

Supplementary Material

E/Z Configurational determination of oximes and related derivatives through quantum mechanics NMR calculations. Scope and limitations of the leading probabilistic methods.

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1. Structures of compounds 1-30

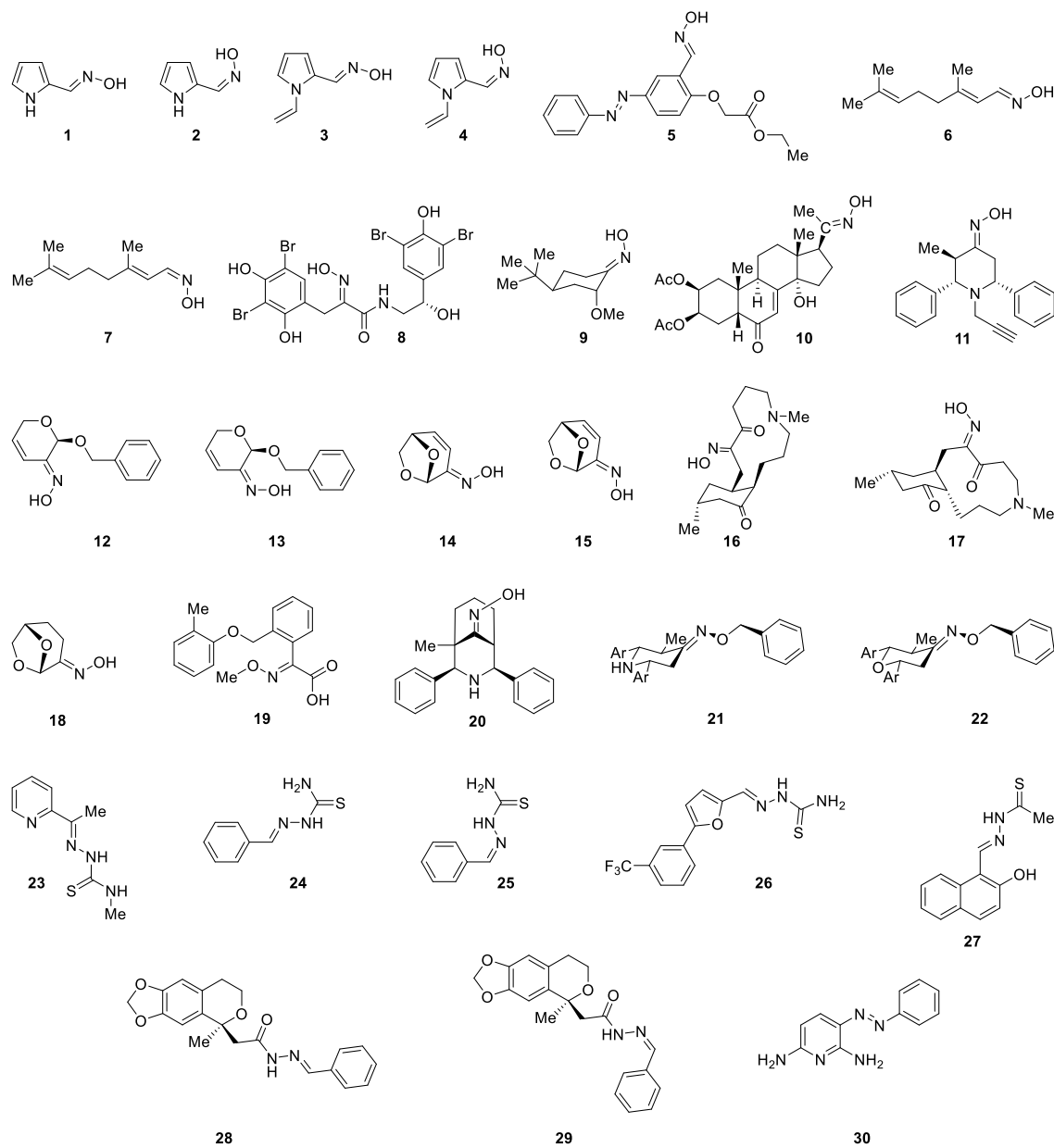
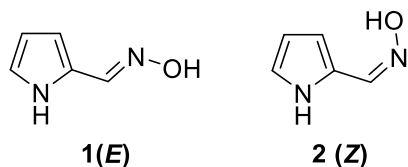


Figure S1. Structures of all compounds under study (1-30).

2. Experimental NMR chemical shifts, and Boltzmann averaged GIAO isotropic magnetic shielding values calculated at the PCM/mPW1PW91/6-31+G//B3LYP/6-31G* level of theory for all compounds under study**

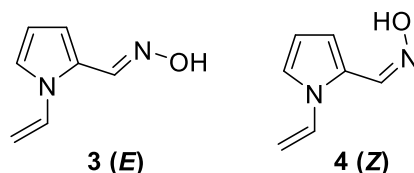
Compounds 1 (E) and 2 (Z)



δ Exp		Shielding tensors	
<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
142.61	138.88	55.91	59.31
124.33	124.33	72.84	73.07
113.76	115.27	84.69	83.23
109.89	109.39	89.48	89.66
121.35	121.90	77.33	76.30
8.03	7.32	23.39	24.12
6.43	6.53	24.91	24.79
6.25	6.28	25.04	24.98
6.88	6.99	24.43	24.27

Experimental NMR data from: *Magn. Reson. Chem.* **2010**, *48*, 685–692.

