100
H	-4.14249300	0.63752700	1.24567400
H	-3.37847300	2.02455300	0.46455600
H	-3.87628000	0.61342900	-0.50397500
C	-2.21479500	-0.89148600	1.50619500
H	-2.68980500	-0.64567500	2.45776900
H	-2.77865600	-1.66682100	0.99299300
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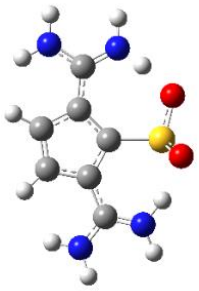
56



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S	0.22307600	1.75323200	-0.40559200
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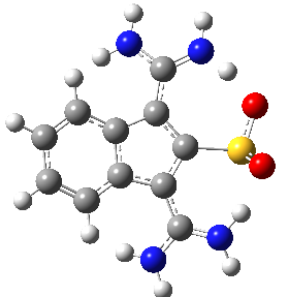
O	0.93158300	2.19388200	0.86232700
C	0.65321100	-2.23215000	0.12216500
C	-0.70869400	-2.21584200	0.14599700
C	1.11307000	-0.88424300	0.00258600
C	2.50198500	-0.54890800	-0.01602800
C	-1.15461300	-0.85923300	0.02857900
C	-2.54327500	-0.51227000	0.06811300
N	-2.97030300	0.71952900	0.21458000
N	-3.45201800	-1.50777600	0.00355600
N	2.96835600	0.62732900	0.34851300
N	3.37954300	-1.49623700	-0.39814100
H	2.28776900	1.36454700	0.67658500
H	3.93518200	0.85852000	0.18674300
H	3.03741900	-2.36383400	-0.76956300
H	4.36758800	-1.38870300	-0.24936000
H	-3.95654600	0.90984200	0.12894500
H	-2.26286700	1.51151600	0.05974300
H	-4.43583900	-1.30467300	-0.00096000
H	-3.15952000	-2.43261400	-0.25200600
H	-1.32767400	-3.08361600	0.32193800
H	1.26954300	-3.10541500	0.27931600

57



0 1

S	2.54943800	-0.18809300	-0.23116000
O	3.13556200	1.19719500	-0.29630800
C	0.71882400	0.02893500	-0.05246500
O	2.85370200	-0.83857500	1.10265400
C	-1.47458700	-0.71694200	-0.02262400
C	-1.49688400	0.69846000	0.02808000
C	-0.08875500	-1.12704500	-0.08147800
C	0.33175800	-2.48852000	-0.17198100
C	-0.12100600	1.16460500	-0.03163800
C	0.24279000	2.54274500	-0.08658000
N	1.44006800	2.99197300	0.23251200
N	-0.69723300	3.44999800	-0.43704000
N	1.46423700	-2.93394500	0.33790100
N	-0.48203200	-3.37459600	-0.77652900
H	2.10722100	-2.25196900	0.81111300
H	1.79802400	-3.85294100	0.09516200
H	-1.24361400	-3.03944400	-1.33933100
H	-0.26042500	-4.35478200	-0.80140400
H	1.66366700	3.94948600	0.00686000
H	2.24039600	2.29363400	0.21699500
H	-0.42725000	4.40873800	-0.57703700
H	-1.51433600	3.13032900	-0.92701500
C	-2.66461500	-1.43830900	0.10582900
C	-2.71829700	1.35180800	0.22802100
C	-3.86074800	-0.76884200	0.25319800
C	-3.88568500	0.62225900	0.31856200
H	-2.66288800	-2.51923800	0.13865900
H	-4.78134700	-1.32973800	0.35267300
H	-4.82532900	1.13678100	0.47461500
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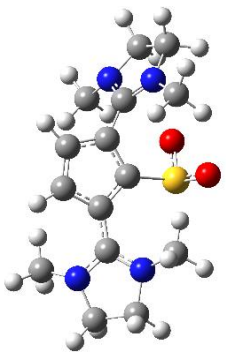

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S	0.23699500	-1.19456900	-1.16273700
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O	0.46647200	-2.48913600	-0.42766000
C	-0.94402100	1.68396100	1.50119300
C	0.42729800	1.75986500	1.60272200
C	-1.26282700	0.59180800	0.63570500
C	-2.56557700	0.20201500	0.24674400
C	-4.72852500	0.35365900	-0.54982400
C	-4.40121100	-1.10502700	-0.24528500
H	-5.65453500	0.68987300	-0.08346900
H	-4.80066000	0.53776500	-1.62636600
H	-4.96752100	-1.48541500	0.61018400
H	-4.57717100	-1.76758200	-1.09244100
C	0.98055200	0.73343400	0.78968700
C	2.37159500	0.50540900	0.45409100
C	4.35253400	-0.60359500	0.18325900
C	4.30969200	0.62119200	-0.73964600
H	5.16519300	-0.56178700	0.91151700
H	4.41993400	-1.53776700	-0.37408200
H	5.19258300	1.25369200	-0.65374000
H	4.17062900	0.32403400	-1.78087200
N	3.10882100	1.33093000	-0.29774900
N	3.06708600	-0.53150900	0.86492600
N	-2.98817200	-1.05639700	0.10038900
N	-3.57329500	1.06669500	-0.01710800
C	-3.38187200	2.44260100	-0.42331700
H	-2.36043300	2.74304900	-0.21540400
H	-3.57626300	2.54592100	-1.49542000
H	-4.06417400	3.09685800	0.12088400
C	-2.37523900	-2.23573100	0.68069200
H	-2.14348900	-2.96793500	-0.08937000
H	-1.43847400	-1.96911100	1.15543500
H	-3.06427000	-2.66564800	1.41360300
C	2.57152600	-1.63148200	1.66499400
H	1.77373500	-1.26855800	2.30754800
H	2.15989800	-2.40693400	1.01497900
H	3.38956100	-2.01029000	2.27847700
C	2.50487800	2.28320600	-1.20730000
H	2.19314100	1.76977300	-2.11971100
H	1.63441300	2.72856800	-0.73430100
H	3.22864700	3.06576600	-1.43412600
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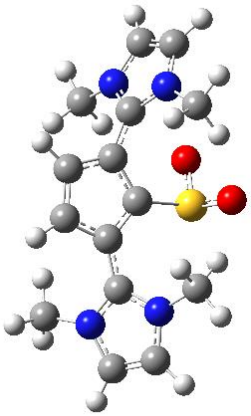

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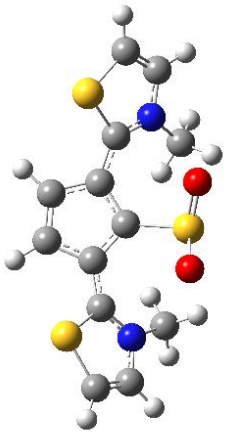
C	-0.06108400	0.03400000	0.11977100
O	0.29901100	-2.44129000	-0.62669100
C	-0.90260100	1.61744600	1.55623100
C	0.47773700	1.66549900	1.63333700
C	-1.25022200	0.59753100	0.62467600
C	-2.57151900	0.21869900	0.24208700
C	-4.68161800	0.30710700	-0.47219800
C	-4.39302800	-0.97881300	-0.19483500
C	0.99751900	0.69386800	0.73929000
C	2.38290300	0.42820200	0.42828300
C	4.33951100	-0.58556600	0.24639600
C	4.41590200	0.57659000	-0.43368900
N	3.20315200	1.20679100	-0.29117100
N	3.08129800	-0.65205600	0.79333200

N	-3.09410700	-1.02169200	0.25606900
N	-3.54764600	1.04099000	-0.19969900
C	-3.38657900	2.46023100	-0.45202900
H	-2.32355900	2.67245700	-0.52947900
H	-3.88651100	2.71496900	-1.38448200
H	-3.80739700	3.04858400	0.36245700
C	-2.43655800	-2.20249700	0.81014200
H	-3.19491500	-2.96879900	0.95149500
H	-1.63568000	-2.55443500	0.15797200
H	-2.00038300	-1.93266100	1.77016300
C	2.51653800	-1.79290700	1.50181800
H	1.95970600	-1.43317300	2.36386900
H	1.84063100	-2.32807700	0.82759400
H	3.33581600	-2.42747800	1.83132600
C	2.73396900	2.31645500	-1.10151200
H	2.24600100	1.90823900	-1.98642700
H	2.01970600	2.90133800	-0.52953100
H	3.58373700	2.93731400	-1.37599300
H	-1.59508400	2.19903500	2.14832900
H	1.05891900	2.30368900	2.28390500
H	5.22027600	1.00496300	-1.00361800
H	5.06748500	-1.36258400	0.39234300
H	-4.99625700	-1.86477400	-0.27576900
H	-5.58155400	0.76059100	-0.84653100

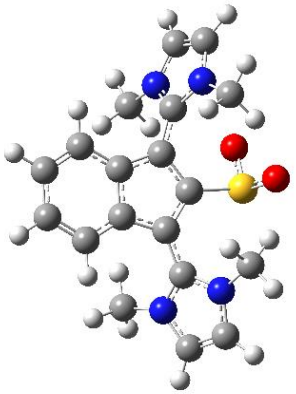
60



0 1

S	-0.00010200	-1.68005900	-0.58486500
O	-1.26376900	-1.57823600	-1.38637400
C	-0.00003200	-0.04679100	0.24847300
O	1.26430000	-1.57889700	-1.38529300
C	0.68270500	2.08501800	0.80001300
C	-0.68277000	2.08500000	0.80008100
C	1.13111200	0.76323500	0.47143300
C	2.49258300	0.46160900	0.21960600
C	4.51366700	-0.60522400	0.16796300
C	4.88147300	0.53945500	-0.41604500
C	-1.13116900	0.76322300	0.47147100
C	-2.49264600	0.46154800	0.21974400
C	-4.88162900	0.53930100	-0.41554100
C	-4.51366600	-0.60540700	0.16831600
N	-3.18711300	-0.63196400	0.54638300
N	3.18717500	-0.63183200	0.54624300
C	2.63034500	-1.77175400	1.25958200
H	1.78313200	-1.43058300	1.84827200
H	2.28721700	-2.51244000	0.54096000
H	3.39882600	-2.17509100	1.91589800
C	-2.63003200	-1.77190400	1.25949400
H	-2.28670800	-2.51235400	0.54072100
H	-1.78291800	-1.43064500	1.84828300
H	-3.39843300	-2.17557100	1.91569800
H	1.32363100	2.91091400	1.07352800
H	-1.32369700	2.91087600	1.07365500
S	3.52792400	1.60420400	-0.54980200
S	-3.52814900	1.60411700	-0.54948300
H	5.85864000	0.80708200	-0.77769100
H	5.13027500	-1.46562900	0.37057500
H	-5.85886600	0.80689300	-0.77702200
H	-5.13019100	-1.46586600	0.37095100

61



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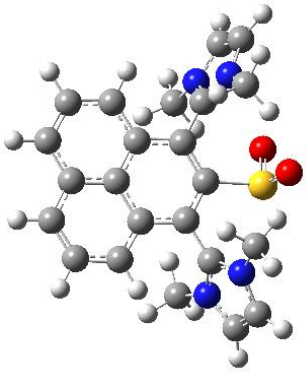
S	-0.21691000	-2.15887800	0.63903100
O	-1.51220700	-1.97707400	1.38277800
C	0.01007300	-0.45445100	0.00608600
O	-0.40952700	-2.94727600	-0.63749100
C	0.92627500	1.61842600	-0.38829400
C	-0.49478700	1.73688500	-0.42401100
C	1.22982700	0.24003800	-0.12189000
C	2.52589200	-0.32598800	0.03737400
C	4.60687100	-0.69763700	0.74872900
C	4.31410100	-1.63234600	-0.17569100
C	-1.03847800	0.43673000	-0.17717800
C	-2.42999200	0.09238100	-0.02890300
C	-4.42992800	-0.79412000	-0.35334400
C	-4.47055700	-0.10676100	0.80707400
N	-3.23044700	0.45687500	0.98315900
N	-3.16720400	-0.64080700	-0.87065100
N	3.03479500	-1.38747200	-0.61830100
N	3.49439400	0.10520200	0.87681800
C	3.32360400	1.15195700	1.86649400
H	2.25918800	1.28149400	2.04348400
H	3.81814600	0.85177200	2.78784600
H	3.73751000	2.09538200	1.51439000
C	2.38088200	-2.07809400	-1.72535100
H	3.14032200	-2.63895500	-2.26473000
H	1.58438600	-2.73193600	-1.36930900
H	1.93863500	-1.33022700	-2.38090000
C	-2.64770400	-1.29014500	-2.06666500
H	-2.08416600	-0.56239100	-2.64625900
H	-1.98708500	-2.10960900	-1.76941500
H	-3.49110400	-1.65069600	-2.65047000
C	-2.73121100	1.04685000	2.21242200
H	-2.15141200	0.29197600	2.74283000
H	-2.10188600	1.90173400	1.97969200
H	-3.57787900	1.36974000	2.81324500
C	1.71858400	2.73998500	-0.64730900
C	-1.08442000	2.97706500	-0.68309900
C	1.11537300	3.95604400	-0.89044900
C	-0.28090500	4.07563000	-0.90228100
H	2.80012900	2.66113800	-0.67217100
H	1.72601200	4.82898800	-1.08515000
H	-0.73077500	5.04060300	-1.10017900
H	-2.16415000	3.07522800	-0.72246800
H	-5.18657200	-1.36972100	-0.85451700
H	-5.26679500	0.02666900	1.51666400
H	4.90326900	-2.44531100	-0.55962300
H	5.49688600	-0.54031400	1.33079200

62



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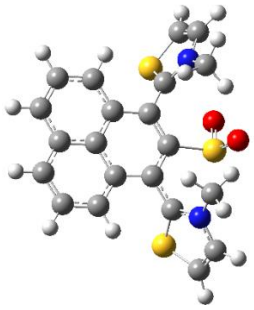
C	-1.15593500	0.16478600	-0.04003800
C	-1.08833800	1.60030000	-0.15122600
C	-2.22144500	2.40673100	-0.22518300
C	-0.00495400	-0.58866500	0.02420700
C	0.20067900	2.22092000	-0.17901800

C	1.39168700	1.43156500	-0.13213900
C	1.24769400	0.00396300	-0.02706200
C	2.62752800	2.06995600	-0.19925100
H	3.54078400	1.48699800	-0.20665300
C	2.70698700	3.46044000	-0.28397100
C	1.58040300	4.23537800	-0.31267100
C	0.30037600	3.63722000	-0.27045400
C	-0.88234200	4.40668100	-0.32849600
C	-2.10559300	3.79402800	-0.30962000
H	-3.00645800	4.39431600	-0.36537500
H	-0.80341200	5.48426300	-0.39962500
H	3.68248800	3.93054100	-0.33397500
H	1.65187600	5.31350300	-0.38307000
H	-3.20664100	1.95796200	-0.22682200
C	-2.46753700	-0.46142900	0.03578500
C	-4.44892100	-1.11279600	0.77557500
C	-4.33412000	-1.51763100	-0.50690200
H	-5.24310800	-1.25040400	1.48667500
H	-5.01165000	-2.06883500	-1.13301000
C	2.43779900	-0.81657800	0.06102800
C	4.09471500	-2.20433500	-0.43940700
C	4.29915100	-1.76351400	0.82015300
H	4.65822800	-2.89492700	-1.04017900
H	5.07611600	-1.99334700	1.52673900
N	-3.11170700	-1.08240900	-0.95752700
N	-3.29665900	-0.43756000	1.08721200
N	2.95361000	-1.59624900	-0.90110700
N	3.26920500	-0.90451700	1.11475300
C	-2.54524600	-1.34031400	-2.27375200
H	-3.35175400	-1.63966000	-2.93848600
H	-2.08642100	-0.42645700	-2.64441500
H	-1.78930000	-2.12287700	-2.18336700
C	-2.88904600	-0.00500400	2.41010900
H	-2.42038400	0.97394700	2.34225200
H	-3.77086400	0.05867200	3.04281600
H	-2.18593000	-0.73556300	2.80757700
C	3.06113200	-0.21458300	2.37390400
H	3.46210000	-0.82256600	3.18094400
H	3.54514900	0.76088500	2.35648400
H	1.99206300	-0.07645400	2.51330000
C	2.37771800	-1.76325300	-2.23098800
H	2.03551500	-0.79202900	-2.58045300
H	3.15473400	-2.14016700	-2.89131800
H	1.52922800	-2.44588700	-2.17246000
S	-0.06120800	-2.41731100	0.35118500
O	-0.19903400	-2.96830200	-1.04819500
O	-1.33453200	-2.53082200	1.13277600

63



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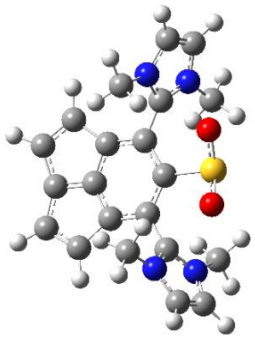
C	1.15182100	0.16135500	0.00195400
C	1.16217500	1.60806600	0.10158000
C	2.33031600	2.34737400	0.23146300
C	-0.04077700	-0.52898800	-0.03473900
C	-0.08928900	2.29937500	0.08098700
C	-1.32335500	1.58208400	0.01785000
C	-1.26280500	0.13823000	-0.01986100
C	-2.51572800	2.29367200	0.04283800
H	-3.46272700	1.77079100	0.03440100
C	-2.51767800	3.68889000	0.08883400
C	-1.34917900	4.39496400	0.13561700
C	-0.10851200	3.71952200	0.14734700
C	1.11268900	4.42230800	0.24402000
C	2.29584700	3.74175000	0.29394600
H	3.22760600	4.28708000	0.38758800
H	1.09143200	5.50362100	0.29669200
H	-3.46545000	4.21424800	0.09810400

H	-1.35615700	5.47662400	0.18410600
H	3.28761400	1.84769100	0.28406200
C	2.42444700	-0.52468300	-0.14232100
C	4.61532400	-1.41177000	-0.81106100
C	4.25112100	-1.75712700	0.43202800
H	5.51917400	-1.68705200	-1.32606600
H	4.79133700	-2.37632800	1.12854500
C	-2.47946300	-0.62183900	-0.15063700
C	-4.15670700	-2.06758400	0.41997400
C	-4.55220100	-1.77799400	-0.82763800
H	-4.63085400	-2.73191700	1.12328600
H	-5.42192900	-2.15286600	-1.33905900
N	3.04199700	-1.21497700	0.80806200
N	-3.01671400	-1.38977100	0.79633600
C	2.43461500	-1.47941200	2.11112800
H	3.21978600	-1.79298200	2.79402200
H	1.97537700	-0.56141200	2.46929100
H	1.66409900	-2.24645100	1.99753500
C	-2.48157200	-1.47197200	2.15812700
H	-2.03573800	-0.51074000	2.39941100
H	-3.30804400	-1.68466300	2.83163400
H	-1.71003000	-2.24150500	2.18814200
S	-0.08326000	-2.37281500	-0.32493600
O	-0.10536700	-2.90189400	1.09103300
O	1.24563800	-2.58813000	-0.97633500
S	3.41292000	-0.42255000	-1.53727100
S	-3.46035700	-0.67326300	-1.56458600

