The Electronic State of Push-Pull Alkenes–an Experimental Dynamic NMR and Theoretical Ab Initio MO Study

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Supporting Information

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Typical Procedure for the Dithiocarboxylation of Acylacetonitriles and Subsequent Alkylation: α-1,3-Dithiolan-2-ylidene-ß-oxo-2-thiophenepropanenitrile (2). Sodium hydride (2.4 g, 0.1 mol) was added in small portions to a solution of thenoylacetonitrile (7.56 g, 0.05 mol) and CS_2 (3.81 g, 0.05 mol) in dry DMSO (100 mL) under N_2 atmosphere with simultaneous stirring and cooling at 10°C during 15 min. The stirring was continued for 2h at room temperature. Finally, 1,2-dibromoethane (9.39 g, 0.05 mol) was added maintaining the temperature below 10°C and stirring was continued for another 2h. The reaction mixture was then poured into cold H_2O (200 mL). The resulting precipitate was filtered and washed with H_2O. Recrystallization from ethanol/charcoal gave **2** (8.0 g, 63% yield) as yellow crystals: mp 151-153°C; IR (KBr) $_{max}$ 2205, 1615 cm^{-1}. Anal. Calcd for $C_{10}H_7NOS_3$: C, 47.41; H, 2.78; N, 5.53; S, 37.97. Found: C, 47.72; H, 2.77; N, 5.53; S, 37.84.

4-Methyl-α–1,3–dithiole-2-ylidene-ß-oxo-benzenepropanenitrile (5). Reaction conditions: Sodium hydride (2.4 g, 0.1 mol), benzoylacetonitrile (7.26 g, 0.05 mol), DMSO (100 mL), CS_2 (3.81 g, 0.05 mol), propargyl bromide (5.95 g, 0.05 mol). Recrystallization from ethanol/charcoal gave **5** (5.4 g, 42% yield) as yellow crystals: mp 176-178°C; IR (KBr) $_{max}$ 2205, 1620 cm^{-1}. Anal. Calcd for $C_{13}H_9NOS_2$: C, 60.21; H, 3.50; N, 5.40; S, 24.73. Found: C, 60.48; H, 3.51; N, 5.42; S, 24.69.

4-Methyl-α–1,3–dithiole-2-ylidene-ß-thioxo-benzenepropanenitrile (11). A solution of **5** (1.30 g, 5 mmol) and Lawesson´s reagent (1.21 g, 3 mmol) in toluene (20 mL) was heated to reflux under argon for 2 h. The solvent was removed and the residue recrystallized from ethanol/charcoal to give **11** (0.95 g, 69% yield) as red-brown crystals: mp 183-185°C; IR (KBr) $_{max}$ 2200, 1565 cm^{-1}; EIMS *m/z* 275 (100) [M^+). Anal. Calcd for $C_{13}H_9NS_3$: C, 56.69; H, 3.29; N, 5.09; S, 34.93. Found: C, 57.00; H, 3.31; N, 4.86; S, 34.63.

Typical Procedure for the Reaction of Acylketene S,S-acetals with α,ω-Diaminoalkanes: ß-Oxo-α-[tetrahydro-2(1H)-pyrimidinylidene]-benzenepropanenitrile (13). A solution of α-[bis(methylthio)methylene]-ß-oxo-benzenepropanenitrile (2.49 g, 0.01 mol) and 1,3-diaminopropane (0.74 g, 0.01 mol) in ethanol (30 mL) was heated to reflux for 3 h. After cooling the precipitate was filtered. Recrystallization from ethanol gave **13** (1.40 g, 62% yield) as colorless crystals: mp 185-

187°C; IR (KBr) $_{max}$ 3340, 3140 (broad), 2200, 1605 cm^{-1}. Anal. Calcd for $C_{13}H_{13}N_3O$: C, 68.71; H, 5.77; N, 18.49. Found: C, 68.39; H, 5.65; N, 18.31.

α-(Hexahydro-2H-1,3-diazepin-2-ylidene)-ß-oxo-benzenepropanenitrile (14). Analogous to **13** using 1,4-diaminobutane (0.88 g, 0.01 mol). Recrystallization from ethanol gave **14** (1.30 g, 54% yield) as colorless crystals: mp 194-195°C; IR (KBr) $_{max}$ 3340, 2190, 1615 cm^{-1}; EIMS *m/z* 241 (M^+), 224, 212, 198, 184, 164, 139, 105. Anal. Calcd for $C_{14}H_{15}N_3O$: C, 69.69; H, 6.27; N, 17.41. Found: C, 69.70; H, 6.36; N, 17.49.

Typical Procedure for the Reaction of Acylketene S,S-acetals with 2-Mercapto-ethanol: α-1,3-Oxathiolane-2-ylidene-ß-oxo-2-furanpropanenitrile (18). A solution of α-[bis(methylthio)methylene]-β-oxo-2-furanpropanenitrile (2.39 g, 0.01 mol) and 2-mercapto-ethanol (0.8 g, 0.01 mol) in ethanol (40 mL) was stirred at refluxing temperature for 2 h. After cooling the precipitate was filtered. Recrystallization from ethanol gave **18** (2.03 g, 92% yield) as nearly colorless crystals: mp 192-193°C; IR (KBr) $_{max}$ 2200, 1615 cm^{-1}; EIMS *m/z* 221 (M^+), 193, 154, 139, 128, 117, 95. Anal. Calcd for $C_{10}H_7NO_3S$: C, 54.29; H, 3.19; N, 6.33; S, 14.49. Found: C, 54.48; H, 3.23; N, 6.45; S, 14.85.

α-1,3-Oxathiolane-2-ylidene-ß-oxo-2-thiophenepropanenitrile (19). Analogous to **18** using α-[bis(methylthio)methylene]-β-oxo-2-thiophenepropanenitrile (2.55 g, 0.01 mol). Recrystallization from ethanol gave **19** (2.20 g, 93% yield) as yellowish crystals: mp 153-154°C; EIMS *m/z* 237 (M^+), 209, 154, 133, 111, 94. Anal. Calcd for $C_{10}H_7NO_2S_2$: C, 50.62; H, 2.97; N, 5.90; S, 27.02. Found: C, 50.61; H, 2.96; N, 5.93; S, 27.10.

α-1,3-Oxathiolane-2-ylidene-ß-oxo-benzenepropanenitrile (20). Analogous to **18** using α-[bis(methylthio)methylene]-β-oxo-2-benzenepropanenitrile (2.49 g, 0.01 mol). Recrystallization from ethanol gave **20** (2.25 g, 97% yield) as yellowish crystals: mp 128-129.5°C. Anal. Calcd for $C_{12}H_9NO_2S$: C, 62.32; H, 3.92; N, 6.06; S, 13.86. Found: C, 62.29; H, 3.94; N, 6.14; S, 14.01.

4-Chloro-α-1,3-oxathiolane-2-ylidene-ß-oxo-benzenepropanenitrile (21). Analogous to **18** using α-[bis(methylthio)methylene]-4-chloro-β-oxo-benzenepropanenitrile (2.84 g, 0.01 mol). Recrystallization from ethanol gave **21** (2.05 g, 77% yield) as yellow crystals: mp 164-165°C; IR (KBr) $_{max}$ 2210, 1605

cm^{-1}; EIMS *m/z* 265 (M^+), 237, 161, 154, 139, 111, 94. Anal. Calcd for $C_{12}H_8ClNO_2S$: C, 54.24; H, 3.03; Cl, 13.34; N, 5.27; S, 12.07. Found: C, 54.30; H, 3.11; Cl, 13.10; N, 5.38; S, 12.28.

ß- Oxo-α-(3-phenyl-2-thiazolidinylidene)-benzenepropanenitrile (26). Sodium hydride (1.2 g, 0.05 mol) was added in small portions to a solution of benzoylacetonitrile (7.25 g, 0.05 mol) in dry DMF (50 mL) under N_2 atmosphere with simultaneous stirring and cooling at 15°C for 20 min and then phenyl isothiocyanate (6.76 g, 0.05 mol). The resulting mixture was stirred for 1 h at room temperature. Finally, 1,2-dibromoethane (9.39 g, 0.05 mol) was added maintaining the temperature below 10°C and stirring was continued for another 2 h. The reaction mixture was poured into cold H_2O (200 mL). The resulting precipitate was filtered and refluxed in pyridine (100 mL) for 1 h. After cooling the solution was diluted with H_2O to yield a precipitate. Recrystallization from ethanol gave **26** (5.10 g, 33% yield) as white needles: mp 244-245°C. Anal. Calcd for $C_{18}H_{14}N_2OS$: C, 70.56; H, 4.61; N, 9.14. Found: C, 70.45; H, 4.50; N, 8.92.

α-(4-Methyl-3-phenyl-2(3H)-thiazolylidene)-ß-thioxo-benzenepropanenitrile (29). A solution of α-(4-methyl-3-phenyl-2(3H)-thiazolylidene)-ß-oxo-benzenepropanenitrile (**28**) [1.59 g, 5 mmol] and Lawesson´s reagent (1.21 g, 3 mmol) in xylene (50 mL) was heated to reflux under argon for 2 h. After cooling the precipitate was collected. Recrystallization from toluene/charcoal gave **29** (1.50 g, 90% yield) as orange crystals: mp 265-267.5°C; IR (KBr) $_{max}$ 2200, 1595 cm^{-1}; EIMS *m/z* 334 (M^+), 333 (M^+-1), 301, 276, 257, 225, 207, 134, 121, 99, 92, 91. Anal. Calcd for $C_{19}H_{14}N_2S_2$: C, 68.23; H, 4.22; N, 8.38; S, 19.17. Found: C, 68.47; H, 4.37; N, 8.28; S, 19.15.

Table S1. ^{13}C NMR chemical shifts (ppm) of compounds 1–29

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-9'	C-11	C-12
1	187.5	94.5	117.7	171.8	150.5	119.4	112.4	147.0	36.3	40.4			
2	187.7	94.9	118.3	176.3	142.6	134.4	134.4	132.9	36.4	40.4			
3	186.1	96.3	118.3	187.6	136.8	128.5	128.3	132.5	36.5	40.4			
4	188.2	96.0	118.2	184.9	138.9	128.7	130.1	135.1	36.6	40.5			
5	181.8 182.2	90.4	118.5 118.8	184.7 185.0	137.2	128.4	128.4	132.0	135.7 141.3	115.7 122.6	15.6 15.9		
6	184.6	104.4	117.4	186.3	137.0	128.9	128.4	132.7	30.1	23.7		30.1	
7	186.8	104.2	117.9	195.2	157.5	117.3	113.5	147.7	35.7	40.7			
8	187.1	105.0	118.3	203.1	152.7	128.0	128.5	136.8	35.9	40.8			
9	187.2	108.3	117.8	218.5	147.0	127.6	127.9	131.1	36.1	41.0			
10	187.9	108.0	117.7	216.3	145.2	129.0	128.2	137.4	36.1	41.0			
11	180.3 180.4	103.0 103.9	117.7 118.1	211.1 210.9	146.8	127.4	127.9	130.1	137.7	117.6 119.4	16.1 15.7		
12	165.5	65.1	121.3	187.7	140.4	127.3	128.0	130.3	43.3	43.3			
13	159.9	68.5	122.2	189.1	141.8	128.0	128.7	130.7	39.1	20.0		39.1	
14	166.9	69.8	121.5	189.0	140.7	127.4	127.8	130.1	43.8	26.5		26.5	43.8
15	164.6	85.6	118.8	206.7	148.3	126.4	127.7	128.6	43.7	43.7			
16	157.2	89.6	118.5	201.5	148.8	126.3	127.7	128.1	38.4	18.3		38.4	
17	163.9	91.0	119.0	203.3	148.9	126.4	127.7	128.3	43.3	25.9		25.9	43.3
18	189.6	84.0	115.7	173.5	150.6	119.0	112.3	146.8	31.1	74.5			
19	189.9	84.3	116.2	177.8	142.8	134.0	128.4	132.6	31.1	74.6			
20	189.8	85.6	116.3	187.8	137.0	128.3	128.3	132.5	31.1	74.6			
21	190.2	85.4	116.1	186.5	138.8	129.8	128.7	135.3	31.1	74.7			
22	173.3	67.7	118.3	190.5	138.5	127.9	128.2	131.6	43.7	68.9			
23	173.1	77.2	116.8	214.3	146.8	126.9	127.8	130.8	44.3	69.1			
24	178.6	78.1	120.3	189.7	138.4	127.8	128.2	131.5	29.4	51.4			
25	179.3	93.8	119.1	212.9	147.3	126.8	127.9	130.0	29.9	52.3			
26[a]	174.4	80.0	117.5	189.9	138.1	128.3	126.3	131.4	27.4	59.7			
27[b]	176.2	96.8	116.7	218.5	147.7	127.3	127.6	129.8	28.8	59.8			
28[c]	167.5	77.1	117.8	188.2	138.6	128.2	127.7	130.6	138.8	107.7	14.9		
29[d]	166.5	94.7	116.3	209.1	136.9	130.2	128.3	131.4	139.9	105.2	15.2		

[a] 140.7 (C5'), 129.9 (C7'), 129.1 (C8'), 127.8 (C6'). [b] 141.5 (C5'), 130.1 (C7'), 129.0 (C8'), 125.6 (C6'). [c] C5' 136.6, 130.0 (C8'), 128.6 (C7'), 127.6 (C6'). [d] 136.9 (C5'), 128.7 (C8'), 127.6 (C7'), 127.2 (C6').

Table S2. ^{1}H NMR chemical shifts (ppm) of compounds 1–29

	H-6	H-7	H-8	H-9	H-10	H-9'	H-11	H-12	NH
1	7.66	7.58	7.69	3.58	3.62				
2	7.68	7.16	8.28	3.60	3.60				
3	7.91	7.55	7.48	3.60	3.60				
4	7.45	7.87		3.62	3.62				
5	7.96	7.45	7.54		6.86	2.46 2.48			
6	7.89	7.46	7.54	3.01	2.37		3.16		
7	7.50	6.58	7.72	3.56	3.62				
8	7.90	7.12	7.66	3.56	3.62				
9	7.61	7.48	7.38	3.60	3.60				
10	7.56	7.35		3.63	3.63				
11	7.63	7.41	7.44		6.83 7.11	2.49 2.56			
12	7.60	7.44	7.44	3.63	3.63				8.70
13	7.55	7.40	7.40	3.32	1.85		3.33		9.12
14	7.56	7.40	7.40	3.43	1.74		1.74	3.43	9.12
15	7.33	7.33	7.33	3.76	3.76				9.85
16	7.32	7.26	7.26	3.41	1.89		3.41		10.24
17	7.29	7.29	7.29	3.54	1.84		1.84	3.54	10.14
18	7.66	6.57	7.66	3.41	4.82				
19	7.67	7.16	8.32	3.41	4.83				
20	7.93	7.47	7.56	3.40	4.82				
21	7.88	7.44		3.41	4.83				
22	7.83	7.46	7.46	3.99	4.82				10.37
23	7.55	7.37	7.37	4.14	4.84				13.16
24	7.82	7.42	7.48	3.43	4.12				11.19
25	7.53	7.40	7.40	3.51	4.26				13.91
26		7.34–7.73		3.25	4.23				
27		7.23–7.51		3.28	4.26				
28		7.34–7.71			6.61	2.01			
29		7.24–7.63			6.65	2.09			

Table S3. ^{13}C NMR chemical shifts (ppm) of 3, 5, 9, 11–16, 20, 22 and 24 calculated at the MP2/6-31G* level of theory

	C-1	C-2	C-3	C-4	C-9	C-10	C-9’	C-11	C-12
3	165.79	96.21	122.63	173.82	39.49	36.51			
5	163.87	89.05	123.58	172.91	124.34	114.87	16.18		
9	162.39	107.51	122.89	202.52	39.77	36.21			
11	159.09	101.67	123.79	196.76	126.4	111.02	16.12		
12	157.83	66.78	118.39	175.94	45.79	44.79			
13	148.86	66.79	121.08	177.32	38.84	21.21		39.67	
14	161.45	71.38	121.08	178.34	46.03	27.84		28.79	47.39
15	156.73	82.83	119.51	198.59	45.92	44.81			
16	146.62	85.27	119.99	193.05	38.02	20.13		39.97	
20	173.59 169.77	85.85 87.18	118.51 120.46	175.14 170.82	31.65 31.85	73.1 76.44			
22	163.53 162.87	68.88 68.29	117.18 120.86	178.77 170.99	44.91 44.24	67.96 70.83			
24	163.31 163.50	79.75 78.88	119.94 121.18	177.91 173.63	51.23 48.56	30.45 31.25			

Table S4. Bond lengths in the GSs and TSs of 1–29 as calculated at the HF/6-31G* level of theory

	ground state					transition state				
	C_1–C_2	C_2–C_3	C_2–C_4	C_1–X_1 [a]	C_1–X_2 [a]	C_1–C_2	C_2–C_3	C_2–C_4	C_1–X_1 [a]	C_1–X_2 [a]
1	1.355	1.440	1.487	1.757	1.762	1.468	1.411	1.419	1.690	1.691
2	1.356	1.438	1.489	1.755	1.762	1.469	1.408	1.421	1.690	1.691
3	1.354	1.439	1.492	1.756	1.762	1.468	1.408	1.425	1.692	1.690
4	1.355	1.438	1.490	1.755	1.761	1.469	1.408	1.424	1.689	1.691
5	1.364	1.435	1.480	1.745 1.749	1.750 1.746	1.464	1.410	1.430	1.679	1.684
6	1.350	1.441	1.503	1.767	1.771	1.470	1.409	1.424	1.704	1.691
7	1.350	1.443	1.485	1.761	1.767	1.480	1.426	1.367	1.707	1.719
8	1.353	1.441	1.498	1.764	1.767	1.478	1.426	1.374	1.708	1.724
9	1.355	1.445	1.481	1.758	1.766	1.478	1.425	1.376	1.695	1.704
10	1.357	1.445	1.479	1.756	1.765	1.481	1.424	1.374	1.694	1.702
11	1.377	1.443	1.455	1.739 1.749	1.750 1.740	1.473	1.425	1.387	1.677	1.684
12	1.399	1.425	1.452	1.330	1.348	1.467	1.409	1.424	1.318	1.312
13	1.422	1.424	1.446	1.326	1.339	1.475	1.409	1.424	1.315	1.314
14	1.409	1.428	1.457	1.335	1.355	1.484	1.410	1.424	1.321	1.314
15	1.422	1.436	1.416	1.321	1.343	1.476	1.425	1.379	1.316	1.309
16	1.447	1.436	1.408	1.316	1.336	1.482	1.426	1.380	1.313	1.313
17	1.434	1.438	1.420	1.322	1.351	1.490	1.426	1.382	1.318	1.310
18	1.357 1.350	1.437 1.436	1.475 1.494	1.755 1.766	1.318 1.315	1.456	1.410	1.417	1.712	1.270
19	1.358 1.348	1.435 1.434	1.476 1.499	1.753 1.766	1.316 1.315	1.457	1.408	1.419	1.712	1.270
20	1.357 1.348	1.436 1.434	1.480 1.502	1.753 1.766	1.319 1.317	1.456	1.408	1.424	1.714	1.270
21	1.357 1.351	1.436 1.434	1.479 1.498	1.754 1.766	1.318 1.314	1.457	1.408	1.422	1.711	1.269
22	1.383 1.374	1.429 1.429	1.460 1.478	1.325 1.345	1.318 1.311	1.458	1.408	1.425	1.300	1.294
23	1.404 1.386	1.439 1.435	1.424 1.451	1.314 1.340	1.314 1.306	1.463	1.423	1.385	1.300	1.290
24	1.383 1.377	1.431 1.431	1.466 1.469	1.326 1.341	1.763 1.756	1.465	1.409	1.425	1.292	1.730
25	1.403 1.392	1.440 1.439	1.432 1.443	1.314 1.337	1.763 1.754	1.473	1.424	1.383	1.292	1.733
26	1.381 1.368	1.434 1.433	1.475 1.492	1.354 1.350	1.768 1.772					
27	1.383 1.370	1.440 1.439	1.460 1.479	1.357 1.356	1.772 1.776					
28	1.391 1.381	1.431 1.430	1.465 1.481	1.353 1.353	1.754 1.756					
29	1.412 1.403	1.439 1.435	1.432 1.447	1.350 1.343	1.743 1.747					

[a] Donor heteroatoms at C_1 (cf. Scheme 2).