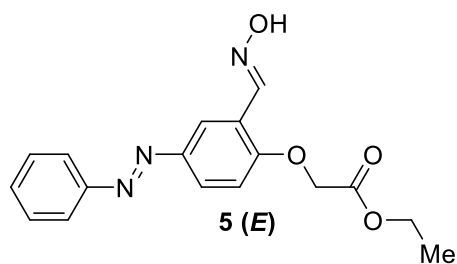
Compounds 3 (E) and 4 (Z)



δ Exp		Shielding tensors	
<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
132.65	130.2	64.33	66.28
100.56	104.04	102.30	95.78
142.96	135.36	53.82	62.55
124.8	122.45	71.93	74.24
115.77	119.63	79.48	77.03
110.74	111.12	87.39	88.03
121.7	121.18	77.58	76.42
4.81	4.98	26.64	26.33
5.20	5.29	26.10	25.98
7.55	7.08	23.03	24.08
8.10	7.49	23.32	24.05
6.49	7.41	24.89	23.78
6.27	6.37	25.01	24.92
7.15	7.08	23.85	24.15

Experimental NMR data from: *Magn. Reson. Chem.* **2009**, *47*, 105–112

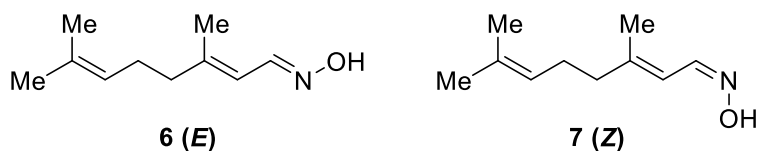
Compound 5 (E)



δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
112.50	87.26	87.98
126.30	76.18	70.50
121.90	71.60	68.00
146.10	52.36	57.24
66.20	130.44	130.06
168.10	29.70	29.57
61.80	133.05	132.93
14.20	180.93	181.06
123.10	75.79	77.76
157.80	40.87	39.96
147.40	51.95	52.18
152.40	46.69	46.83
123.00	74.69	74.62
129.00	69.83	69.92
130.80	67.03	66.98
6.93	24.60	24.50
7.97	23.16	23.07
8.37	22.44	21.49
8.64	22.46	23.08
4.81	26.81	26.77
4.30	27.21	27.24
1.31	30.21	30.23
7.90	23.17	23.15
7.50	23.68	23.68
7.47	23.69	23.71

Experimental NMR data from: *Magn. Reson. Chem.* **2012**, 50, 765–771

Compounds 6 (E) and 7 (Z)

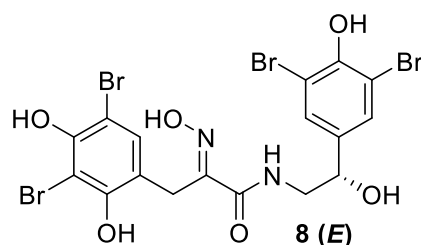


δ Exp	Shielding tensors			
	<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
149.00	145.70	48.81	52.76	
117.90	112.90	78.77	85.58	
147.90	150.20	46.58	43.61	
40.10	40.30	152.81	152.61	

26.20	26.20	165.79	165.59
123.30	123.30	72.70	72.83
132.30	132.30	63.50	63.27
17.70	17.70	177.92	177.84
25.70	25.70	169.12	169.08
17.20	17.20	177.76	178.01
8.07	7.37	23.16	24.07
5.93	6.53	25.42	24.63
2.16	2.18	29.39	29.34
2.16	2.17	29.29	29.26
5.08	5.09	26.08	26.05
1.61	1.61	29.84	29.83
1.69	1.69	29.85	29.84
1.83	1.88	29.61	29.60

Experimental NMR data from: *J. Mol. Struct.* **2021**, 1227, 129427

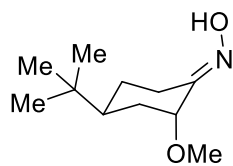
Compound 8 (E)



δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
116.90	80.22	80.84
152.40	46.17	46.26
102.40	81.01	80.54
150.10	48.86	48.60
100.50	81.68	81.05
131.90	65.06	65.26
24.40	169.42	159.95
150.60	42.83	43.99
164.70	34.96	39.04
46.60	149.04	148.78
69.20	121.32	121.64
137.70	64.98	64.17
129.80	69.45	69.60
111.70	73.13	72.76
149.60	48.61	49.24
7.16	23.86	24.18
3.63	27.79	28.04
3.32	27.73	27.60
4.63	26.74	26.64
7.45	24.18	24.15