64



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C	-1.25469500	1.71199100	-0.37520500
C	-2.15695000	2.84269900	-0.22705300
C	-1.38784400	4.00164200	-0.23294000
C	0.00002600	3.66545100	-0.41741100
C	0.00001000	2.29111100	-0.52577000
C	1.38790200	4.00161200	-0.23294200
C	2.15698200	2.84265000	-0.22705000
C	1.25470100	1.71196300	-0.37520300
H	-3.23409100	2.80751000	-0.14923000
H	-1.80253600	4.99386100	-0.10930100
H	1.80261700	4.99382100	-0.10930100
H	3.23412200	2.80743700	-0.14922500
C	-1.23401400	0.31836300	-0.25158400
C	-0.00001500	-0.36127300	-0.20871600
C	1.23399400	0.31833400	-0.25157700
C	2.50779700	-0.37650700	-0.05375900
C	4.41526500	-1.03011100	0.84723400
C	4.38415800	-1.48710200	-0.42003300
H	5.15723400	-1.14402000	1.61641000
H	5.09464200	-2.07209200	-0.97505100
C	-2.50782100	-0.37647100	-0.05377700
C	-4.41527200	-1.03013500	0.84720100
C	-4.38413100	-1.48715300	-0.42005600
H	-5.15724600	-1.14406300	1.61637000
H	-5.09458700	-2.07217600	-0.97507500
N	-3.20377700	-1.04682000	-0.97559100
N	3.25684700	-0.31716300	1.04936000
N	3.20380100	-1.04679500	-0.97558000
N	-3.25688900	-0.31714000	1.04933000
S	-0.00004800	-2.19436100	0.00161000
O	1.25763200	-2.37759200	0.80710200
O	-1.25754500	-2.37751700	0.80739500
C	2.75936100	0.15909600	2.32916500
H	2.02671000	-0.55825700	2.69784000
H	3.59625000	0.23964700	3.01803300
H	2.29993800	1.13535900	2.19746600

C	2.69154600	-1.40577600	-2.28374300
H	3.52899100	-1.59450800	-2.95077900
H	2.06657100	-2.29483500	-2.19934400
H	2.09780600	-0.58107600	-2.66949600
C	-2.69153700	-1.40572500	-2.28378400
H	-2.09789900	-0.58095600	-2.66954600
H	-2.06646700	-2.29472100	-2.19943600
H	-3.52899500	-1.59452900	-2.95078400
C	-2.75942400	0.15913700	2.32914000
H	-3.59632500	0.23969300	3.01799300
H	-2.02677300	-0.55821200	2.69782400
H	-2.30000400	1.13540100	2.19743600

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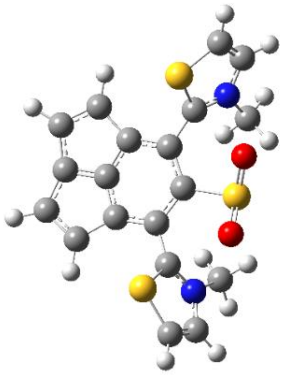
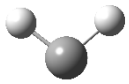


0 1

C	1.25293500	1.74357000	0.30272100
C	2.15208400	2.87595000	0.16411000
C	1.38377300	4.03316600	0.20367300
C	-0.00004600	3.69299800	0.40366300
C	-0.00002800	2.31695600	0.49140600
C	-1.38387900	4.03313400	0.20371300
C	-2.15215100	2.87589500	0.16408200
C	-1.25297600	1.74353700	0.30271600
H	3.22645100	2.84366000	0.06218700
H	1.79518700	5.02742700	0.08726000
H	-1.79531900	5.02738500	0.08731400
H	-3.22651500	2.84357600	0.06213400
C	1.23548400	0.34674100	0.17509000
C	0.00000500	-0.33613700	0.14780600
C	-1.23549400	0.34670800	0.17508900
C	-2.51347400	-0.32424700	-0.05976200
C	-4.73283200	-1.00466800	-0.84553100
C	-4.40882700	-1.51386400	0.35004600
H	-5.64154800	-1.16279700	-1.39960500
H	-4.99337200	-2.17722900	0.96576600
C	2.51347400	-0.32419700	-0.05975500
C	4.73282200	-1.00463200	-0.84553800
C	4.40883600	-1.51379900	0.35005700
H	5.64153100	-1.16277200	-1.39962100
H	4.99339100	-2.17715000	0.96578300
N	3.17435000	-1.09190900	0.79618000
N	-3.17434500	-1.09196400	0.79617300
S	0.00005700	-2.17039400	-0.01446300
O	-1.26532700	-2.38228700	-0.79439000
O	1.26546600	-2.38220400	-0.79437400
C	-2.58880800	-1.56557300	2.04185500
H	-3.39066400	-1.81878600	2.73021400
H	-1.96592000	-2.43536800	1.83420800
H	-1.97597300	-0.77378100	2.46408300
C	2.58881800	-1.56551100	2.04186900
H	1.97598000	-0.77371700	2.46408900
H	1.96593500	-2.43531300	1.83423700
H	3.39067900	-1.81870800	2.73022900
S	3.46439100	-0.00039700	-1.43553600
S	-3.46440400	-0.00043200	-1.43553200

2.2 Cartesian coordinates of the optimized geometries of all singlet carbenes and their energies (Sum of electronic and thermal Free Energies) in Hartree in singlet state at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory.

1S

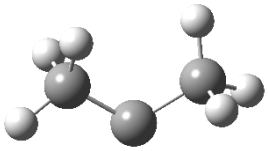


Energy= -39.119524 Hartree

0 1

C	0.00000000	0.00000000	0.17385600
H	0.00000000	0.86289700	-0.52156900
H	0.00000000	-0.86289700	-0.52156900

2S

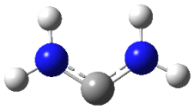


Energy= -117.711578 Hartree

0 1

C	0.00000000	0.00000000	0.65841200
C	0.00000000	1.21575400	-0.15529300
H	0.32376000	1.12294100	-1.20285400
H	-1.08707900	1.42029500	-0.17330300
H	0.44671500	2.08152800	0.33268100
C	0.00000000	-1.21575400	-0.15529300
H	-0.32376000	-1.12294100	-1.20285400
H	1.08707900	-1.42029500	-0.17330300
H	-0.44671500	-2.08152800	0.33268100

3S

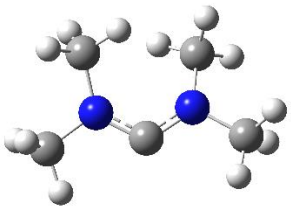


Energy= -149.919786 Hartree

0 1

C	-0.00000100	0.59666900	0.00002200
N	-1.11154800	-0.13712900	-0.00014000
H	-2.00216100	0.32562800	0.00056600
H	-1.12899900	-1.15574400	-0.00011300
N	1.11154600	-0.13712900	0.00011600
H	1.12904400	-1.15576000	0.00019000
H	2.00214300	0.32566800	-0.00060100

4S



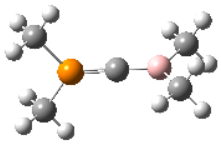
Energy= -306.978192 Hartree

0 1

C	-0.00001800	-0.81774100	-0.00005500
N	-1.15224900	-0.13461100	-0.04018400
N	1.15222600	-0.13463600	0.04009800
C	-2.36582200	-0.91199000	-0.22321200
H	-2.08499700	-1.93061600	-0.46920200
H	-2.97320400	-0.91052400	0.68832200
H	-2.96881000	-0.49727800	-1.03593900
C	-1.41006200	1.23835300	0.38876700
H	-0.59425400	1.60761200	1.00185300
H	-1.57192700	1.92507300	-0.44618000
H	-2.31328900	1.24345800	1.00167100
C	1.41013600	1.23832600	-0.38874600
H	1.57219500	1.92493600	0.44625900
H	2.31328500	1.24340100	-1.00177400
H	0.59430800	1.60777000	-1.00168500
C	2.36577200	-0.91204000	0.22327500
H	2.97330900	-0.91047300	-0.68815300
H	2.96861600	-0.49740200	1.03614600

H	2.08489200	-1.93068500	0.46911200

5S

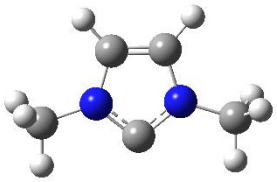


Energy= -563.743396 Hartree

0 1

C	0.37198600	-0.00007500	-0.00033800
B	1.82238600	0.00006200	-0.00003100
P	-1.20055600	-0.00000800	-0.00022700
C	2.62736300	-0.00022700	1.36472000
H	3.28439700	-0.87453800	1.41288400
H	3.28433800	0.87410700	1.41327800
H	1.99946800	-0.00044600	2.25607200
C	2.62791800	0.00020200	-1.36444200
H	3.28484600	0.87460100	-1.41246300
H	3.28503700	-0.87404600	-1.41256700
H	2.00040500	0.00019400	-2.25606200
C	-2.26417900	-1.47346700	-0.00010000
H	-2.89844200	-1.48843300	0.88655800
H	-2.89931300	-1.48791700	-0.88614400
H	-1.62047100	-2.34951400	-0.00066800
C	-2.26408300	1.47352200	0.00036300
H	-2.89881400	1.48859800	-0.88595800
H	-2.89875000	1.48794600	0.88674300
H	-1.62032000	2.34952900	0.00066100

6S

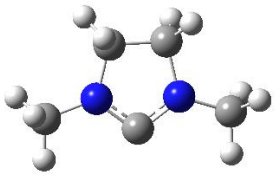


Energy= -304.636073 Hartree

0 1

N	1.05644000	0.12233800	-0.00001300
C	0.00000000	0.97176200	-0.00006100
N	-1.05643800	0.12234200	0.00000600
C	-2.43180700	0.56833400	0.00001900
H	-2.95388500	0.21103100	0.88873500
H	-2.42574200	1.65422700	-0.00010700
H	-2.95395400	0.21082200	-0.88857100
C	2.43180700	0.56833500	0.00002800
H	2.42573800	1.65422700	-0.00011100
H	2.95386500	0.21104400	0.88876000
H	2.95398000	0.21081400	-0.88854400
C	0.67244700	-1.20580100	0.00000100
H	1.37325700	-2.02295200	-0.00005300
C	-0.67244900	-1.20580000	-0.00001100
H	-1.37326500	-2.02294600	0.00009100

7S



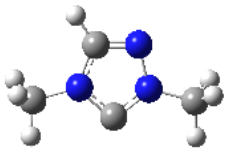
Energy= -305.816719 Hartree

0 1

N	-1.06683900	0.20276500	0.07112800
C	-0.00000200	1.00726400	-0.00009100
N	1.06684900	0.20275400	-0.07131000
C	-0.75971900	-1.22324900	-0.06812100
H	-1.08952400	-1.58989100	-1.04614200
H	-1.25949900	-1.81485300	0.70052200
C	0.75972000	-1.22324000	0.06812100
H	1.08952200	-1.58974300	1.04619800
H	1.25949400	-1.81496100	-0.70043300
C	2.42834200	0.65861700	-0.00530700
H	3.02382000	0.22769300	-0.81500800
H	2.43052400	1.74111100	-0.09807200
H	2.89526100	0.38258900	0.94664500
C	-2.42834600	0.65861500	0.00546300

H	-2.43052200	1.74110200	0.09831100
H	-2.89548100	0.38266100	-0.94640300
H	-3.02363800	0.22762200	0.81526600

8S

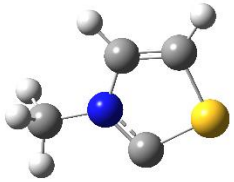


Energy= -320.691189 Hartree

0 1

N	-1.03467200	-0.13379700	0.00001900
C	-0.00593200	-0.98807800	-0.00011600
N	1.04785300	-0.12059700	-0.00015200
C	-2.43425500	-0.48824400	0.00001400
H	-2.49885200	-1.57190700	0.00014900
H	-2.92122500	-0.08618700	0.88746700
H	-2.92117500	-0.08642000	-0.88757400
C	2.43886000	-0.52194400	0.00014000
H	2.94714400	-0.15140800	0.89037500
H	2.46582300	-1.60731700	-0.00165800
H	2.94832700	-0.14838500	-0.88814700
N	-0.69722300	1.19691600	0.00007600
C	0.59210800	1.16711400	-0.00005500
H	1.22356300	2.04087700	-0.00011200

9S

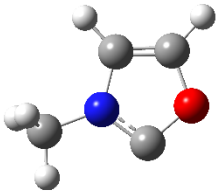


Energy= -608.234172 Hartree

0 1

C	-0.08528200	-1.14572600	-0.00004800
N	-0.89578600	-0.08298400	-0.00002400
C	-0.32545500	1.18718900	-0.00001000
H	-0.96008700	2.06031500	-0.00000900
C	1.01116200	1.14586400	-0.00001000
H	1.69023100	1.98155300	-0.00000400
C	-2.34491600	-0.23714700	-0.00002000
H	-2.77335100	0.22541700	-0.88944700
H	-2.56282000	-1.29981000	-0.00021600
H	-2.77332600	0.22508600	0.88959200
S	1.50730000	-0.51954700	0.00004900

10S

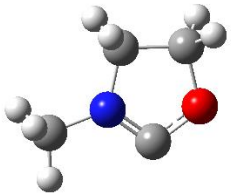


Energy= -285.232831 Hartree

0 1

C	0.09324400	-1.17611700	-0.00012300
N	-0.61082400	-0.03633300	-0.00005300
C	0.21180200	1.08746300	-0.00002100
H	-0.16079600	2.09630200	-0.00004300
C	1.45301300	0.60820000	-0.00007300
C	-2.05750000	0.00274300	-0.00003800
H	-2.42490100	0.51498900	-0.88925700
H	-2.41407500	-1.02308300	-0.00038900
H	-2.42494200	0.51440500	0.88950200
O	1.38412600	-0.75633700	0.00027000
H	2.42412200	1.06868100	-0.00007100

11S



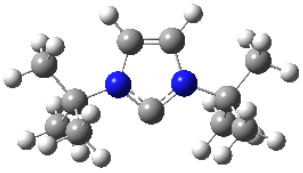
Energy= -286.425148 Hartree

0 1

C	-0.01486600	-1.21097700	0.00000100
N	0.67033300	-0.08038200	-0.00006300
C	-0.14314900	1.13715100	0.00006300

H	0.06697800	1.74034100	-0.88542800
C	-1.54094100	0.53750100	-0.00006200
C	2.10957000	-0.01068100	-0.00000300
H	2.47083400	0.51503100	0.88719500
H	2.49808500	-1.02506800	-0.00012400
H	2.47089100	0.51526200	-0.88703900
O	-1.31145000	-0.90095300	0.00005200
H	-2.11895200	0.78327600	-0.88834200
H	0.06692600	1.74010500	0.88573100
H	-2.11918100	0.78338700	0.88803600

12S

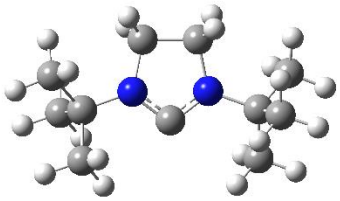


Energy= -540.306232 Hartree

0 1

N	-1.06221200	-0.28620600	-0.00000600
C	-0.00000100	0.55261600	0.00003000
N	1.06221200	-0.28620800	-0.00001400
C	-0.67264300	-1.61448400	-0.00006800
C	0.67264100	-1.61448300	-0.00007400
C	-2.45376000	0.22109600	0.00001200
C	-3.43697800	-0.94264500	-0.00003100
H	-3.32427400	-1.56699000	-0.88753300
H	-4.45190900	-0.54600300	-0.00000900
H	-3.32426700	-1.56706300	0.88741800
C	-2.65660300	1.06866000	-1.25302600
H	-1.94040300	1.88792900	-1.26842500
H	-3.66848400	1.47704600	-1.27141700
H	-2.50902900	0.46652100	-2.15115600
C	-2.65660400	1.06857300	1.25310900
H	-1.94036700	1.88780900	1.26858600
H	-2.50908800	0.46636000	2.15119900
H	-3.66846700	1.47700600	1.27150000
C	2.45376000	0.22109500	0.00000700
C	3.43698200	-0.94264400	-0.00004300
H	3.32427200	-1.56699000	-0.88754300
H	3.32427800	-1.56706200	0.88740700
H	4.45191300	-0.54600200	-0.00003100
C	2.65660300	1.06856300	1.25311000
H	1.94038800	1.88781800	1.26858000
H	3.66847700	1.47696500	1.27152300
H	2.50904900	0.46635000	2.15119500
C	2.65660300	1.06867200	-1.25302200
H	1.94037600	1.88791800	-1.26842700
H	2.50906900	0.46653200	-2.15115900
H	3.66847100	1.47709000	-1.27138900
H	-1.35392300	-2.44422800	-0.00009800
H	1.35391900	-2.44422900	-0.00011100

13S



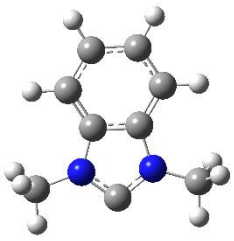
Energy= -541.483612 Hartree

0 1

N	-1.07012400	-0.22775300	-0.13183300
C	0.00000200	0.56652900	0.00000000
N	1.07012600	-0.22775500	0.13183400
C	-0.75483200	-1.64799900	0.08569200
H	-1.25735300	-2.29408500	-0.63055400
H	-1.04476300	-1.95995500	1.09477300
C	0.75483300	-1.64800000	-0.08569000
H	1.25735300	-2.29408600	0.63055600
H	1.04476400	-1.95995700	-1.09477100
C	-2.44989100	0.27265100	-0.00561300
C	-2.81446100	0.39835700	1.47545300
H	-2.73395200	-0.56223300	1.98805100
H	-3.84029600	0.75242900	1.59159200

H	-2.14388300	1.10623600	1.96316600
C	-3.40307500	-0.69970700	-0.69841500
H	-3.11323800	-0.84963800	-1.73988300
H	-4.41441600	-0.29319800	-0.68219900
H	-3.43240400	-1.67090500	-0.20261500
C	-2.55231700	1.63557400	-0.68068900
H	-2.28456700	1.56050800	-1.73537400
H	-1.87788600	2.34991100	-0.21610200
H	-3.57744200	2.00235400	-0.60441600
C	2.44989200	0.27265100	0.00561200
C	3.40307700	-0.69970200	0.69841900
H	3.43239200	-1.67090800	0.20263500
H	3.11325200	-0.84961400	1.73989300
H	4.41442100	-0.29320200	0.68218300
C	2.55231300	1.63557800	0.68068400
H	1.87790800	2.34992300	0.21607100
H	3.57744500	2.00234400	0.60444200
H	2.28452500	1.56052100	1.73536000
C	2.81446000	0.39835100	-1.47545400
H	2.14386600	1.10621100	-1.96317400
H	2.73397400	-0.56224500	-1.98804300
H	3.84028700	0.75244700	-1.59159500