Table S5. Barrier to rotation about the central C=C partial double bond and some characteristic bond lengths (Å) in the GSs of model compounds a1–f6

	ΔE (kJ mol^{-1})	C_1–C_2	C_2–C_3	C_2–C_4	C_1–X_1 [a]	C_1–X_2 [a]
a1	205.3	1.348	1.437	1.437	1.755	1.755
a2	164.7	1.350	1.431	1.431	1.310	1.310
a3	113.9	1.380	1.422	1.422	1.345	1.345
a4	186.6	1.348	1.433	1.434	1.756	1.315
a5	143.6	1.365	1.428	1.429	1.757	1.341
a6	131.9	1.365	1.426	1.426	1.313	1.340
b1	148.0	1.364	1.468	1.468	1.754	1.754
b2	85.9	1.366	1.464	1.464	1.308	1.308
b3	107.9	1.411	1.435	1.435	1.332	1.332
b4	123.0	1.363	1.471	1.459	1.309	1.758
b5	117.8	1.393	1.444	1.449	1.323	1.756
b6	92.9	1.392	1.440	1.455	1.325	1.310
c1	70.7	1.387	1.459	1.459	1.751	1.751
c2	21.9	1.388	1.447	1.447	1.297	1.297
c3	45.7	1.446	1.422	1.422	1.323	1.323
c4	54.4	1.385	1.444	1.458	1.751	1.301
c5	46.6	1.427	1.438	1.427	1.757	1.310
c6	31.1	1.422	1.443	1.419	1.302	1.313
d1	178.0	1.354	1.475	1.438	1.752	1.758
d2	124.9	1.356	1.471	1.432	1.306	1.314
d3	109.2	1.395	1.439	1.424	1.332	1.345
d4-1	146.9	1.353	1.479	1.435	1.310	1.762
d4-2	163.2	1.354	1.466	1.435	1.316	1.753
d5-1	122.9	1.374	1.456	1.430	1.754	1.340
d5-2	136.4	1.379	1.451	1.429	1.758	1.327
d6-1	96.3	1.373	1.462	1.428	1.310	1.342
d6-2	126.4	1.380	1.445	1.427	1.314	1.326
e1	132.6	1.364	1.451	1.445	1.746	1.759
e2	84.9	1.367	1.442	1.438	1.299	1.311
e3	73.5	1.416	1.404	1.433	1.322	1.340
e4-1	108.3	1.362	1.451	1.440	1.304	1.760
e4-2	119.8	1.366	1.440	1.442	1.316	1.746
e5-1	80.9	1.390	1.427	1.437	1.749	1.335
e5-2	97.7	1.399	1.417	1.437	1.757	1.315
e6-1	59.9	1.387	1.431	1.434	1.303	1.336
e6-2	90.3	1.399	1.411	1.435	1.311	1.314
f1	103.7	1.376	1.444	1.479	1.748	1.756
f2	48.9	1.378	1.436	1.474	1.300	1.304
f3	75.2	1.431	1.403	1.452	1.324	1.329
f4-1	87.6	1.374	1.444	1.467	1.302	1.755

f4-2	80.4	1.376	1.434	1.484	1.307	1.752
f5-1	83.1	1.413	1.411	1.462	1.312	1.757
f5-2	78.2	1.410	1.422	1.457	1.319	1.753
f6-1	59.3	1.413	1.406	1.470	1.314	1.307
f6-2	59.2	1.406	1.426	1.451	1.321	1.304

[a] Donor heteroatoms at C_1 (cf. Scheme 3).

Discussion of the results of ab initio calculations on compound 20 at various levels of theory

The level of theory necessary for the correct calculation of the geometries and molecular properties of the push-pull alkenes can be gauged by the level of agreement between the calculated and experimental ^{13}C NMR chemical shifts. Using compound **20** as a test structure, the magnetic shieldings were calculated using the GIAO method implemented within the Gaussian program at the HF, B3LYP and MP2 levels of theory using various basis sets. TMS was used as a standard and it was calculated at the same levels of theory and the chemical shifts were obtained by the difference of the calculated shielding values to that calculated for TMS (at that same level of theory).

The strong electron delocalization in the push-pull alkenes, together with the presence of hetero atoms, required the application of large and flexible basis sets. The calculated chemical shifts for compound **20** progressively improved in comparison to experimental values upon expanding from DZSV to TZSV basis sets (cf. Table S6). The explicit consideration of diffuse functions, however, did not lead to improvements in the accuracy of the results, and came at the cost of dramatic increases in the required CPU time.

Selection of a suitable method, though, is crucially dependent on correct consideration of electron delocalization. Methods with electron correlation correction led to more accurate chemical shifts for all carbons except C-1 and C-4 in comparison to experimental values (cf. Table S7). The MP2 method was found to be more accurate than the density functional method tried.

The accuracy of the calculated shifts for C-1 and C-4 was found to increase with the size of the basis set used, however, incorporating a more flexible TZSV basis set at the MP2 level of theory is prohibitive even with the computer architecture presently available. By using a TZSV basis set for the carbonyl oxygen attached to C-4 whilst using a DZSV basis set for the remainder of the atoms in the molecule, the accuracies of the resulting chemical shifts were increased significantly, especially for C-1 and C-4 at both the HF and MP2 levels of theory (cf. Table S8).

Push-pull alkenes are strongly polar molecules, therefore explicit consideration of solvent effects in the theoretical calculation of molecular properties should increase the accuracy of the results. Incorporating the solvent directly in GIAO calculations, however, is not possible within the Gaussian program package but the effect of the solvent can be simulated by optimizing the structure of the compound using the SCRF method. The resulting structure should thus lead to more accurate calculated chemical shifts in comparison to a structure optimized without consideration of the influence of the solvent (cf. Table S9). Scrutinizing the structure of compound **20** optimized with the effect of the solvent influence revealed that the largest effect was on the carbonyl bond length. Explicit lengthening

of this bond was found to increase the resulting accuracies of the chemical shifts of the corresponding structures (cf. Table S10).

To summarize the results of the test calculations for compound **20**, a calculation method with explicit consideration of electron correlation correction was found to be necessary for the correct description of the molecular properties based on the divergence between the observed and the calculated chemical shifts. Employing a TZSV basis set and incorporation of the solvent influence led to improved results, and this is especially necessary generally when strong electron-withdrawing groups or atoms are present.

Table S6. HF calculated[a] ^{13}C NMR chemical shifts (ppm) for compound 20 using various basis sets

	C-1	C-2	C-3	C-4	C-9	C-10	Σ Error[b]
experimental	189.8	85.6	116.3	187.8	31.1	74.6	
3-21G	173.2	87.8	108.0	179.6	31.4	65.8	44.5
	182.8	86.3	106.6	182.6	28.4	63.9	35.8
6-31G*	183.6	84.8	106.2	178.9	26.9	65.1	39.6
	190.9	84.3	104.5	184.4	26.2	63.2	33.8
6-311G**	190.9	88.2	116.6	184.6	30.0	67.7	15.1
	198.6	87.6	115.0	190.4	29.5	65.8	25.1
6-31+G**	185.3	85.3	108.0	181.7	27.9	65.9	31.1
	193.2	85.0	106.1	186.4	27.4	64.3	29.6
6-311+G**	192.8	88.6	118.2	186.9	30.8	67.7	15.8
	200.5	88.1	116.6	192.9	30.1	66.0	27.5

Table S7. Calculated[a] ^{13}C NMR chemical shifts (ppm) at various levels of theory for compound 20 using the 6-31G* basis set

	C-1	C-2	C-3	C-4	C-9	C-10	Σ Error[b]
experimental	189.8	85.6	116.3	187.8	31.1	74.6	
HF	183.6	84.8	106.2	178.9	26.9	65.1	39.6
	190.9	84.3	104.5	184.4	26.2	63.2	33.8
B3LYP	180.5	86.1	107.8	175.4	34.6	74.6	34.3
	184.9	84.5	104.8	177.7	34.3	71.1	34.2
MP2	169.8	87.2	120.5	170.8	31.8	76.4	45.4
	173.6	85.9	118.5	175.1	31.6	73.1	33.4

Table S8. Effect of basis set extension for the carbonyl oxygen on the calculated[a] ^{13}C NMR chemical shifts (ppm) at various levels of theory for compound 20

	C-1	C-2	C-3	C-4	C-9	C-10	Σ Error[b]
experimental	189.8	85.6	116.3	187.8	31.1	74.6	
HF/6-31G*	183.6	84.8	106.2	178.9	26.9	65.1	39.6
	190.9	84.3	104.5	184.4	26.2	63.2	33.8
HF/6-31G*, C=O 6-311G*	183.7	84.8	106.2	181.3	26.9	64.9	37.3
	191.0	84.3	104.5	186.3	26.3	63.2	31.9
MP2/6-31G*	169.8	87.2	120.5	170.8	31.8	76.4	45.4
	173.6	85.9	118.5	175.1	31.6	73.1	33.4
MP2/6-31G*, C=O 6-311G*	170.2	86.8	120.7	174.2	31.4	76.1	40.7
	174.0	85.5	118.7	177.7	31.2	72.8	30.3

Table S9. Effect of solvent inclusion in the calculation[a] of the ^{13}C NMR chemical shifts (ppm) at the HF/6-31G* level of theory for compound 20

	C-1	C-2	C-3	C-4	C-9	C-10	Σ Error[b]
experimental	189.8	85.6	116.3	187.8	31.1	74.6	
without $CDCl_3$	183.6	84.8	106.2	178.9	26.9	65.1	39.6
	190.9	84.3	104.5	184.4	26.2	63.2	33.8
with $CDCl_3$	184.3	84.2	106.5	180.5	26.6	66.4	36.7
	190.7	84.4	104.5	186.5	25.9	64.4	30.5

Table S10. Effect of the bond length of the carbonyl group on the calculated[a] ^{13}C NMR chemical shifts (ppm) at various levels of theory for compound 20

	C-1	C-2	C-3	C-4	C-9	C-10	Σ Error[b]
experimental	189.8	85.6	116.3	187.8	31.1	74.6	
HF/6-31G*	183.6	84.8	106.2	178.9	26.9	65.1	39.6
	190.9	84.3	104.5	184.4	26.2	63.2	33.8
C=O –0.05Å	182.5	84.9	106.4	162.9	26.8	65.1	56.8
	189.1	82.9	104.8	168.9	26.2	63.0	49.6
C=O +0.05Å	184.6	85.1	106.0	196.2	27.1	65.1	37.9
	192.7	85.3	104.2	200.7	26.2	63.4	44.3
MP2/6-31G*	173.6	85.9	118.5	175.1	31.6	73.1	33.4
C=O +0.01Å	173.8	86.1	118.4	176.8	31.7	73.1	31.6
C=O +0.05Å	174.8	87.2	118.2	183.2	31.7	73.3	24.9

Tables S6–S10:

[a] Two sets of theoretical ^{13}C chemical shifts arise due to two conceivable ground states (*E* and *Z* isomers). [b] Sum over all differences compared to the experimental values.

Table S11. ^{13}C NMR chemical shifts (ppm) of compounds 1–29 calculated at the HF/6-31G* level of theory

	C-1	C-2	C-3	C-4	C-9	C-10	C-9'	C-11	C-12
1	203.1	100.4	114.1	177.0	36.8	34.9	–	–	–
2	204.1	100.4	114.5	180.1	36.8	35.0	–	–	–
3	202.5	101.3	115.2	188.3	36.8	35.1	–	–	–
4	204.3	100.4	115.1	187.2	36.8	35.1	–	–	–
5	205.0 204.7	94.5 95.0	115.0 114.7	188.7 188.6	137.7 143.3	123.6 117.3	16.7 16.6	–	–
6	193.9	110.9	114.0	187.1	27.6	23.7	–	28.0	–
7	191.4	110.7	113.6	236.5	36.9	35.6	–	–	–
8	182.1	110.9	113.2	146.9	37.1	36.2	–	–	–
9	195.1	113.0	114.2	257.3	37.0	35.5	–	–	–
10	197.4	112.2	114.1	255.1	37.1	35.4	–	–	–
11	205.4 205.3	106.8 107.3	114.5 114.2	253.3 253.4	139.0 141.0	121.2 118.8	16.6 16.5	–	–
12	180.3	61.1	119.6	194.5	41.5	40.4	–	–	–
13	173.1	61.3	120.0	196.1	36.7	21.4	–	35.9	–
14	186.5	66.1	120.5	196.2	42.6	28.8	–	29.2	43.6
15	179.3	81.0	118.1	250.6	41.6	41.6	–	–	–
16	170.9	84.1	117.6	246.5	35.2	20.4	–	36.9	–
17	185.2	86.3	118.7	251.9	42.1	28.1	–	28.9	44.1
18	198.1 191.6	88.2 87.4	116.6 115.9	184.6 174.2	30.0 30.1	67.7 68.1	–	–	–
19	199.3 190.2	87.9 86.6	113.9 115.6	181.5 177.1	29.3 30.4	66.2 67.9	–	–	–
20	198.6 191.0	88.2 87.6	115.0 116.6	190.4 184.6	29.5 30.0	65.8 67.7	–	–	–
21	198.6 192.4	86.9 86.9	114.8 116.7	189.4 183.1	29.4 30.3	66.4 68.3	–	–	–
22	181.9 181.3	64.6 63.6	117.1 119.7	195.9 186.0	39.9 39.4	61.8 63.9	–	–	–
23	181.8 181.1	82.9 78.6	115.5 118.6	255.0 254.5	40.1 39.3	61.9 64.1	–	–	–
24	193.9 194.1	76.2 76.9	118.5 117.3	194.8 189.6	46.3 44.2	29.2 29.9	–	–	–
25	196.3 195.3	91.9 92.4	117.4 116.7	254.5 254.2	46.9 44.1	29.3 30.8	–	–	–
26	190.6 195.9	79.7 78.9	118.8 115.6	187.7 192.3	27.4 28.0	56.6 58.2	–	–	–
27	189.5 195.3	91.9 98.9	117.8 113.5	253.7 262.6	28.5 29.1	60.9 58.1	–	–	–
28	197.5 191.1	76.4 75.6	119.7 116.8	189.1 195.3	147.4 143.5	106.1 109.9	17.2 16.6	–	–
29	204.9 194.5	87.3 93.2	120.2 116.5	250.2 253.3	148.1 145.1	110.8 109.6	17.5 17.2	–	–

Table S12. Depiction of the ground and transition states (for restricted rotation about the central C=C partial double bond) in compounds 2, 4–8, 10, 11 and 15–29