Experimental NMR data from: *Eur. J. Org. Chem.* **2020**, 2583–2591

Compound 9 (E)

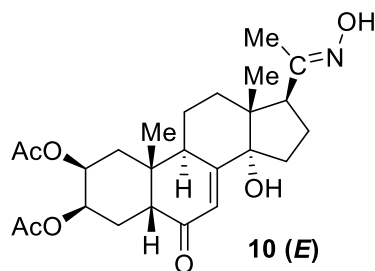


9 (E)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
159.70	35.55	35.39
78.10	116.23	126.48
33.90	159.63	161.78
40.80	153.23	153.11
26.30	166.94	166.00
20.80	172.37	164.27
32.00	161.39	160.66
27.40	168.75	169.00
55.80	140.74	139.91
3.78	28.06	26.72
3.23	28.34	28.24
3.23	28.24	29.51
1.92	29.55	29.04
2.17	29.38	29.42
1.70	29.65	29.76
0.87	30.70	30.69

Experimental NMR data from: *Magn. Reson. Chem.* **2000**, 38, 627–638

Compound 10 (E)



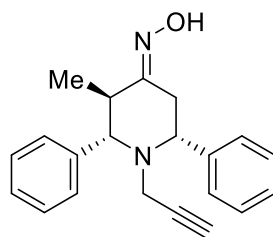
10 (E)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
15.58	178.28	173.25
17.13	177.38	177.10
20.50	173.14	173.33
21.08	173.98	173.99
21.12	173.94	173.97
21.39	171.88	170.79
23.84	170.65	170.46
29.09	161.59	161.30
29.71	163.98	163.39
31.78	162.95	163.02
33.78	157.27	157.35

33.94	160.14	159.82
38.35	153.77	153.77
47.75	144.10	141.38
50.94	142.83	142.81
51.40	140.06	150.37
67.00	127.23	127.38
68.71	126.03	125.90
83.85	107.93	108.06
121.48	75.64	75.77
158.24	36.44	36.05
164.26	31.17	31.63
170.33	27.54	27.71
170.74	27.15	27.20
202.45	-4.03	-4.21
0.61	30.85	30.66
1.01	30.52	30.52
1.90	29.60	29.65
2.00	29.52	29.52
2.10	29.43	29.44
2.36	29.28	29.27
3.11	28.35	27.25
5.03	26.32	26.33
5.32	26.08	26.07
5.87	25.62	25.64

Experimental NMR data from: *Canadian Journal of Chemistry*, **2017**, 95, 130–133

Compound 11 (*E*)



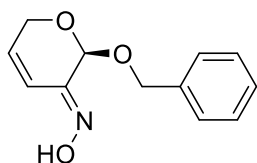
11 (*E*)

δ Exp	Shielding tensors	
<i>E</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
12.70	181.81	177.17
71.80	123.92	128.98
43.00	149.03	153.49
159.50	36.96	35.51
33.80	159.82	155.90
63.80	130.73	132.07
40.00	154.30	151.60
77.60	119.53	116.21
73.90	124.73	126.18
141.80	55.26	51.81
142.80	53.08	52.90
0.82	30.81	30.10
2.70	28.88	27.88

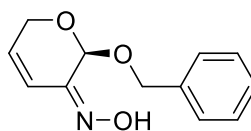
3.59	27.97	28.92
3.46	27.93	27.25
3.79	27.56	27.25
2.94	28.51	28.18
2.83	28.72	28.39
2.22	29.51	29.13
2.16	29.34	29.59
7.39	23.68	23.67
7.39	23.81	23.76
7.39	23.90	23.93
7.39	23.68	23.51
7.39	23.73	23.72
7.39	23.92	23.93

Experimental NMR data from: *Spectrochim. Acta A Mol. Biomol.* **2015**, 139, 108–118.

Compounds 12 (*E*) and 13 (*Z*)



12 (*E*)

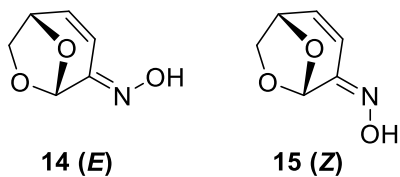


13 (*Z*)

δ Exp		Shielding tensors	
<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
95.10	89.80	99.84	104.33
148.00	150.50	48.34	45.41
113.50	120.10	84.84	76.65
135.80	133.50	59.19	62.40
60.40	59.30	134.02	135.21
69.80	70.30	127.01	124.21
137.30	137.50	58.35	58.13
128.60	128.50	72.61	70.84
128.10	128.20	70.64	71.13
128.00	128.00	72.13	71.37
5.28	5.98	26.48	25.57
6.82	6.20	24.28	25.10
6.34	6.26	24.76	24.91
4.49	4.45	26.95	26.92
4.25	4.17	27.28	27.36
4.71	4.80	26.61	26.66
7.33	7.34	23.80	23.67
7.33	7.34	23.85	23.85
7.33	7.34	23.94	23.94