14S

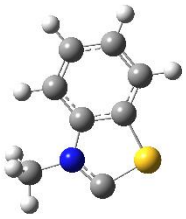


Energy= -458.205594 Hartree

0 1

C	0.16936700	0.69625000	-0.00003000
C	0.16937700	-0.69624000	-0.00000600
C	1.34989300	-1.41779800	-0.00005400
C	2.53393300	-0.69717600	-0.00012100
C	2.53392400	0.69718700	-0.00013800
C	1.34988400	1.41780600	-0.00009700
C	-2.00253100	-0.00001000	0.00003900
H	1.35370900	-2.49980600	-0.00005500
H	3.47763300	-1.22677400	-0.00016100
H	3.47761800	1.22679700	-0.00017900
H	1.35371000	2.49981300	-0.00009800
N	-1.16666600	-1.06949800	0.00006400
N	-1.16667600	1.06949000	0.00005300
C	-1.62242700	-2.43917800	0.00004100
H	-1.26710100	-2.96444300	-0.88838500
H	-1.26629800	-2.96471700	0.88798200
H	-2.70813600	-2.42618300	0.00053000
C	-1.62244500	2.43916900	0.00018300
H	-1.26668900	2.96450400	0.88839600
H	-1.26674900	2.96463800	-0.88797300
H	-2.70815400	2.42617300	0.00021800

15S



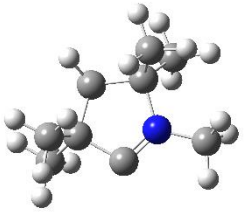
Energy= -761.802511 Hartree

0 1

C	0.37103200	-0.83015300	-0.00004200
C	0.02470100	0.51545700	0.00003800
C	0.99906800	1.50435000	0.00022800
C	2.32437800	1.11383800	0.00032100
C	2.67447000	-0.23531200	0.00023200
C	1.70228000	-1.21695800	0.00005300
C	-2.14171400	-0.39817300	-0.00020800
H	0.73305800	2.55255200	0.00030900
H	3.10090700	1.86749100	0.00046800
H	3.71930800	-0.51682500	0.00030600
H	1.97346200	-2.26451900	-0.00001800
N	-1.36748300	0.68617600	-0.00007400
C	-1.94614400	2.02071000	0.00001100

H	-1.63285600	2.56895700	0.88941100
H	-1.63233500	2.56928800	-0.88899800
H	-3.02485100	1.90864400	-0.00032300
S	-1.10704600	-1.77071100	-0.00027800

16S

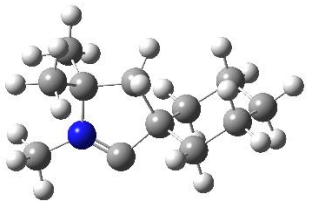


Energy= -407.579435 Hartree

0 1

C	0.59061500	1.27839100	0.09721300
N	-0.65049800	0.89692500	0.05792900
C	0.45058300	-1.10604500	-0.41783700
H	0.65555000	-2.03512200	0.11514700
H	0.52072100	-1.32343200	-1.48496300
C	-0.94672700	-0.56675200	-0.09294400
C	-1.75266400	1.83533400	0.19613400
H	-2.38934000	1.56445800	1.03946200
H	-1.32504000	2.81776500	0.36557300
H	-2.36129600	1.85368900	-0.70846200
C	1.43495500	0.02704300	-0.04472900
C	2.49471000	0.23602900	-1.12302900
H	3.15722300	1.05873900	-0.85379900
H	3.09540400	-0.66838800	-1.25146900
H	2.03549500	0.47744400	-2.08354400
C	2.12377900	-0.22279300	1.30097200
H	2.74162500	0.63210200	1.57581100
H	1.40227000	-0.38183500	2.10379200
H	2.76148500	-1.10787600	1.23884300
C	-1.93671500	-0.80868600	-1.22569000
H	-2.02543900	-1.88043100	-1.40925600
H	-2.93272700	-0.43259700	-0.98744400
H	-1.59582000	-0.33420500	-2.14703000
C	-1.50120400	-1.12260000	1.21714900
H	-2.45686500	-0.66510200	1.47674700
H	-1.66666200	-2.19667100	1.12132700
H	-0.80708900	-0.95653800	2.04033000

17S



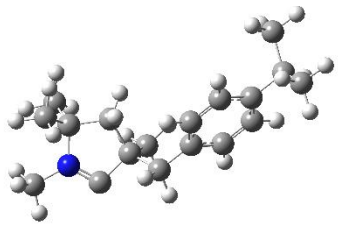
Energy= -524.222684 Hartree

0 1

C	-0.54026600	-1.22672800	-0.80114000
N	-1.67948100	-0.70209600	-0.46264600
C	-0.19582500	0.58010100	0.80615800
H	0.18157000	1.60140600	0.76319400
H	-0.08136000	0.24199500	1.83767000
C	-1.67391000	0.52053600	0.40354200
C	-2.94716700	-1.23881000	-0.93029600
H	-3.51302600	-0.48052600	-1.47327200
H	-2.72506900	-2.06889800	-1.59243800
H	-3.55072900	-1.59137800	-0.09328800
C	-2.59248100	0.34259500	1.60614700
H	-2.46296700	1.18195700	2.29091000
H	-3.64437100	0.31270900	1.31812300
H	-2.35205400	-0.57489200	2.14526600
C	-2.10537500	1.73734800	-0.41263500
H	-3.13386400	1.64375300	-0.76405100
H	-2.04969100	2.63473800	0.20526700
H	-1.45863500	1.87800000	-1.27827200
C	0.53961200	-0.38563100	-0.15355200
C	1.52639000	-1.29941400	0.58445000
C	1.29317600	0.35182700	-1.27717100
C	2.73815000	-0.54202500	1.11647200
H	1.85414500	-2.07535600	-0.11224300
H	1.00646000	-1.81292300	1.39768000
C	2.52114900	1.10334700	-0.77154300

H	1.59839700	-0.39154800	-2.01826000
H	0.61687800	1.03842300	-1.79233100
C	3.46796500	0.18130000	-0.01048800
H	3.41435000	-1.23398300	1.62379400
H	2.42086000	0.18759900	1.86977700
H	3.03866600	1.56663900	-1.61491000
H	2.21334900	1.92301800	-0.11386700
H	4.31511100	0.74811300	0.38299700
H	3.87984600	-0.56083600	-0.70289300

18S

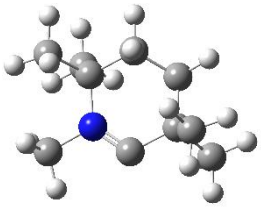


Energy= -756.327712 Hartree

0 1

C	2.99556100	-1.32610800	-0.36083600
N	3.78396400	-0.29551000	-0.30470400
C	1.72602900	0.68269300	0.20052000
H	1.23589100	1.08978300	1.08468300
H	1.24493100	1.13635400	-0.66562500
C	3.22328100	1.00923400	0.17788700
C	5.19256000	-0.37995600	-0.65550700
H	5.81937800	-0.07577000	0.18385000
H	5.40406000	-1.41297500	-0.91028100
H	5.41797500	0.26004700	-1.50907200
C	1.63379800	-0.85734300	0.11780700
C	0.57331500	-1.33844100	-0.89475800
H	0.85260000	-0.96318300	-1.88231700
H	0.64174800	-2.42596900	-0.94921200
C	1.40009500	-1.49250600	1.49192400
H	1.40339900	-2.58030100	1.41628800
H	2.18441700	-1.21082800	2.19539200
H	0.44429000	-1.17110200	1.90688100
C	3.54974200	2.13528000	-0.79563700
H	3.01008300	3.03696500	-0.50255600
H	4.61371700	2.37652900	-0.80275500
H	3.24481400	1.87231500	-1.80963100
C	3.77866400	1.33776500	1.56206700
H	4.85907800	1.48676200	1.53706800
H	3.32817900	2.26091800	1.92936000
H	3.55849900	0.54457200	2.27531800
C	-0.84050900	-0.92444200	-0.58711600
C	-1.38184900	0.24633600	-1.10847000
C	-1.65545400	-1.69583000	0.23170300
C	-2.67222300	0.64151900	-0.80513400
H	-0.78601800	0.85643200	-1.77733200
C	-2.94824300	-1.30075900	0.53516500
H	-1.27586100	-2.62724800	0.63453700
C	-3.47989500	-0.12329200	0.02887200
H	-3.05598200	1.55945900	-1.23477500
H	-3.55942200	-1.92611500	1.17638300
C	-4.89248500	0.29968400	0.36570100
H	-5.30367200	-0.46605500	1.02968200
C	-4.91935000	1.62955600	1.11948900
H	-5.94005800	1.89100300	1.40574100
H	-4.31176500	1.58193400	2.02415400
H	-4.53029000	2.43981300	0.49935700
C	-5.77847900	0.35791300	-0.87891400
H	-5.78432100	-0.59846100	-1.40326600
H	-6.80675800	0.60755200	-0.60970100
H	-5.42399800	1.11833700	-1.57782000

19S



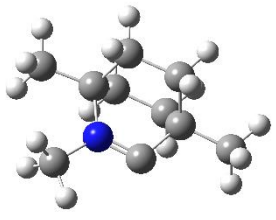
Energy= -446.845584 Hartree

0 1

C	0.64352600	1.19776600	0.02902600

C	-1.29209300	-0.43573400	-0.00064600
C	1.04972200	-1.33346100	0.26264200
C	-0.27770100	-1.48408400	-0.44854000
H	1.74899700	-2.10622300	-0.06765700
N	-0.62848900	0.91732300	0.00740000
H	0.91560600	-1.48358200	1.33678700
C	1.63692000	0.05840000	0.00917600
C	2.69611900	0.36926000	1.06938000
H	3.46854100	-0.40495700	1.07193300
H	3.16163000	1.33460500	0.87370300
H	2.25257700	0.40802000	2.06642900
C	2.30446600	0.11719200	-1.37338300
H	1.60885400	-0.13518100	-2.17537900
H	2.68384300	1.11976500	-1.56811300
H	3.13869000	-0.58738400	-1.41181700
H	-0.70993400	-2.47225700	-0.27683500
H	-0.13154600	-1.39097500	-1.52759500
C	-1.80469100	-0.74222600	1.40730900
H	-0.99130300	-0.76085800	2.13107500
H	-2.53209900	-0.00195600	1.73947000
H	-2.29725800	-1.71615700	1.41748300
C	-2.45795300	-0.44603700	-0.98738200
H	-3.28899500	0.17900300	-0.66352400
H	-2.13614900	-0.11438700	-1.97562000
H	-2.83099300	-1.46712700	-1.08102200
C	-1.55412200	2.05567200	0.02637600
H	-2.30467200	1.93642200	0.80823300
H	-2.06174300	2.16051800	-0.93219300
H	-0.95977700	2.94095800	0.21908400

20S

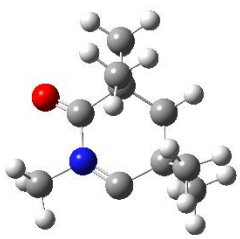


Energy= -445.663473 Hartree

0 1

C	1.12754800	-0.66483300	-1.25273300
C	1.45015000	0.17506900	0.00000000
C	-1.03503100	-0.49063900	0.00000200
C	-0.35233600	-1.07127700	-1.24479000
H	1.36341500	-0.07699300	-2.14100200
H	1.78146800	-1.53979400	-1.27128600
H	-0.86754700	-0.70701300	-2.13538900
H	-0.47112100	-2.15644600	-1.22815600
C	0.52310000	1.36814100	-0.00001100
C	-0.35233800	-1.07126000	1.24480400
H	-0.86755300	-0.70698700	2.13539700
H	-0.47111900	-2.15642800	1.22818300
C	1.12754500	-0.66481100	1.25274800
H	1.36340400	-0.07695100	2.14100700
H	1.78146700	-1.53976800	1.27132200
N	-0.71922300	0.96870200	-0.00000800
C	2.90619100	0.60916000	-0.00000200
H	3.12396000	1.21650300	-0.87943000
H	3.12395900	1.21651600	0.87941800
H	3.57697000	-0.25458800	0.00000600
C	-2.52073500	-0.79563800	0.00000300
H	-3.02094200	-0.40315500	0.88537500
H	-3.02094000	-0.40317000	-0.88537600
H	-2.65430300	-1.87840600	0.00001200
C	-1.79657800	1.95043000	-0.00001700
H	-2.42317900	1.84599900	-0.88643700
H	-2.42318100	1.84601200	0.88640300
H	-1.32530200	2.92770500	-0.00002400

21S

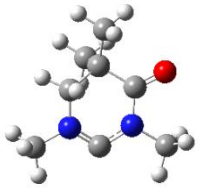


Energy= -520.897973 Hartree

0 1

C	-0.98541800	1.28817900	0.19864300
C	1.28371700	0.36750600	-0.17152000
C	-0.61909600	-1.14564900	-0.58565400
C	0.79669400	-1.05329200	-0.01648100
H	-1.02360200	-2.14097100	-0.38119000
N	0.32352900	1.40664200	0.08297300
H	-0.53369000	-1.07257100	-1.67361500
C	-1.58851000	-0.05793200	-0.10009100
C	-2.61320100	0.21499700	-1.21452700
H	-3.11675500	-0.71679300	-1.48462600
H	-3.35685400	0.93845100	-0.88434800
H	-2.12893700	0.60982800	-2.10949300
C	-2.37769900	-0.48996600	1.14628400
H	-1.73593800	-0.71849400	1.99485500
H	-3.05967300	0.30390400	1.44796700
H	-2.96067000	-1.38439300	0.91568000
C	0.86981800	-1.37692700	1.48575700
H	0.42599700	-2.35614700	1.67191100
H	1.91026500	-1.40443400	1.81107700
H	0.34710200	-0.64492800	2.09862200
C	1.72472600	-1.99750000	-0.77390100
H	2.74822000	-1.91711900	-0.41261200
H	1.38518400	-3.02605600	-0.63959100
H	1.72778900	-1.77552800	-1.84159800
O	2.42119300	0.67126200	-0.40599900
C	0.92906900	2.73715200	0.24742200
H	1.68405900	2.71122800	1.03162000
H	1.41012600	3.04503000	-0.67867400
H	0.12254200	3.41299300	0.50560600

22S

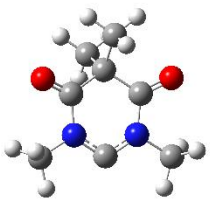


Energy= -497.710831 Hartree

0 1

C	-0.89480200	-1.03480400	-0.59715700
C	0.49172100	-1.08304800	0.02156800
C	1.12514500	0.29147300	-0.10749100
C	-1.11768000	1.30750500	0.09842400
N	0.25121500	1.36730000	-0.04337400
N	-1.64427600	0.11951900	-0.11426800
O	2.32100600	0.45810500	-0.17802400
C	0.40412400	-1.39890200	1.52108000
H	-0.01522600	-2.39676900	1.66406500
H	1.39691800	-1.37741300	1.97002200
H	-0.22762600	-0.68309400	2.04763900
C	1.34765500	-2.12174400	-0.69007000
H	1.43441100	-1.90059800	-1.75483000
H	2.35181200	-2.13849100	-0.27221700
H	0.90348000	-3.11284700	-0.57824000
C	-3.08539500	-0.03745500	-0.04699600
H	-3.35270000	-0.80451000	0.68331900
H	-3.51593300	0.91445800	0.24648700
H	-3.48270600	-0.33266500	-1.02194700
C	0.87527900	2.68579800	0.03669800
H	0.07806600	3.40903900	0.16777700
H	1.57109700	2.72741100	0.87413000
H	1.43207500	2.89653500	-0.87525700
H	-0.82336000	-0.98112800	-1.68966300
H	-1.44320900	-1.94543900	-0.34993400

23S



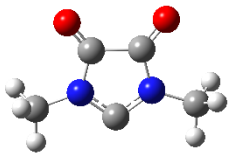
Energy= -571.767855 Hartree

0 1

C	-1.26523400	0.30474700	-0.12061800

C	-0.00000100	1.11437200	0.05533800
C	1.26523600	0.30475000	-0.12060300
C	0.00000200	-1.79217400	0.04081300
N	1.14676800	-1.08211900	-0.00865700
N	-1.14676500	-1.08212100	-0.00866100
O	-2.34067100	0.82099400	-0.28580800
O	2.34067000	0.82099900	-0.28580800
C	0.00000300	2.30803000	-0.89645500
H	-0.89056800	2.90861500	-0.72695500
H	0.89057200	2.90861400	-0.72694700
H	0.00000700	1.98112800	-1.93678500
C	-0.00000900	1.59979000	1.52309300
H	-0.00001200	0.76413000	2.22482200
H	0.88898900	2.20344000	1.69987900
H	-0.88901100	2.20343800	1.69987000
C	-2.40666700	-1.82779300	-0.02272000
H	-2.92457500	-1.67403400	-0.96783500
H	-2.15733900	-2.87458100	0.10815400
H	-3.05329100	-1.48100600	0.78143300
C	2.40667100	-1.82779000	-0.02271900
H	2.15734400	-2.87458000	0.10814100
H	2.92458300	-1.67401900	-0.96783100
H	3.05329100	-1.48101100	0.78144000

24S

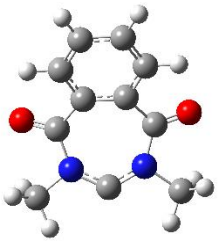


Energy= -453.923412 Hartree

0 1

C	-0.00000700	1.40091700	-0.00001400
N	1.08896900	0.58255900	-0.00006600
C	-0.77060500	-0.76556300	-0.00000600
C	0.77060300	-0.76555600	-0.00004600
C	2.45777700	1.06044400	0.00004000
H	2.98161800	0.70186300	-0.88508900
H	2.42532400	2.14572200	-0.00034600
H	2.98130400	0.70251500	0.88562400
N	-1.08898100	0.58253000	-0.00000600
C	-2.45778400	1.06045200	0.00003700
H	-2.42528400	2.14572600	0.00051800
H	-2.98138500	0.70262400	-0.88554500
H	-2.98156900	0.70179200	0.88516500
O	1.51215200	-1.69998700	-0.00000300
O	-1.51212900	-1.70001700	0.00001700

25S



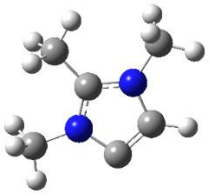
Energy= -684.831218 **Hartree**

0 1

C	0.88072600	0.69483700	0.05737300
C	0.88077900	-0.69473100	0.05753300
C	-0.29365100	-1.57973300	0.26228600
C	-0.29375800	1.57980700	0.26202100
C	-2.18436900	-0.00010500	-0.35480400
C	2.08792800	-1.37576500	-0.10299000
H	2.06862000	-2.45527600	-0.06842200
C	3.26860000	-0.69363200	-0.29473400
H	4.19115500	-1.24158200	-0.43605600
C	3.26855000	0.69381200	-0.29490000
H	4.19106600	1.24179300	-0.43635800
C	2.08783200	1.37591000	-0.10330900
H	2.06845200	2.45542700	-0.06898700
N	-1.58545700	-1.18690000	-0.14456100
N	-1.58562900	1.18676100	-0.14437200
O	-0.13733400	2.70312400	0.67682100
O	-0.13718500	-2.70300600	0.67717300
C	-2.50090700	-2.34063700	-0.25445500
H	-2.69294000	-2.76475500	0.72907900

H	-3.41765600	-1.96771600	-0.69289100
H	-2.05269900	-3.11235400	-0.87741300
C	-2.50132000	2.34034700	-0.25388200
H	-3.41818300	1.96727300	-0.69194600
H	-2.69301800	2.76441600	0.72973900
H	-2.05349700	3.11215300	-0.87700500