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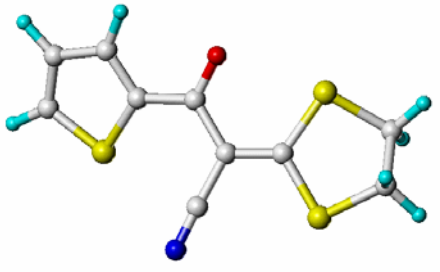
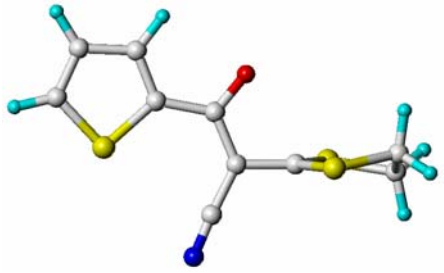
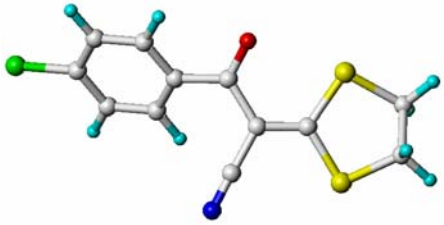
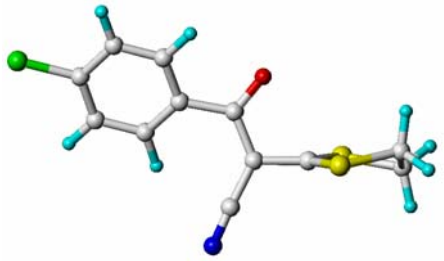
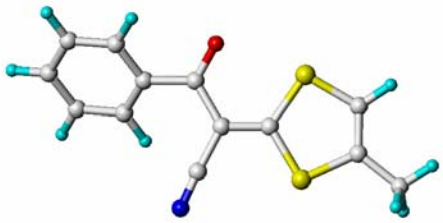
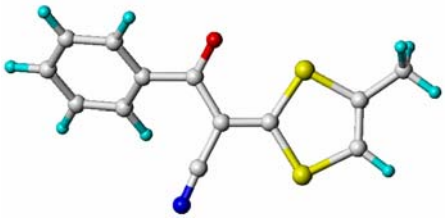
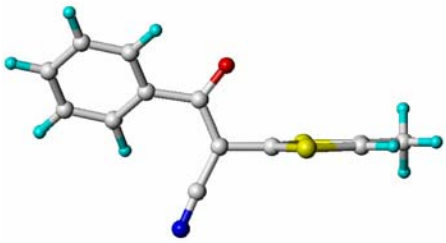
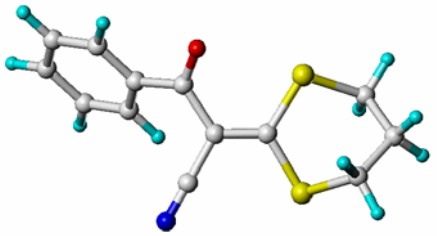
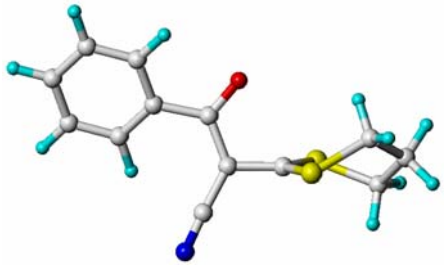
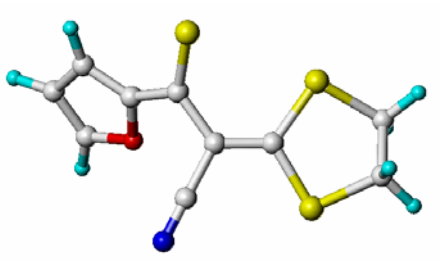
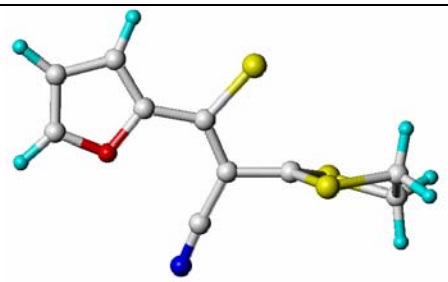
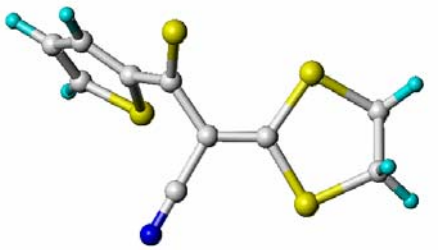
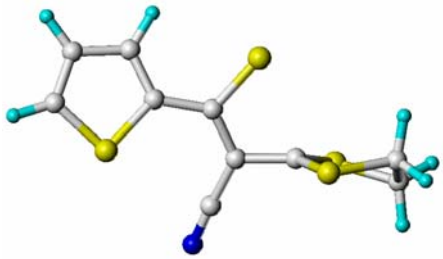
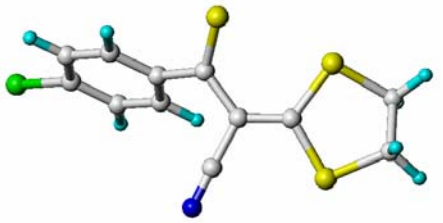
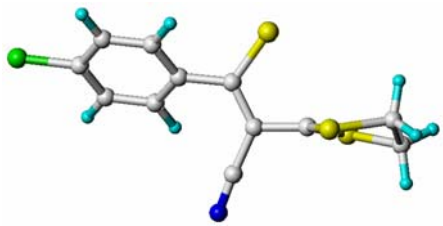
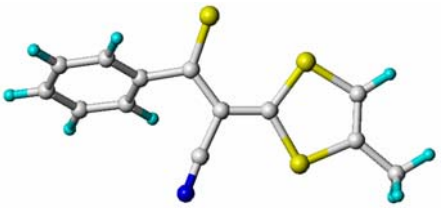
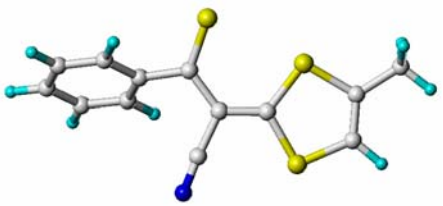
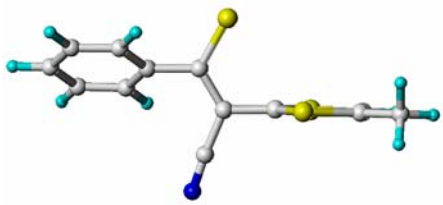
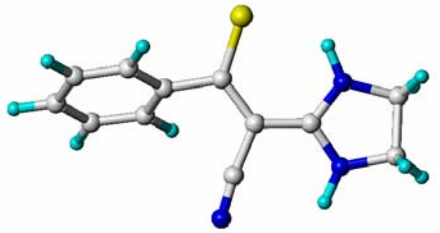
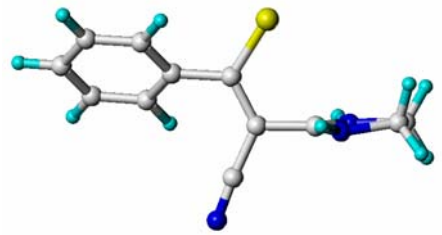
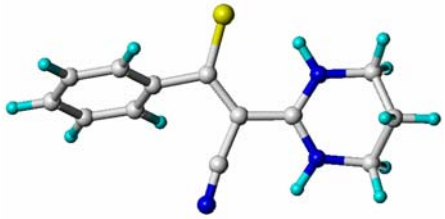
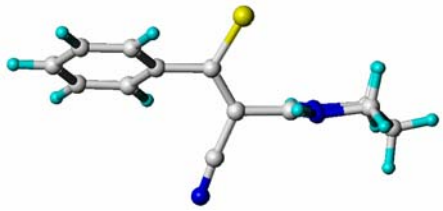
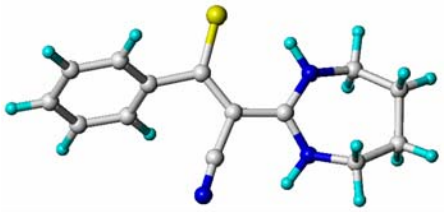
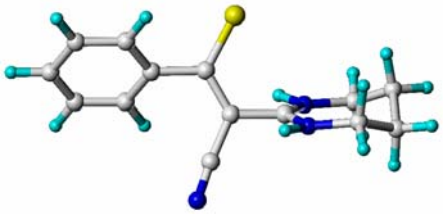
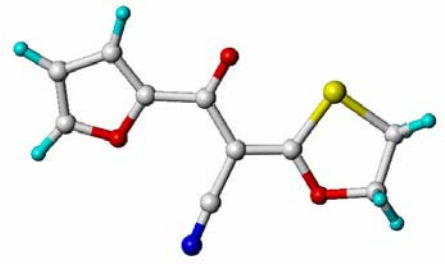
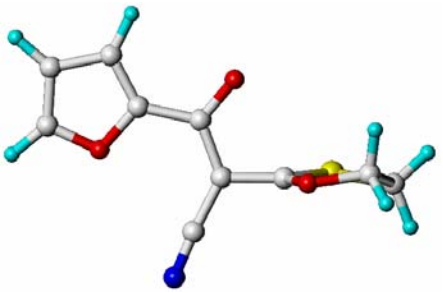
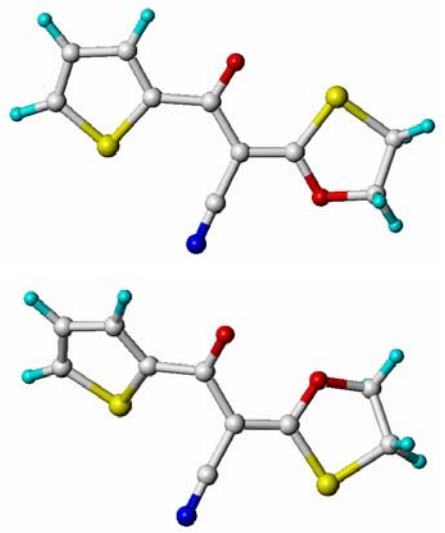
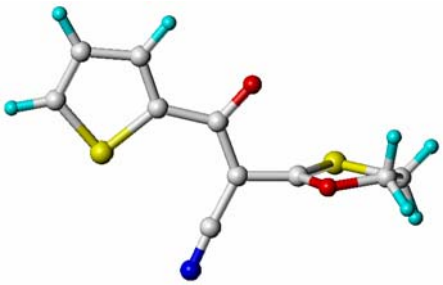
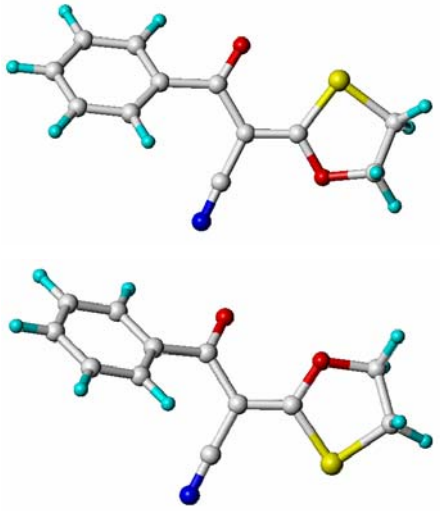
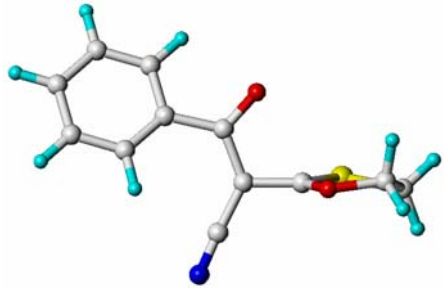
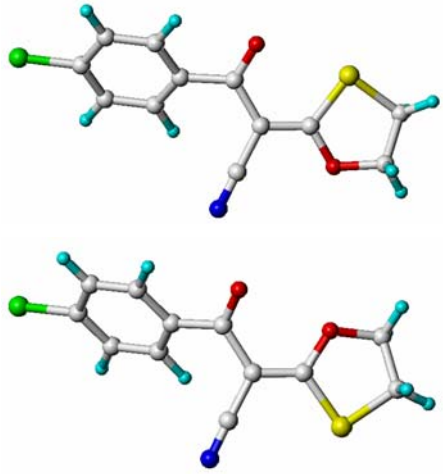
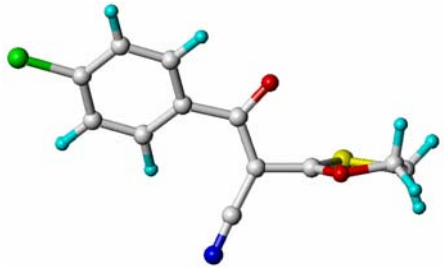
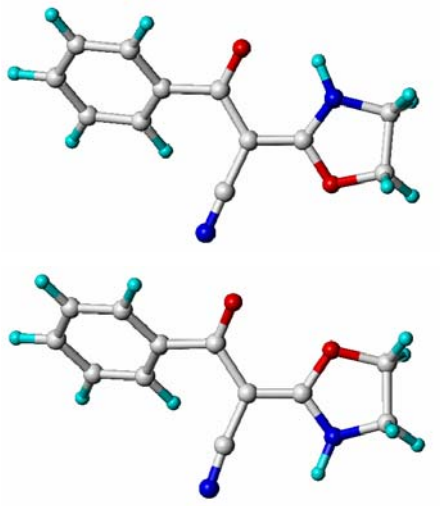
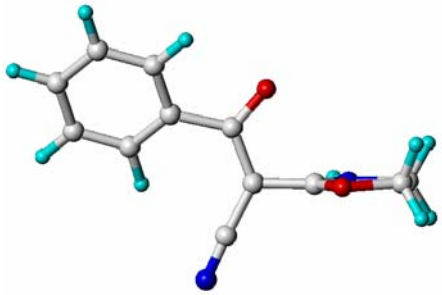
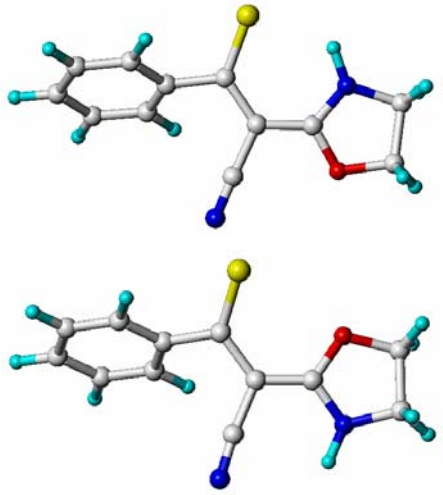
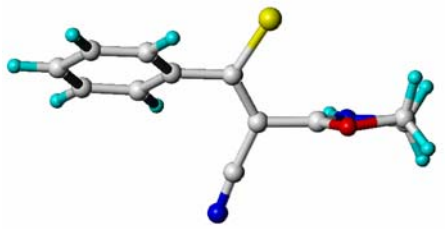
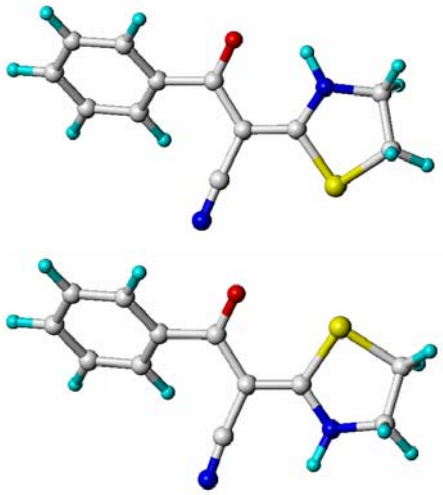
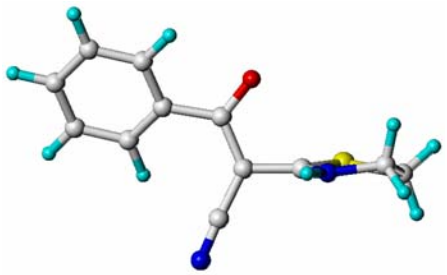
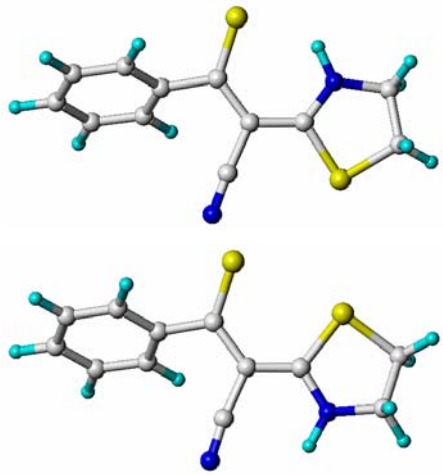
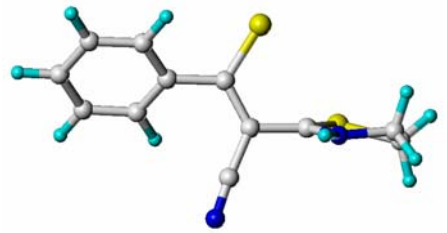
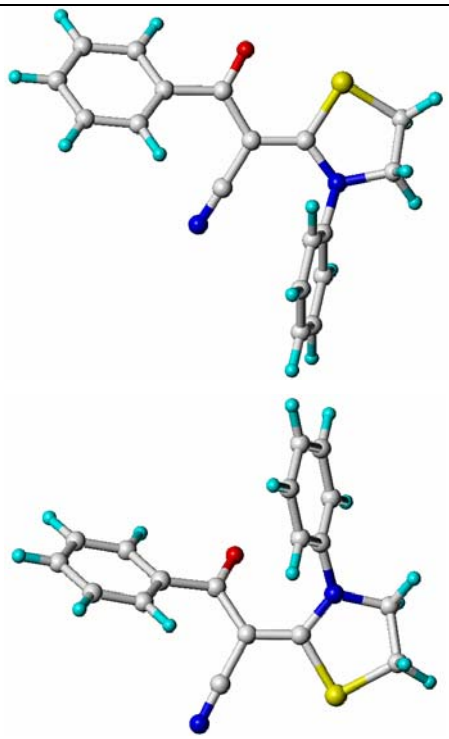
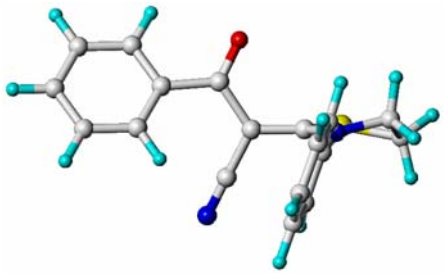
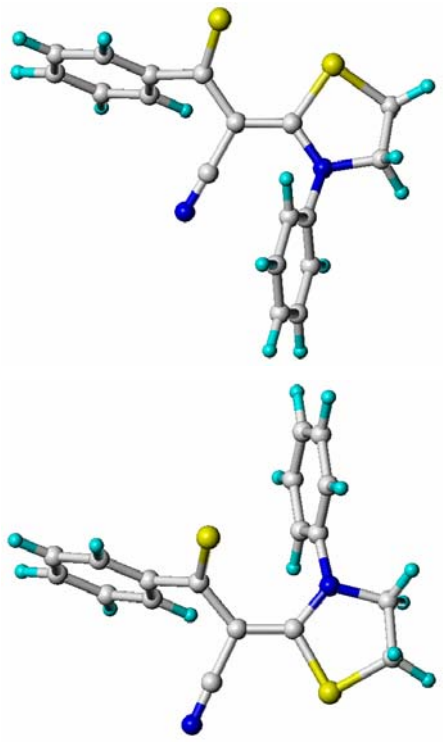
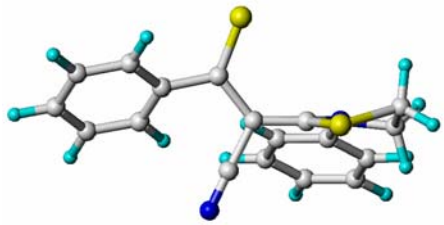
2		
4		
5	 	
6		

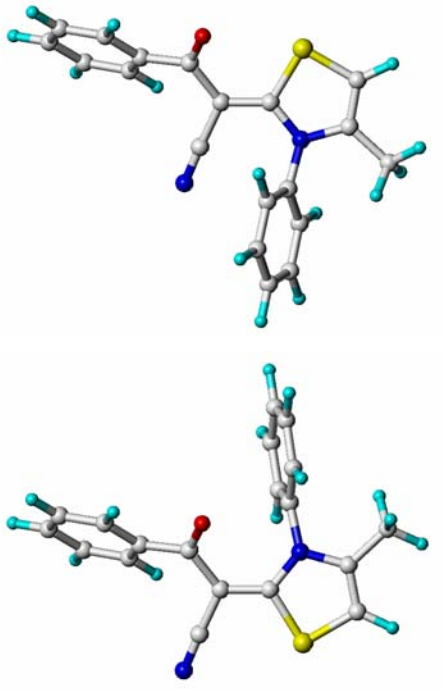
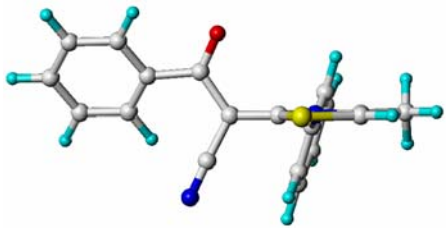
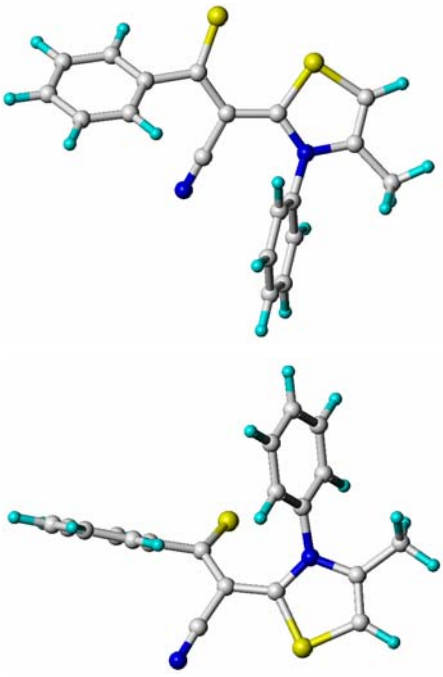
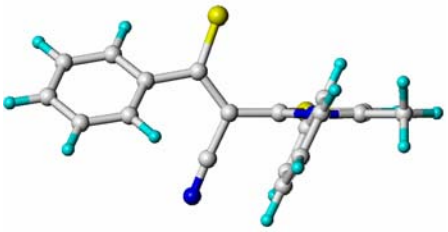
	ground state	transition state
7		
8		
10		
11	 	
15		

	ground state	transition state
16		
17		
18		
19		

	ground state	transition state
20		
21		
22		

	ground state	transition state
23		
24		
25		

	ground state	transition state
26		
27		

	ground state	transition state
28		
29		

Coordinates and computed total energies for the ground states (GS) and transition states of compounds 1 – 29

1

GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.354720(1)					
3	3	S	2	1.756590(2)	1	124.741(22)			
4	4	C	3	1.816480(3)	2	95.475(23)	1	-166.832(42)	0
5	5	C	4	1.517180(4)	3	108.311(24)	2	-35.563(43)	0
6	6	S	2	1.761860(5)	1	120.849(25)	3	-179.162(44)	0
7	7	C	1	1.439610(6)	2	117.975(26)	3	-177.108(45)	0
8	8	N	7	1.136840(7)	1	176.998(27)	2	22.916(46)	0
9	9	C	1	1.486700(8)	2	120.956(28)	3	-0.187(47)	0
10	10	C	9	1.471890(9)	1	120.943(29)	2	162.500(48)	0
11	11	C	10	1.347550(10)	9	128.853(30)	1	169.707(49)	0
12	12	C	11	1.429560(11)	10	105.964(31)	9	178.869(50)	0
13	13	C	12	1.345360(12)	11	105.464(32)	10	-0.306(51)	0
14	14	O	13	1.332120(13)	12	111.103(33)	11	0.135(52)	0
15	15	O	9	1.200440(14)	1	120.271(34)	2	-17.195(53)	0
16	16	H	4	1.082510(15)	3	107.341(35)	2	-156.076(54)	0
17	17	H	4	1.081990(16)	3	109.785(36)	2	85.834(55)	0
18	18	H	5	1.081480(17)	4	111.375(37)	3	-73.893(56)	0
19	19	H	5	1.081970(18)	4	111.807(38)	3	163.843(57)	0
20	20	H	11	1.069180(19)	10	125.759(39)	9	-1.180(58)	0
21	21	H	12	1.069700(20)	11	127.730(40)	10	179.713(59)	0
22	22	H	13	1.068160(21)	12	132.823(41)	11	-179.894(60)	0

E(RHF) = -1381.90420307

TS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.467980(1)					
3	3	S	2	1.689750(2)	1	121.363(22)			
4	4	C	3	1.821910(3)	2	97.336(23)	1	-172.244(42)	0
5	5	C	4	1.525310(4)	3	108.526(24)	2	-26.628(43)	0
6	6	S	2	1.690860(5)	1	121.351(25)	3	-179.625(44)	0
7	7	C	1	1.410910(6)	2	116.166(26)	3	96.082(45)	0
8	8	N	7	1.142820(7)	1	175.340(27)	2	-1.693(46)	0
9	9	C	1	1.418690(8)	2	112.044(28)	3	-86.216(47)	0
10	10	C	9	1.475840(9)	1	121.426(29)	2	-179.701(48)	0
11	11	C	10	1.345020(10)	9	129.077(30)	1	178.861(49)	0
12	12	C	11	1.433160(11)	10	105.956(31)	9	179.962(50)	0
13	13	C	12	1.343530(12)	11	105.479(32)	10	-0.012(51)	0
14	14	O	13	1.334870(13)	12	111.003(33)	11	0.000(52)	0
15	15	O	9	1.224220(14)	1	120.248(34)	2	0.128(53)	0
16	16	H	4	1.080980(15)	3	108.796(35)	2	-147.673(54)	0
17	17	H	4	1.081830(16)	3	107.843(36)	2	94.326(55)	0
18	18	H	5	1.081620(17)	4	111.402(37)	3	-82.292(56)	0
19	19	H	5	1.081000(18)	4	111.280(38)	3	155.741(57)	0

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 20  20  H    11   1.068850( 19)  10  125.613( 39)   9   -0.035( 58)   0
 21  21  H    12   1.070090( 20)  11  127.768( 40)  10  179.990( 59)   0
 22  22  H    13   1.068250( 21)  12  132.923( 41)  11  180.000( 60)   0
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E(RHF) =  -1381.83888920
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2

GS

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                    Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------------
  1   1  C
  2   2  C     1   1.355700(  1)
  3   3  S     2   1.755380(  2)   1  124.817( 22)
  4   4  C     3   1.816650(  3)   2   95.497( 23)   1 -167.039( 42)   0
  5   5  C     4   1.517110(  4)   3  108.335( 24)   2  -35.473( 43)   0
  6   6  S     2   1.761710(  5)   1  120.766( 25)   3 -179.189( 44)   0
  7   7  C     1   1.437620(  6)   2  117.772( 26)   3 -177.216( 45)   0
  8   8  N     7   1.137400(  7)   1  177.971( 27)   2   14.047( 46)   0
  9   9  C     1   1.488600(  8)   2  121.136( 28)   3    0.039( 47)   0
 10  10  C     9   1.485050(  9)   1  122.471( 29)   2  162.113( 48)   0
 11  11  C    10   1.356710( 10)   9  121.248( 30)   1  169.195( 49)   0
 12  12  C    11   1.423790( 11)  10  113.409( 31)   9  176.263( 50)   0
 13  13  C    12   1.349730( 12)  11  111.953( 32)  10   -0.768( 51)   0
 14  14  S    13   1.712810( 13)  12  112.699( 33)  11    0.880( 52)   0
 15  15  O     9   1.200550( 14)   1  118.748( 34)   2  -17.304( 53)   0
 16  16  H     4   1.082520( 15)   3  107.330( 35)   2 -155.982( 54)   0
 17  17  H     4   1.082000( 16)   3  109.789( 36)   2   85.936( 55)   0
 18  18  H     5   1.081450( 17)   4  111.401( 37)   3  -73.866( 56)   0
 19  19  H     5   1.081940( 18)   4  111.839( 38)   3  163.805( 57)   0
 20  20  H    11   1.071800( 19)  10  122.097( 39)   9   -3.162( 58)   0
 21  21  H    12   1.072850( 20)  11  124.040( 40)  10  179.450( 59)   0
 22  22  H    13   1.071460( 21)  12  127.498( 41)  11  179.973( 60)   0
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E(RHF) =  -1704.56390888
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TS