Experimental NMR data from: *J. Org. Chem.* **2001**, 66, 8859–8866

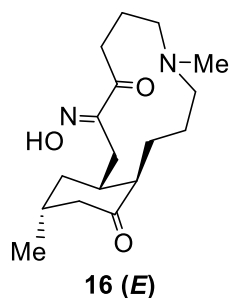
Compounds 14 (E) and 15 (Z)



δ Exp		Shielding tensors	
<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
70.22	69.09	125.39	126.59
72.10	71.35	121.02	121.20
100.09	93.07	93.44	101.62
115.57	122.30	81.89	73.49
137.90	135.70	57.34	60.42
150.06	152.60	45.92	42.81
3.85	3.87	27.62	27.64
4.87	4.90	26.74	26.76
5.73	6.60	25.98	24.84
6.60	6.53	24.50	24.66
6.80	6.15	24.38	25.17

Experimental NMR data from: *Chem. Nat. Compd.* **2003**, 39, 563–568

Compound 16 (E)

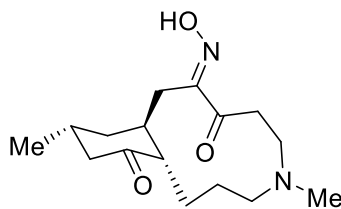


δ Exp	Shielding tensors	
<i>E</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
58.60	138.75	141.73
24.00	169.64	172.36
36.00	159.85	155.31
199.60	-1.64	-10.10
159.30	36.01	34.19
26.80	167.83	164.43
34.10	159.83	155.81
36.70	158.90	159.04
56.50	140.57	138.42
24.10	170.50	168.02
22.00	171.48	172.18
53.00	141.80	141.40
214.00	-18.44	-16.36
46.10	149.02	145.34
30.80	161.72	162.01
21.40	174.26	173.41
41.30	155.79	156.08

2.25	29.29	28.86
2.13	29.53	29.64
2.12	29.27	29.73
1.64	30.05	29.75
3.29	28.69	28.39
2.60	28.96	28.92
3.23	28.33	29.07
2.54	29.24	29.61
3.28	28.37	29.00
1.93	29.60	29.62
1.44	30.12	30.07
2.27	29.34	29.25
2.15	29.46	29.49
1.33	30.38	30.32
1.24	30.41	30.47
1.82	29.83	29.89
1.61	30.04	29.98
2.52	29.24	29.10
2.65	28.91	29.42
1.96	29.69	29.53
2.20	29.22	29.36
0.92	30.55	30.59
2.02	29.51	29.49

Experimental NMR data from: *J. Org. Chem.* **2020**, 85, 6803–6807

Compound 17 (*E*)



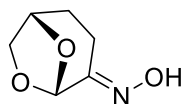
17 (*E*)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
54.60	145.23	141.13
22.70	171.44	171.50
34.30	161.71	152.62
199.70	-1.56	-7.76
160.00	35.27	35.91
30.20	163.99	156.65
36.90	155.11	155.23
39.10	156.36	159.26
58.30	138.42	139.38
25.30	167.48	170.17
27.90	167.12	166.73
54.20	139.61	141.75
213.40	-17.22	-16.91
48.10	146.64	147.09
29.50	162.86	162.45

21.00	174.55	174.33
42.10	154.92	155.51
2.48	28.90	29.23
2.00	29.78	29.37
1.93	29.63	29.66
1.84	29.81	29.71
3.22	28.16	28.55
2.87	29.14	28.60
3.19	28.48	29.05
2.76	29.10	29.11
2.54	29.15	29.32
1.67	29.81	29.83
1.67	29.88	29.87
2.16	29.48	29.20
2.16	29.41	29.46
1.50	30.15	30.07
1.36	30.54	30.32
1.71	30.09	29.78
1.67	30.25	30.02
2.37	29.49	29.28
2.44	29.06	29.25
2.09	29.54	29.47
2.20	29.24	29.34
0.87	30.63	30.63
1.97	29.56	29.54

Experimental NMR data from: *J. Org. Chem.* **2020**, 85, 6803–6807

Compound 18 (E)

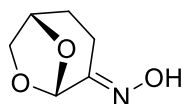


18 (E)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
15.86	176.58	169.85
27.41	165.03	163.16
67.15	128.50	128.09
73.16	120.50	120.29
100.08	93.38	102.13
153.95	40.68	40.27
1.75	29.89	29.87
2.05	29.55	29.51
2.25	29.25	28.95
3.05	28.39	29.46
3.87	27.60	27.60
3.93	27.49	27.45
4.67	27.03	27.02
5.51	26.17	24.98

Experimental NMR data from: *Chem. Nat. Compd.* **2003**, 39, 563–568

Compound 19 (E)