26S

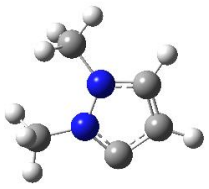


Energy= -343.891420 Hartree

0 1

N	1.06560300	-0.34763200	0.00022400
C	0.67165800	-1.69497900	0.00200900
C	0.03806900	0.51050900	-0.00250900
N	-1.07082200	-0.22407000	-0.00354300
C	0.12393600	1.99100200	0.00109100
H	0.61831100	2.35510700	0.90456900
H	0.69693200	2.35290200	-0.85501100
H	-0.86566500	2.44116500	-0.04332600
C	-0.69117400	-1.56760600	-0.00009400
H	-1.45818600	-2.32437800	-0.00087500
C	-2.42941500	0.27516800	0.00164000
H	-2.63957700	0.83709300	0.91180600
H	-2.61931200	0.90732200	-0.86558900
H	-3.10136800	-0.57783000	-0.04078200
C	2.45132600	0.07243100	-0.00004100
H	2.68787000	0.64876200	-0.89629500
H	2.68025500	0.67447200	0.88109700
H	3.05086200	-0.83185100	0.01507000

27S

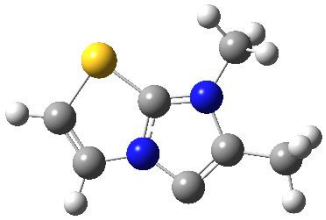


Energy= -304.584172 Hartree

0 1

N	0.21657700	-0.70924000	0.02150000
C	-0.96766000	-1.31939500	0.09550300
C	1.51479600	-1.33882100	-0.05180200
H	1.33821500	-2.40148100	0.07170900
H	1.98492800	-1.16029400	-1.02055000
H	2.17461200	-0.98671800	0.74280500
N	0.12176400	0.66671500	-0.12988400
C	-1.88785100	-0.22809200	0.03860700
H	-2.96093100	-0.31941900	0.06936500
C	-1.19779800	0.94401900	-0.08315500
H	-1.52834700	1.96926700	-0.14471200
C	1.22416700	1.56781300	0.09913600
H	1.55921200	1.53986900	1.13883000
H	2.06143400	1.32772100	-0.55444300
H	0.88856700	2.57558900	-0.13405000

28S



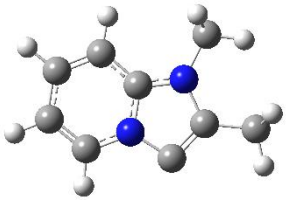
Energy= -778.996614 Hartree

0 1

C	0.31291700	0.28871900	-0.00417300
C	-1.68824500	-0.62780200	-0.00076600
N	-0.97110200	0.60463300	-0.01539400
C	-1.51380700	1.94355400	0.01386000
H	-1.79591500	2.22891400	1.02833500
H	-0.77516700	2.64967200	-0.36226700
H	-2.39332000	1.99198900	-0.62402100
N	0.41033200	-1.05275600	0.00555200
C	-0.84226500	-1.70239700	0.00823700
C	-3.17532500	-0.60839300	-0.00569200
H	-3.59370500	-0.08121900	0.85678200

H	-3.58884800	-0.15004400	-0.90922000
H	-3.51884100	-1.63949100	0.03163300
C	2.61092500	-0.49447500	-0.00176900
H	3.68437700	-0.56462200	-0.00259400
C	1.72126200	-1.49274200	0.00396200
H	1.91392000	-2.55297200	0.00766400
S	1.84000700	1.08849000	-0.00246100

29S

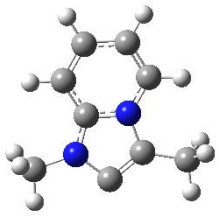


Energy= -458.165913 Hartree

0 1

C	-0.27636800	0.45322900	-0.00022500
C	-1.33541300	1.36606900	-0.00022700
C	-2.60636100	0.86394900	-0.00008500
C	-2.82081300	-0.53145400	0.00008300
C	-1.76219900	-1.38245000	0.00011700
C	1.64099000	-0.66262100	-0.00003900
H	-1.14127600	2.42957900	-0.00030200
H	-3.45274900	1.53757000	-0.00006500
H	-3.82327900	-0.93385300	0.00018900
H	-1.83308300	-2.45968700	0.00025300
N	1.04877100	0.61815800	-0.00033400
C	1.70374600	1.90593900	0.00046900
H	1.43368900	2.48026200	-0.88719100
H	1.43680100	2.47773300	0.89071800
H	2.77849900	1.75369800	-0.00168500
N	-0.49201100	-0.90040800	0.00003700
C	0.69965700	-1.65423200	0.00017100
C	3.12064500	-0.80962100	-0.00014500
H	3.58684900	-0.36485700	-0.88421700
H	3.58706600	-0.36453500	0.88365000
H	3.34685800	-1.87300400	0.00001900

30S

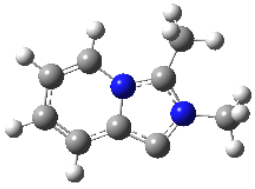


Energy= -458.168328 Hartree

0 1

C	-0.12197200	-0.70408100	-0.00002600
C	-1.32423300	-1.41126300	0.00004400
C	-2.49780200	-0.70617500	0.00005900
C	-2.47419600	0.70224900	0.00001000
C	-1.28793100	1.36620000	-0.00003400
C	2.05072400	0.00378500	-0.00004700
H	-1.30869900	-2.49179400	0.00009100
H	-3.44452800	-1.22862100	0.00010900
H	-3.39385000	1.26922600	0.00002200
H	-1.20033000	2.44173600	-0.00005200
N	1.16646700	-1.07849700	-0.00007900
C	1.58819900	-2.46214500	0.00003600
H	1.22840600	-2.98108200	0.89053000
H	1.22597200	-2.98194300	-0.88896200
H	2.67335200	-2.45946100	-0.00142300
C	1.52745200	2.54267600	0.00001800
H	1.13636900	3.05788000	-0.88368400
H	1.13634000	3.05788000	0.88370800
H	2.60953600	2.64949200	0.00003700
N	-0.11918200	0.66699700	-0.00003300
C	1.20749800	1.09328600	0.00000700

31S

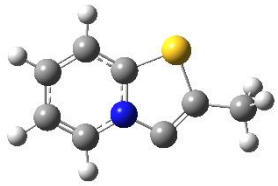


Energy= -458.160378 Hartree

0 1

C	-1.29081800	1.34749500	0.00007100
C	-2.56097800	0.90077600	0.00002500
C	-2.85851900	-0.49461900	-0.00008100
C	-1.84467400	-1.39697200	-0.00009100
H	-1.01524400	2.39126700	0.00013400
H	-3.36191000	1.62734400	0.00005800
H	-3.88968500	-0.81869500	-0.00012300
H	-2.02691700	-2.46297700	-0.00010500
C	1.72809700	1.93286400	0.00004500
H	1.45749900	2.51953500	-0.88233700
H	1.45908900	2.51849400	0.88361900
H	2.80845100	1.81136000	-0.00102000
C	0.70660500	-1.66328100	0.00013600
C	3.04684400	-0.84187200	0.00000300
H	3.50802100	-0.41201500	-0.88991300
H	3.50800900	-0.41210000	0.88996700
H	3.19379600	-1.91649800	-0.00004300
C	-0.49980700	-0.97530900	-0.00001600
N	-0.26069700	0.42344700	-0.00000200
N	1.61220200	-0.62116200	0.00001200
C	1.05630900	0.61396700	-0.00014300

32S

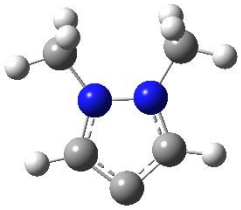


Energy= -761.769536 Hartree

0 1

C	0.39236900	-0.62548800	-0.00000200
C	1.61270700	-1.30048000	-0.00000500
C	2.77010000	-0.57195300	-0.00000700
C	2.71102000	0.83143300	-0.00000700
C	1.50356700	1.45548500	-0.00000200
C	-1.84910100	0.39633200	0.00000300
H	1.62284000	-2.38100900	-0.00000400
H	3.72767300	-1.07512500	-0.00001000
H	3.61302800	1.42587200	-0.00001000
H	1.36190800	2.52494700	-0.00000200
N	0.34541700	0.74304900	0.00000200
C	-0.92026800	1.37272200	0.00000000
C	-3.33212100	0.54934900	-0.00000300
H	-3.79029800	0.09680400	-0.88256100
H	-3.79030400	0.09680000	0.88255100
H	-3.56437500	1.61243200	-0.00000200
S	-1.18300200	-1.25915400	0.00001000

33S

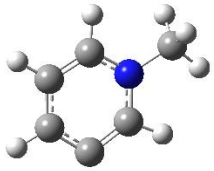


Energy= -304.559236 Hartree

0 1

C	1.14571700	1.06650400	0.01371300
C	1.14570500	-1.06650500	-0.01370800
H	1.32767800	2.13368100	0.02477600
H	1.32765800	-2.13368400	-0.02477000
C	2.03604200	-0.00000600	-0.00001500
N	-0.15775100	-0.67391800	-0.01152800
N	-0.15774900	0.67392600	0.01153800
C	-1.36692800	-1.45708000	0.01307700
H	-1.99783300	-1.24485200	-0.85103500
H	-1.07146500	-2.50233900	-0.02297300
H	-1.93492600	-1.28730900	0.92906300
C	-1.36693200	1.45707900	-0.01307500
H	-1.99777500	1.24495500	0.85110800
H	-1.07147500	2.50234500	0.02281600
H	-1.93499000	1.28719300	-0.92900200

34S

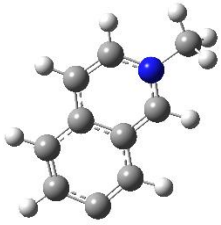


Energy= -287.340682 Hartree

0 1

C	-1.23344900	1.11767000	-0.00154700
C	-1.88123800	-0.11643300	0.00602200
C	-1.21386100	-1.35076700	0.00172300
C	0.16225700	-1.19576800	-0.00611800
H	-1.77862900	2.05378700	-0.00268300
H	-2.96925600	-0.09928500	0.01603200
H	0.84418400	-2.04191400	-0.01423000
C	0.13563300	1.15140700	-0.00491300
H	0.71621200	2.06305000	-0.00620200
N	0.82034300	-0.00400800	-0.00563000
C	2.28149200	0.04401600	0.00758100
H	2.66685600	-0.96693400	-0.08559400
H	2.64081700	0.64219200	-0.82780600
H	2.63240800	0.47641300	0.94340100

35S

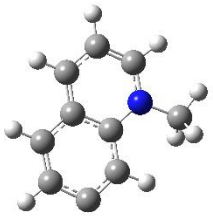


Energy= -440.871806 Hartree

0 1

C	-2.77089500	-1.18680100	0.00002700
C	-1.43333900	-1.54131800	-0.00005500
C	-0.36538800	-0.61340900	-0.00008800
C	-0.63248500	0.79486700	0.00004400
C	-1.96983400	1.19287300	0.00013000
C	-2.96093700	0.23441300	0.00005500
H	1.22614300	-2.06299700	-0.00029500
H	-1.14370900	-2.59383600	-0.00006000
C	0.96064600	-1.01292500	-0.00021100
C	0.46843900	1.67382500	0.00001800
H	-2.20766200	2.25209600	0.00020100
H	-3.98412300	0.60732300	0.00001500
C	1.73900400	1.20244100	-0.00010100
H	0.30748200	2.74391100	0.00006200
H	2.61151600	1.83633900	-0.00011100
N	1.97362300	-0.14721100	-0.00022500
C	3.34742700	-0.65021500	0.00029200
H	3.52310400	-1.24933800	0.89186900
H	3.52129400	-1.25568100	-0.88731800
H	4.03477000	0.19015900	-0.00345900

36S



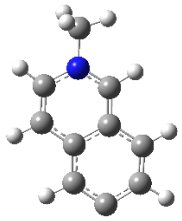
Energy= -440.878531 Hartree

0 1

C	-2.33932800	-1.32699500	0.00020200
C	-0.95305600	-1.49131900	0.00014400
C	-0.04890300	-0.43148800	-0.00001000
C	-0.52167200	0.92011600	-0.00005900
C	-1.92501600	1.11873100	-0.00005000
C	-2.76358200	0.04873400	0.00005800
H	-0.55440400	-2.50047900	0.00027600
C	0.38726200	1.96173200	-0.00003700
H	-2.29493000	2.13970000	-0.00012600
H	-3.83166900	0.25312700	0.00006400
C	1.75131800	1.71556300	0.00003400
H	0.01759300	2.98040200	-0.00006200
H	2.47779000	2.51407700	0.00006300
C	2.17962700	0.41293100	0.00000700

H	3.22910400	0.15609500	0.00002000
N	1.32374700	-0.61538900	-0.00007300
C	1.85470500	-1.97632400	-0.00015000
H	1.51186400	-2.50767100	0.88535900
H	1.51075000	-2.50795200	-0.88504400
H	2.93953700	-1.92965600	-0.00087700

37S

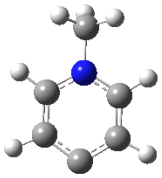


Energy= -440.874943 Hartree

0 1

C	-3.06994000	0.41228000	0.00015600
C	-1.95227300	1.25459900	0.00006200
C	-0.63400800	0.81214100	-0.00004700
C	-0.36881900	-0.59816900	-0.00005800
C	-1.46706600	-1.49192100	-0.00007200
C	-2.73303500	-0.98797100	-0.00004500
H	0.35830400	2.74107500	-0.00010400
H	-2.09560800	2.33513700	0.00012700
C	0.50040100	1.66834300	-0.00007800
C	0.93643100	-1.03218900	-0.00003100
H	-1.27517600	-2.56125000	-0.00010200
H	-3.54925100	-1.70714400	-0.00011700
H	1.17908800	-2.08675100	0.00001200
C	1.75393800	1.17089100	-0.00007400
H	2.64165900	1.78612000	-0.00010300
N	1.97158200	-0.18613200	-0.00004900
C	3.34540700	-0.67472200	0.00017800
H	3.86627800	-0.32202200	0.88947100
H	3.34053900	-1.76083200	-0.00040100
H	3.86687600	-0.32110100	-0.88839300

38S

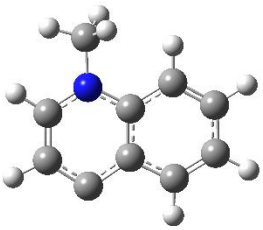


Energy= -287.339980 Hartree

0 1

C	0.13536700	-1.16399800	-0.01244400
C	-1.23140700	-1.17288100	0.00465900
C	-2.02894200	-0.00222300	0.01366700
C	-1.23518900	1.17035000	0.00515500
C	0.13199800	1.16560700	-0.01197400
N	0.81723100	0.00202700	-0.02296000
H	0.74493700	-2.05977000	-0.02096900
H	-1.70282300	-2.15177100	0.00693300
H	-1.70925600	2.14797000	0.00751100
H	0.73817900	2.06351200	-0.02027600
C	2.27464600	0.00033800	0.01971300
H	2.64948600	0.91727300	-0.42792000
H	2.62654600	-0.06720900	1.04913600
H	2.65347800	-0.84734800	-0.54635600

39C



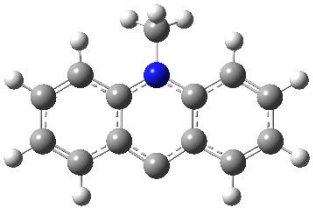
Energy= -440.903334 Hartree

0 1

C	2.73546700	-0.22335500	0.00000000
C	1.81751400	-1.23671000	-0.00000300
C	0.42654600	-0.98926200	-0.00000200
C	0.01621800	0.36497000	0.00000000
C	0.95824500	1.40772400	0.00000400
C	2.29488800	1.10656200	0.00000500

H	3.79590400	-0.43939600	0.00000000
H	2.11599600	-2.27667600	-0.00000500
C	-0.47610400	-2.10384700	-0.00000100
H	0.64783300	2.44226100	0.00000900
H	3.01803500	1.91274200	0.00000900
C	-2.21346500	-0.38834500	0.00000000
C	-1.82158600	-1.70104300	0.00000300
H	-3.25603000	-0.09288500	-0.00000100
H	-2.61804100	-2.43909900	0.00000600
N	-1.33670700	0.62966500	-0.00000200
C	-1.82020400	2.00249600	-0.00000400
H	-1.47298800	2.52995800	0.88785900
H	-1.47295700	2.52996600	-0.88785000
H	-2.90592000	1.99034100	-0.00002400

40C

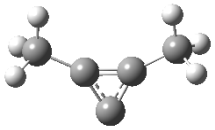


Energy= -594.463396 Hartree

0 1

C	3.61610200	-0.97798700	-0.06251800
C	2.42937400	-1.64781300	0.03363700
C	1.18596900	-0.97620800	0.06276200
C	1.19466200	0.44098200	0.01418900
C	2.42060200	1.12370200	-0.09997700
C	3.59653100	0.41959900	-0.13823400
C	0.00005400	-1.75636400	0.13027200
C	-1.19463800	0.44090000	0.01416000
C	-1.18589900	-0.97627700	0.06269300
C	-2.42928900	-1.64790300	0.03352100
H	-2.38470400	-2.72774500	0.08419900
C	-3.61602800	-0.97808200	-0.06259100
C	-3.59649000	0.41951600	-0.13816900
C	-2.42057000	1.12363300	-0.09987300
H	4.55707900	-1.51110900	-0.08965500
H	2.38480200	-2.72765300	0.08436800
H	2.45801200	2.19786000	-0.19397000
H	4.52763400	0.96433100	-0.23760200
H	-4.55699700	-1.51121700	-0.08975600
H	-4.52760800	0.96424000	-0.23743900
H	-2.45795300	2.19781400	-0.19368400
N	-0.00002200	1.12076300	0.06815700
C	-0.00023900	2.57088300	0.19450600
H	-0.00070100	3.06368100	-0.77992800
H	-0.87324100	2.88629800	0.75535700
H	0.87299700	2.88667800	0.75473700

41S

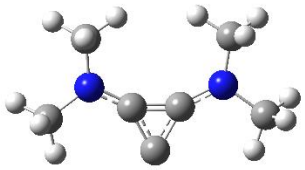


Energy= -193.893635 Hartree

0 1

C	-0.00006700	1.39510900	0.00000300
C	0.66199400	0.15948800	0.00003100
C	-0.66193700	0.15937700	-0.00004000
C	-1.96750000	-0.52100300	-0.00001600
H	-1.88135300	-1.60669400	-0.00131300
H	-2.53524300	-0.20565500	0.87719300
H	-2.53652300	-0.20355000	-0.87562600
C	1.96751400	-0.52098700	-0.00000200
H	2.53576000	-0.20490700	-0.87661800
H	2.53610800	-0.20442400	0.87621100
H	1.88122800	-1.60666800	0.00029800

42S

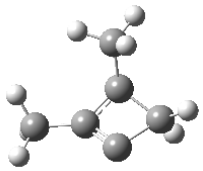


Energy= -383.105959 Hartree

0 1

C	0.00000100	-1.72286600	-0.01871000
C	-0.67228800	-0.50532300	-0.08104400
C	0.67227300	-0.50531300	-0.08108600
N	1.87016800	0.08674600	-0.13263000
N	-1.87017800	0.08674700	-0.13262400
C	2.01491600	1.51429100	0.03027200
H	2.86510200	1.86843300	-0.55559600
H	1.12078000	2.01877300	-0.32813400
H	2.18023500	1.79385000	1.07772500
C	3.04726200	-0.72581600	0.10249100
H	2.79186200	-1.76905500	-0.06540200
H	3.84553800	-0.43591800	-0.58350700
H	3.41256900	-0.61382600	1.12934100
C	-2.01487100	1.51430400	0.03024700
H	-2.86554900	1.86829100	-0.55499200
H	-2.17937600	1.79400300	1.07779100
H	-1.12107300	2.01881400	-0.32897400
C	-3.04728800	-0.72579300	0.10250400
H	-3.84545900	-0.43611900	-0.58371100
H	-2.79181000	-1.76906500	-0.06506600
H	-3.41277800	-0.61354700	1.12926000