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                    Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------------
  1   1  C
  2   2  C     1   1.468590(  1)
  3   3  S     2   1.690250(  2)   1  121.391( 22)
  4   4  C     3   1.821780(  3)   2   97.307( 23)   1 -172.065( 42)   0
  5   5  C     4   1.525240(  4)   3  108.534( 24)   2  -26.582( 43)   0
  6   6  S     2   1.690810(  5)   1  121.309( 25)   3 -179.273( 44)   0
  7   7  C     1   1.407860(  6)   2  116.525( 26)   3   96.211( 45)   0
  8   8  N     7   1.143810(  7)   1  176.826( 27)   2   -3.604( 46)   0
  9   9  C     1   1.421010(  8)   2  111.892( 28)   3  -86.287( 47)   0
 10  10  C     9   1.488510(  9)   1  122.925( 29)   2 -179.831( 48)   0
 11  11  C    10   1.353030( 10)   9  121.795( 30)   1  178.634( 49)   0
 12  12  C    11   1.427600( 11)  10  113.392( 31)   9  179.673( 50)   0
 13  13  C    12   1.347850( 12)  11  112.068( 32)  10   -0.063( 51)   0
 14  14  S    13   1.717370( 13)  12  112.513( 33)  11    0.083( 52)   0
 15  15  O     9   1.224470( 14)   1  118.693( 34)   2    0.035( 53)   0
 16  16  H     4   1.080970( 15)   3  108.791( 35)   2 -147.618( 54)   0
 17  17  H     4   1.081820( 16)   3  107.858( 36)   2   94.382( 55)   0
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18	18	H	5	1.081620(17)	4	111.401(37)	3	-82.205(56)	0		
19	19	H	5	1.081000(18)	4	111.285(38)	3	155.823(57)	0		
20	20	H	11	1.071520(19)	10	121.835(39)	9	-0.242(58)	0		
21	21	H	12	1.073360(20)	11	123.985(40)	10	179.959(59)	0		
22	22	H	13	1.071530(21)	12	127.554(41)	11	179.980(60)	0		

E(RHF) = -1704.49982134

3

GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.353690(1)					
3	3	S	2	1.756340(2)	1	124.561(25)			
4	4	C	3	1.816400(3)	2	95.425(26)	1	-166.594(48)	0
5	5	C	4	1.517620(4)	3	108.284(27)	2	-35.809(49)	0
6	6	S	2	1.762030(5)	1	121.013(28)	3	-179.269(50)	0
7	7	C	1	1.438640(6)	2	118.268(29)	3	-176.603(51)	0
8	8	N	7	1.137410(7)	1	178.607(30)	2	9.079(52)	0
9	9	C	1	1.492500(8)	2	121.593(31)	3	-0.277(53)	0
10	10	C	9	1.496120(9)	1	120.757(32)	2	161.307(54)	0
11	11	C	10	1.392780(10)	9	117.417(33)	1	149.866(55)	0
12	12	C	11	1.381330(11)	10	120.311(34)	9	177.841(56)	0
13	13	C	12	1.387630(12)	11	119.895(35)	10	-1.212(57)	0
14	14	C	13	1.384180(13)	12	120.122(36)	11	0.126(58)	0
15	15	C	14	1.385340(14)	13	120.037(37)	12	0.814(59)	0
16	16	O	9	1.198890(15)	1	119.075(38)	2	-19.012(60)	0
17	17	H	4	1.082470(16)	3	107.341(39)	2	-156.260(61)	0
18	18	H	4	1.081990(17)	3	109.845(40)	2	85.621(62)	0
19	19	H	5	1.081430(18)	4	111.382(41)	3	-73.792(63)	0
20	20	H	5	1.081930(19)	4	111.810(42)	3	163.913(64)	0
21	21	H	11	1.073350(20)	10	119.100(43)	9	-2.179(65)	0
22	22	H	12	1.074920(21)	11	119.947(44)	10	179.138(66)	0
23	23	H	13	1.075360(22)	12	119.954(45)	11	-179.695(67)	0
24	24	H	14	1.074670(23)	13	120.246(46)	12	-179.390(68)	0
25	25	H	15	1.073240(24)	14	119.120(47)	13	-179.827(69)	0

E(RHF) = -1383.97905588

TS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.336720(1)					
3	3	S	2	1.813140(2)	1	124.783(25)			
4	4	C	3	1.886810(3)	2	94.511(26)	1	-166.058(48)	0
5	5	C	4	1.517220(4)	3	108.219(27)	2	-38.309(49)	0
6	6	S	2	1.818610(5)	1	120.949(28)	3	-179.727(50)	0
7	7	C	1	1.423430(6)	2	118.865(29)	3	-85.978(51)	0
8	8	N	7	1.140840(7)	1	178.620(30)	2	32.419(52)	0
9	9	C	1	1.490690(8)	2	121.066(31)	3	90.000(53)	0
10	10	C	9	1.488240(9)	1	120.143(32)	2	177.197(54)	0
11	11	C	10	1.389650(10)	9	116.681(33)	1	143.607(55)	0
12	12	C	11	1.379290(11)	10	120.431(34)	9	177.838(56)	0

13	13	C	12	1.385490(12)	11	119.818(35)	10	-1.330(57)	0
14	14	C	13	1.382980(13)	12	120.052(36)	11	-0.196(58)	0
15	15	C	14	1.383510(14)	13	120.136(37)	12	0.967(59)	0
16	16	O	9	1.218520(15)	1	119.505(38)	2	-3.678(60)	0
17	17	H	4	1.079550(16)	3	105.911(39)	2	-158.171(61)	0
18	18	H	4	1.077770(17)	3	108.767(40)	2	83.244(62)	0
19	19	H	5	1.077210(18)	4	112.059(41)	3	-69.907(63)	0
20	20	H	5	1.078790(19)	4	112.201(42)	3	164.769(64)	0
21	21	H	11	1.070330(20)	10	118.800(43)	9	-2.153(65)	0
22	22	H	12	1.071330(21)	11	119.972(44)	10	179.043(66)	0
23	23	H	13	1.071870(22)	12	120.020(45)	11	-179.830(67)	0
24	24	H	14	1.071200(23)	13	120.204(46)	12	-179.032(68)	0
25	25	H	15	1.069380(24)	14	119.214(47)	13	-179.380(69)	0

E(RHF) = -1383.88007229

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.354850(1)					
3	3	S	2	1.755200(2)	1	124.578(25)			
4	4	C	3	1.816660(3)	2	95.456(26)	1	-166.757(48)	0
5	5	C	4	1.517490(4)	3	108.300(27)	2	-35.619(49)	0
6	6	S	2	1.760940(5)	1	120.940(28)	3	-179.228(50)	0
7	7	C	1	1.438330(6)	2	118.308(29)	3	-176.672(51)	0
8	8	N	7	1.137400(7)	1	178.828(30)	2	5.026(52)	0
9	9	C	1	1.490350(8)	2	121.572(31)	3	-0.286(53)	0
10	10	C	9	1.497260(9)	1	120.867(32)	2	161.866(54)	0
11	11	C	10	1.392190(10)	9	117.353(33)	1	150.591(55)	0
12	12	C	11	1.380330(11)	10	120.756(34)	9	177.706(56)	0
13	13	C	12	1.385170(12)	11	119.030(35)	10	-1.190(57)	0
14	14	C	13	1.381530(13)	12	121.255(36)	11	0.127(58)	0
15	15	C	14	1.384640(14)	13	119.196(37)	12	0.765(59)	0
16	16	O	9	1.198680(15)	1	119.318(38)	2	-18.460(60)	0
17	17	H	4	1.082420(16)	3	107.339(39)	2	-156.086(61)	0
18	18	H	4	1.081920(17)	3	109.795(40)	2	85.809(62)	0
19	19	H	5	1.081370(18)	4	111.401(41)	3	-73.897(63)	0
20	20	H	5	1.081880(19)	4	111.806(42)	3	163.785(64)	0
21	21	H	11	1.073040(20)	10	119.216(43)	9	-2.263(65)	0
22	22	H	12	1.073030(21)	11	120.792(44)	10	179.183(66)	0
23	23	Cl	13	1.739900(22)	12	119.335(45)	11	-179.642(67)	0
24	24	H	14	1.072830(23)	13	120.272(46)	12	-179.399(68)	0
25	25	H	15	1.072730(24)	14	118.518(47)	13	-179.797(69)	0

E(RHF) = -1842.87827643

TS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.469110(1)					
3	3	S	2	1.688990(2)	1	121.053(25)			
4	4	C	3	1.821750(3)	2	97.350(26)	1	-172.748(48)	0

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  5   5  C    4   1.525320(  4)   3  108.471( 27)   2  -26.480( 49)   0
  6   6  S    2   1.690860(  5)   1  121.629( 28)   3 -179.717( 50)   0
  7   7  C    1   1.408460(  6)   2  116.610( 29)   3   97.432( 51)   0
  8   8  N    7   1.143740(  7)   1  177.333( 30)   2  -12.036( 52)   0
  9   9  C    1   1.423600(  8)   2  111.915( 31)   3  -89.771( 53)   0
 10  10  C    9   1.501070(  9)   1  122.002( 32)   2  179.683( 54)   0
 11  11  C   10   1.391660( 10)   9  116.993( 33)   1  155.325( 55)   0
 12  12  C   11   1.381320( 11)  10  120.967( 34)   9  179.180( 56)   0
 13  13  C   12   1.384140( 12)  11  119.009( 35)  10   -0.917( 57)   0
 14  14  C   13   1.380950( 13)  12  121.172( 36)  11    0.000( 58)   0
 15  15  C   14   1.385560( 14)  13  119.258( 37)  12    0.580( 59)   0
 16  16  O    9   1.223100( 15)   1  118.838( 38)   2   -0.953( 60)   0
 17  17  H    4   1.080950( 16)   3  108.792( 39)   2 -147.506( 61)   0
 18  18  H    4   1.081800( 17)   3  107.841( 40)   2   94.481( 62)   0
 19  19  H    5   1.081610( 18)   4  111.409( 41)   3  -82.114( 63)   0
 20  20  H    5   1.080970( 19)   4  111.283( 42)   3  155.895( 64)   0
 21  21  H   11   1.072550( 20)  10  118.844( 43)   9   -0.551( 65)   0
 22  22  H   12   1.073340( 21)  11  120.809( 44)  10  179.428( 66)   0
 23  23  Cl  13   1.743820( 22)  12  119.375( 45)  11 -179.722( 67)   0
 24  24  H   14   1.073120( 23)  13  120.258( 46)  12 -179.381( 68)   0
 25  25  H   15   1.071980( 24)  14  118.472( 47)  13 -179.642( 69)   0
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E(RHF) =  -1842.81371753
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GS

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                    Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------------
  1   1  C
  2   2  C    1   1.364310(  1)
  3   3  S    2   1.745400(  2)   1  125.128( 26)
  4   4  C    3   1.753150(  3)   2   95.274( 27)   1 -177.717( 50)   0
  5   5  C    4   1.319040(  4)   3  119.268( 28)   2   -1.681( 51)   0
  6   6  S    2   1.749580(  5)   1  121.324( 29)   3 -179.765( 52)   0
  7   7  C    5   1.502410(  6)   4  127.262( 30)   3 -179.301( 53)   0
  8   8  C    1   1.435050(  7)   2  117.437( 31)   3 -176.969( 54)   0
  9   9  N    8   1.138070(  8)   1  177.267( 32)   2    5.242( 55)   0
 10  10  C    1   1.480230(  9)   2  120.813( 33)   3   -0.258( 56)   0
 11  11  C   10   1.497200( 10)   1  121.363( 34)   2  172.422( 57)   0
 12  12  C   11   1.392800( 11)  10  117.161( 35)   1  146.004( 58)   0
 13  13  C   12   1.381450( 12)  11  120.348( 36)  10  178.020( 59)   0
 14  14  C   13   1.387480( 13)  12  119.907( 37)  11   -1.330( 60)   0
 15  15  C   14   1.384010( 14)  13  120.065( 38)  12    0.108( 61)   0
 16  16  C   15   1.385610( 15)  14  120.098( 39)  13    0.888( 62)   0
 17  17  O   10   1.202660( 16)   1  118.880( 40)   2   -8.293( 63)   0
 18  18  H    4   1.073460( 17)   3  116.605( 41)   2  179.043( 64)   0
 19  19  H    7   1.084930( 18)   5  110.994( 42)   4  119.989( 65)   0
 20  20  H    7   1.082480( 19)   5  109.956( 43)   4    0.049( 66)   0
 21  21  H    7   1.084880( 20)   5  111.037( 44)   4 -119.942( 67)   0
 22  22  H   12   1.073400( 21)  11  119.122( 45)  10   -1.976( 68)   0
 23  23  H   13   1.074970( 22)  12  119.925( 46)  11  179.090( 69)   0
 24  24  H   14   1.075370( 23)  13  119.982( 47)  12 -179.639( 70)   0
 25  25  H   15   1.074720( 24)  14  120.240( 48)  13 -179.264( 71)   0
 26  26  H   16   1.072920( 25)  15  119.064( 49)  14 -179.716( 72)   0
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E(RHF) =  -1421.83432136
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TS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.463850(1)					
3	3	S	2	1.679300(2)	1	123.349(26)			
4	4	C	3	1.729380(3)	2	97.174(27)	1	-178.609(50)	0
5	5	C	4	1.334480(4)	3	116.859(28)	2	-0.112(51)	0
6	6	S	2	1.684450(5)	1	122.580(29)	3	-178.661(52)	0
7	7	C	5	1.504470(6)	4	126.521(30)	3	179.987(53)	0
8	8	C	1	1.410310(7)	2	116.352(31)	3	-89.601(54)	0
9	9	N	8	1.143820(8)	1	177.022(32)	2	-6.864(55)	0
10	10	C	1	1.429840(9)	2	113.245(33)	3	84.979(56)	0
11	11	C	10	1.502120(10)	1	121.574(34)	2	178.825(57)	0
12	12	C	11	1.392500(11)	10	117.023(35)	1	152.396(58)	0
13	13	C	12	1.382120(12)	11	120.571(36)	10	179.163(59)	0
14	14	C	13	1.387210(13)	12	119.959(37)	11	-1.044(60)	0
15	15	C	14	1.383870(14)	13	119.861(38)	12	0.023(61)	0
16	16	C	15	1.386410(15)	14	120.199(39)	13	0.671(62)	0
17	17	O	10	1.221090(16)	1	119.289(40)	2	-1.785(63)	0
18	18	H	4	1.072730(17)	3	118.558(41)	2	179.859(64)	0
19	19	H	7	1.084190(18)	5	110.972(42)	4	120.022(65)	0
20	20	H	7	1.082130(19)	5	109.892(43)	4	0.145(66)	0
21	21	H	7	1.084100(20)	5	110.914(44)	4	-119.684(67)	0
22	22	H	12	1.072940(21)	11	118.755(45)	10	-0.584(68)	0
23	23	H	13	1.075500(22)	12	119.916(46)	11	179.335(69)	0
24	24	H	14	1.075740(23)	13	120.086(47)	12	-179.704(70)	0
25	25	H	15	1.075200(24)	14	120.188(48)	13	-179.347(71)	0
26	26	H	16	1.072320(25)	15	119.041(49)	14	-179.700(72)	0

E(RHF) = -1421.77918214

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.349590(1)					
3	3	C	1	1.502640(2)	2	122.462(28)			
4	4	C	3	1.495060(3)	1	120.063(29)	2	146.916(54)	0
5	5	C	4	1.392870(4)	3	117.697(30)	1	155.657(55)	0
6	6	C	5	1.381180(5)	4	120.282(31)	3	177.950(56)	0
7	7	C	6	1.387850(6)	5	119.896(32)	4	-0.976(57)	0
8	8	C	7	1.384280(7)	6	120.164(33)	5	0.122(58)	0
9	9	C	8	1.385150(8)	7	119.976(34)	6	0.666(59)	0
10	10	C	1	1.440900(9)	2	119.657(35)	3	-176.158(60)	0
11	11	N	10	1.137070(10)	1	179.192(36)	2	162.179(61)	0
12	12	O	3	1.196160(11)	1	119.201(37)	2	-33.176(62)	0
13	13	S	2	1.766770(12)	1	122.459(38)	3	-0.134(63)	0
14	14	C	13	1.819070(13)	2	100.158(39)	1	-152.878(64)	0
15	15	C	14	1.530290(14)	13	114.783(40)	2	-67.985(65)	0
16	16	C	15	1.530530(15)	14	112.799(41)	13	37.422(66)	0
17	17	S	2	1.770710(16)	1	119.601(42)	3	-178.684(67)	0
18	18	H	5	1.073250(17)	4	119.059(43)	3	-2.079(68)	0
19	19	H	6	1.074900(18)	5	119.965(44)	4	179.263(69)	0

20	20	H	7	1.075370(19)	6	119.932(45)	5	-179.786(70)	0		
21	21	H	8	1.074670(20)	7	120.246(46)	6	-179.560(71)	0		
22	22	H	9	1.073560(21)	8	119.186(47)	7	-179.904(72)	0		
23	23	H	14	1.080810(22)	13	108.365(48)	2	56.569(73)	0		
24	24	H	14	1.082790(23)	13	104.310(49)	2	170.583(74)	0		
25	25	H	15	1.085080(24)	14	108.178(50)	13	159.500(75)	0		
26	26	H	15	1.084990(25)	14	110.165(51)	13	-83.492(76)	0		
27	27	H	16	1.082270(26)	15	111.247(52)	14	152.842(77)	0		
28	28	H	16	1.080450(27)	15	111.174(53)	14	-87.455(78)	0		

E(RHF) = -1423.00276442

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.066936	0.681818	0.095702
2	6	-1.354814	0.314891	0.036619
3	6	0.901625	-0.448976	-0.133278
4	6	2.397048	-0.344137	-0.122302
5	6	3.114983	-1.493556	0.196033
6	6	4.497095	-1.475861	0.211298
7	6	5.178401	-0.311236	-0.110617
8	6	4.472431	0.831127	-0.446458
9	6	3.086520	0.817314	-0.450026
10	6	0.374482	1.956216	0.611353
11	7	0.567391	3.006551	1.021597
12	8	0.374282	-1.537167	-0.331967
13	16	-2.186985	-0.086621	1.468853
14	6	-3.442071	-1.265159	0.855510
15	6	-4.440790	-0.751046	-0.181588
16	6	-3.888648	0.377144	-1.051636
17	16	-2.116942	0.302558	-1.472836
18	1	2.575503	-2.392198	0.425397
19	1	5.042362	-2.366648	0.467874
20	1	6.254010	-0.296595	-0.103237
21	1	4.996151	1.733482	-0.706174
22	1	2.555300	1.709527	-0.718886
23	1	-2.863665	-2.086106	0.454397
24	1	-3.943594	-1.617341	1.746741
25	1	-4.736038	-1.591583	-0.798734
26	1	-5.334628	-0.378299	0.305427
27	1	-4.395991	0.419760	-2.006270
28	1	-4.031772	1.331270	-0.561917

E(RHF) = -1422.93601103

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.349610(1)					
3	3	S	2	1.760760(2)	1	125.557(22)			
4	4	C	3	1.816040(3)	2	95.193(23)	1	-161.277(42)	0
5	5	C	4	1.518010(4)	3	107.561(24)	2	-38.763(43)	0

6	6	S	2	1.766880(5)	1	120.555(25)	3	-177.805(44)	0
7	7	C	1	1.443220(6)	2	117.820(26)	3	-178.132(45)	0
8	8	N	7	1.136830(7)	1	178.138(27)	2	65.021(46)	0
9	9	C	1	1.485500(8)	2	125.648(28)	3	0.460(47)	0
10	10	C	9	1.451160(9)	1	116.349(29)	2	137.893(48)	0
11	11	C	10	1.354520(10)	9	132.058(30)	1	163.586(49)	0
12	12	C	11	1.424240(11)	10	106.342(31)	9	179.816(50)	0
13	13	C	12	1.347480(12)	11	105.464(32)	10	-0.167(51)	0
14	14	O	13	1.327940(13)	12	111.188(33)	11	0.053(52)	0
15	15	S	9	1.633220(14)	1	122.636(34)	2	-43.507(53)	0
16	16	H	4	1.082330(15)	3	107.307(35)	2	-158.972(54)	0
17	17	H	4	1.081700(16)	3	110.092(36)	2	82.575(55)	0
18	18	H	5	1.081290(17)	4	111.243(37)	3	-72.903(56)	0
19	19	H	5	1.082080(18)	4	111.732(38)	3	164.916(57)	0
20	20	H	11	1.068710(19)	10	125.788(39)	9	-0.675(58)	0
21	21	H	12	1.069560(20)	11	127.675(40)	10	179.576(59)	0
22	22	H	13	1.068330(21)	12	132.615(41)	11	-179.841(60)	0