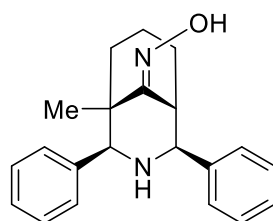


18 (E)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
164.70	34.41	33.45
156.31	47.41	45.01
156.10	42.17	42.62
134.44	59.08	59.32
133.01	69.98	70.28
130.32	68.63	68.51
127.53	67.99	69.02
127.22	71.98	72.13
126.81	72.18	70.61
126.56	68.86	68.72
125.79	70.19	70.22
125.72	72.36	71.86
120.14	79.32	79.45
111.34	88.49	88.32
66.96	128.49	127.14
61.31	133.24	133.68
16.11	176.70	176.68
7.43	23.53	23.30
7.30	23.72	23.72
7.25	23.86	23.80
7.11	23.93	23.64
7.11	24.10	24.08
7.11	24.16	24.13
6.87	24.72	24.62
6.81	24.42	24.39
4.98	26.44	26.16
3.76	27.42	27.42
2.22	29.19	29.11

Experimental NMR data from: *J. Agric. Food Chem.* **2008**, 56, 1545–1552

Compound 20 (E)



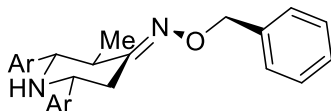
20 (E)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
164.83	31.38	34.03
142.10	50.29	50.74

140.60	53.07	52.62
71.61	119.87	119.37
63.10	125.92	126.03
40.85	150.09	146.31
35.39	152.20	142.59
35.27	152.36	149.12
28.81	166.24	165.14
21.78	174.27	173.99
21.00	174.06	169.48
7.57	23.62	23.58
4.32	27.44	27.45
3.99	27.19	27.28
3.73	27.64	29.05
3.10	30.16	29.95
1.98	29.77	29.88
1.75	29.70	29.84
1.48	29.44	29.46
1.35	29.89	29.87
0.92	31.04	30.40

Experimental NMR data from: *Bioorg. Med. Chem. Lett.* **2010**, 20, 642–1647

Compound 21 (*E*)



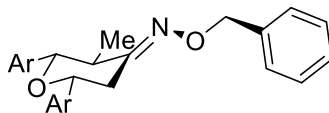
21 (*E*)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
69.50	124.60	126.52
60.94	132.40	130.18
43.37	147.94	146.00
34.77	157.89	147.74
160.15	35.68	38.24
75.65	118.97	118.58
11.91	182.42	179.36
138.46	58.84	58.39
142.84	53.71	54.47
143.90	52.56	52.62
3.41	28.01	27.92
3.74	27.74	27.65
2.40	29.04	28.95
1.93	29.66	29.22
3.51	27.99	29.18
5.03	26.43	26.52
0.80	30.77	30.50
7.34	24.00	24.01

7.34 23.95 23.95

Experimental NMR data from: *Bioorg. Med. Chem. Lett.* **2009**, 19, 2981–2985

Compound 22 (*E*)

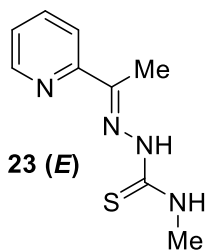


22 (*E*)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
86.86	107.39	108.68
78.66	115.72	113.83
42.99	148.01	146.13
34.35	157.65	148.18
158.28	37.60	40.42
75.80	119.08	118.48
11.17	183.06	179.97
138.17	59.34	58.83
140.51	56.09	57.30
141.77	54.40	54.59
4.22	27.25	27.36
4.56	26.83	26.91
2.56	28.98	28.89
2.12	29.60	29.23
3.69	27.87	29.04
5.14	26.40	26.51
0.91	30.81	30.51

Experimental NMR data from: *Bioorg. Med. Chem. Lett.* **2009**, 19, 2981–2985

Compound 23 (*E*)



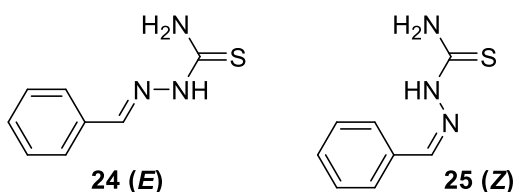
23 (*E*)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
154.50	43.69	44.93
123.90	79.42	74.11
136.20	62.35	61.55
120.30	75.10	75.31
148.80	49.51	50.02
147.60	51.85	62.89
11.40	186.79	172.23
178.80	20.69	19.63

31.20	164.50	165.11
7.95	23.06	23.74
7.69	23.55	23.34
7.27	24.04	23.91
8.58	22.70	22.48
2.38	29.04	29.23
3.26	28.45	28.53

Experimental NMR data from: *Transition Met. Chem.* **1992**, 17, 384–386

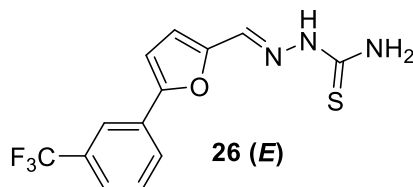
Compounds 24 (*E*) and 25 (*Z*)