43S

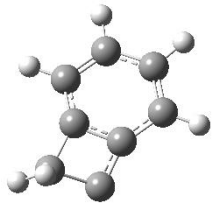


Energy= -233.153547 Hartree

0 1

C	-0.04093600	-1.20706300	0.64766600
C	0.55066700	0.18974100	-0.30520100
C	1.23673600	-1.10890400	-0.23774000
C	-0.74807800	-0.27767700	-0.06242800
C	-2.11480000	0.27630400	-0.08737200
H	-2.56667800	0.11786400	-1.06888400
H	-2.73483200	-0.21627100	0.66016700
H	-2.11356600	1.35183100	0.10124100
C	1.13859100	1.49201900	0.12134000
H	1.67167400	1.36233900	1.06870400
H	1.85960100	1.84890700	-0.61597800
H	0.37251900	2.25477600	0.25899600
H	1.17298400	-1.73697600	-1.11675000
H	2.20521800	-1.16900000	0.25491500

44S

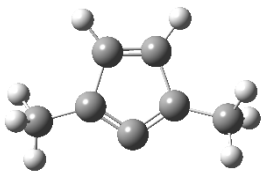


Energy= -308.127796 Hartree

0 1

C	-1.66643600	-0.92461700	-0.54045700
C	-0.68170700	0.51108700	0.19213400
C	-2.16552800	0.36995900	0.16033100
C	-0.41915300	-0.86612700	0.12042600
H	-2.60235400	0.19683300	1.13961000
H	-2.77076700	1.05086700	-0.43453500
C	0.33431900	1.44001200	-0.06048400
C	1.61239100	0.93693200	-0.09428500
C	0.88976500	-1.37910300	0.10952300
C	1.88907100	-0.44797400	0.02693100
H	1.10137200	-2.43975600	0.14534900
H	2.92320700	-0.76849700	0.01154800
H	2.44791500	1.61684500	-0.20679100
H	0.14429300	2.50269800	-0.13989100

45S

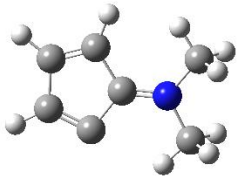


Energy= -271.213256 Hartree

0 1

C	0.00001700	0.94995000	-0.00003300
C	-0.64266600	-1.23195200	-0.19697500
C	0.64261100	-1.23195300	0.19697500
C	-1.11120400	0.20427900	-0.15485400
C	1.11121200	0.20425000	0.15480300
H	1.29238300	-2.09562900	0.26397300
H	-1.29247200	-2.09560700	-0.26390500
C	2.52578200	0.57213500	-0.08043700
H	2.60522600	1.57207100	-0.50418300
H	3.08816000	0.55687900	0.85869700
H	3.00914400	-0.14998300	-0.74377300
C	-2.52575300	0.57217000	0.08047000
H	-2.60521000	1.57230000	0.50374600
H	-3.08833600	0.55635500	-0.85853000
H	-3.00889200	-0.14966700	0.74428400

46S

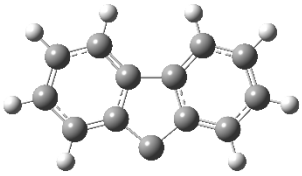


Energy= -326.564738 Hartree

0 1

C	0.89962200	-1.29807900	0.00012500
C	0.97354900	1.18012100	-0.00004100
C	2.21477400	0.68474100	-0.00007700
C	0.11219600	-0.02413700	0.00006900
C	2.15771400	-0.81491800	-0.00004600
H	3.11959800	1.28242300	-0.00006500
H	0.68379200	2.21747100	-0.00025200
N	-1.18470900	-0.00841600	0.00000500
C	-1.98947800	1.20322100	0.00000700
H	-2.62666200	1.20944800	-0.88480900
H	-2.62549700	1.21026700	0.88566000
H	-1.36111700	2.08473500	-0.00083400
C	-1.95769300	-1.25081000	0.00000600
H	-2.59004800	-1.27194100	0.88836000
H	-2.58913700	-1.27258900	-0.88898300
H	-1.24626600	-2.07298300	0.00057900
H	3.06419800	-1.40875700	0.00005300

47S

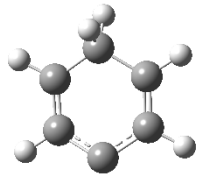


Energy= -499.819351 Hartree

0 1

C	0.00000000	1.83275300	0.00000000
C	0.00000000	-0.44821400	0.74096900
C	0.00000000	-0.44821400	-0.74096900
C	0.00000000	0.90832900	1.13728900
C	0.00000000	0.90832900	-1.13728900
C	0.00000100	1.24004800	-2.47707500
C	-0.00000100	-1.45602400	-1.66613000
C	-0.00000100	-1.45602400	1.66613000
C	0.00000100	1.24004800	2.47707500
C	0.00000100	0.21754400	-3.42792100
C	0.00000000	-1.10336200	-3.02410400
C	0.00000100	0.21754400	3.42792100
C	0.00000000	-1.10336200	3.02410400
H	0.00000100	2.28243000	2.76953400
H	0.00000100	0.45615000	4.48341200
H	0.00000000	-1.88702500	3.77185200
H	-0.00000100	-2.49974400	1.37641500
H	-0.00000100	-2.49974400	-1.37641500
H	0.00000000	-1.88702500	-3.77185200
H	0.00000100	0.45615000	-4.48341200
H	0.00000100	2.28243000	-2.76953400

48S

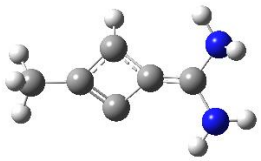


Energy= -231.963588 Hartree

0 1

C	1.23899700	0.56203500	-0.04297900
C	1.20705600	-0.78319700	-0.06800200
C	-0.00101200	-1.52538300	0.16536700
C	-1.20816200	-0.78172300	-0.06821700
C	-1.23818800	0.56355800	-0.04281800
H	2.18221200	1.10013700	-0.04297500
H	2.14463300	-1.32809500	-0.12451600
H	-2.14650600	-1.32520700	-0.12464400
H	-2.18068700	1.10291000	-0.04266800
C	0.00093900	1.36135700	0.06147000
H	0.00134700	2.15031300	-0.70326000
H	0.00121500	1.92005400	1.00913700

49S

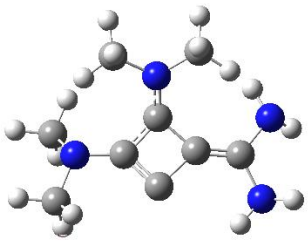


Energy= -342.617062 Hartree

0 1

C	0.86403700	0.89581800	-0.36162500
C	0.88063100	-0.91325500	-0.23610000
C	-0.25944200	-0.04148600	-0.09463200
C	1.85768100	0.04510400	0.09467500
C	-1.58215700	0.01034400	0.02027400
N	-2.41825500	-1.10348100	0.08823300
H	-1.91965000	-1.98049500	0.12092400
H	-3.09352000	-1.03895600	0.83985700
N	-2.27290900	1.21636200	0.13677200
H	-1.67633300	2.01447300	-0.03654600
H	-3.09899000	1.24641500	-0.44743500
C	3.32379300	0.07300100	0.25138400
H	3.71291900	1.05217400	-0.02461500
H	3.60039500	-0.12415900	1.28982100
H	3.80852400	-0.68850400	-0.36402500
H	0.99753800	-1.68827500	-0.99687300

50S



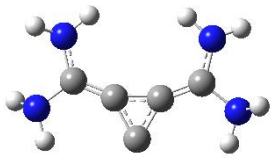
Energy= -571.110414 Hartree

0 1

C	0.04862800	-1.37966700	-0.69385800
C	-0.02449900	0.42907800	0.07963200
C	-1.07812100	-0.55334500	-0.11882700
C	0.98002900	-0.57614300	-0.05907100
C	-2.35628300	-0.81221900	0.13144100
N	-3.27362600	0.04923800	0.76261300
H	-3.91569500	-0.48111100	1.33961900
H	-2.82307400	0.75034300	1.33379300
N	-2.91799200	-2.05448000	-0.19763900
H	-3.78272000	-1.95788500	-0.71770900
H	-2.25522900	-2.61020700	-0.72659300
N	2.37389900	-0.54031000	0.00165500
C	2.99908700	-1.68210000	-0.64344800
H	4.07790700	-1.52633400	-0.67302200
H	2.79005200	-2.62180700	-0.11456800
H	2.61758300	-1.77853300	-1.65728800
C	2.89313300	-0.30599000	1.34002000
H	2.40690700	0.56237500	1.78483300
H	2.72745800	-1.16491400	2.00571900
H	3.96478800	-0.10980600	1.28564200
N	-0.00773600	1.74377200	-0.13252400

C	1.23522800	2.46252900	-0.34541000
H	1.27753800	2.83917300	-1.37082400
H	1.29830000	3.31328600	0.33687100
H	2.07892500	1.79712200	-0.19304900
C	-1.21540000	2.50027600	-0.39754600
H	-1.32662600	3.30917000	0.32936600
H	-1.16282900	2.94332700	-1.39522600
H	-2.08591400	1.85375100	-0.36389500

51S

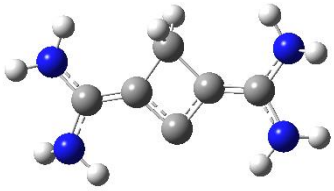


Energy= -414.026466 Hartree

0 1

C	-0.00011100	-1.61230900	-0.00035300
C	0.70539800	-0.38846900	0.02625800
C	-0.70530000	-0.38827900	-0.02759100
C	1.96105300	0.10286800	0.01331500
C	-1.96102400	0.10288200	-0.01339600
N	3.05730300	-0.72865000	-0.13536600
H	3.81542100	-0.54004400	0.50768900
H	2.79425700	-1.70527100	-0.14530700
N	2.28117200	1.44041900	0.14179400
H	3.05514700	1.74823000	-0.43118600
H	1.49161600	2.06572800	0.10991400
N	-2.28152400	1.44035500	-0.14173100
H	-3.05497800	1.74811600	0.43197300
H	-1.49206500	2.06583100	-0.11082900
N	-3.05695100	-0.72882700	0.13642900
H	-3.81579100	-0.54042800	-0.50583000
H	-2.79369900	-1.70539500	0.14629400

52S

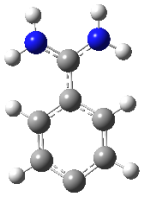


Energy= -453.338614 Hartree

0 1

C	-0.00000100	0.96013200	-0.10083700
C	-0.00002000	-1.23645400	0.04525000
H	0.00001600	-1.81540600	0.97551500
H	-0.00006300	-1.92664200	-0.80523700
C	0.98601200	-0.07371700	-0.02526500
C	-0.98599800	-0.07368800	-0.02518300
C	2.34068500	0.05747700	-0.00015500
C	-2.34068900	0.05746900	-0.00006500
N	3.21641700	-0.99438300	-0.07649900
H	4.07859700	-0.89479400	0.43795300
H	2.80044000	-1.90964500	-0.00971000
N	2.91461500	1.29732400	0.10977700
H	3.72636700	1.45361800	-0.47071200
H	2.21189900	2.02762000	0.04293700
N	-2.91462900	1.29732400	0.10974500
H	-2.21187600	2.02757400	0.04285000
H	-3.72633700	1.45359200	-0.47080800
N	-3.21637200	-0.99437900	-0.07635900
H	-2.80046300	-1.90967100	-0.00968000
H	-4.07872800	-0.89475500	0.43777100

53S



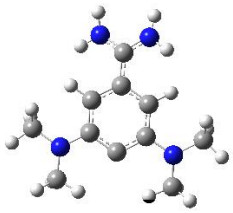
Energy= -380.762010 Hartree

0 1

C	0.58362400	1.19926300	0.14189700

C	1.95490900	1.17512300	0.14526200
C	2.73998500	-0.00001500	-0.00019300
C	1.95484500	-1.17512400	-0.14558800
C	0.58356300	-1.19922900	-0.14206600
H	0.06219400	2.13869900	0.30972600
H	2.46189300	2.12764700	0.28509800
H	2.46178600	-2.12766500	-0.28546300
H	0.06204800	-2.13863200	-0.30981600
C	-0.14656400	0.00002800	-0.00004100
C	-1.55919300	0.00000400	0.00015200
N	-2.26581900	-1.10196400	0.28978600
H	-1.77067000	-1.93441600	0.56025700
H	-3.22528800	-1.19570600	0.00170500
N	-2.26604000	1.10188000	-0.28954400
H	-1.77083900	1.93448000	-0.55949600
H	-3.22513000	1.19587900	-0.00024700

54S

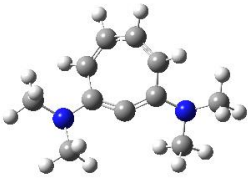


Energy= -648.522746 Hartree

0 1

C	-1.26256500	0.59826500	-0.03902400
C	-1.14810500	-0.78746600	-0.11296700
C	0.10051800	-1.43551900	-0.14248600
C	1.24651800	-0.61813700	-0.15024000
C	1.16556700	0.77024500	-0.07913200
H	-2.22026600	1.07760400	0.11186000
H	2.04917600	1.39054300	-0.13972500
C	-0.09709100	1.38257600	-0.02885000
C	-0.19587400	2.79010200	0.05839600
N	0.80538900	3.54305700	0.54143700
H	1.62407000	3.07335400	0.88978700
H	0.88568000	4.51568800	0.29578100
N	-1.29876200	3.44726600	-0.33434800
H	-2.04603400	2.91217900	-0.74358200
H	-1.51434800	4.35989200	0.03126700
N	-2.31163400	-1.57123500	-0.16982400
N	2.50564300	-1.22629000	-0.27498700
C	-2.25878200	-2.92488700	0.33950300
H	-2.43669400	-2.96347300	1.42525700
H	-3.01875800	-3.53225900	-0.15617900
H	-1.27158100	-3.32796800	0.13873200
C	-3.58898600	-0.93100800	-0.02565700
H	-4.37631600	-1.66852600	-0.17685400
H	-3.74061300	-0.47685200	0.96860400
H	-3.72212700	-0.14967800	-0.77768400
C	2.65201200	-2.60124800	0.15391400
H	3.49152200	-3.05906500	-0.37274700
H	2.83532600	-2.67896500	1.23651400
H	1.73389200	-3.13268500	-0.07312000
C	3.68316100	-0.42043400	-0.10568500
H	3.75585900	0.03250900	0.89816000
H	4.56499200	-1.04148000	-0.25554100
H	3.72353700	0.38467900	-0.84310600

55S



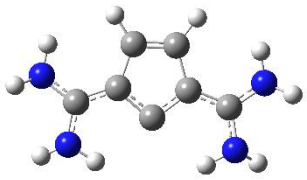
Energy= -537.850691 Hartree

0 1

C	0.61911100	2.27008100	0.58814000
C	-0.39070300	2.31723800	-0.43749600
C	-1.22032900	1.33086100	-0.83460700
C	1.34597800	1.20413400	0.98305800
C	-1.21987500	0.04121600	-0.15483800
C	1.21075700	-0.08723000	0.33153800
C	-0.02181400	-0.52191000	0.05905300

H	0.85613400	3.22531000	1.04521600
H	-0.52797600	3.28826100	-0.90265600
H	-1.94485600	1.55116200	-1.61110200
H	2.10540900	1.34599000	1.74659200
N	-2.41823700	-0.50638100	0.26695400
N	2.36630100	-0.82740400	0.08120100
C	-3.62800800	-0.21179900	-0.46918000
H	-3.65221600	-0.69236200	-1.45787900
H	-4.48545300	-0.56632300	0.10102100
H	-3.74544400	0.86189400	-0.60327000
C	-2.35009600	-1.83105500	0.84080200
H	-1.58324500	-1.86446300	1.61053700
H	-3.31091000	-2.07467800	1.29278300
H	-2.10118700	-2.59089200	0.08702300
C	3.57352600	-0.12211500	-0.30081200
H	3.57380600	0.14563500	-1.36726000
H	3.69101800	0.79086200	0.27537900
H	4.43995200	-0.75668700	-0.10984400
C	2.18661800	-2.07498600	-0.62630900
H	1.95098500	-1.92647300	-1.68865400
H	3.10406500	-2.66034900	-0.55283500
H	1.36247900	-2.62699800	-0.17823200

56S

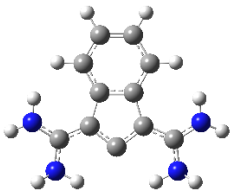


Energy= -491.470910 Hartree

0 1

C	0.00000200	0.66754200	0.04291000
C	-0.67579400	-1.61251600	-0.07194100
C	0.67579200	-1.61252100	-0.07194700
C	-1.10624800	-0.22050500	-0.00608400
C	-2.40505200	0.26677500	0.01006000
C	1.10626100	-0.22052000	-0.00614200
C	2.40504700	0.26676500	0.01001500
N	2.62330000	1.59722400	-0.10659700
N	3.50162500	-0.52362100	0.13700900
N	-2.62327900	1.59722800	-0.10641700
N	-3.50163400	-0.52366300	0.13690800
H	-1.73734200	2.10137800	-0.05185800
H	-3.40645100	1.99008500	0.39245500
H	-3.35258200	-1.51769900	0.09613700
H	-4.37301900	-0.19593300	-0.24693200
H	3.40625600	1.99008100	0.39262300
H	1.73732300	2.10131400	-0.05212500
H	4.37306700	-0.19601500	-0.24678000
H	3.35261700	-1.51768400	0.09694800
H	1.29789400	-2.49790700	-0.12408100
H	-1.29789000	-2.49791400	-0.12394900

57S



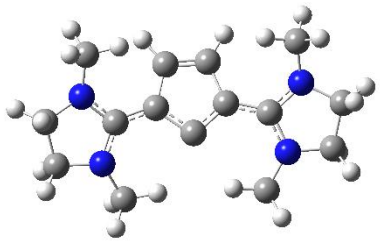
Energy= -645.044266 Hartree

0 1

C	-0.00000500	-1.48642800	-0.01585700
C	0.71018200	0.78661000	-0.00550100
C	-0.71018300	0.78661200	-0.00550600
C	1.12019900	-0.61968900	-0.00592700
C	2.39951900	-1.16485200	0.02178100
C	-1.12020000	-0.61968700	-0.00593600
C	-2.39952600	-1.16485200	0.02175900
N	-2.55766600	-2.49278500	-0.20025800
N	-3.52607000	-0.45756700	0.26211700
N	2.55767100	-2.49279000	-0.20025100
N	3.52606600	-0.45757600	0.26216100
H	1.64353400	-2.94878100	-0.21403800
H	3.29018400	-2.96347900	0.30900400
H	3.45537300	0.53566200	0.38452100