E(RHF) = -1704.53294824

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.089675	0.527535	-0.271338
2	6	-0.151766	0.516938	1.206849
3	16	1.272024	0.679834	2.155362
4	6	0.431869	0.460892	3.747236
5	6	-0.923713	1.151191	3.659264
6	16	-1.627785	0.801728	2.014987
7	6	-0.318852	1.777880	-0.918152
8	7	-0.511068	2.808636	-1.363604
9	6	0.090448	-0.720473	-0.799954
10	6	0.277686	-0.986025	-2.213035
11	6	0.310269	-2.144281	-2.904960
12	6	0.526717	-1.785655	-4.271324
13	6	0.604455	-0.442946	-4.282173
14	8	0.457626	0.055960	-3.056294
15	16	0.035828	-1.996459	0.349605
16	1	1.046477	0.896015	4.523450
17	1	0.324438	-0.600319	3.929886
18	1	-0.831064	2.223123	3.769547
19	1	-1.606673	0.774813	4.408104
20	1	0.190908	-3.122476	-2.491221
21	1	0.609262	-2.439875	-5.113655
22	1	0.757406	0.268579	-5.064284

E(RHF) = -1704.48838241

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.342860(1)					
3	3	S	2	1.763660(2)	1	124.365(22)			

4	4	C	3	1.815490(3)	2	95.202(23)	1	-162.271(42)	0
5	5	C	4	1.519390(4)	3	107.555(24)	2	-38.248(43)	0
6	6	S	2	1.766880(5)	1	121.559(25)	3	-178.125(44)	0
7	7	C	1	1.441030(6)	2	119.210(26)	3	-177.736(45)	0
8	8	N	7	1.137130(7)	1	179.253(27)	2	95.709(46)	0
9	9	C	1	1.498470(8)	2	125.152(28)	3	0.692(47)	0
10	10	C	9	1.460330(9)	1	116.249(29)	2	122.328(48)	0
11	11	C	10	1.360840(10)	9	126.997(30)	1	159.101(49)	0
12	12	C	11	1.421420(11)	10	113.284(31)	9	178.426(50)	0
13	13	C	12	1.351820(12)	11	112.249(32)	10	-0.395(51)	0
14	14	S	13	1.711040(13)	12	112.569(33)	11	0.563(52)	0
15	15	S	9	1.627460(14)	1	120.992(34)	2	-58.973(53)	0
16	16	H	4	1.082200(15)	3	107.418(35)	2	-158.414(54)	0
17	17	H	4	1.081510(16)	3	110.041(36)	2	83.054(55)	0
18	18	H	5	1.081160(17)	4	111.181(37)	3	-72.966(56)	0
19	19	H	5	1.082070(18)	4	111.614(38)	3	164.981(57)	0
20	20	H	11	1.071680(19)	10	122.570(39)	9	-2.096(58)	0
21	21	H	12	1.072750(20)	11	123.882(40)	10	179.539(59)	0
22	22	H	13	1.071330(21)	12	127.330(41)	11	-179.526(60)	0

E(RHF) = -2027.19118707

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.135442	0.571518	-0.094736
2	6	-1.544524	0.151536	-0.009220
3	16	-2.283539	-0.197514	1.509080
4	6	-3.865875	-0.722696	0.798560
5	6	-4.167923	0.186183	-0.386590
6	16	-2.616444	0.439979	-1.307847
7	6	0.121090	1.964857	-0.255581
8	7	0.273015	3.087974	-0.375809
9	6	0.741085	-0.485083	-0.148950
10	6	2.198068	-0.372896	-0.095208
11	6	3.070553	-1.312789	-0.539618
12	6	4.435452	-0.961418	-0.329527
13	6	4.565475	0.235154	0.280011
14	16	3.053658	0.976736	0.600994
15	16	-0.033370	-2.004023	-0.336868
16	1	-4.628050	-0.642075	1.561644
17	1	-3.776334	-1.756622	0.491741
18	1	-4.536102	1.150355	-0.063369
19	1	-4.888706	-0.263380	-1.055402
20	1	2.747857	-2.224028	-1.002141
21	1	5.263256	-1.579046	-0.620072
22	1	5.474334	0.729941	0.557646

E(RHF) = -2027.14747103

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							

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  2   2  C     1   1.354990(  1)
  3   3  S     2   1.757510(  2)   1  125.866( 25)
  4   4  C     3   1.816810(  3)   2   95.275( 26)   1 -161.598( 48)   0
  5   5  C     4   1.517340(  4)   3  107.647( 27)   2  -38.514( 49)   0
  6   6  S     2   1.766260(  5)   1  120.238( 28)   3 -177.853( 50)   0
  7   7  C     1   1.444740(  6)   2  117.076( 29)   3 -178.587( 51)   0
  8   8  N     7   1.137020(  7)   1  178.465( 30)   2   33.556( 52)   0
  9   9  C     1   1.481340(  8)   2  126.537( 31)   3    0.535( 53)   0
 10  10  C     9   1.488240(  9)   1  116.359( 32)   2  144.482( 54)   0
 11  11  C    10   1.393700( 10)   9  120.656( 33)   1  142.013( 55)   0
 12  12  C    11   1.381710( 11)  10  120.417( 34)   9  178.189( 56)   0
 13  13  C    12   1.386630( 12)  11  120.131( 35)  10   -1.100( 57)   0
 14  14  C    13   1.384840( 13)  12  119.953( 36)  11    0.517( 58)   0
 15  15  C    14   1.383240( 14)  13  119.989( 37)  12    0.656( 59)   0
 16  16  S     9   1.628830( 15)   1  122.205( 38)   2  -35.953( 60)   0
 17  17  H     4   1.082330( 16)   3  107.254( 39)   2 -158.770( 61)   0
 18  18  H     4   1.081810( 17)   3  110.052( 40)   2   82.872( 62)   0
 19  19  H     5   1.081330( 18)   4  111.303( 41)   3  -73.047( 63)   0
 20  20  H     5   1.082030( 19)   4  111.788( 42)   3  164.682( 64)   0
 21  21  H    11   1.072760( 20)  10  119.479( 43)   9   -2.456( 65)   0
 22  22  H    12   1.074840( 21)  11  119.717( 44)  10  178.989( 66)   0
 23  23  H    13   1.075220( 22)  12  120.029( 45)  11 -179.627( 67)   0
 24  24  H    14   1.074720( 23)  13  120.274( 46)  12 -179.696( 68)   0
 25  25  H    15   1.074170( 24)  14  119.334( 47)  13 -179.987( 69)   0
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E(RHF) =  -1706.60438521
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TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.036833	0.601915	0.018840
2	6	-0.019593	0.596837	1.497041
3	16	1.442362	0.563824	2.372464
4	6	0.667418	0.363291	4.002064
5	6	-0.642412	1.141847	4.001764
6	16	-1.434245	0.907678	2.377288
7	6	-0.091387	1.890879	-0.585400
8	7	-0.131211	2.949894	-1.006350
9	6	-0.002632	-0.635185	-0.581408
10	6	0.018602	-0.779492	-2.064215
11	6	0.893597	-1.690962	-2.650598
12	6	0.933619	-1.836469	-4.024436
13	6	0.080865	-1.096190	-4.829635
14	6	-0.807813	-0.206068	-4.253268
15	6	-0.834828	-0.041860	-2.877802
16	16	-0.029179	-2.002737	0.437737
17	1	1.346979	0.734526	4.756676
18	1	0.499771	-0.693875	4.160487
19	1	-0.477621	2.200910	4.147781
20	1	-1.316024	0.778834	4.765337
21	1	1.536068	-2.280730	-2.025412
22	1	1.623219	-2.533338	-4.465942
23	1	0.106334	-1.217849	-5.897867
24	1	-1.480442	0.363213	-4.869064
25	1	-1.534441	0.647552	-2.445050

E(RHF) = -1706.55812810

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.356700(1)					
3	3	S	2	1.756130(2)	1	125.911(25)			
4	4	C	3	1.817070(3)	2	95.315(26)	1	-161.868(48)	0
5	5	C	4	1.517180(4)	3	107.670(27)	2	-38.293(49)	0
6	6	S	2	1.765100(5)	1	120.132(28)	3	-177.851(50)	0
7	7	C	1	1.444610(6)	2	117.018(29)	3	-178.593(51)	0
8	8	N	7	1.137010(7)	1	178.631(30)	2	31.547(52)	0
9	9	C	1	1.479120(8)	2	126.545(31)	3	0.497(53)	0
10	10	C	9	1.489260(9)	1	116.397(32)	2	145.885(54)	0
11	11	C	10	1.392890(10)	9	120.712(33)	1	141.761(55)	0
12	12	C	11	1.380840(11)	10	120.846(34)	9	177.988(56)	0
13	13	C	12	1.384090(12)	11	119.274(35)	10	-1.092(57)	0
14	14	C	13	1.382270(13)	12	121.077(36)	11	0.560(58)	0
15	15	C	14	1.382440(14)	13	119.144(37)	12	0.576(59)	0
16	16	S	9	1.628500(15)	1	122.516(38)	2	-34.471(60)	0
17	17	H	4	1.082280(16)	3	107.237(39)	2	-158.563(61)	0
18	18	H	4	1.081770(17)	3	109.999(40)	2	83.108(62)	0
19	19	H	5	1.081310(18)	4	111.339(41)	3	-73.134(63)	0
20	20	H	5	1.081970(19)	4	111.788(42)	3	164.558(64)	0
21	21	H	11	1.072500(20)	10	119.625(43)	9	-2.586(65)	0
22	22	H	12	1.073000(21)	11	120.551(44)	10	179.040(66)	0
23	23	Cl	13	1.739240(22)	12	119.455(45)	11	-179.482(67)	0
24	24	H	14	1.072890(23)	13	120.291(46)	12	-179.722(68)	0
25	25	H	15	1.073770(24)	14	118.762(47)	13	-179.943(69)	0

E(RHF) = -2165.50350548

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.859920	0.541639	0.163025
2	6	-2.301661	0.215254	0.076861
3	16	-3.137617	-0.463455	1.394586
4	6	-4.686291	-0.754247	0.491292
5	6	-4.864980	0.372747	-0.518543
6	16	-3.231876	0.753983	-1.232483
7	6	-0.559041	1.864468	0.597118
8	7	-0.381511	2.933872	0.950666
9	6	-0.000335	-0.473852	-0.178617
10	6	1.477560	-0.293358	-0.118299
11	6	2.270459	-1.305368	0.416340
12	6	3.642726	-1.165723	0.487826
13	6	4.232734	-0.015166	-0.005814
14	6	3.470612	0.992560	-0.562143
15	6	2.093788	0.851706	-0.609618
16	16	-0.684017	-1.943483	-0.710481
17	1	-5.501459	-0.780996	1.201017

18	1	-4.606114	-1.715932	0.001991
19	1	-5.246358	1.270924	-0.051769
20	1	-5.528391	0.080277	-1.320295
21	1	1.808139	-2.204426	0.775006
22	1	4.248576	-1.942934	0.912855
23	17	5.965125	0.159249	0.068598
24	1	3.940671	1.874882	-0.952053
25	1	1.510632	1.637196	-1.050102

E(RHF) = -2165.45825182

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.377370(1)					
3	3	S	2	1.738620(2)	1	127.061(26)			
4	4	C	3	1.752000(3)	2	95.671(27)	1	-176.087(50)	0
5	5	C	4	1.319570(4)	3	119.004(28)	2	-2.500(51)	0
6	6	S	2	1.750180(5)	1	119.797(29)	3	-179.066(52)	0
7	7	C	5	1.502800(6)	4	127.234(30)	3	-178.894(53)	0
8	8	C	1	1.443460(7)	2	114.954(31)	3	-177.573(54)	0
9	9	N	8	1.137570(8)	1	176.296(32)	2	13.618(55)	0
10	10	C	1	1.455450(9)	2	126.804(33)	3	0.624(56)	0
11	11	C	10	1.494580(10)	1	117.073(34)	2	166.765(57)	0
12	12	C	11	1.391750(11)	10	120.149(35)	1	130.708(58)	0
13	13	C	12	1.382730(12)	11	120.330(36)	10	178.246(59)	0
14	14	C	13	1.385960(13)	12	120.151(37)	11	-1.437(60)	0
15	15	C	14	1.384800(14)	13	119.870(38)	12	0.504(61)	0
16	16	C	15	1.383660(15)	14	120.076(39)	13	0.808(62)	0
17	17	S	10	1.640830(16)	1	123.589(40)	2	-12.796(63)	0
18	18	H	4	1.073330(17)	3	116.507(41)	2	178.645(64)	0
19	19	H	7	1.084790(18)	5	110.953(42)	4	119.915(65)	0
20	20	H	7	1.082370(19)	5	109.939(43)	4	-0.011(66)	0
21	21	H	7	1.084710(20)	5	111.016(44)	4	-120.010(67)	0
22	22	H	12	1.073290(21)	11	119.536(45)	10	-2.121(68)	0
23	23	H	13	1.074960(22)	12	119.677(46)	11	178.953(69)	0
24	24	H	14	1.075220(23)	13	120.078(47)	12	-179.435(70)	0
25	25	H	15	1.074820(24)	14	120.257(48)	13	-179.498(71)	0
26	26	H	16	1.074400(25)	15	119.433(49)	14	179.987(72)	0

E(RHF) = -1744.45944489

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.141708	0.534981	-0.117165
2	6	-0.030748	0.393469	1.345206
3	16	1.441263	0.231180	2.150100
4	6	0.811719	0.202458	3.772401
5	6	-0.513595	0.333459	3.848950
6	16	-1.367263	0.491721	2.353383
7	6	-0.278152	1.883647	-0.558206
8	7	-0.380663	2.986182	-0.832686

9	6	-0.081785	-0.605102	-0.903976
10	16	0.110855	-2.141863	-0.211590
11	6	-0.219499	-0.470443	-2.386058
12	6	0.692901	-1.107069	-3.223508
13	6	0.577855	-0.995107	-4.596330
14	6	-0.466384	-0.271587	-5.152855
15	6	-1.390354	0.344425	-4.327889
16	6	-1.263427	0.253263	-2.951093
17	6	1.762901	0.037468	4.926459
18	1	2.496940	0.835122	4.941769
19	1	2.289691	-0.907409	4.858522
20	1	1.216014	0.058483	5.859804
21	1	-1.076621	0.342591	4.761609
22	1	-1.989897	0.732758	-2.322501
23	1	-2.209245	0.898450	-4.750245
24	1	-0.560285	-0.194111	-6.221429
25	1	1.296968	-1.480160	-5.231867
26	1	1.485051	-1.688781	-2.792766

E(RHF) = -1744.42204899

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.399370(1)					
3	3	N	2	1.330340(2)	1	126.663(27)			
4	4	C	3	1.450210(3)	2	111.975(28)	1	-172.953(52)	0
5	5	C	4	1.535650(4)	3	101.245(29)	2	-19.339(53)	0
6	6	N	2	1.348490(5)	1	124.699(30)	3	-179.383(54)	0
7	7	C	1	1.425170(6)	2	115.089(31)	3	-173.775(55)	0
8	8	N	7	1.141050(7)	1	175.044(32)	2	2.177(56)	0
9	9	C	1	1.452200(8)	2	120.400(33)	3	2.869(57)	0
10	10	O	9	1.215380(9)	1	121.056(34)	2	-4.611(58)	0
11	11	C	9	1.501690(10)	1	120.754(35)	2	176.188(59)	0
12	12	C	11	1.389350(11)	9	123.406(36)	1	-37.934(60)	0
13	13	C	12	1.386210(12)	11	120.229(37)	9	-177.248(61)	0
14	14	C	13	1.383730(13)	12	120.145(38)	11	-0.622(62)	0
15	15	C	14	1.387410(14)	13	119.943(39)	12	0.869(63)	0
16	16	C	15	1.381760(15)	14	119.941(40)	13	0.110(64)	0
17	17	H	16	1.073270(16)	15	120.517(41)	14	178.560(65)	0
18	18	H	15	1.075250(17)	14	120.140(42)	13	179.663(66)	0
19	19	H	14	1.075540(18)	13	120.018(43)	12	-179.415(67)	0
20	20	H	13	1.074970(19)	12	119.639(44)	11	179.495(68)	0
21	21	H	12	1.072770(20)	11	120.676(45)	9	1.829(69)	0
22	22	H	5	1.085560(21)	4	111.448(46)	3	-95.116(70)	0
23	23	H	5	1.080670(22)	4	112.756(47)	3	142.012(71)	0
24	24	H	4	1.080950(23)	3	111.290(48)	2	-139.339(72)	0
25	25	H	4	1.085260(24)	3	111.126(49)	2	99.217(73)	0
26	26	H	3	0.997270(25)	2	119.516(50)	1	-7.185(74)	0
27	27	H	6	0.995680(26)	2	120.405(51)	1	-16.645(75)	0

E(RHF) = -699.045798066

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.020257	0.693410	0.504514
2	6	0.034858	0.588113	1.966395
3	7	1.137332	0.526409	2.685770
4	6	0.871364	0.233407	4.087826
5	6	-0.660783	0.435708	4.165679
6	7	-1.011351	0.550754	2.757492
7	6	0.110096	1.988303	-0.036356
8	7	0.208072	3.060915	-0.422588
9	6	-0.008229	-0.578193	-0.136923
10	8	0.070407	-1.590091	0.547583
11	6	-0.077182	-0.714254	-1.631746
12	6	-0.685973	0.216787	-2.465110
13	6	-0.735697	0.003625	-3.834101
14	6	-0.173431	-1.136143	-4.381974
15	6	0.430123	-2.073494	-3.556534
16	6	0.468253	-1.867304	-2.190288
17	1	0.913885	-2.594064	-1.538879
18	1	0.863413	-2.963512	-3.977184
19	1	-0.208187	-1.296501	-5.445157
20	1	-1.213341	0.729030	-4.467975
21	1	-1.130850	1.104310	-2.059829
22	1	-0.925681	1.340686	4.697226
23	1	-1.164946	-0.402718	4.624440
24	1	1.409745	0.908749	4.737031
25	1	1.156590	-0.784684	4.319550
26	1	2.015098	0.374475	2.242145
27	1	-1.936210	0.598630	2.394950

E(RHF) = -699.006316891

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.422210(1)					
3	3	N	2	1.340240(2)	1	120.207(30)			
4	4	C	3	1.451780(3)	2	124.281(31)	1	-176.743(58)	0
5	5	C	4	1.521130(4)	3	109.375(32)	2	-30.783(59)	0
6	6	C	5	1.521030(5)	4	108.937(33)	3	52.513(60)	0
7	7	N	2	1.327100(6)	1	121.613(34)	3	178.796(61)	0
8	8	C	1	1.445760(7)	2	122.062(35)	3	-179.690(62)	0
9	9	C	8	1.503440(8)	1	120.318(36)	2	175.552(63)	0
10	10	C	9	1.392220(9)	8	117.349(37)	1	142.731(64)	0
11	11	C	10	1.381980(10)	9	120.477(38)	8	178.165(65)	0
12	12	C	11	1.387280(11)	10	119.955(39)	9	-1.417(66)	0
13	13	C	12	1.383770(12)	11	119.915(40)	10	0.126(67)	0
14	14	C	13	1.386150(13)	12	120.143(41)	11	0.895(68)	0
15	15	O	8	1.219260(14)	1	122.214(42)	2	-5.419(69)	0
16	16	C	1	1.423670(15)	2	115.215(43)	3	4.092(70)	0
17	17	N	16	1.141880(16)	1	174.711(44)	2	-0.305(71)	0
18	18	H	3	0.995450(17)	2	117.061(45)	1	-3.394(72)	0
19	19	H	4	1.082050(18)	3	107.889(46)	2	-151.619(73)	0
20	20	H	4	1.086710(19)	3	110.440(47)	2	90.874(74)	0

21	21	H	5	1.084750(20)	4	109.562(48)	3	-67.569(75)	0
22	22	H	5	1.083920(21)	4	110.229(49)	3	173.559(76)	0
23	23	H	6	1.082150(22)	5	110.937(50)	4	-170.229(77)	0
24	24	H	6	1.086680(23)	5	110.259(51)	4	70.679(78)	0
25	25	H	7	1.001350(24)	2	114.537(52)	1	3.980(79)	0
26	26	H	10	1.073350(25)	9	119.042(53)	8	-1.695(80)	0
27	27	H	11	1.075300(26)	10	119.907(54)	9	179.071(81)	0
28	28	H	12	1.075570(27)	11	120.052(55)	10	-179.570(82)	0
29	29	H	13	1.075030(28)	12	120.208(56)	11	-179.233(83)	0
30	30	H	14	1.072980(29)	13	119.183(57)	12	-179.764(84)	0

E(RHF) = -738.084633361

TS

1	6	-0.045778	-0.716934	0.147746
2	6	-0.011652	-0.776560	1.621528
3	7	1.122680	-0.998854	2.247829
4	6	1.281925	-0.995581	3.696414
5	6	0.191130	-0.128900	4.313271
6	6	-1.168973	-0.557867	3.777020
7	7	-1.112700	-0.620433	2.321792
8	6	0.045068	0.607767	-0.365629
9	6	0.047785	0.887866	-1.843551
10	6	-0.414134	2.136364	-2.252533
11	6	-0.429562	2.478023	-3.591802
12	6	0.037774	1.581058	-4.541151
13	6	0.517947	0.345812	-4.142879
14	6	0.520702	-0.002151	-2.800711
15	8	0.113294	1.551171	0.411669
16	6	-0.302707	-1.932402	-0.517704
17	7	-0.506052	-2.948387	-1.003984
18	1	1.922223	-1.090000	1.661935
19	1	2.263082	-0.602254	3.924197
20	1	1.231150	-2.012035	4.071975
21	1	0.368240	0.908818	4.054994
22	1	0.209938	-0.220251	5.392619
23	1	-1.933899	0.155311	4.051764
24	1	-1.454896	-1.526903	4.171733
25	1	-1.928209	-0.411972	1.790281
26	1	-0.752678	2.829581	-1.506933
27	1	-0.798231	3.441789	-3.895388
28	1	0.031155	1.846353	-5.583699
29	1	0.890841	-0.350121	-4.872866
30	1	0.900280	-0.962934	-2.513532