δ Exp		Shielding tensors	
<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
178.40	178.90	20.92	19.17
142.50	133.70	55.93	66.38
153.30	151.90	44.82	45.39
120.20	126.60	78.19	71.97
136.50	138.30	61.88	61.27
124.10	124.10	74.38	74.87
149.30	148.40	47.68	49.48
8.08	7.41	23.83	24.48
8.26	7.77	23.22	23.83
7.81	8.06	23.48	23.34
7.35	7.54	23.98	23.94
8.55	8.79	22.67	22.52

Experimental NMR data from: *Magn. Reson. Chem.* **2014**, 52, 98–105

Compound 26 (*E*)

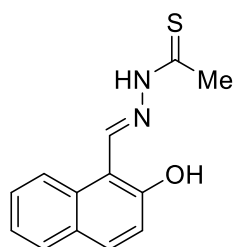


δ Exp	Shielding tensors	
<i>E</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
177.70	21.24	20.46
131.60	64.98	65.48
149.80	49.21	50.17
115.20	80.77	79.42
110.10	89.21	89.15
152.60	43.27	43.13
130.20	67.41	68.86

120.30	76.90	76.19
125.00	69.78	74.43
124.50	72.87	72.02
127.60	69.13	68.26
130.00	65.88	66.26
124.10	71.44	70.91
8.00	24.08	24.61
7.11	24.44	24.41
7.35	24.27	24.25
8.12	23.11	23.16
7.68	23.61	23.56
8.14	23.64	23.57
7.68	23.15	22.98

Experimental NMR data from: *Magn. Reson. Chem.* **2014**, 52, 98–105

Compound 27 (*E*)

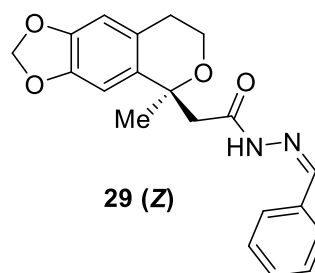
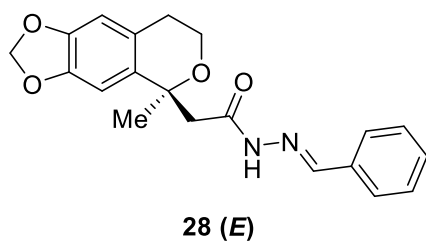


27 (*E*)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
173.30	21.14	17.40
143.10	56.95	57.75
109.70	88.73	87.41
156.70	39.96	44.21
118.40	80.12	81.09
132.50	63.09	63.54
128.00	69.34	69.65
128.70	68.52	68.93
123.50	75.33	74.65
127.90	70.24	69.85
122.90	78.82	75.09
131.40	64.47	66.67
9.05	22.65	23.41
7.87	23.97	24.13
7.85	23.40	23.35
7.36	23.79	23.74
7.56	23.57	23.58
8.50	23.13	23.67

Experimental NMR data from: *Magn. Reson. Chem.* **2014**, 52, 98–105

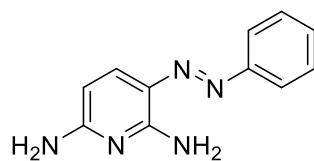
Compounds 28 (E) and 29 (Z)



δ Exp		Shielding tensors	
<i>E</i> -Isomer	<i>Z</i> -Isomer	<i>E</i> -Isomer	<i>Z</i> -Isomer
75.97	75.88	116.23	116.70
146.25	145.77	52.74	52.65
146.37	145.89	52.73	52.65
132.34	134.58	65.10	63.31
126.48	125.79	69.58	69.72
166.45	172.87	31.99	28.93
133.48	133.85	62.56	66.55
108.25	106.25	89.72	89.59
105.39	105.51	91.69	91.51
127.46	126.91	70.27	70.31
128.39	128.54	71.19	69.71
130.12	129.76	68.45	68.60
147.10	143.75	54.15	58.96
59.72	59.86	134.95	135.05
29.18	29.24	163.66	163.18
48.37	42.49	145.63	150.06
100.80	100.60	94.43	94.12
27.20	28.36	168.28	168.45
6.50	6.52	24.78	24.75
6.59	6.66	24.62	24.70
7.70	7.61	23.52	23.62
7.40	7.40	23.80	23.69
7.40	7.40	23.96	23.81
8.00	7.70	23.18	24.12
4.10	4.00	27.51	27.67
2.80	2.75	28.85	28.87
2.90	3.46	28.77	28.28
2.90	3.10	28.68	28.82
5.90	5.80	25.41	25.38
1.56	1.63	30.04	30.04

Experimental NMR data from: *Magn. Reson. Chem.* **1998**, 36, 533–538

Compound 30 (*E*)



30 (*E*)