H	4.41345200	-0.82177200	-0.04043900
H	-3.29022600	-2.96348000	0.30892200
H	-1.64353100	-2.94878100	-0.21402800
H	-4.41346100	-0.82177100	-0.04046100
H	-3.45537600	0.53567600	0.38443800
C	1.39365000	1.99449000	-0.04480800
C	-1.39364400	1.99449600	-0.04481200
C	0.69254900	3.19251800	-0.07155500
C	-0.69253800	3.19252100	-0.07155600
H	2.47530700	2.04538400	-0.08501800
H	1.23294300	4.13026800	-0.10338000
H	-1.23292800	4.13027300	-0.10338000
H	-2.47530100	2.04539800	-0.08502000

58S

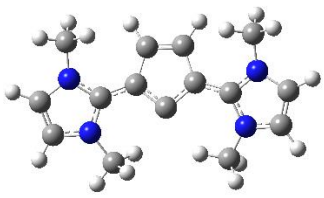


Energy= -803.233407 Hartree

0 1

C	-0.00004700	0.46998600	-0.09294600
C	0.67518500	-1.60449100	0.85850700
C	-0.67505900	-1.60451000	0.85859200
C	1.11424300	-0.34850500	0.25292600
C	2.44793100	-0.00164200	0.01593200
C	4.72802500	-0.21784600	-0.36386600
C	4.39324800	1.23596700	-0.09423200
H	5.56683000	-0.58201800	0.22992200
H	4.95613100	-0.38858700	-1.42320400
H	4.70092800	1.54133900	0.91447700
H	4.84605700	1.92098200	-0.81130000
C	-1.11421400	-0.34859500	0.25294100
C	-2.44793700	-0.00176200	0.01598200
C	-4.39326300	1.23592500	-0.09341900
C	-4.72805400	-0.21775900	-0.36379500
H	-4.70098200	1.54083500	0.91541100
H	-4.84602400	1.92129000	-0.81018600
H	-5.56676000	-0.58229100	0.22991600
H	-4.95635000	-0.38791300	-1.42318700
N	-3.48821900	-0.89231000	-0.01209000
N	-2.94568100	1.24615500	-0.19588900
N	2.94567200	1.24617100	-0.19679700
N	3.48824000	-0.89215300	-0.01151700
C	3.35327600	-2.27436500	-0.42361800
H	2.32218800	-2.48644600	-0.68741400
H	3.98411200	-2.45172600	-1.29944400
H	3.66246500	-2.96016700	0.36739300
C	2.26095700	2.47009600	0.15570900
H	2.63117200	3.27499100	-0.48135300
H	1.19623700	2.31548200	-0.00931300
H	2.44855100	2.73234000	1.20445100
C	-2.26090000	2.46982200	0.15738300
H	-1.19616900	2.31517200	-0.00752600
H	-2.63085700	3.27509200	-0.47935100
H	-2.44869800	2.73154700	1.20621500
C	-3.35338300	-2.27401600	-0.42588400
H	-3.98144300	-2.44946600	-1.30413000
H	-2.32167200	-2.48681100	-0.68650400
H	-3.66601800	-2.96056000	0.36313200
H	1.29528700	-2.35897300	1.32228300
H	-1.29511400	-2.35896900	1.32248200

59S



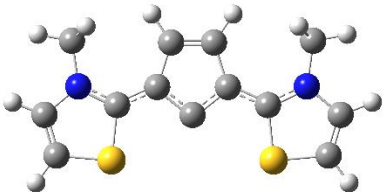
Energy= -800.863423 Hartree

0 1

C	-0.01071200	0.43189400	-0.03568300
C	0.67737700	-1.72179100	0.68945000
C	-0.67990000	-1.72875500	0.69161900

C	1.10517000	-0.41036200	0.22725500
C	2.43985600	-0.00469400	0.02556600
C	4.67010500	-0.04477100	-0.30426800
C	4.29321600	1.23937400	-0.24068200
C	-1.11737100	-0.41952200	0.23456400
C	-2.44656300	-0.01194000	0.03522300
C	-4.27738300	1.26064300	-0.24021200
C	-4.66994200	-0.01807200	-0.32805500
N	-3.54372900	-0.80409300	-0.16033900
N	-2.91612400	1.26721000	-0.01130300
N	2.92830700	1.26698700	-0.04244500
N	3.52950400	-0.81328800	-0.14655200
C	3.50682500	-2.24821600	-0.32599200
H	2.61015000	-2.53074500	-0.87223100
H	4.38645800	-2.53685700	-0.89837600
H	3.51567900	-2.77292100	0.62927400
C	2.17545800	2.49019900	0.17274100
H	2.47816900	3.22680200	-0.57146200
H	1.11799700	2.23413300	0.05299500
H	2.37194100	2.87814400	1.17446200
C	-2.14531100	2.47296900	0.21437300
H	-1.47952000	2.32202900	1.06020000
H	-1.51912700	2.69610700	-0.64535500
H	-2.84753200	3.28327600	0.41166200
C	-3.53043000	-2.23856500	-0.34054900
H	-4.40828400	-2.52173100	-0.91825900
H	-2.63165100	-2.52646500	-0.88101600
H	-3.54790000	-2.76317800	0.61477300
H	1.29057500	-2.53408300	1.05194100
H	-1.28700700	-2.54519400	1.05559900
H	-5.64175300	-0.44458200	-0.49844100
H	-4.84286500	2.17188400	-0.31342600
H	4.86967900	2.14347300	-0.32052100
H	5.63691500	-0.48815200	-0.45944600

60S

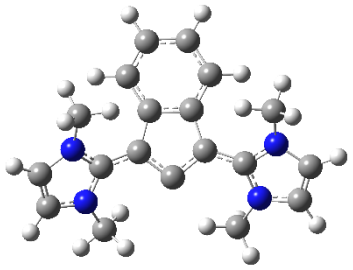


Energy= -1408.069078 Hartree

0 1

C	0.00000100	-0.29384400	-0.00001700
C	0.67595700	1.98168800	-0.00001300
C	-0.67595700	1.98168800	-0.00005500
C	1.11523800	0.58574400	0.00000900
C	2.37698800	0.01477300	0.00000700
C	4.66567800	-0.29467100	0.00003800
C	4.28779400	-1.57099500	0.00011400
C	-1.11523700	0.58574200	-0.00000900
C	-2.37698700	0.01477200	-0.00002400
C	-4.28779400	-1.57099400	-0.00013700
C	-4.66567700	-0.29466900	-0.00003000
N	-3.60040600	0.59852500	0.00003400
N	3.60040700	0.59852400	-0.00004100
C	3.79817500	2.03401000	-0.00005200
H	3.35088200	2.48117200	0.88679300
H	4.86623700	2.23619000	-0.00024700
H	3.35057300	2.48117900	-0.88673300
C	-3.79817500	2.03401100	0.00025300
H	-3.35050800	2.48105500	0.88696500
H	-3.35094500	2.48129600	-0.88656100
H	-4.86623700	2.23619000	0.00054800
H	1.28139600	2.87512200	0.00001800
H	-1.28139700	2.87512100	-0.00009500
S	2.54802300	-1.72179400	0.00008400
S	-2.54802400	-1.72179500	-0.00015500
H	4.93089900	-2.43397000	0.00016100
H	5.67023900	0.09757800	0.00001200
H	-4.93090100	-2.43396800	-0.00020200
H	-5.67023900	0.09757900	0.00000500

61S

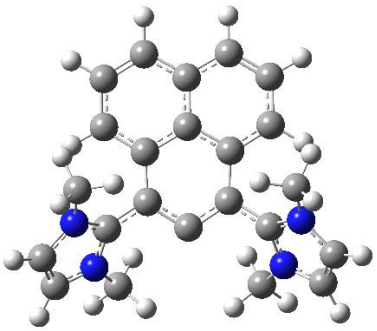


Energy= -954.433780 Hartree

0 1

C	-0.00989900	-0.98065100	0.01596300
C	0.71084300	1.25836700	-0.36299000
C	-0.70968200	1.26584000	-0.36246700
C	1.11013600	-0.11312400	-0.08333400
C	2.42899000	-0.56671600	0.12570900
C	4.58603300	-0.68315000	0.75139800
C	4.27309300	-1.84258500	0.15389400
C	-1.12159200	-0.10281200	-0.08764100
C	-2.43863400	-0.55378800	0.11605400
C	-4.26328100	-1.85672900	0.14917700
C	-4.58629000	-0.70692700	0.76070700
N	-3.46033000	0.09818900	0.74340100
N	-2.94735300	-1.75880300	-0.25394400
N	2.94950300	-1.77248800	-0.22677000
N	3.44605200	0.10371000	0.74072400
C	3.28514700	1.28415600	1.56632700
H	2.22854700	1.41596600	1.78043100
H	3.83102000	1.13877500	2.49752300
H	3.65138100	2.17930400	1.06628600
C	2.26291300	-2.78368300	-1.01002100
H	2.66781700	-3.75985400	-0.74784300
H	1.20347600	-2.72479700	-0.75897800
H	2.40906100	-2.59964400	-2.07614100
C	-2.24426600	-2.76573000	-1.02124000
H	-1.60968900	-2.27076500	-1.75218200
H	-1.59814500	-3.35764900	-0.37792400
H	-2.98392100	-3.39313300	-1.51787300
C	-3.30950300	1.28419100	1.56216000
H	-3.86109600	1.14329900	2.49054600
H	-2.25457800	1.42108400	1.78250200
H	-3.67544400	2.17494600	1.05392000
C	1.40266500	2.40393800	-0.74610200
C	-1.39234100	2.41701500	-0.74332000
C	0.70582200	3.55139400	-1.09101000
C	-0.68614900	3.55858500	-1.08908700
H	2.48390000	2.40046100	-0.81913200
H	1.24760700	4.44003900	-1.39181500
H	-1.22003600	4.45268400	-1.38764600
H	-2.47384800	2.42291600	-0.81321600
H	-4.85394600	-2.73307900	-0.04828200
H	-5.50831600	-0.38768300	1.21197100
H	4.87218500	-2.71448400	-0.03874600
H	5.50487800	-0.34818500	1.19765900

62S



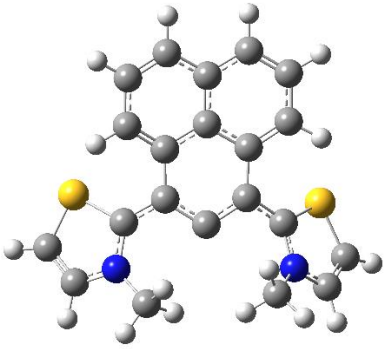
Energy= -1107.996983 Hartree

0 1

C	-1.17938300	-0.28416200	-0.18136600
C	-1.23784700	1.16358400	-0.26310700
C	-2.41776300	1.88796500	-0.39651000
C	0.00004600	-1.04149400	-0.22431000
C	-0.00006900	1.87681200	-0.29156300
C	1.23776600	1.16368500	-0.26308100
C	1.17941300	-0.28406800	-0.18133900
C	2.41762200	1.88816700	-0.39648500
H	3.36351900	1.36594600	-0.47347100
C	2.40716900	3.28186000	-0.48392500

C	1.23255300	3.98174000	-0.46787600
C	-0.00012900	3.29488000	-0.39752900
C	-1.23286900	3.98163700	-0.46788500
C	-2.40742700	3.28166100	-0.48394200
H	-3.34810700	3.81216800	-0.58194200
H	-1.22881900	5.06185800	-0.54713500
H	3.34780500	3.81244600	-0.58192200
H	1.22841400	5.06196100	-0.54713200
H	-3.36361500	1.36565900	-0.47349800
C	-2.36360700	-1.04045100	0.07299800
C	-4.23898400	-1.83047600	1.01698200
C	-3.89284800	-2.67610000	0.03157800
H	-5.06490600	-1.85528600	1.70467900
H	-4.36411900	-3.57885300	-0.31297000
C	2.36369200	-1.04027800	0.07303200
C	3.89310000	-2.67576900	0.03150100
C	4.23907700	-1.83024800	1.01704700
H	4.36448100	-3.57843400	-0.31312900
H	5.06494800	-1.85507200	1.70480500
N	-2.74915900	-2.17735900	-0.55479300
N	-3.29452400	-0.82276200	1.04077800
N	2.74939600	-2.17707000	-0.55487600
N	3.29450800	-0.82263700	1.04091900
C	-2.07301500	-2.76861600	-1.68882500
H	-2.80149600	-3.33496100	-2.26813400
H	-1.64524300	-1.97304200	-2.29322800
H	-1.25861400	-3.40601700	-1.35375800
C	-3.17097000	0.16520900	2.09151500
H	-3.60987600	1.11729200	1.79756800
H	-3.66002600	-0.21516700	2.98580500
H	-2.11365500	0.32729800	2.29138000
C	3.17079100	0.16516700	2.09179400
H	3.65953500	-0.21543600	2.98616000
H	3.60991400	1.11724100	1.79814700
H	2.11344300	0.32736000	2.29138200
C	2.07339500	-2.76825100	-1.68903300
H	1.64543400	-1.97265100	-2.29326300
H	2.80201100	-3.33430300	-2.26846000
H	1.25914800	-3.40592500	-1.35410700

63S



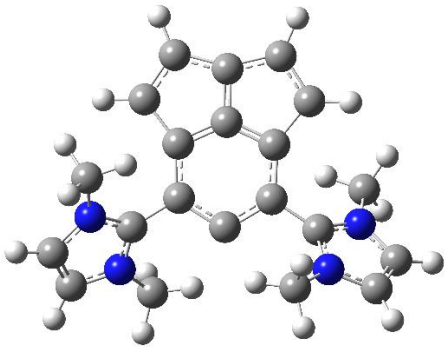
Energy= -1715.192829 Hartree

0 1

C	1.20735800	-0.03627000	0.27707300
C	1.11573600	1.42127300	0.13033400
C	2.20503600	2.26439400	0.02933400
C	0.09950100	-0.88480500	0.44119000
C	-0.18506800	2.00613500	0.18837900
C	-1.34361000	1.19058500	0.35666300
C	-1.16667900	-0.26851200	0.35048300
C	-2.55645600	1.81520000	0.56611800
H	-3.43175600	1.23080000	0.80811400
C	-2.68902100	3.20903500	0.51173000
C	-1.60435900	3.99772800	0.27352200
C	-0.32466200	3.41714100	0.13243100
C	0.82184900	4.22529800	-0.02803500
C	2.05771800	3.65393100	-0.07054500
H	2.94176400	4.27361200	-0.16089000
H	0.70197900	5.30028400	-0.08528200
H	-3.66428300	3.65458700	0.66652100
H	-1.69876900	5.07563600	0.22348300
H	3.20849200	1.86846600	0.06937600
C	2.40712600	-0.72662900	0.01065000
C	4.47324000	-1.75573500	-0.96070800
C	3.89610000	-2.49407700	-0.01295800
H	5.36961500	-1.97789000	-1.51226000

H	4.22646500	-3.45148900	0.35692900
C	-2.23494300	-1.10950200	0.00500600
C	-3.37907700	-3.06976600	-0.46080500
C	-4.18212200	-2.23540600	-1.11665200
H	-3.48366000	-4.13972300	-0.37730100
H	-5.07703100	-2.47684000	-1.66226100
N	2.77782900	-1.91368500	0.55230600
N	-2.32844400	-2.45747100	0.19509600
C	2.16383600	-2.49610300	1.73510500
H	2.93927800	-3.02725700	2.28808900
H	1.74761600	-1.69805000	2.34235100
H	1.35453800	-3.16608700	1.46653300
C	-1.45223300	-3.24498000	1.04299500
H	-1.15871300	-2.65681700	1.90697100
H	-2.00478100	-4.13114400	1.35728300
H	-0.54616800	-3.51375100	0.50707400
S	3.60613800	-0.26970500	-1.18604600
S	-3.64025700	-0.59528500	-0.92860400

64S



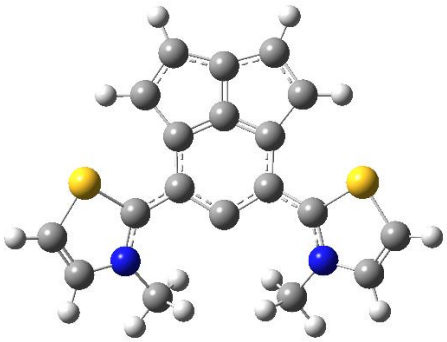
Energy= -1030.549742 Hartree

0 1

C	1.24820800	1.40554600	0.15700400
C	2.14314700	2.54695700	0.29276900
C	1.37804100	3.71102700	0.19732000
C	-0.00056200	3.36610000	0.00074600
C	-0.00048200	1.98387900	0.00222800
C	-1.37882200	3.71042500	-0.19926300
C	-2.14359100	2.54605200	-0.29375400
C	-1.24867200	1.40504800	-0.15458300
H	3.20897100	2.52564500	0.47145400
H	1.79554800	4.70713100	0.27760800
H	-1.79628600	4.70630400	-0.28250100
H	-3.20917200	2.52424100	-0.47383500
C	1.20302100	-0.00988400	0.12711300
C	0.00019300	-0.75032700	0.00104500
C	-1.20294000	-0.01039100	-0.12522200
C	-2.42730400	-0.78308500	-0.16608500
C	-4.49512100	-1.50537200	0.25937300
C	-3.96506800	-2.31104600	-0.67892800
H	-5.45642300	-1.52197600	0.74026300
H	-4.37814200	-3.16377700	-1.18692600
C	2.42764100	-0.78230800	0.16653500
C	3.96610900	-2.31006600	0.67783400
C	4.49490000	-1.50467300	-0.26142200
H	4.37988100	-3.16261800	1.18556400
H	5.45557100	-1.52139900	-0.74357000
N	3.53467400	-0.56453300	-0.57305200
N	-3.53534000	-0.56510500	0.57196500
N	-2.69060800	-1.85756400	-0.93350900
N	2.69198000	-1.85652100	0.93394900
C	3.65701000	0.40202300	-1.65268900
H	2.66307800	0.72754000	-1.94270000
H	4.22102600	1.27374100	-1.32980800
H	4.15573400	-0.07760700	-2.49324900
C	1.79386900	-2.40544200	1.93837300
H	1.92338500	-1.87773600	2.88322900
H	0.77794000	-2.27614200	1.56374700
H	2.02680800	-3.46031600	2.06884400
C	-1.79134900	-2.40671300	-1.93678500
H	-1.92064900	-1.88001400	-2.88223600
H	-0.77580200	-2.27627500	-1.56150600
H	-2.02332300	-3.46190700	-2.06641400
C	-3.65917300	0.40187300	1.65105900
H	-2.66557400	0.72641200	1.94332000
H	-4.22149800	1.27412400	1.32667200

H	-4.16034600	-0.07704700	2.49056000

65S



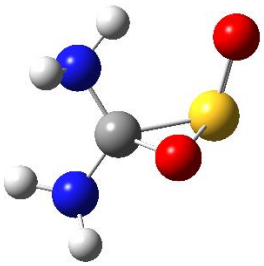
Energy= -1637.738234 Hartree

0 1

C	1.25552300	1.49287700	0.27909700
C	2.15462000	2.62933500	0.21234200
C	1.38175800	3.79257600	0.26025400
C	0.00010900	3.44512400	0.38910400
C	0.00007200	2.06200500	0.41615500
C	-1.38081800	3.79255500	0.25946100
C	-2.15425400	2.62895300	0.21123500
C	-1.25589200	1.49287500	0.27875500
H	3.23241700	2.61778400	0.17343600
H	1.80068300	4.78935500	0.20391800
H	-1.79961500	4.78934800	0.20216900
H	-3.23201600	2.61792900	0.17146100
C	1.21969900	0.06504500	0.19718500
C	-0.00003400	-0.67637000	0.19520400
C	-1.21981600	0.06494800	0.19714800
C	-2.42618900	-0.65066300	-0.04208700
C	-4.69570900	-1.39207000	-0.73719200
C	-3.96101300	-2.35688600	-0.18106200
H	-5.70308500	-1.46586900	-1.10758400
H	-4.24800900	-3.38132500	-0.00787800
C	2.42607500	-0.65047800	-0.04219700
C	4.69513200	-1.39249100	-0.73812900
C	3.96110600	-2.35660700	-0.17989300
H	5.70223000	-1.46663900	-1.10920800
H	4.24848300	-3.38070500	-0.00532200
N	2.70335700	-1.94147000	0.21934600
N	-2.70302300	-1.94212500	0.21778800
C	-1.82601400	-2.85716200	0.93646000
H	-2.45168000	-3.62348200	1.39323900
H	-1.10337500	-3.29574900	0.25578300
H	-1.27537800	-2.30375300	1.68928400
C	1.82715200	-2.85530400	0.94052200
H	1.27620400	-2.30027700	1.69192800
H	1.10481000	-3.29635100	0.26112100
H	2.45342300	-3.61993500	1.39929500
S	3.80333000	0.08823400	-0.79463800
S	-3.80435900	0.08896900	-0.79197200

2.3. Cartesian coordinates of the optimized geometries of Oxathiirane-S-oxides, *N*-Heterocyclic ketones, SO_2 and SO molecules and their energies (sum of electronic and thermal Free Energies) in Hartree in singlet state at CAM-B3LYP-GD3BJ/6-311++G(2d,p) level of theory.