E(RHF) = -738.051457355

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.408790(1)					
3	3	N	2	1.334740(2)	1	122.005(33)			
4	4	C	3	1.460370(3)	2	124.433(34)	1	-147.503(64)	0
5	5	C	4	1.523690(4)	3	114.637(35)	2	-78.204(65)	0

6	6	C	5	1.525030(5)	4	112.946(36)	3	69.541(66)	0
7	7	C	6	1.522700(6)	5	113.082(37)	4	-58.294(67)	0
8	8	N	2	1.355420(7)	1	120.489(38)	3	-179.215(68)	0
9	9	C	1	1.427630(8)	2	115.936(39)	3	-169.665(69)	0
10	10	N	9	1.141070(9)	1	175.621(40)	2	-3.341(70)	0
11	11	C	1	1.457080(10)	2	122.507(41)	3	6.998(71)	0
12	12	C	11	1.502020(11)	1	120.300(42)	2	169.877(72)	0
13	13	C	12	1.392290(12)	11	117.420(43)	1	144.474(73)	0
14	14	C	13	1.381930(13)	12	120.444(44)	11	177.999(74)	0
15	15	C	14	1.387270(14)	13	119.933(45)	12	-1.371(75)	0
16	16	C	15	1.383990(15)	14	119.974(46)	13	0.149(76)	0
17	17	C	16	1.385800(16)	15	120.106(47)	14	0.874(77)	0
18	18	O	11	1.215550(17)	1	121.964(48)	2	-10.982(78)	0
19	19	H	3	1.000650(18)	2	112.427(49)	1	2.002(79)	0
20	20	H	4	1.081610(19)	3	105.483(50)	2	161.317(80)	0
21	21	H	4	1.086380(20)	3	109.786(51)	2	46.017(81)	0
22	22	H	5	1.086490(21)	4	108.990(52)	3	-53.273(82)	0
23	23	H	5	1.086470(22)	4	108.105(53)	3	-169.390(83)	0
24	24	H	6	1.086500(23)	5	109.434(54)	4	-178.794(84)	0
25	25	H	6	1.086480(24)	5	110.039(55)	4	63.718(85)	0
26	26	H	7	1.086450(25)	6	110.049(56)	5	-56.382(86)	0
27	27	H	7	1.081750(26)	6	109.380(57)	5	-173.987(87)	0
28	28	H	8	0.996300(27)	2	113.366(58)	1	2.652(88)	0
29	29	H	13	1.073320(28)	12	119.058(59)	11	-1.923(89)	0
30	30	H	14	1.075200(29)	13	119.922(60)	12	179.074(90)	0
31	31	H	15	1.075520(30)	14	120.025(61)	13	-179.600(91)	0
32	32	H	16	1.074940(31)	15	120.214(62)	14	-179.300(92)	0
33	33	H	17	1.073020(32)	16	119.203(63)	15	-179.836(93)	0

E(RHF) = -777.112284366

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.070379	0.631239	-0.084476
2	6	0.127237	0.537987	1.395476
3	7	1.316232	0.428132	1.961054
4	6	1.727013	-0.093727	3.264401
5	6	0.953019	0.419148	4.465464
6	6	-0.512707	-0.001678	4.452337
7	6	-1.345005	0.786254	3.456137
8	7	-1.012821	0.598506	2.046266
9	6	0.524129	1.841447	-0.647112
10	7	0.895272	2.847723	-1.047187
11	6	-0.189257	-0.615228	-0.721501
12	6	-0.284523	-0.728967	-2.218258
13	6	0.021535	-1.964356	-2.782942
14	6	-0.059344	-2.153279	-4.149943
15	6	-0.468428	-1.112203	-4.970321
16	6	-0.794181	0.113532	-4.416357
17	6	-0.700206	0.306719	-3.046694
18	8	-0.331281	-1.624678	-0.044064
19	1	2.034901	0.380432	1.272462
20	1	2.770517	0.172289	3.365875
21	1	1.666065	-1.177102	3.229715
22	1	1.035751	1.500735	4.529712
23	1	1.437517	0.011567	5.347119

24	1	-0.947405	0.174049	5.431395
25	1	-0.599738	-1.065296	4.250327
26	1	-1.275939	1.845611	3.685958
27	1	-2.384531	0.502695	3.548219
28	1	-1.782758	0.681799	1.420105
29	1	0.316021	-2.767628	-2.135445
30	1	0.189228	-3.109515	-4.575098
31	1	-0.536503	-1.258166	-6.033997
32	1	-1.121239	0.921463	-5.046083
33	1	-0.960390	1.262644	-2.635941

E(RHF) = -777.074159724

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.421930(1)					
3	3	N	2	1.342550(2)	1	123.132(27)			
4	4	C	3	1.454080(3)	2	111.391(28)	1	-170.705(52)	0
5	5	C	4	1.536550(4)	3	101.222(29)	2	-19.293(53)	0
6	6	N	2	1.320500(5)	1	127.883(30)	3	179.504(54)	0
7	7	C	1	1.435580(6)	2	112.615(31)	3	6.121(55)	0
8	8	N	7	1.139770(7)	1	173.888(32)	2	4.913(56)	0
9	9	C	1	1.415600(8)	2	125.900(33)	3	-176.206(57)	0
10	10	S	9	1.677590(9)	1	126.071(34)	2	-4.200(58)	0
11	11	C	9	1.498220(10)	1	116.868(35)	2	175.392(59)	0
12	12	C	11	1.390480(11)	9	120.661(36)	1	-56.073(60)	0
13	13	C	12	1.384680(12)	11	120.374(37)	9	-177.678(61)	0
14	14	C	13	1.384090(13)	12	120.110(38)	11	-1.113(62)	0
15	15	C	14	1.386320(14)	13	119.789(39)	12	0.828(63)	0
16	16	C	15	1.382720(15)	14	120.211(40)	13	0.490(64)	0
17	17	H	16	1.073290(16)	15	120.196(41)	14	178.523(65)	0
18	18	H	15	1.075160(17)	14	120.135(42)	13	179.936(66)	0
19	19	H	14	1.075350(18)	13	120.104(43)	12	-179.349(67)	0
20	20	H	13	1.075010(19)	12	119.638(44)	11	179.165(68)	0
21	21	H	12	1.074290(20)	11	120.073(45)	9	1.234(69)	0
22	22	H	5	1.084260(21)	4	111.802(46)	3	-97.623(70)	0
23	23	H	5	1.080500(22)	4	112.829(47)	3	139.244(71)	0
24	24	H	4	1.080460(23)	3	111.157(48)	2	-139.238(72)	0
25	25	H	4	1.084890(24)	3	110.963(49)	2	99.370(73)	0
26	26	H	3	0.995600(25)	2	121.174(50)	1	-13.598(74)	0
27	27	H	6	1.000440(26)	2	120.465(51)	1	-5.334(75)	0

E(RHF) = -1021.67609465

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.041022	0.703571	0.430648
2	6	-0.057896	0.718237	1.906166
3	7	1.011556	0.807343	2.667604
4	6	0.691799	0.592843	4.074551
5	6	-0.853802	0.676349	4.067736

6	7	-1.142283	0.714271	2.639475
7	6	-0.019634	1.993276	-0.174046
8	7	-0.007153	3.056275	-0.587732
9	6	0.044858	-0.527068	-0.186617
10	16	0.173446	-1.952588	0.745615
11	6	0.023348	-0.608966	-1.677428
12	6	-0.907578	0.105166	-2.424539
13	6	-0.930055	0.001600	-3.805875
14	6	-0.011963	-0.803479	-4.456409
15	6	0.919746	-1.518930	-3.719174
16	6	0.928721	-1.434677	-2.339531
17	1	1.632019	-2.007793	-1.766992
18	1	1.633151	-2.149818	-4.218486
19	1	-0.024033	-0.878152	-5.529252
20	1	-1.662763	0.551745	-4.368372
21	1	-1.628389	0.730462	-1.932640
22	1	-1.218138	1.573554	4.549788
23	1	-1.313952	-0.186298	4.527714
24	1	1.143095	1.353954	4.694087
25	1	1.041992	-0.381075	4.389732
26	1	1.909948	0.621721	2.279928
27	1	-2.042031	0.580363	2.236327

E(RHF) = -1021.65192282

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.446700(1)					
3	3	N	2	1.316290(2)	1	122.494(30)			
4	4	C	3	1.453540(3)	2	124.762(31)	1	-179.215(58)	0
5	5	C	4	1.520510(4)	3	109.872(32)	2	-27.638(59)	0
6	6	C	5	1.520780(5)	4	108.797(33)	3	51.474(60)	0
7	7	N	2	1.335770(6)	1	119.115(34)	3	179.787(61)	0
8	8	C	1	1.408080(7)	2	127.112(35)	3	0.302(62)	0
9	9	C	8	1.500750(8)	1	116.556(36)	2	175.313(63)	0
10	10	C	9	1.390740(9)	8	120.129(37)	1	122.302(64)	0
11	11	C	10	1.382990(10)	9	120.256(38)	8	178.903(65)	0
12	12	C	11	1.386200(11)	10	120.228(39)	9	-1.474(66)	0
13	13	C	12	1.384120(12)	11	119.758(40)	10	0.476(67)	0
14	14	C	13	1.384720(13)	12	120.118(41)	11	0.775(68)	0
15	15	S	8	1.685940(14)	1	127.439(42)	2	-4.440(69)	0
16	16	C	1	1.435530(15)	2	113.022(43)	3	-177.434(70)	0
17	17	N	16	1.140210(16)	1	173.886(44)	2	2.156(71)	0
18	18	H	3	1.005190(17)	2	115.778(45)	1	1.079(72)	0
19	19	H	4	1.081450(18)	3	107.523(46)	2	-148.820(73)	0
20	20	H	4	1.085680(19)	3	109.839(47)	2	94.183(74)	0
21	21	H	5	1.084630(20)	4	109.739(48)	3	-68.589(75)	0
22	22	H	5	1.083630(21)	4	110.304(49)	3	172.388(76)	0
23	23	H	6	1.081800(22)	5	111.105(50)	4	-170.392(77)	0
24	24	H	6	1.085930(23)	5	110.457(51)	4	70.001(78)	0
25	25	H	7	0.995500(24)	2	117.432(52)	1	1.442(79)	0
26	26	H	10	1.073520(25)	9	119.548(53)	8	-1.033(80)	0
27	27	H	11	1.075230(26)	10	119.644(54)	9	179.077(81)	0
28	28	H	12	1.075370(27)	11	120.120(55)	10	-179.348(82)	0

29	29	H	13	1.075110(28)	12	120.235(56)	11	-179.499(83)	0
30	30	H	14	1.074540(29)	13	119.660(57)	12	179.865(84)	0

E(RHF) = -1060.71495029

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.101302	0.582943	0.178546
2	6	-0.112466	0.598040	1.660811
3	7	1.017218	0.620662	2.328880
4	6	1.089542	0.457252	3.773693
5	6	-0.120787	1.135437	4.402963
6	6	-1.400136	0.624513	3.751180
7	7	-1.257022	0.668986	2.299597
8	6	0.140222	-0.613191	-0.465561
9	6	0.117123	-0.657677	-1.959994
10	6	1.146578	-1.294336	-2.648832
11	6	1.139363	-1.343236	-4.030123
12	6	0.089293	-0.784472	-4.743462
13	6	-0.949352	-0.171039	-4.066399
14	6	-0.931743	-0.100288	-2.682616
15	16	0.443714	-2.046808	0.411553
16	6	-0.314004	1.860520	-0.417258
17	7	-0.495045	2.913634	-0.817058
18	1	1.831694	0.433449	1.785759
19	1	2.008502	0.912221	4.116119
20	1	1.119499	-0.600031	4.014534
21	1	-0.044212	2.208406	4.266226
22	1	-0.148370	0.935138	5.467143
23	1	-2.245767	1.240922	4.024264
24	1	-1.609647	-0.395054	4.053834
25	1	-2.073815	0.602694	1.733301
26	1	1.944297	-1.751649	-2.095907
27	1	1.947605	-1.826156	-4.549669
28	1	0.079991	-0.832733	-5.817847
29	1	-1.773124	0.255704	-4.609833
30	1	-1.746129	0.376237	-2.170385

E(RHF) = -1060.69743575

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.433800(1)					
3	3	N	2	1.321570(2)	1	122.729(33)			
4	4	C	3	1.462410(3)	2	125.401(34)	1	-149.787(64)	0
5	5	C	4	1.522810(4)	3	115.044(35)	2	-76.173(65)	0
6	6	C	5	1.524300(5)	4	112.670(36)	3	69.819(66)	0
7	7	C	6	1.521840(6)	5	112.865(37)	4	-59.309(67)	0
8	8	N	2	1.350890(7)	1	119.391(38)	3	-179.190(68)	0
9	9	C	1	1.437740(8)	2	113.611(39)	3	-169.626(69)	0
10	10	N	9	1.139880(9)	1	174.776(40)	2	2.046(70)	0

11	11	C	1	1.420450(10)	2	127.317(41)	3	8.913(71)	0
12	12	C	11	1.499300(11)	1	116.573(42)	2	170.465(72)	0
13	13	C	12	1.390990(12)	11	120.271(43)	1	125.280(73)	0
14	14	C	13	1.383070(13)	12	120.286(44)	11	178.675(74)	0
15	15	C	14	1.385950(14)	13	120.204(45)	12	-1.555(75)	0
16	16	C	15	1.384490(15)	14	119.797(46)	13	0.544(76)	0
17	17	C	16	1.384150(16)	15	120.092(47)	14	0.826(77)	0
18	18	S	11	1.677710(17)	1	127.123(48)	2	-9.749(78)	0
19	19	H	3	1.003580(18)	2	113.750(49)	1	2.844(79)	0
20	20	H	4	1.081140(19)	3	105.210(50)	2	162.925(80)	0
21	21	H	4	1.085690(20)	3	109.210(51)	2	47.913(81)	0
22	22	H	5	1.086390(21)	4	109.224(52)	3	-53.135(82)	0
23	23	H	5	1.086160(22)	4	107.928(53)	3	-169.272(83)	0
24	24	H	6	1.086240(23)	5	109.545(54)	4	-179.567(84)	0
25	25	H	6	1.086400(24)	5	110.089(55)	4	62.831(85)	0
26	26	H	7	1.086270(25)	6	109.976(56)	5	-56.434(86)	0
27	27	H	7	1.081400(26)	6	109.515(57)	5	-174.120(87)	0
28	28	H	8	0.995970(27)	2	113.801(58)	1	3.952(88)	0
29	29	H	13	1.073310(28)	12	119.541(59)	11	-1.443(89)	0
30	30	H	14	1.075140(29)	13	119.651(60)	12	178.985(90)	0
31	31	H	15	1.075340(30)	14	120.107(61)	13	-179.322(91)	0
32	32	H	16	1.075020(31)	15	120.241(62)	14	-179.499(92)	0
33	33	H	17	1.074420(32)	16	119.610(63)	15	179.815(93)	0

E(RHF) = -1099.74072849

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.147564	0.546996	-0.077154
2	6	0.150157	0.565728	1.412926
3	7	1.332482	0.618241	1.993026
4	6	1.786908	0.420564	3.369030
5	6	0.828964	0.867381	4.456995
6	6	-0.493632	0.106627	4.423683
7	6	-1.462064	0.655991	3.392909
8	7	-1.019294	0.607793	2.001869
9	6	0.664926	1.736542	-0.669742
10	7	1.098554	2.714907	-1.065875
11	6	-0.186565	-0.617709	-0.742228
12	6	-0.228052	-0.604916	-2.237204
13	6	0.383970	-1.625982	-2.959795
14	6	0.347150	-1.625162	-4.341647
15	6	-0.326195	-0.621623	-5.022102
16	6	-0.955873	0.385029	-4.311965
17	6	-0.899596	0.398324	-2.927738
18	16	-0.533139	-2.065642	0.089483
19	1	2.070039	0.549831	1.325786
20	1	2.718094	0.965338	3.452639
21	1	2.008664	-0.633868	3.496979
22	1	0.654642	1.938056	4.392174
23	1	1.330747	0.687562	5.402113
24	1	-0.987738	0.190173	5.386213
25	1	-0.319575	-0.950389	4.246143
26	1	-1.697662	1.688075	3.633166
27	1	-2.385686	0.093899	3.425830
28	1	-1.761660	0.519138	1.343074

29	1	0.881648	-2.416318	-2.431965
30	1	0.835575	-2.412563	-4.887417
31	1	-0.362557	-0.628420	-6.097013
32	1	-1.488522	1.162104	-4.830169
33	1	-1.393949	1.184337	-2.388227

E(RHF) = -1099.71964633

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.356980(1)					
3	3	S	2	1.754910(2)	1	127.496(22)			
4	4	C	3	1.818620(3)	2	90.255(23)	1	-171.237(42)	0
5	5	C	4	1.517610(4)	3	103.931(24)	2	-23.863(43)	0
6	6	O	2	1.318170(5)	1	119.740(25)	3	-178.816(44)	0
7	7	C	1	1.474780(6)	2	119.391(26)	3	-0.230(45)	0
8	8	C	7	1.471530(7)	1	121.608(27)	2	171.004(46)	0
9	9	C	8	1.347810(8)	7	128.568(28)	1	173.109(47)	0
10	10	C	9	1.429450(9)	8	105.978(29)	7	179.310(48)	0
11	11	C	10	1.345460(10)	9	105.439(30)	8	-0.191(49)	0
12	12	O	11	1.331710(11)	10	111.107(31)	9	0.086(50)	0
13	13	O	7	1.204790(12)	1	120.084(32)	2	-8.890(51)	0
14	14	C	1	1.437480(13)	2	116.695(33)	3	-177.705(52)	0
15	15	N	14	1.136530(14)	1	177.664(34)	2	24.872(53)	0
16	16	H	4	1.081500(15)	3	110.070(35)	2	96.032(54)	0
17	17	H	4	1.080590(16)	3	109.636(36)	2	-143.771(55)	0
18	18	H	5	1.078210(17)	4	113.488(37)	3	151.638(56)	0
19	19	H	5	1.082210(18)	4	111.687(38)	3	-83.725(57)	0
20	20	H	9	1.069090(19)	8	125.712(39)	7	-0.706(58)	0
21	21	H	10	1.069750(20)	9	127.750(40)	8	179.821(59)	0
22	22	H	11	1.068200(21)	10	132.839(41)	9	-179.936(60)	0

E(RHF) = -1059.25166913

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.081580	-0.557981	-0.045434
2	6	-0.090733	-0.578427	1.410315
3	16	1.330940	-0.584592	2.363284
4	6	0.380755	-0.763386	3.902868
5	6	-1.051309	-0.416305	3.495177
6	8	-1.171142	-0.619031	2.076051
7	6	-0.052976	0.776578	-0.521645
8	6	-0.040241	1.086623	-1.962206
9	6	-0.044631	2.283259	-2.576385
10	6	-0.027360	2.004263	-3.981762
11	6	-0.014098	0.664238	-4.081242
12	8	-0.021209	0.094454	-2.874435
13	8	-0.031899	1.703785	0.280065
14	6	-0.210739	-1.800904	-0.699422
15	7	-0.309356	-2.845969	-1.150454

16	1	0.471489	-1.777844	4.262962
17	1	0.751919	-0.082826	4.654357
18	1	-1.792604	-1.046179	3.956845
19	1	-1.285274	0.623270	3.664125
20	1	-0.058564	3.233895	-2.087850
21	1	-0.025559	2.706327	-4.789299
22	1	0.000517	-0.002801	-4.915521

E(RHF) = -1059.19228179

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.358100(1)					
3	3	S	2	1.753130(2)	1	127.620(22)			
4	4	C	3	1.818970(3)	2	90.309(23)	1	-171.818(42)	0
5	5	C	4	1.517540(4)	3	104.006(24)	2	-23.431(43)	0
6	6	O	2	1.317930(5)	1	119.558(25)	3	-178.892(44)	0
7	7	C	1	1.476230(6)	2	119.676(26)	3	-0.119(45)	0
8	8	C	7	1.485480(7)	1	123.232(27)	2	172.416(46)	0
9	9	C	8	1.357220(8)	7	120.721(28)	1	175.565(47)	0
10	10	C	9	1.423410(9)	8	113.521(29)	7	178.078(48)	0
11	11	C	10	1.349500(10)	9	111.890(30)	8	-0.357(49)	0
12	12	S	11	1.712720(11)	10	112.785(31)	9	0.488(50)	0
13	13	O	7	1.205120(12)	1	118.446(32)	2	-7.345(51)	0
14	14	C	1	1.434740(13)	2	116.443(33)	3	-178.393(52)	0
15	15	N	14	1.137260(14)	1	178.924(34)	2	20.471(53)	0
16	16	H	4	1.080600(15)	3	109.649(35)	2	-143.359(54)	0
17	17	H	4	1.081490(16)	3	110.023(36)	2	96.488(55)	0
18	18	H	5	1.082160(17)	4	111.712(37)	3	-84.005(56)	0
19	19	H	5	1.078140(18)	4	113.515(38)	3	151.307(57)	0
20	20	H	9	1.071540(19)	8	121.971(39)	7	-1.574(58)	0
21	21	H	10	1.072910(20)	9	124.039(40)	8	179.747(59)	0
22	22	H	11	1.071570(21)	10	127.464(41)	9	179.915(60)	0