δ Exp	Shielding tensors	
	<i>E</i> -Isomer	<i>Z</i> -Isomer
153.60	48.54	36.71
124.00	72.07	72.86
138.10	53.34	70.90
100.00	99.83	103.51
160.90	39.43	38.92
152.70	45.82	40.96
121.00	77.05	80.35
129.00	70.01	69.69
127.70	70.66	73.47
7.72	23.56	25.07
6.03	25.30	26.03
7.69	23.41	24.39
7.42	23.79	23.78
7.26	23.92	24.07

Experimental NMR data from: *Magn. Reson. Chem.* **2005**, 43, 256–260

3. Cartesian Coordinates found at the B3LYP/6-31G* level of theory and energies found at the PCM/mPW1PW91/6-31+G level of theory of all significant conformers for all compounds under study**

Comp_01E_c01			H	0.279814	-1.580535	-0.000038	
B3LYP/6-31G* Geometry			H	-2.213097	-2.091889	-0.000379	
N	0.816322	-0.978058	0.000311	H	-3.497518	0.310311	0.000318
C	2.183174	-0.924729	0.000076	H	-1.548066	2.200163	0.000478
C	2.559116	0.406613	-0.000461	H	1.175361	2.134876	-0.000115
C	1.371008	1.179689	0.000170	H	3.165539	-1.164547	0.000718
C	0.295733	0.298766	0.000255	Number of Imaginary Frequencies= 0			
C	-1.124344	0.552316	0.000020	SCF Energy (PCM/mPW1PW91/6-31+G**) = -378.746651029			
N	-1.964145	-0.421720	-0.000462	Comp_02Z_c02			
O	-3.286513	0.060940	0.000070	B3LYP/6-31G* Geometry			
H	0.239909	-1.806622	0.000095	N	-1.313149	-1.046729	-0.000186
H	2.778094	-1.826840	0.000250	C	-2.400053	-0.219993	-0.000181
H	3.574880	0.777344	-0.000848	C	-1.940218	1.085210	0.000097
H	1.295403	2.258963	0.000242	C	-0.526439	1.039808	0.000377
H	-1.463467	1.590020	0.000680	C	-0.141799	-0.300356	0.000011
H	-3.806079	-0.757864	-0.000279	C	1.130342	-0.982408	0.000329
Number of Imaginary Frequencies= 0			N	2.333652	-0.521911	0.000182	
SCF Energy (PCM/mPW1PW91/6-31+G**) = -378.744858061			O	2.358411	0.884753	-0.000459	
Comp_01E_c02			H	-1.350132	-2.055055	-0.000750	
B3LYP/6-31G* Geometry			H	-3.404978	-0.617393	-0.000506	
N	1.239052	-1.081430	-0.000032	H	-2.559033	1.972180	0.000195
C	2.488475	-0.522368	0.000013	H	0.156457	1.873741	0.000698
C	2.335555	0.852740	0.000028	H	1.105446	-2.072835	0.000813
C	0.947077	1.127256	-0.000039	H	3.310438	1.068262	-0.000537
C	0.274082	-0.089136	-0.000010	Number of Imaginary Frequencies= 0			
C	-1.130479	-0.428417	-0.000047	SCF Energy (PCM/mPW1PW91/6-31+G**) = -378.742542235			
N	-2.045374	0.473910	0.000093	Comp_03E_c01			
O	-3.319383	-0.126087	-0.000027	B3LYP/6-31G* Geometry			
H	1.044810	-2.071571	0.000365	N	-1.087058	-0.111273	-0.083013
H	3.376238	-1.138065	0.000008	C	-2.003979	0.920327	-0.060221
H	3.138874	1.576862	0.000002	C	-1.323404	2.114272	0.023369
H	0.468434	2.096142	-0.000125	C	0.060699	1.814003	0.056149
H	-1.409493	-1.487215	-0.000264	C	0.200105	0.437138	-0.011663
H	-3.907804	0.644738	0.000130	C	-1.399676	-1.480185	-0.173981
Number of Imaginary Frequencies= 0			C	-2.564088	-2.033547	0.172404	
SCF Energy (PCM/mPW1PW91/6-31+G**) = -378.741093779			C	1.395310	-0.378726	0.030904	
Comp_02Z_c01			N	2.560576	0.160421	-0.040456	
B3LYP/6-31G* Geometry			O	3.557983	-0.826482	0.056892	
N	-0.454086	-0.887147	-0.000237	H	-3.059373	0.715131	-0.152197
C	-1.800795	-1.092855	-0.000160	H	-1.775045	3.096712	0.045677
C	-2.429165	0.143541	0.000197	H	0.884390	2.509463	0.130885
C	-1.415169	1.126234	0.000276	H	-0.601030	-2.084801	-0.589148
C	-0.184430	0.468704	-0.000167	H	-3.380064	-1.468806	0.610903
C	1.135007	1.047126	-0.000301	H	-2.720823	-3.094394	0.015201
N	2.306108	0.507245	-0.000166	H	1.312060	-1.461388	0.143023
O	2.230141	-0.913195	0.000346	H	4.371595	-0.303795	-0.016965