3-OXO

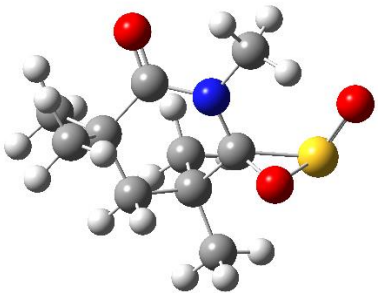


Energy= -698.577299 Hartree

0 1

C	-0.75439100	0.07985100	0.01461500
S	0.94699100	-0.53654300	-0.27098900
O	-0.12856300	-0.59335700	1.08194300
O	1.93598600	0.53784000	-0.13181700
N	-0.83853700	1.47840200	-0.00190900
H	0.07755400	1.90394400	0.10616500
H	-1.46842000	1.82578000	0.71326300
N	-1.86454700	-0.59515500	-0.48143900
H	-2.57820700	-0.01043500	-0.88496400
H	-2.19424400	-1.35228500	0.09609700

21-OXO

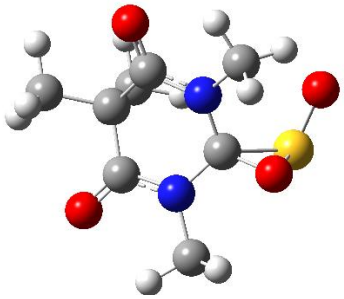


Energy= -1069.584009 Hartree

0 1

C	0.81624700	0.09091800	-0.20524800
C	-1.29883600	-1.09075500	0.21921900
C	-1.26845100	1.31953500	-0.57691900
C	-2.13344800	0.11672400	-0.19643000
H	-1.82048700	2.24294600	-0.38742200
N	0.06826200	-1.08852100	-0.00417400
H	-1.06593400	1.29709200	-1.65075300
C	0.08152000	1.38418800	0.13698100
C	0.83409400	2.61053700	-0.37957900
H	0.25425000	3.50283400	-0.14078000
H	1.81213600	2.72483200	0.08904500
H	0.97560400	2.56889200	-1.45812900
C	-0.04549200	1.48952300	1.66080600
H	-0.47879400	0.60029200	2.11489800
H	0.93695100	1.64211600	2.11062300
H	-0.66838600	2.34432600	1.92649600
C	-3.13249900	0.44789600	0.91596200
H	-3.83199400	1.20635300	0.56009100
H	-3.69310800	-0.44338900	1.19073500
H	-2.64771500	0.83279700	1.81126100
C	-2.92396400	-0.34586400	-1.43118600
H	-3.57847100	-1.17755700	-1.17627400
H	-3.53152100	0.48021400	-1.80569000
H	-2.25447300	-0.66399700	-2.23250800
O	-1.84263900	-2.09067300	0.63514700
S	2.63437400	0.12755600	0.05824600
O	3.25831200	-1.15282300	0.37377000
O	1.64718400	0.10794400	-1.34793900
C	0.71476600	-2.40461000	0.00035200
H	1.52296600	-2.41257200	-0.72151300
H	1.11282300	-2.65241400	0.98206900
H	-0.03814900	-3.13815200	-0.26643800

23-OXO

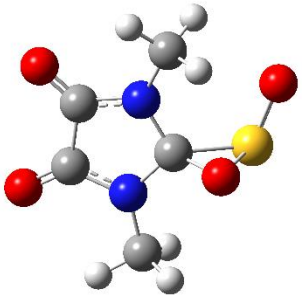


Energy= -1120.430341 Hartree

0 1

C	0.84609900	0.27161000	-0.42573700
C	-0.95087500	-1.33801000	-0.33366900
C	-1.38051500	1.14921600	-0.11380400
C	-1.76243300	-0.24818000	0.35246800
N	0.34916100	-1.01576500	-0.65647200
C	-1.45826200	-0.32924000	1.86404500
H	-2.02743300	0.43679700	2.38938100
H	-1.75503600	-1.30882300	2.23690500
H	-0.39975800	-0.19054900	2.08630400
C	-3.24808300	-0.47990700	0.10644900
H	-3.52862100	-1.46545300	0.46953000
H	-3.82571800	0.28487200	0.61983900
H	-3.48259400	-0.43024300	-0.95644400
O	-1.40653100	-2.43509500	-0.54874600
S	2.23951700	0.40045900	0.86186700
O	2.66048400	-0.92626800	1.31073100
O	2.09791600	0.51791800	-0.89673600
C	1.21516600	-2.02048400	-1.27501500
H	1.58493500	-1.65374500	-2.23016000
H	2.05290800	-2.25563900	-0.62437800
H	0.60337300	-2.90299600	-1.42618000
O	-2.15602200	2.07474200	-0.07242200
N	-0.08201500	1.31993200	-0.54138100
C	0.40220300	2.67223400	-0.79683800
H	0.86461900	3.10422100	0.09332000
H	1.12329800	2.65688100	-1.60755900
H	-0.45884100	3.27435100	-1.06547600

24-OXO

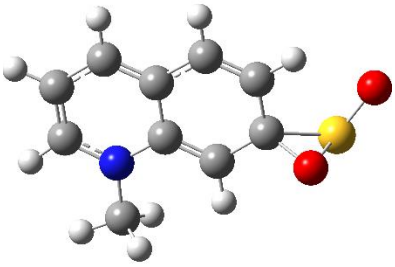


Energy= -1002.591612 Hartree

0 1

S	2.04282100	-0.61005700	-0.39450300
O	1.33612600	-0.47838100	1.20680900
C	0.36302800	-0.21283500	0.27730500
O	2.77046900	0.58444700	-0.80492300
N	-0.72150600	-1.09569800	0.14699400
C	-1.50581400	1.05835700	-0.10666300
C	-1.88100600	-0.42901200	-0.15682500
C	-0.59746000	-2.53593700	0.17517400
H	-0.07864900	-2.90732500	-0.71060800
H	-0.06384900	-2.84972200	1.07033800
H	-1.60524600	-2.94331300	0.18671100
N	-0.16111300	1.08560400	0.16578100
C	0.56564900	2.30964200	0.46010100
H	1.18954600	2.16053400	1.33823300
H	1.18990700	2.60909700	-0.37741400
H	-0.17973000	3.07594400	0.65829000
O	-2.95050000	-0.91056100	-0.39591900
O	-2.23423900	1.99762800	-0.24815200

36-OXO

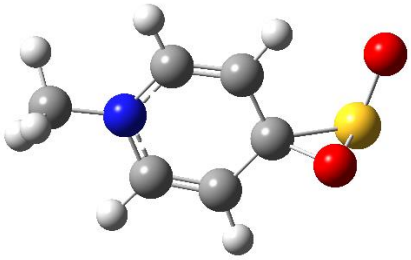


Energy= -989.574373 Hartree

0 1

C	-1.35748100	0.05354500	0.35979700
C	-0.15426400	0.85160100	0.24313500
C	1.05756700	0.26151800	0.08236300
C	1.19861200	-1.18195500	0.05577200
C	-0.00208000	-1.96151800	0.24142100
C	-1.20097700	-1.39756400	0.40043700
H	-0.27235800	1.92212800	0.29513100
C	2.41940900	-1.74930600	-0.11969100
H	0.09850500	-3.04005800	0.25570600
H	-2.09544200	-1.98869000	0.54016700
C	3.57752300	-0.94945100	-0.27642200
H	2.50341300	-2.82916300	-0.13459000
H	4.55363100	-1.38545100	-0.42226600
S	-2.96415900	0.59658800	-0.47322000
O	-3.89091200	-0.51138800	-0.73216400
O	-2.41229000	0.60251600	1.13575600
C	3.43809000	0.39261600	-0.23181400
H	4.27827500	1.06377600	-0.33615100
N	2.23221200	0.99618800	-0.05215300
C	2.15152200	2.44192300	-0.00620900
H	1.50922700	2.81211500	-0.80736300
H	1.73732900	2.76844400	0.94923400
H	3.14657300	2.86070400	-0.12476500

38-OXO

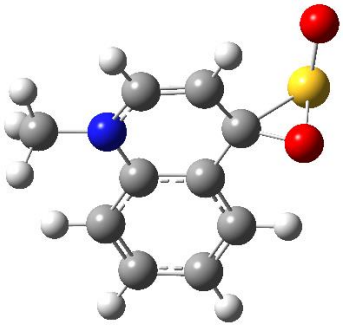


Energy= -836.029090 Hartree

0 1

C	1.41007300	-1.16575700	0.20386800
C	0.09533100	-1.02134400	0.40052000
C	-0.54080200	0.28473300	0.25553000
C	0.38194100	1.36741900	-0.06642300
C	1.68799100	1.12895200	-0.23945500
N	2.23623600	-0.12390500	-0.14507300
H	1.89493200	-2.12700700	0.30618500
H	-0.51853900	-1.87304400	0.65156500
H	0.00302600	2.37534800	-0.15504800
H	2.38329700	1.92486100	-0.46919700
S	-2.28160400	0.25523800	-0.39283600
O	-1.61499700	0.59003900	1.14009700
O	-2.79874800	-1.11437900	-0.48770900
C	3.67402500	-0.30431300	-0.16904500
H	4.12152600	0.42820200	-0.83841100
H	4.11582200	-0.19099500	0.82451200
H	3.91055900	-1.29724900	-0.54778600

39-OXO



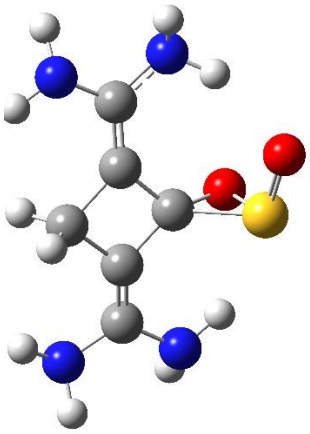
Energy= -989.599324 Hartree

0 1

C	-1.60197300	-2.59980100	0.03748200
C	-0.39597800	-1.96318000	0.24999200
C	-0.29297000	-0.57854700	0.19710700
C	-1.44375100	0.18971800	-0.04610400
C	-2.65986900	-0.46164900	-0.25975000
C	-2.73144200	-1.83976800	-0.22348700
H	-1.66367300	-3.67884000	0.07873300
H	0.49287900	-2.53761500	0.47343400
C	1.00695500	0.08738700	0.38625000
H	-3.55766600	0.10793800	-0.44671800
H	-3.68514800	-2.32358200	-0.39152800
C	-0.18851800	2.18274100	0.32296300

C	0.94935000	1.52678800	0.56873700
H	-0.23795200	3.25922200	0.40758200
H	1.84573800	2.05924800	0.84390400
N	-1.36255800	1.57694000	-0.04767500
C	-2.54675100	2.37926100	-0.27101600
H	-2.98490300	2.16449500	-1.24689500
H	-3.30200600	2.20450500	0.49931400
H	-2.26711200	3.42891200	-0.24869100
S	2.51861100	-0.52879000	-0.52565400
O	3.50970900	0.53110000	-0.72128000
O	1.99399900	-0.63109000	1.09653200

52-OXO

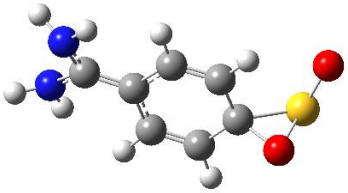


Energy= -1002.030529 Hartree

0 1

C	0.10142100	-0.27255600	0.14047600
C	0.34405400	1.77744400	-0.43530000
H	0.48234900	2.64617600	0.21869800
H	0.34915200	2.11116500	-1.47811100
C	-0.81465100	0.85877000	-0.04874900
C	1.25458700	0.59387500	-0.12594100
C	-2.12576200	1.08205400	0.14346900
C	2.57278800	0.43633100	0.02770200
N	-2.69880000	2.31417800	-0.13918000
H	-3.40656400	2.59693100	0.52475200
H	-2.03468800	3.05156500	-0.31946300
N	-3.01955000	0.15990300	0.64751600
H	-3.94242300	0.25144700	0.24489300
H	-2.69537000	-0.79726400	0.56643900
N	3.17300100	-0.77907300	0.33541800
H	3.93823900	-0.68154300	0.99013700
H	2.51768400	-1.47965300	0.65487700
N	3.48286800	1.47876900	-0.09315500
H	4.33038100	1.22261200	-0.58181600
H	3.08462100	2.33021300	-0.45965500
S	-0.24830800	-2.01222400	-0.44874500
O	-1.69421200	-2.20674400	-0.66944500
O	0.04324900	-1.30925800	1.08882300

53-OXO



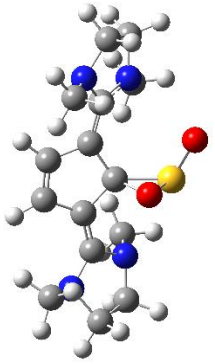
Energy= -929.464144 Hartree

0 1

C	-0.75395500	1.13379400	0.26569000
C	0.57240900	1.03490400	0.41208400
C	1.23788500	-0.26309900	0.35246300
C	0.37100700	-1.42989200	0.23238900
C	-0.95307800	-1.29823700	0.08281100
H	-1.18536800	2.12752700	0.27027800
H	1.19566700	1.90853600	0.53876800
H	0.83318200	-2.40628500	0.29487500
H	-1.54884500	-2.20178000	0.03051100
C	-1.60804900	-0.01337800	0.06388700
C	-2.96097000	0.10789300	-0.11982400
N	-3.76142900	-0.89935100	-0.60135700
H	-3.31411000	-1.76965100	-0.83253100
H	-4.66539000	-0.99727300	-0.16363900
N	-3.67436900	1.24940100	0.15135000
H	-3.16103000	2.03718200	0.50754100
H	-4.39722900	1.48899500	-0.51081900

S	2.91023100	-0.23931200	-0.47872400
O	3.36868000	1.12257700	-0.76690900
O	2.41863400	-0.42764000	1.13411300

58-OXO

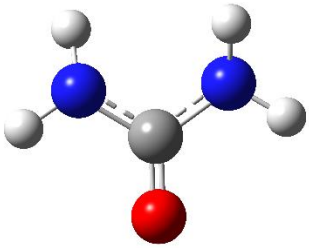


Energy= -1351.885746 Hartree

0 1

S	-0.14706500	-1.67255400	0.99208700
O	-0.19426800	-0.17625900	1.67219800
C	-0.07341300	-0.00566400	0.19877900
O	1.12910200	-2.35449600	1.21976000
C	0.63534500	2.00620400	-0.74196000
C	-0.70856300	2.01411300	-0.81325500
C	1.13284000	0.73697200	-0.24499600
C	2.45489000	0.37614500	-0.24236000
C	4.73748400	0.52653900	0.09569900
C	4.41651200	-0.82898700	-0.50360700
H	5.58208100	1.01781800	-0.38730700
H	4.95645000	0.43915300	1.16716800
H	4.74522700	-0.89539200	-1.54836700
H	4.86785700	-1.65415100	0.04840400
C	-1.24504400	0.74484700	-0.34933300
C	-2.53335100	0.32466400	-0.30026500
C	-4.36540100	-1.09118000	-0.10165500
C	-4.74328000	0.31274400	0.31753600
H	-4.81429500	-1.34081100	-1.07070400
H	-4.66698000	-1.84836400	0.62233700
H	-5.71958200	0.62052300	-0.05502700
H	-4.73939100	0.41141400	1.41132000
N	-3.67651100	1.12162400	-0.26768900
N	-2.91334600	-1.01685300	-0.23140900
N	2.96598100	-0.87360600	-0.44549300
N	3.50086500	1.27984800	-0.09202400
C	3.36045200	2.39522100	0.82672900
H	2.42976100	2.92415600	0.66094800
H	3.38245500	2.05266900	1.86869000
H	4.18667900	3.08845500	0.66730200
C	2.32543700	-1.82382200	-1.32751200
H	2.34805800	-2.82323400	-0.89959100
H	1.29180500	-1.53543700	-1.48822200
H	2.83459900	-1.82788400	-2.29931100
C	-2.37607100	-1.93610400	-1.22140700
H	-1.34034200	-1.70074600	-1.43733700
H	-2.43213000	-2.95922300	-0.84856900
H	-2.94306300	-1.87043200	-2.15901500
C	-3.59432200	2.46570300	0.27308000
H	-3.04089200	2.48519800	1.21876800
H	-3.11366400	3.14587900	-0.42260100
H	-4.60700800	2.82846100	0.44356500
H	1.27232200	2.77729600	-1.14954700
H	-1.28560400	2.79008400	-1.28848500

3-Ketone



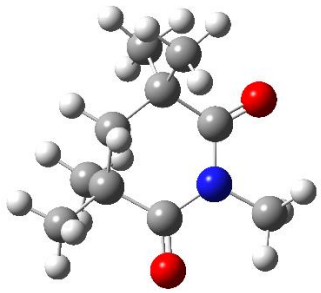
Energy= -225.225723 Hartree

0 1

C	0.00000400	0.14053200	-0.00001400
O	0.00011100	1.35144200	-0.00000100
N	-1.15658500	-0.60664300	-0.07035500
H	-1.99200300	-0.06231400	0.07664200
H	-1.15929200	-1.51789300	0.35981900
N	1.15644200	-0.60677800	0.07025600