E(RHF) = -1381.91188764

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.372654	0.562678	-0.066041
2	6	1.771537	0.159834	-0.115088
3	16	2.707635	-0.176658	1.278490
4	6	4.217641	-0.405656	0.292016
5	6	3.704679	-0.549055	-1.141033
6	8	2.404915	0.063606	-1.211087
7	6	-0.466841	-0.581751	-0.079861
8	6	-1.949725	-0.506534	-0.035216
9	6	-2.727293	-1.612653	-0.087329
10	6	-4.123861	-1.325388	-0.019666
11	6	-4.364491	-0.002931	0.084060
12	16	-2.922485	0.929188	0.099387
13	8	0.066332	-1.685515	-0.123038

14	6	0.097258	1.941520	-0.132200
15	7	-0.069203	3.071863	-0.177173
16	1	4.743955	-1.292356	0.612001
17	1	4.858995	0.454871	0.415166
18	1	3.558838	-1.580120	-1.423179
19	1	4.318663	-0.045464	-1.868218
20	1	-2.308483	-2.595630	-0.169181
21	1	-4.892593	-2.073889	-0.047696
22	1	-5.316685	0.483949	0.150427

E(RHF) = -1381.85336308

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.357060(1)					
3	3	C	1	1.479560(2)	2	120.158(25)			
4	4	C	3	1.497820(3)	1	121.580(26)	2	-175.887(48)	0
5	5	C	4	1.393120(4)	3	116.964(27)	1	-146.455(49)	0
6	6	C	5	1.381320(5)	4	120.396(28)	3	-178.075(50)	0
7	7	C	6	1.387510(6)	5	119.899(29)	4	1.357(51)	0
8	8	C	7	1.383800(7)	6	120.036(30)	5	-0.129(52)	0
9	9	C	8	1.385860(8)	7	120.141(31)	6	-0.904(53)	0
10	10	O	3	1.203100(9)	1	118.937(32)	2	4.752(54)	0
11	11	C	1	1.436130(10)	2	116.682(33)	3	177.338(55)	0
12	12	N	11	1.137220(11)	1	179.369(34)	2	-18.320(56)	0
13	13	O	2	1.319030(12)	1	119.736(35)	3	-178.764(57)	0
14	14	C	13	1.420810(13)	2	114.486(36)	1	-163.436(58)	0
15	15	C	14	1.518400(14)	13	106.983(37)	2	-33.344(59)	0
16	16	S	2	1.753490(15)	1	127.472(38)	3	0.543(60)	0
17	17	H	5	1.073320(16)	4	119.091(39)	3	1.902(61)	0
18	18	H	6	1.075020(17)	5	119.924(40)	4	-179.076(62)	0
19	19	H	7	1.075420(18)	6	119.994(41)	5	179.632(63)	0
20	20	H	8	1.074750(19)	7	120.239(42)	6	179.302(64)	0
21	21	H	9	1.072370(20)	8	119.011(43)	7	179.887(65)	0
22	22	H	14	1.082330(21)	13	108.236(44)	2	87.093(66)	0
23	23	H	14	1.078090(22)	13	106.601(45)	2	-155.021(67)	0
24	24	H	15	1.080580(23)	14	111.937(46)	13	151.378(68)	0
25	25	H	15	1.081330(24)	14	111.815(47)	13	-85.745(69)	0

E(RHF) = -1061.32541641

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.415314	0.628375	-0.026158
2	6	-1.796789	0.185215	0.097071
3	6	0.482009	-0.459910	0.165873
4	6	1.972097	-0.308334	0.103069
5	6	2.710313	-1.451790	-0.192045
6	6	4.089708	-1.399320	-0.260015
7	6	4.750192	-0.204579	-0.014199
8	6	4.025584	0.932460	0.298260

9	6	2.641366	0.884041	0.354091
10	8	-0.003555	-1.565953	0.373443
11	6	-0.214376	1.992586	-0.308752
12	7	-0.107872	3.107056	-0.542429
13	8	-2.448608	0.319410	1.178970
14	6	-3.731009	-0.330238	1.235612
15	6	-4.218718	-0.540425	-0.197774
16	16	-2.697430	-0.497452	-1.191828
17	1	2.187767	-2.373030	-0.362369
18	1	4.649102	-2.286390	-0.498202
19	1	5.824006	-0.162465	-0.062159
20	1	4.533030	1.858676	0.499566
21	1	2.100597	1.775228	0.604267
22	1	-3.566342	-1.262189	1.753688
23	1	-4.371856	0.311317	1.816276
24	1	-4.712920	-1.493872	-0.308989
25	1	-4.882482	0.246413	-0.525329

E(RHF) = -1061.26612121

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.356750(1)					
3	3	S	2	1.753650(2)	1	127.313(25)			
4	4	C	3	1.818620(3)	2	90.171(26)	1	-170.354(48)	0
5	5	C	4	1.517840(4)	3	103.865(27)	2	-24.448(49)	0
6	6	O	2	1.317510(5)	1	119.813(28)	3	-178.826(50)	0
7	7	C	1	1.435590(6)	2	117.132(29)	3	-176.582(51)	0
8	8	N	7	1.137240(7)	1	179.642(30)	2	56.328(52)	0
9	9	C	1	1.478610(8)	2	120.087(31)	3	-0.548(53)	0
10	10	C	9	1.497430(9)	1	121.335(32)	2	168.488(54)	0
11	11	C	10	1.392390(10)	9	117.179(33)	1	150.469(55)	0
12	12	C	11	1.380290(11)	10	120.805(34)	9	177.913(56)	0
13	13	C	12	1.385110(12)	11	119.016(35)	10	-1.197(57)	0
14	14	C	13	1.381250(13)	12	121.238(36)	11	0.123(58)	0
15	15	C	14	1.384950(14)	13	119.232(37)	12	0.772(59)	0
16	16	Cl	13	1.740440(15)	12	119.335(38)	11	-179.643(60)	0
17	17	O	9	1.202600(16)	1	119.191(39)	2	-12.049(61)	0
18	18	H	4	1.080500(17)	3	109.598(40)	2	-144.287(62)	0
19	19	H	4	1.081430(18)	3	110.133(41)	2	95.483(63)	0
20	20	H	5	1.082010(19)	4	111.718(42)	3	-83.482(64)	0
21	21	H	5	1.078140(20)	4	113.484(43)	3	151.810(65)	0
22	22	H	11	1.072950(21)	10	119.176(44)	9	-2.024(66)	0
23	23	H	12	1.073070(22)	11	120.798(45)	10	179.190(67)	0
24	24	H	14	1.072860(23)	13	120.275(46)	12	-179.405(68)	0
25	25	H	15	1.072220(24)	14	118.478(47)	13	-179.880(69)	0

E(RHF) = -1520.22593650

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	1.187506	0.632148	-0.129041
2	6	2.563749	0.153373	-0.117919
3	16	3.500243	0.014794	1.307217
4	6	4.976648	-0.481996	0.369369
5	6	4.429471	-0.851957	-1.009470
6	8	3.170979	-0.176353	-1.182544
7	6	0.978181	1.984432	-0.461024
8	7	0.854568	3.092099	-0.716221
9	6	0.291766	-0.466036	-0.007891
10	6	-1.196845	-0.295926	0.015179
11	6	-1.967067	-1.405428	-0.319891
12	6	-3.346832	-1.340659	-0.311175
13	6	-3.960719	-0.154780	0.053196
14	6	-3.219280	0.956135	0.405281
15	6	-1.836201	0.881613	0.382519
16	17	-5.701633	-0.064496	0.073562
17	8	0.771114	-1.590212	0.080271
18	1	5.455032	-1.326220	0.842673
19	1	5.669567	0.345791	0.329065
20	1	4.210962	-1.904991	-1.095003
21	1	5.061254	-0.533039	-1.820914
22	1	-1.471066	-2.319059	-0.583523
23	1	-3.939129	-2.195158	-0.577622
24	1	-3.711096	1.865344	0.693331
25	1	-1.272623	1.749376	0.662890

E(RHF) = -1520.16732993

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.374390(1)					
3	3	O	2	1.311340(2)	1	124.233(26)			
4	4	C	3	1.424720(3)	2	110.344(27)	1	-173.516(50)	0
5	5	C	4	1.528210(4)	3	103.929(28)	2	-17.995(51)	0
6	6	N	2	1.345490(5)	1	125.851(29)	3	-178.113(52)	0
7	7	C	1	1.428970(6)	2	114.446(30)	3	-178.274(53)	0
8	8	N	7	1.140350(7)	1	175.151(31)	2	5.820(54)	0
9	9	C	1	1.477870(8)	2	122.496(32)	3	-3.069(55)	0
10	10	C	9	1.503210(9)	1	119.175(33)	2	164.372(56)	0
11	11	C	10	1.392290(10)	9	117.456(34)	1	148.405(57)	0
12	12	C	11	1.381770(11)	10	120.437(35)	9	178.077(58)	0
13	13	C	12	1.387590(12)	11	119.940(36)	10	-1.166(59)	0
14	14	C	13	1.383890(13)	12	119.990(37)	11	0.101(60)	0
15	15	C	14	1.386060(14)	13	120.062(38)	12	0.787(61)	0
16	16	O	9	1.199250(15)	1	121.438(39)	2	-16.441(62)	0
17	17	H	4	1.081140(16)	3	108.182(40)	2	101.437(63)	0
18	18	H	4	1.077580(17)	3	107.879(41)	2	-139.779(64)	0
19	19	H	5	1.081000(18)	4	112.604(42)	3	140.556(65)	0
20	20	H	5	1.085150(19)	4	112.340(43)	3	-95.801(66)	0
21	21	H	6	0.995790(20)	2	120.742(44)	1	-14.218(67)	0
22	22	H	11	1.073350(21)	10	118.942(45)	9	-1.790(68)	0
23	23	H	12	1.075230(22)	11	119.938(46)	10	179.202(69)	0
24	24	H	13	1.075560(23)	12	120.018(47)	11	-179.684(70)	0
25	25	H	14	1.075000(24)	13	120.214(48)	12	-179.345(71)	0

26 26 H 15 1.073440(25) 14 119.161(49) 13 -179.702(72) 0

E(RHF) = -718.853138416

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.015389	0.705361	0.534324
2	6	0.206669	0.517322	1.962690
3	8	1.380364	0.365864	2.485351
4	6	1.287840	0.096898	3.889152
5	6	-0.214205	0.232908	4.206002
6	7	-0.723346	0.489732	2.870205
7	6	0.030790	2.029615	0.056812
8	7	0.052079	3.124019	-0.275533
9	6	-0.043761	-0.546448	-0.146451
10	6	-0.217503	-0.652557	-1.633054
11	6	0.248453	-1.814342	-2.243146
12	6	0.114698	-1.994280	-3.607026
13	6	-0.505089	-1.020849	-4.376683
14	6	-0.987241	0.129205	-3.776280
15	6	-0.841933	0.316055	-2.410408
16	8	0.072338	-1.568491	0.517370
17	1	1.667433	-0.898578	4.052714
18	1	1.903651	0.817554	4.401884
19	1	-0.638221	-0.674560	4.611677
20	1	-0.433724	1.059036	4.868256
21	1	-1.684789	0.550106	2.617313
22	1	0.710378	-2.566512	-1.633494
23	1	0.487396	-2.891208	-4.068837
24	1	-0.613744	-1.160592	-5.437765
25	1	-1.475900	0.883246	-4.366786
26	1	-1.225210	1.212946	-1.965015

E(RHF) = -718.819592805

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.386360(1)					
3	3	O	2	1.305800(2)	1	124.813(26)			
4	4	C	3	1.426780(3)	2	110.583(27)	1	-172.888(50)	0
5	5	C	4	1.529160(4)	3	103.957(28)	2	-16.703(51)	0
6	6	N	2	1.340160(5)	1	125.076(29)	3	-177.483(52)	0
7	7	C	1	1.435330(6)	2	112.776(30)	3	179.191(53)	0
8	8	N	7	1.139780(7)	1	174.195(31)	2	10.092(54)	0
9	9	C	1	1.450610(8)	2	126.363(32)	3	-3.654(55)	0
10	10	C	9	1.495850(9)	1	115.736(33)	2	161.122(56)	0
11	11	C	10	1.392310(10)	9	120.493(34)	1	134.190(57)	0
12	12	C	11	1.382540(11)	10	120.424(35)	9	178.556(58)	0
13	13	C	12	1.386320(12)	11	120.197(36)	10	-1.348(59)	0
14	14	C	13	1.384460(13)	12	119.813(37)	11	0.539(60)	0
15	15	C	14	1.384100(14)	13	120.045(38)	12	0.775(61)	0

16	16	S	9	1.644810(15)	1	124.884(39)	2	-19.568(62)	0
17	17	H	4	1.080680(16)	3	107.966(40)	2	102.859(63)	0
18	18	H	4	1.077310(17)	3	107.765(41)	2	-138.469(64)	0
19	19	H	5	1.080920(18)	4	112.583(42)	3	138.531(65)	0
20	20	H	5	1.084590(19)	4	112.477(43)	3	-97.712(66)	0
21	21	H	6	0.995820(20)	2	121.368(44)	1	-12.304(67)	0
22	22	H	11	1.072810(21)	10	119.366(45)	9	-1.726(68)	0
23	23	H	12	1.075130(22)	11	119.674(46)	10	179.009(69)	0
24	24	H	13	1.075390(23)	12	120.101(47)	11	-179.444(70)	0
25	25	H	14	1.075030(24)	13	120.252(48)	12	-179.522(71)	0
26	26	H	15	1.074240(25)	14	119.438(49)	13	-179.973(72)	0

E(RHF) = -1041.48264512

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.041434	0.633995	0.524070
2	6	0.282381	0.458274	1.956090
3	8	1.448444	0.198830	2.443528
4	6	1.347464	-0.080516	3.845344
5	6	-0.053443	0.429768	4.223821
6	7	-0.604712	0.625091	2.891040
7	6	-0.109446	1.988975	0.115923
8	7	-0.235430	3.096051	-0.129802
9	6	-0.009163	-0.514535	-0.249023
10	6	-0.232416	-0.406470	-1.721719
11	6	0.571992	-1.138401	-2.591708
12	6	0.383754	-1.050791	-3.958158
13	6	-0.628871	-0.255839	-4.474152
14	6	-1.447087	0.456166	-3.615478
15	6	-1.245059	0.388844	-2.246284
16	16	0.128631	-2.042362	0.480403
17	1	1.450865	-1.147448	3.964514
18	1	2.152017	0.435544	4.341180
19	1	-0.626469	-0.301069	4.775059
20	1	-0.035605	1.363471	4.769873
21	1	-1.562562	0.799482	2.679621
22	1	1.338944	-1.772396	-2.190438
23	1	1.020923	-1.609799	-4.619766
24	1	-0.780388	-0.196921	-5.537264
25	1	-2.241213	1.066893	-4.005726
26	1	-1.890407	0.944574	-1.592739

E(RHF) = -1041.46348063

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.382960(1)					
3	3	S	2	1.763320(2)	1	122.984(26)			
4	4	C	3	1.821810(3)	2	91.362(27)	1	-171.856(50)	0
5	5	C	4	1.526280(4)	3	105.060(28)	2	-23.667(51)	0

6	6	N	2	1.326310(5)	1	126.102(29)	3	179.312(52)	0
7	7	C	1	1.430650(6)	2	117.030(30)	3	6.165(53)	0
8	8	N	7	1.139040(7)	1	177.835(31)	2	-3.556(54)	0
9	9	C	1	1.465950(8)	2	120.511(32)	3	-176.704(55)	0
10	10	C	9	1.499590(9)	1	121.025(33)	2	173.336(56)	0
11	11	C	10	1.392750(10)	9	117.224(34)	1	145.274(57)	0
12	12	C	11	1.381590(11)	10	120.425(35)	9	178.072(58)	0
13	13	C	12	1.387380(12)	11	119.909(36)	10	-1.389(59)	0
14	14	C	13	1.383890(13)	12	120.007(37)	11	0.151(60)	0
15	15	C	14	1.385820(14)	13	120.135(38)	12	0.896(61)	0
16	16	O	9	1.212890(15)	1	120.635(39)	2	-7.327(62)	0
17	17	H	4	1.080980(16)	3	109.132(40)	2	95.915(63)	0
18	18	H	4	1.079840(17)	3	109.435(41)	2	-144.546(64)	0
19	19	H	5	1.081620(18)	4	111.559(42)	3	150.964(65)	0
20	20	H	5	1.085780(19)	4	110.959(43)	3	-87.828(66)	0
21	21	H	11	1.073300(20)	10	119.100(44)	9	-1.917(67)	0
22	22	H	12	1.075110(21)	11	119.926(45)	10	179.044(68)	0
23	23	H	13	1.075460(22)	12	120.009(46)	11	-179.618(69)	0
24	24	H	14	1.074810(23)	13	120.230(47)	12	-179.321(70)	0
25	25	H	15	1.072620(24)	14	119.106(48)	13	-179.913(71)	0
26	26	H	6	1.000420(25)	2	117.325(49)	1	-2.404(72)	0

E(RHF) = -1041.51441380

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.404019	0.554668	-0.179992
2	6	1.806923	0.134546	-0.129975
3	16	2.735511	0.036001	1.326831
4	6	4.268257	-0.348402	0.411402
5	6	3.819406	-0.769839	-0.994538
6	7	2.490831	-0.194980	-1.174915
7	6	0.165111	1.902056	-0.513817
8	7	0.029316	3.003375	-0.792667
9	6	-0.497199	-0.535010	-0.000753
10	6	-1.983907	-0.334682	0.045707
11	6	-2.782588	-1.410469	-0.333128
12	6	-4.160613	-1.307720	-0.302900
13	6	-4.758019	-0.131563	0.126245
14	6	-3.972039	0.936191	0.523391
15	6	-2.589902	0.837906	0.481142
16	8	-0.041758	-1.666220	0.097443
17	1	4.886455	0.537185	0.381499
18	1	4.808488	-1.138664	0.909933
19	1	4.488286	-0.399397	-1.757916
20	1	3.741424	-1.846105	-1.082394
21	1	-2.307779	-2.321230	-0.643485
22	1	-4.767826	-2.141943	-0.606336
23	1	-5.830347	-0.050881	0.154890
24	1	-4.430026	1.846226	0.867029
25	1	-1.997724	1.673567	0.799053
26	1	2.017217	-0.229885	-2.054746

E(RHF) = -1041.46515942

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.403420(1)					
3	3	S	2	1.762540(2)	1	121.679(26)			
4	4	C	3	1.820820(3)	2	91.391(27)	1	-171.305(50)	0
5	5	C	4	1.525690(4)	3	105.124(28)	2	-23.231(51)	0
6	6	N	2	1.314170(5)	1	127.216(29)	3	179.177(52)	0
7	7	C	1	1.439510(6)	2	114.402(30)	3	5.289(53)	0
8	8	N	7	1.138160(7)	1	176.797(31)	2	3.213(54)	0
9	9	C	1	1.431500(8)	2	125.834(32)	3	-176.312(55)	0
10	10	C	9	1.497080(9)	1	117.094(33)	2	172.767(56)	0
11	11	C	10	1.391390(10)	9	120.096(34)	1	126.994(57)	0
12	12	C	11	1.382840(11)	10	120.273(35)	9	178.586(58)	0
13	13	C	12	1.385960(12)	11	120.172(36)	10	-1.557(59)	0
14	14	C	13	1.384530(13)	12	119.842(37)	11	0.554(60)	0
15	15	C	14	1.383990(14)	13	120.104(38)	12	0.834(61)	0
16	16	S	9	1.669150(15)	1	125.845(39)	2	-6.953(62)	0
17	17	H	4	1.080940(16)	3	109.045(40)	2	96.445(63)	0
18	18	H	4	1.079770(17)	3	109.459(41)	2	-144.087(64)	0
19	19	H	5	1.081150(18)	4	111.792(42)	3	149.593(65)	0
20	20	H	5	1.084880(19)	4	111.230(43)	3	-88.693(66)	0
21	21	H	11	1.073290(20)	10	119.583(44)	9	-1.652(67)	0
22	22	H	12	1.075050(21)	11	119.663(45)	10	178.939(68)	0
23	23	H	13	1.075280(22)	12	120.087(46)	11	-179.361(69)	0
24	24	H	14	1.074880(23)	13	120.257(47)	12	-179.548(70)	0
25	25	H	15	1.074160(24)	14	119.524(48)	13	179.764(71)	0
26	26	H	6	1.004120(25)	2	118.308(49)	1	-0.910(72)	0