H	1.15945200	-1.51818700	-0.35955000
H	1.99192800	-0.06238200	-0.07612500

21-Ketone

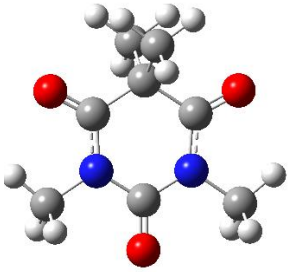


Energy= -596.229323 Hartree

0 1

C	-1.29912700	0.67812600	-0.15901600
C	1.15264300	0.73711300	0.14348400
C	-0.00082800	-1.39220900	-0.61417800
C	1.31714500	-0.74171700	-0.18330800
H	0.05014700	-2.46705800	-0.42435500
N	-0.07973500	1.34781700	-0.06313000
H	-0.10914000	-1.27969500	-1.69609100
C	-1.26909000	-0.82954600	0.02576800
C	-2.49026500	-1.44353400	-0.65256000
H	-2.49492600	-2.52290900	-0.48982000
H	-3.40996300	-1.02321900	-0.25163500
H	-2.47974400	-1.25914900	-1.72737800
C	-1.35681000	-1.08784600	1.53879900
H	-0.58773800	-0.56082700	2.10195800
H	-2.32569400	-0.75772000	1.91376600
H	-1.25603500	-2.15548600	1.74083500
C	1.95741900	-1.44533800	1.01895500
H	2.21005800	-2.47075700	0.74410700
H	2.86990000	-0.92805500	1.31018100
H	1.29782600	-1.48353800	1.88336400
C	2.31012300	-0.80205600	-1.35452500
H	3.27078000	-0.38024300	-1.06452000
H	2.45596300	-1.84148600	-1.65436700
H	1.93695500	-0.25010000	-2.21915900
O	2.09413200	1.40319400	0.50673900
O	-2.32652400	1.29371400	-0.31229200
C	-0.10304500	2.80686900	0.00897700
H	-1.03275900	3.14977400	-0.43023300
H	-0.04085400	3.13993900	1.04479200
H	0.75351900	3.20138000	-0.52949000

23-Ketone



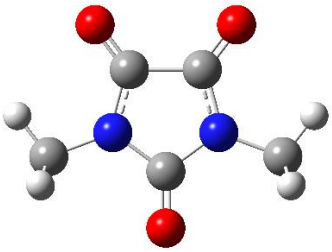
Energy= -647.079632 Hartree

0 1

C	1.54723000	0.00001500	0.00037900
C	-0.54260600	1.28345000	-0.00249800
C	-0.54258200	-1.28345700	-0.00239200
C	-1.34948400	-0.00001100	0.00098600
N	0.83509500	1.18991100	-0.00028000
C	-2.23790300	-0.00008200	-1.25242900
H	-2.86209100	-0.89099800	-1.24862400
H	-2.86208200	0.89084000	-1.24872300
H	-1.63958600	-0.00013800	-2.16527800
C	-2.22420200	0.00004600	1.26438900
H	-2.84853100	0.89091500	1.26725100
H	-2.84850200	-0.89084300	1.26734700
H	-1.61606900	0.00010500	2.17075100
O	-1.09829700	2.35543800	-0.00539000
O	2.75365000	0.00002300	0.00117700
C	1.63678400	2.41216400	-0.00063600
H	2.27356000	2.43583100	0.88060300
H	2.26843300	2.43928400	-0.88554100
H	0.95001400	3.25046400	0.00267500
O	-1.09823100	-2.35546400	-0.00505200
N	0.83511500	-1.18989100	-0.00041800

C	1.63681400	-2.41214000	-0.00087000
H	2.26913500	-2.43867900	-0.88530400
H	2.27291900	-2.43637100	0.88084600
H	0.95004600	-3.25044700	0.00143400

24-Ketone

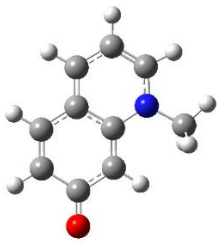


Energy= -529.241481 Hartree

0 1

O	-0.00003900	2.31057600	0.00005100
C	-0.00000900	1.11273800	-0.00005000
N	1.12240300	0.29014900	-0.00049600
C	-0.77254000	-1.04012200	-0.00012900
C	0.77255700	-1.04010500	-0.00000300
C	2.47847700	0.79783300	0.00007200
H	2.64640200	1.42493600	-0.87339500
H	2.66399400	1.38265900	0.89919200
H	3.14435700	-0.06101600	-0.02618400
N	-1.12241200	0.29011200	0.00014900
C	-2.47848400	0.79779800	0.00022500
H	-2.64768000	1.42101000	0.87625400
H	-2.66271900	1.38661600	-0.89652500
H	-3.14438600	-0.06116500	0.02183700
O	1.49926400	-1.98799600	0.00021100
O	-1.49921300	-1.98804400	-0.00019300

36-Ketone

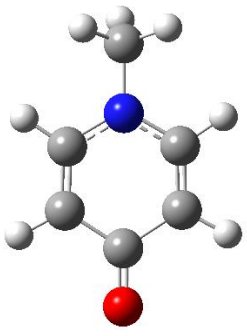


Energy= -516.203742 Hartree

0 1

C	2.28352100	0.38034800	-0.00000600
C	0.99400900	1.02776900	0.00010300
C	-0.16368900	0.30819200	-0.00002800
C	-0.15232000	-1.13841100	-0.00009100
C	1.12880600	-1.78821100	-0.00005600
C	2.27056300	-1.08852900	0.00001800
H	1.00884300	2.10640000	0.00029400
C	-1.32575300	-1.83309500	-0.00007500
H	1.13947600	-2.87232400	-0.00006700
H	3.23784100	-1.57457800	0.00006800
C	-2.56360600	-1.16453900	-0.00003000
H	-1.29650600	-2.91617900	-0.00007400
H	-3.50066100	-1.69951900	-0.00002200
O	3.34242300	1.00393700	0.00029300
C	-2.55955700	0.19167900	-0.00004400
H	-3.47295800	0.76876800	-0.00005000
N	-1.41603200	0.91362000	-0.00009800
C	-1.48474000	2.36470300	-0.00005800
H	-0.99062900	2.76449500	0.88568800
H	-0.98966000	2.76453400	-0.88523500
H	-2.52631600	2.67212700	-0.00065700

38-Ketone



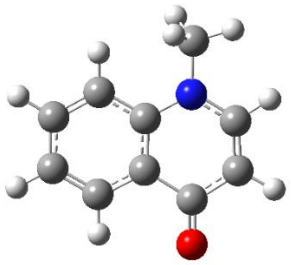
Energy= -362.661047 Hartree

0 1

C	0.57121600	-1.17426400	-0.02491400
C	-0.77321900	-1.21651300	-0.00471100

C	-1.57221000	-0.00000100	0.00901500
C	-0.77321900	1.21651200	-0.00471500
C	0.57121500	1.17426200	-0.02491900
N	1.26772200	0.00000000	-0.04306900
H	1.17669500	-2.07105500	-0.03264900
H	-1.28735300	-2.16714400	-0.00286000
H	-1.28736300	2.16713800	-0.00286600
H	1.17669200	2.07105400	-0.03265900
O	-2.79734100	0.00000100	0.02682700
C	2.71735500	0.00000200	0.04657800
H	3.11329600	0.88182600	-0.45298600
H	3.05258500	0.00005200	1.08579100
H	3.11329000	-0.88187100	-0.45290200

39-Ketone

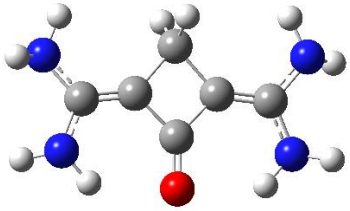


Energy= -516.228749 Hartree

0 1

C	-2.75086400	0.28668200	-0.00000300
C	-1.69825300	1.16962300	-0.00000200
C	-0.37949600	0.71813400	-0.00001900
C	-0.12463600	-0.66045600	-0.00003400
C	-1.20081500	-1.55752600	-0.00004700
C	-2.49178600	-1.08246300	-0.00003000
H	-3.77083700	0.64747500	0.00001100
H	-1.85003100	2.24105800	0.00000800
C	0.72132800	1.70406800	-0.00004200
H	-1.02876400	-2.62343700	-0.00008100
H	-3.31319000	-1.78794200	-0.00004300
C	2.20797700	-0.21725600	-0.00005200
C	2.04152900	1.11839600	-0.00005300
H	3.19652600	-0.65698300	-0.00006800
H	2.89966000	1.77424100	-0.00007000
N	1.18567700	-1.11517400	-0.00005500
C	1.47151200	-2.53722600	0.00020500
H	1.05931000	-3.01942900	0.88786500
H	1.05956100	-3.01972600	-0.88741000
H	2.54874400	-2.67730700	0.00038300
O	0.51503700	2.90955100	0.00003200

52-Ketone

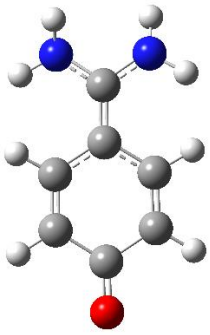


Energy= -528.666869 Hartree

0 1

C	0.00004200	0.72079900	0.00018800
C	-0.00004800	-1.42734400	0.00013700
H	0.00233800	-2.06248800	-0.89118000
H	-0.00249500	-2.06255000	0.89140500
C	-1.03642700	-0.30012800	-0.00572100
C	1.03640800	-0.30021400	0.00601600
C	-2.37476900	-0.15880200	-0.00480300
C	2.37475700	-0.15883400	0.00474400
N	-3.27523100	-1.19427800	0.13838300
H	-4.11732400	-1.10212200	-0.41166700
H	-2.87118800	-2.11653800	0.08802500
N	-2.94413800	1.08807100	-0.14665500
H	-3.74734200	1.25749900	0.44207400
H	-2.25793800	1.83653200	-0.11963500
N	2.94407700	1.08805200	0.14637200
H	3.74730100	1.25744000	-0.44233000
H	2.25785900	1.83650100	0.11940200
N	3.27522900	-1.19428200	-0.13870300
H	4.11742800	-1.10212000	0.41119000
H	2.87120400	-2.11654400	-0.08817500
O	0.00010300	1.95107200	0.00021800

53-Ketone

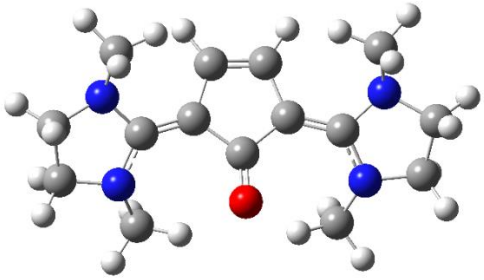


Energy= -456.091220 Hartree

0 1

C	-0.16062800	1.21699600	0.10026300
C	-1.50554500	1.22881700	0.10341700
C	-2.28706100	0.00000100	-0.00001000
C	-1.50554700	-1.22881800	-0.10341400
C	-0.16062900	-1.21699400	-0.10028700
H	0.36206200	2.15919600	0.22456900
H	-2.06250500	2.15124600	0.20417100
H	-2.06250800	-2.15124800	-0.20415300
H	0.36206200	-2.15919000	-0.22461600
C	0.59260400	0.00000100	-0.00002100
C	1.97376700	0.00000000	0.00000300
N	2.72607700	-1.11189700	0.24112600
H	2.24207700	-1.96960100	0.44221600
H	3.58937200	-1.21013100	-0.27005600
N	2.72608600	1.11189400	-0.24109400
H	2.24210100	1.96961000	-0.44217000
H	3.58938100	1.21010600	0.27009200
O	-3.51361900	0.00000100	0.00000200

58-Ketone



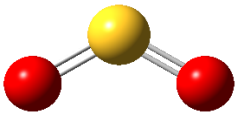
Energy= -878.542290 Hartree

0 1

O	-0.00005000	1.40805600	-0.89357300
C	-0.00002100	0.41534400	-0.14724400
C	0.67338800	-1.51602400	1.01426500
C	-0.67339700	-1.51601400	1.01429600
C	1.16881200	-0.34349500	0.31256200
C	2.49449900	-0.06544500	0.05868200
C	4.74885000	-0.40287300	-0.35259900
C	4.50060100	1.06232400	-0.07241900
H	5.59906800	-0.81076400	0.19426200
H	4.91065400	-0.57658100	-1.42435500
H	4.82457300	1.33640500	0.93987700
H	4.99200900	1.72598200	-0.78330500
C	-1.16882800	-0.34350300	0.31257700
C	-2.49451300	-0.06544900	0.05868800
C	-4.50053900	1.06244700	-0.07249300
C	-4.74890400	-0.40278400	-0.35245400
H	-4.82448300	1.33671200	0.93976100
H	-4.99190900	1.72602900	-0.78347800
H	-5.59909100	-0.81054200	0.19455600
H	-4.91084100	-0.57663200	-1.42416500
N	-3.49752200	-1.02173400	0.06539100
N	-3.05141300	1.15979900	-0.17406600
N	3.05147700	1.15979800	-0.17395600
N	3.49746900	-1.02179000	0.06529700
C	3.27641700	-2.34313300	-0.49117800
H	2.28347800	-2.70265200	-0.25164700
H	3.38637100	-2.32650800	-1.58288600
H	4.01089200	-3.03617100	-0.07910200
C	2.46334700	2.38352800	0.33331000
H	3.08338100	3.21823200	0.00763700
H	1.46214800	2.50063800	-0.07113000
H	2.42753700	2.37370100	1.42932500
C	-2.46312600	2.38354100	0.33298100
H	-1.46193800	2.50048300	-0.07154300

H	-3.08308900	3.21826600	0.00722400
H	-2.42724300	2.37387500	1.42899500
C	-3.27656900	-2.34313500	-0.49098100
H	-3.38643900	-2.32657100	-1.58269900
H	-2.28368900	-2.70274900	-0.25134700
H	-4.01115300	-3.03606100	-0.07891400
H	1.28974500	-2.19701000	1.58242700
H	-1.28974500	-2.19699600	1.58247400

SO_2

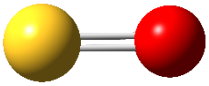


Energy= -548.660825 Hartree

0 1

S	0.00000000	0.00000000	0.36433800
O	0.00000000	-1.23551900	-0.36433800
O	0.00000000	1.23551900	-0.36433800

SO

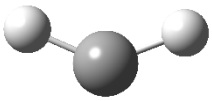


Energy= -473.360117 Hartree

0 1

S	0.00000000	0.00000000	0.49506300
O	0.00000000	0.00000000	-0.99012600

1T

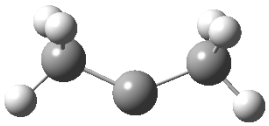


Energy= -39.139519 Hartree

0 3

C	0.00000000	0.00000000	0.10272800
H	0.00000000	0.99761300	-0.30818300
H	0.00000000	-0.99761300	-0.30818300

2T

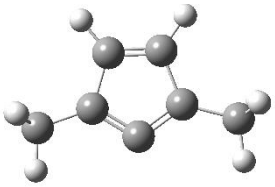


Energy= -117.712698 Hartree

0 3

C	0.00000000	0.00000000	0.47630200
C	0.00000000	1.34246900	-0.10501000
H	0.88516100	1.51515100	-0.73430200
H	-0.88521200	1.51521900	-0.73422300
H	0.00004600	2.11212700	0.66967800
C	0.00000000	-1.34246900	-0.10501000
H	-0.88516100	-1.51515100	-0.73430200
H	0.88521200	-1.51521900	-0.73422300
H	-0.00004600	-2.11212700	0.66967800

45T



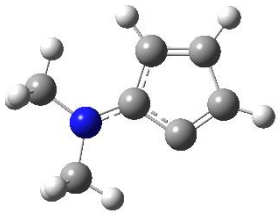
Energy= -271.243178 Hartree

0 3

C	-0.00003500	0.93233600	-0.00000600
C	-0.67512600	-1.22834100	-0.00002600
C	0.67518800	-1.22834100	0.00002600
C	-1.14580500	0.16711500	-0.00004700
C	1.14581000	0.16707300	0.00004000
H	1.32730100	-2.09014100	0.00006000
H	-1.32723800	-2.09014500	-0.00005900
C	2.56437200	0.59539200	-0.00000600
H	2.65285700	1.68011500	0.00011900
H	3.08701200	0.20406900	0.87745000
H	3.08681600	0.20431900	-0.87770400
C	-2.56439800	0.59534500	0.00001200
H	-2.65294400	1.68006400	-0.00024300

H	-3.08706000	0.20388400	-0.87736900
H	-3.08677600	0.20435900	0.87778800

46T

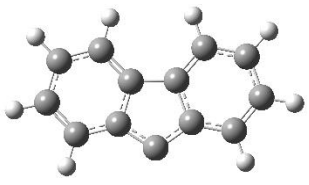


Energy= -326.569579 Hartree

0 3

C	0.95060700	-1.14819900	0.00003300
C	0.97442200	1.13353600	0.00003000
C	2.26415600	0.64798700	0.00008200
C	0.09641200	0.01011100	-0.00002000
C	2.25389700	-0.80119800	-0.00006000
H	3.16123000	1.25076800	0.00016400
H	0.69011600	2.17317100	0.00010600
N	-1.24950200	-0.02092000	-0.00008600
C	-2.05386500	1.17606400	-0.00009200
H	-2.69489000	1.20415000	-0.88577000
H	-2.69355300	1.20517600	0.88653100
H	-1.42253700	2.05762100	-0.00110400
C	-1.97325900	-1.27060100	0.00008100
H	-2.60921300	-1.34412700	0.88678100
H	-2.60883700	-1.34461000	-0.88685000
H	-1.27006700	-2.09902100	0.00046200
H	3.12004400	-1.44289000	-0.00004500

47T

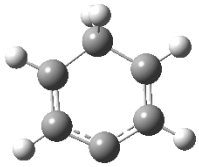


Energy= -499.828266 Hartree

0 3

C	0.00000000	1.73638400	0.00000000
C	0.00000000	-0.41214500	0.73420600
C	0.00000000	-0.41214500	-0.73420600
C	0.00000000	0.94269100	1.17469000
C	0.00000000	0.94269100	-1.17469000
C	0.00000000	1.24393400	-2.53259300
C	0.00000000	-1.43577000	-1.65532400
C	0.00000000	-1.43577000	1.65532400
C	0.00000000	1.24393400	2.53259300
C	0.00000000	0.20017600	-3.44284400
C	0.00000000	-1.12293100	-3.01236900
C	0.00000000	0.20017600	3.44284400
C	0.00000000	-1.12293100	3.01236900
H	0.00000000	2.27259800	2.86827000
H	0.00000000	0.41507900	4.50375700
H	0.00000000	-1.92149200	3.74306300
H	0.00000000	-2.47106700	1.33637400
H	0.00000000	-2.47106700	-1.33637400
H	0.00000000	-1.92149200	-3.74306300
H	0.00000000	0.41507900	-4.50375700
H	0.00000000	2.27259800	-2.86827000

48T



Energy= -231.974802 Hartree

0 3

C	1.25703800	0.55307700	0.00004500
C	1.23707100	-0.80581600	-0.00001300
C	0.00000200	-1.44909700	-0.00025400
C	-1.23706800	-0.80582000	-0.00001300
C	-1.25704100	0.55307300	0.00004500
H	2.20288800	1.08172200	0.00062100
H	2.16207200	-1.37010300	0.00063700
H	-2.16206600	-1.37011100	0.00063800
H	-2.20289300	1.08171300	0.00062000

C	-0.00000300	1.36767800	-0.00022100
H	-0.00000300	2.04928200	-0.86465700
H	-0.00000300	2.04892000	0.86460700