E(RHF) = -1364.14185638

TS

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.352806	0.520349	-0.184393
2	6	1.792116	0.212358	-0.129203
3	16	2.710072	0.080372	1.334895
4	6	4.288557	0.061466	0.414446
5	6	3.922156	-0.255560	-1.039693
6	7	2.527942	0.147599	-1.189290
7	6	0.062009	1.864904	-0.552778
8	7	-0.091393	2.952412	-0.862301
9	6	-0.536999	-0.524580	-0.014182
10	6	-2.000553	-0.246233	0.038167
11	6	-2.891879	-1.070776	-0.644087
12	6	-4.250928	-0.822287	-0.597480
13	6	-4.741157	0.236022	0.152687
14	6	-3.864821	1.048239	0.851145
15	6	-2.501334	0.813961	0.787995
16	16	0.049796	-2.116459	0.100535
17	1	4.754433	1.032186	0.503595
18	1	4.945433	-0.686624	0.831081
19	1	4.539514	0.289802	-1.738647
20	1	3.995457	-1.315464	-1.248351

21	1	-2.512482	-1.902225	-1.205864
22	1	-4.927606	-1.458605	-1.139124
23	1	-5.799569	0.422216	0.195477
24	1	-4.237634	1.863962	1.443924
25	1	-1.831991	1.446227	1.340118
26	1	2.080874	0.158657	-2.083695

E(RHF) = -1364.10961207

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.367780(1)					
3	3	S	2	1.772020(2)	1	120.878(36)			
4	4	C	3	1.813320(3)	2	92.075(37)	1	-171.863(70)	0
5	5	C	4	1.522290(4)	3	104.121(38)	2	-24.592(71)	0
6	6	N	2	1.349680(5)	1	128.479(39)	3	-178.884(72)	0
7	7	C	1	1.492450(6)	2	123.468(40)	3	-158.978(73)	0
8	8	C	7	1.498550(7)	1	119.483(41)	2	-153.294(74)	0
9	9	C	8	1.392510(8)	7	117.906(42)	1	-155.497(75)	0
10	10	C	9	1.381470(9)	8	120.374(43)	7	-178.015(76)	0
11	11	C	10	1.387850(10)	9	119.914(44)	8	0.876(77)	0
12	12	C	11	1.384180(11)	10	120.087(45)	9	-0.129(78)	0
13	13	C	12	1.385540(12)	11	119.981(46)	10	-0.582(79)	0
14	14	C	1	1.433440(13)	2	117.473(47)	3	8.986(80)	0
15	15	N	14	1.139080(14)	1	179.494(48)	2	-36.417(81)	0
16	16	O	7	1.198470(15)	1	120.431(49)	2	28.564(82)	0
17	17	C	6	1.428750(16)	2	125.659(50)	1	21.302(83)	0
18	18	C	17	1.385170(17)	6	119.975(51)	2	-125.446(84)	0
19	19	C	18	1.383440(18)	17	119.762(52)	6	-175.914(85)	0
20	20	C	19	1.386070(19)	18	120.280(53)	17	-0.815(86)	0
21	21	C	20	1.384590(20)	19	119.768(54)	18	0.423(87)	0
22	22	C	21	1.385520(21)	20	120.176(55)	19	0.571(88)	0
23	23	H	4	1.080320(22)	3	109.419(56)	2	-144.837(89)	0
24	24	H	4	1.081520(23)	3	109.934(57)	2	95.114(90)	0
25	25	H	5	1.084700(24)	4	110.672(58)	3	-84.465(91)	0
26	26	H	5	1.079990(25)	4	111.920(59)	3	154.098(92)	0
27	27	H	9	1.073170(26)	8	118.932(60)	7	1.980(93)	0
28	28	H	10	1.075140(27)	9	119.976(61)	8	-179.297(94)	0
29	29	H	11	1.075550(28)	10	119.967(62)	9	179.856(95)	0
30	30	H	12	1.074930(29)	11	120.216(63)	10	179.730(96)	0
31	31	H	13	1.073530(30)	12	119.328(64)	11	-179.893(97)	0
32	32	H	18	1.073920(31)	17	119.644(65)	6	5.803(98)	0
33	33	H	19	1.074890(32)	18	119.593(66)	17	-179.762(99)	0
34	34	H	20	1.074950(33)	19	120.116(67)	18	-179.381(100)	0
35	35	H	21	1.074950(34)	20	120.213(68)	19	179.803(101)	0
36	36	H	22	1.074780(35)	21	120.379(69)	20	178.985(102)	0

E(RHF) = -1271.03410816

TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.231992	-0.649280	0.619688
2	6	0	1.064940	-1.201843	0.219165
3	16	0	1.347876	-2.913101	0.156102
4	6	0	3.130739	-2.688044	-0.130449
5	6	0	3.290354	-1.231082	-0.567600
6	7	0	2.111468	-0.499043	-0.082091
7	6	0	-1.201144	-0.666765	-0.417512
8	6	0	-2.612118	-0.191836	-0.211559
9	6	0	-3.589352	-0.747053	-1.034151
10	6	0	-4.910453	-0.357048	-0.920091
11	6	0	-5.269511	0.612237	0.004924
12	6	0	-4.302093	1.184995	0.811731
13	6	0	-2.978920	0.783500	0.708458
14	6	0	-0.319310	-0.223117	1.960045
15	7	0	-0.322114	0.109764	3.054673
16	8	0	-0.876080	-1.088026	-1.522762
17	6	0	2.104113	0.937350	-0.211902
18	6	0	1.475929	1.513444	-1.302360
19	6	0	1.520170	2.889461	-1.448346
20	6	0	2.187805	3.669408	-0.516623
21	6	0	2.808578	3.077882	0.571512
22	6	0	2.769058	1.702271	0.728181
23	1	0	3.476047	-3.371235	-0.891742
24	1	0	3.662758	-2.888226	0.788654
25	1	0	3.315775	-1.133463	-1.645927
26	1	0	4.182519	-0.780091	-0.159476
27	1	0	-3.296075	-1.481036	-1.759557
28	1	0	-5.657379	-0.802098	-1.553226
29	1	0	-6.296350	0.920950	0.092206
30	1	0	-4.572169	1.944278	1.523627
31	1	0	-2.245829	1.244542	1.340304
32	1	0	0.940193	0.895280	-1.998922
33	1	0	1.027721	3.349693	-2.285070
34	1	0	2.216822	4.737432	-0.634154
35	1	0	3.313626	3.682589	1.301998
36	1	0	3.228732	1.233270	1.579016

E(RHF) = -1271.00759035

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GS

Z-MATRIX (ANGSTROMS AND DEGREES)

CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.369840(1)					
3	3	S	2	1.775840(2)	1	119.611(36)			
4	4	C	3	1.810110(3)	2	91.277(37)	1	-166.162(70)	0
5	5	C	4	1.516030(4)	3	104.275(38)	2	-28.658(71)	0
6	6	N	2	1.356770(5)	1	129.577(39)	3	178.132(72)	0
7	7	C	1	1.479420(6)	2	128.184(40)	3	164.100(73)	0
8	8	C	7	1.488920(7)	1	116.613(41)	2	143.377(74)	0
9	9	C	8	1.395070(8)	7	120.974(42)	1	147.156(75)	0
10	10	C	9	1.381220(9)	8	120.598(43)	7	178.364(76)	0
11	11	C	10	1.387040(10)	9	120.182(44)	8	-0.684(77)	0
12	12	C	11	1.384290(11)	10	119.853(45)	9	0.512(78)	0
13	13	C	12	1.383640(12)	11	119.968(46)	10	0.386(79)	0
14	14	C	1	1.438560(13)	2	116.029(47)	3	-7.331(80)	0

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 15  15  N    14   1.138660( 14)   1  179.342( 48)   2    3.311( 81)   0
 16  16  S     7   1.632990( 15)   1  121.632( 49)   2  -40.581( 82)   0
 17  17  C     6   1.433420( 16)   2  124.353( 50)   1  -24.514( 83)   0
 18  18  C    17   1.385440( 17)   6  120.485( 51)   2  -54.084( 84)   0
 19  19  C    18   1.385650( 18)  17  119.804( 52)   6 -176.167( 85)   0
 20  20  C    19   1.384550( 19)  18  120.161( 53)  17    1.122( 86)   0
 21  21  C    20   1.386110( 20)  19  119.820( 54)  18   -0.201( 87)   0
 22  22  C    21   1.383740( 21)  20  120.198( 55)  19   -0.503( 88)   0
 23  23  H     4   1.080290( 22)   3  109.795( 56)   2 -149.004( 89)   0
 24  24  H     4   1.081180( 23)   3  109.520( 57)   2   90.963( 90)   0
 25  25  H     5   1.086200( 24)   4  110.997( 58)   3  -84.550( 91)   0
 26  26  H     5   1.080930( 25)   4  111.761( 59)   3  154.380( 92)   0
 27  27  H     9   1.072180( 26)   8  119.354( 60)   7   -2.221( 93)   0
 28  28  H    10   1.074980( 27)   9  119.698( 61)   8  179.168( 94)   0
 29  29  H    11   1.075390( 28)  10  120.071( 62)   9 -179.842( 95)   0
 30  30  H    12   1.074950( 29)  11  120.268( 63)  10  179.883( 96)   0
 31  31  H    13   1.073280( 30)  12  119.268( 64)  11  179.524( 97)   0
 32  32  H    18   1.074690( 31)  17  119.939( 65)   6    3.976( 98)   0
 33  33  H    19   1.074860( 32)  18  119.635( 66)  17 -179.424( 99)   0
 34  34  H    20   1.074890( 33)  19  120.085( 67)  18  179.859(100)   0
 35  35  H    21   1.074810( 34)  20  120.142( 68)  19 -179.700(101)   0
 36  36  H    22   1.074010( 35)  21  120.730( 69)  20 -178.231(102)   0
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E(RHF) =  -1593.65881571

TS
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                    Z-MATRIX (ANGSTROMS AND DEGREES)
 CD Cent Atom  N1     Length/X     N2    Alpha/Y     N3     Beta/Z      J
 ---------------------------------------------------------------------
  1   1  C
  2   2  C     1   1.369840(  1)
  3   3  S     2   1.775840(  2)   1  119.611( 36)
  4   4  C     3   1.810110(  3)   2   91.277( 37)   1 -166.162( 70)   0
  5   5  C     4   1.516030(  4)   3  104.275( 38)   2  -28.658( 71)   0
  6   6  N     2   1.356770(  5)   1  129.577( 39)   3  178.132( 72)   0
  7   7  C     1   1.479420(  6)   2  128.184( 40)   3   84.100( 73)   0
  8   8  C     7   1.488920(  7)   1  116.613( 41)   2 -175.461( 74)   0
  9   9  C     8   1.395070(  8)   7  120.974( 42)   1  137.156( 75)   0
 10  10  C     9   1.381220(  9)   8  120.598( 43)   7  178.364( 76)   0
 11  11  C    10   1.387040( 10)   9  120.182( 44)   8   -0.684( 77)   0
 12  12  C    11   1.384290( 11)  10  119.853( 45)   9    0.512( 78)   0
 13  13  C    12   1.383640( 12)  11  119.968( 46)  10    0.386( 79)   0
 14  14  C     1   1.438560( 13)   2  116.029( 47)   3  -87.331( 80)   0
 15  15  N    14   1.138660( 14)   1  179.342( 48)   2    3.308( 81)   0
 16  16  S     7   1.632990( 15)   1  121.632( 49)   2    0.581( 82)   0
 17  17  C     6   1.433420( 16)   2  124.353( 50)   1  -24.514( 83)   0
 18  18  C    17   1.385440( 17)   6  120.485( 51)   2   24.835( 84)   0
 19  19  C    18   1.385650( 18)  17  119.804( 52)   6 -176.167( 85)   0
 20  20  C    19   1.384550( 19)  18  120.161( 53)  17    1.122( 86)   0
 21  21  C    20   1.386110( 20)  19  119.820( 54)  18   -0.201( 87)   0
 22  22  C    21   1.383740( 21)  20  120.198( 55)  19   -0.503( 88)   0
 23  23  H     4   1.080290( 22)   3  109.795( 56)   2 -149.004( 89)   0
 24  24  H     4   1.081180( 23)   3  109.520( 57)   2   90.963( 90)   0
 25  25  H     5   1.086200( 24)   4  110.997( 58)   3  -84.550( 91)   0
 26  26  H     5   1.080930( 25)   4  111.761( 59)   3  154.380( 92)   0
 27  27  H     9   1.072180( 26)   8  119.354( 60)   7   -2.221( 93)   0
 28  28  H    10   1.074980( 27)   9  119.698( 61)   8  179.168( 94)   0
 29  29  H    11   1.075390( 28)  10  120.071( 62)   9 -179.842( 95)   0
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30	30	H	12	1.074950(29)	11	120.269(63)	10	179.883(96)	0
31	31	H	13	1.073280(30)	12	119.268(64)	11	179.524(97)	0
32	32	H	18	1.074690(31)	17	119.939(65)	6	3.976(98)	0
33	33	H	19	1.074860(32)	18	119.635(66)	17	-179.424(99)	0
34	34	H	20	1.074890(33)	19	120.085(67)	18	179.859(100)	0
35	35	H	21	1.074810(34)	20	120.142(68)	19	-179.700(101)	0
36	36	H	22	1.074010(35)	21	120.730(69)	20	-178.231(102)	0

E(RHF) = -1593.65193634

28

GS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.238242	-1.295442	-0.135709
2	6	0	-1.141141	-1.250182	-0.108997
3	7	0	-1.960174	-0.166412	-0.179554
4	6	0	-3.337453	-0.475463	-0.118080
5	6	0	-3.572997	-1.768991	0.023649
6	16	0	-2.100075	-2.702955	0.079465
7	6	0	-4.367676	0.608525	-0.207329
8	6	0	0.832751	-2.549581	0.211598
9	7	0	1.275019	-3.562052	0.492015
10	6	0	1.091460	-0.268203	-0.779569
11	6	0	2.520674	-0.124904	-0.349655
12	6	0	3.430724	0.385820	-1.271293
13	6	0	4.752028	0.577667	-0.915845
14	6	0	5.172759	0.278242	0.372237
15	6	0	4.270847	-0.214542	1.299515
16	6	0	2.949273	-0.421063	0.938247
17	8	0	0.663220	0.420330	-1.665485
18	1	0	-4.528228	-2.244000	0.095548
19	1	0	-4.294412	1.143133	-1.147140
20	1	0	-4.258324	1.328968	0.594234
21	1	0	-5.352304	0.164997	-0.140958
22	1	0	3.089020	0.626733	-2.259728
23	1	0	5.451877	0.961151	-1.636388
24	1	0	6.200546	0.429758	0.650714
25	1	0	4.593133	-0.442196	2.299441
26	1	0	2.257760	-0.803429	1.664967
27	6	0	-1.522978	1.180261	0.087351
28	6	0	-1.524986	2.130336	-0.917936
29	6	0	-1.174778	3.435335	-0.621597
30	6	0	-0.809428	3.783909	0.669607
31	6	0	-0.797808	2.825669	1.669041
32	6	0	-1.162512	1.520263	1.380021
33	1	0	-1.768024	1.839225	-1.921355
34	1	0	-1.171441	4.174643	-1.401481
35	1	0	-0.529820	4.797448	0.893693
36	1	0	-0.514077	3.090533	2.671245
37	1	0	-1.166180	0.770992	2.150878

E(RHF) = -1308.89274474

TS

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.337517	-0.546327	0.652608
2	6	0	-1.042009	-0.882800	0.307812
3	7	0	-1.988748	-0.038451	-0.033506
4	6	0	-3.227721	-0.618957	-0.306526
5	6	0	-3.241446	-1.943452	-0.170099
6	16	0	-1.660632	-2.477977	0.319221
7	6	0	-4.386880	-2.885221	-0.393162
8	6	0	0.551532	-0.130198	1.984039
9	7	0	0.659079	0.205357	3.072389
10	6	0	1.269839	-0.740657	-0.404673
11	6	0	2.740134	-0.476309	-0.230215
12	6	0	3.613193	-1.222458	-1.018213
13	6	0	4.979120	-1.029795	-0.932008
14	6	0	5.490599	-0.069213	-0.071743
15	6	0	4.629725	0.692571	0.698434
16	6	0	3.260053	0.488782	0.624157
17	8	0	0.871912	-1.139830	-1.492445
18	1	0	-4.032332	0.019204	-0.605087
19	1	0	-4.153347	-3.601610	-1.172613
20	1	0	-5.268263	-2.331774	-0.692565
21	1	0	-4.621134	-3.435241	0.511353
22	1	0	3.204809	-1.947093	-1.695932
23	1	0	5.643276	-1.621049	-1.537155
24	1	0	6.553127	0.086147	-0.006634
25	1	0	5.019076	1.446059	1.359451
26	1	0	2.611191	1.093119	1.226779
27	6	0	-1.779319	1.380520	-0.204503
28	6	0	-1.040510	1.822731	-1.287024
29	6	0	-0.878443	3.185551	-1.466888
30	6	0	-1.453376	4.081278	-0.577831
31	6	0	-2.187920	3.619508	0.501880
32	6	0	-2.353463	2.257625	0.695385
33	1	0	-0.588499	1.111335	-1.952920
34	1	0	-0.300939	3.544918	-2.298507
35	1	0	-1.322627	5.138196	-0.723127
36	1	0	-2.622827	4.312630	1.198074
37	1	0	-2.902768	1.884022	1.540132

E(RHF) = -1308.87593223

29
GS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.331694	-1.193251	0.009281
2	6	0	-1.070091	-1.282373	0.021903
3	7	0	-1.982680	-0.290541	0.083754
4	6	0	-3.324007	-0.729036	0.050187
5	6	0	-3.427930	-2.044482	-0.068088
6	16	0	-1.872888	-2.816794	-0.126919
7	6	0	-4.461639	0.243906	0.115872
8	6	0	0.987835	-2.314455	-0.601091
9	7	0	1.464982	-3.228730	-1.086343
10	6	0	1.143720	-0.271988	0.771914
11	6	0	2.542850	-0.062812	0.296210

12	6	0	3.602064	0.006602	1.198368
13	6	0	4.890267	0.231466	0.750685
14	6	0	5.136906	0.413113	-0.601623
15	6	0	4.090186	0.358026	-1.506166
16	6	0	2.803677	0.109440	-1.061106
17	16	0	0.626698	0.458543	2.159910
18	1	0	-4.331091	-2.613104	-0.133399
19	1	0	-4.412600	0.968618	-0.687525
20	1	0	-4.466588	0.784558	1.054490
21	1	0	-5.391982	-0.301890	0.031986
22	1	0	3.410009	-0.124068	2.245426
23	1	0	5.700626	0.266837	1.456319
24	1	0	6.139087	0.594133	-0.947264
25	1	0	4.273395	0.501429	-2.555774
26	1	0	1.997672	0.066200	-1.769335
27	6	0	-1.674494	1.092566	-0.184464
28	6	0	-1.238002	1.441951	-1.451767
29	6	0	-0.999620	2.772899	-1.749298
30	6	0	-1.214199	3.747402	-0.787777
31	6	0	-1.660718	3.389785	0.473485
32	6	0	-1.885281	2.058729	0.782041
33	1	0	-1.086967	0.681034	-2.195274
34	1	0	-0.657358	3.045893	-2.730698
35	1	0	-1.031756	4.780812	-1.020328
36	1	0	-1.819526	4.141838	1.224236
37	1	0	-2.199300	1.769700	1.766012

E(RHF) = -1631.5243238

TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.343031	-0.446019	0.458458
2	6	0	1.046471	-0.849265	0.265428
3	7	0	2.048028	-0.011838	0.090909
4	6	0	3.311382	-0.604500	0.067369
5	6	0	3.284366	-1.925023	0.224292
6	16	0	1.636961	-2.452153	0.407303
7	6	0	4.437054	-2.884273	0.218257
8	6	0	-0.525366	0.384960	1.606908
9	7	0	-0.585552	1.030866	2.545176
10	6	0	-1.362454	-0.893825	-0.375325
11	6	0	-2.757882	-0.427360	-0.097207
12	6	0	-3.788842	-1.356355	0.011828
13	6	0	-5.083064	-0.938337	0.258932
14	6	0	-5.371363	0.413774	0.369458
15	6	0	-4.355705	1.343867	0.238995
16	6	0	-3.053465	0.925918	0.015907
17	16	0	-1.090931	-1.890447	-1.715602
18	1	0	4.161937	0.023468	-0.092495
19	1	0	4.495489	-3.429953	1.153242
20	1	0	5.365900	-2.344967	0.080668
21	1	0	4.337060	-3.603432	-0.586718
22	1	0	-3.570431	-2.400967	-0.101829
23	1	0	-5.868181	-1.666872	0.355281
24	1	0	-6.380696	0.737688	0.551382
25	1	0	-4.570955	2.394705	0.314031

26	1	0	-2.273202	1.657167	-0.084461
27	6	0	1.891243	1.400079	-0.172262
28	6	0	2.334337	2.316240	0.762262
29	6	0	2.223257	3.667838	0.480258
30	6	0	1.668948	4.082891	-0.719264
31	6	0	1.222410	3.150067	-1.643280
32	6	0	1.335179	1.796757	-1.375897
33	1	0	2.734765	1.980821	1.700956
34	1	0	2.556265	4.390250	1.202151
35	1	0	1.579006	5.132467	-0.932355
36	1	0	0.788298	3.472474	-2.571580
37	1	0	0.990076	1.060937	-2.078778

E(RHF) = -1631.51877044