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -456.113393117

Comp_03E_c02
B3LYP/6-31G* Geometry

N 0.906934 0.259261 -0.003824
C 2.179887 -0.273580 -0.003912
C 2.095650 -1.646779 0.000492
C 0.719367 -1.979338 0.003223
C -0.009473 -0.798418 0.000305
C 0.581492 1.631685 -0.006523
C 1.454468 2.641939 0.007412
C -1.452880 -0.725978 0.001657
N -2.151077 0.354123 -0.000409
O -3.524375 0.042274 0.000648
H 3.045669 0.369903 -0.009365
H 2.932486 -2.331516 0.000772
H 0.287172 -2.971220 0.006591
H -0.487338 1.801112 -0.020503
H 2.531835 2.515651 0.024729
H 1.081318 3.659486 0.001616
H -1.962064 -1.692811 0.004269
H -3.936150 0.920329 0.000413

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -456.116163897

Comp_03E_c03
B3LYP/6-31G* Geometry

N -1.229222 0.309029 -0.128327
C -2.329701 -0.525079 -0.065384
C -1.897196 -1.821195 0.095205
C -0.480627 -1.791472 0.118437
C -0.073591 -0.473984 -0.021351
C -1.355947 1.711100 -0.187500
C -0.530886 2.614491 0.346851
C 1.263486 0.061477 -0.183411
N 2.286528 -0.623170 0.186915
O 3.472441 0.055534 -0.153440
H -3.326322 -0.109350 -0.108531
H -2.530708 -2.694040 0.174591
H 0.194553 -2.633004 0.181640
H -2.249315 2.023364 -0.722612
H 0.342282 2.349337 0.931300
H -0.735796 3.669901 0.205513
H 1.396473 1.035854 -0.655689
H 4.154938 -0.539383 0.194112

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -456.111897246

Comp_03E_c04
B3LYP/6-31G* Geometry

N -1.033943 0.529324 -0.000053

C -2.374356 0.184459 -0.000100
C -2.508985 -1.182305 0.000008
C -1.201379 -1.712772 0.000084
C -0.287764 -0.661989 0.000078
C -0.685032 1.900451 -0.000118
C 0.512953 2.483923 0.000208
C 1.134886 -0.918124 0.000045
N 2.106505 -0.077446 -0.000008
O 3.334517 -0.772055 -0.000116
H -3.125318 0.961368 -0.000158
H -3.440617 -1.730527 0.000043
H -0.922789 -2.758507 0.000198
H -1.582352 2.512155 -0.000446
H 1.441893 1.931029 0.000522
H 0.545931 3.568509 0.000110
H 1.376826 -1.983886 0.000106
H 3.980410 -0.048707 -0.000254

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -456.109246954

Comp_04Z_c01
B3LYP/6-31G* Geometry

N 1.058928 0.030342 -0.095281
C 1.562884 1.311858 -0.073119
C 0.514894 2.199869 0.020718
C -0.682043 1.444678 0.056804
C -0.343980 0.097854 -0.013137
C 1.832599 -1.140985 -0.201455
C 3.100417 -1.264585 0.197710
C -1.145706 -1.103145 0.052505
N -2.426323 -1.255564 0.059901
O -3.114800 -0.033074 -0.018106
H 2.623612 1.481473 -0.179341
H 0.601583 3.277665 0.041236
H -1.689823 1.818188 0.133581
H 1.318481 -1.967272 -0.680344
H 3.639779 -0.468538 0.700375
H 3.632062 -2.192166 0.019303
H -0.630118 -2.057806 0.123649
H -4.039797 -0.323671 -0.006108

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -456.114451848

Comp_04Z_c02
B3LYP/6-31G* Geometry

N -0.674935 0.309240 0.075921
C -1.980022 -0.025649 0.371122
C -2.130476 -1.389933 0.278550
C -0.875334 -1.918835 -0.108793
C 0.026130 -0.868885 -0.208304
C -0.214499 1.629197 -0.129050
C -1.000103 2.672510 -0.404986
C 1.426806 -1.035843 -0.581573

N 2.527950 -0.488196 -0.205442
O 2.346622 0.514731 0.768546
H -2.688545 0.742417 0.640884
H -3.037075 -1.943127 0.482220
H -0.626121 -2.960777 -0.261787
H 0.857065 1.727201 -0.017731
H -2.072776 2.593122 -0.548180
H -0.560133 3.658958 -0.499159
H 1.609014 -1.853471 -1.278487
H 3.259483 0.795146 0.938726

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -456.108780417**

Comp_04Z_c03
B3LYP/6-31G* Geometry

N -1.208926 0.131554 -0.125136
C -1.718249 1.409782 -0.033729
C -0.676217 2.299122 0.093763
C 0.523658 1.548097 0.072800
C 0.194984 0.204564 -0.071596
C -2.050022 -0.999826 -0.150707
C -1.813327 -2.189339 0.407371
C 1.021159 -0.957432 -0.320172
N 2.297261 -1.110504 -0.219644
O 2.945414 0.049321 0.243973
H -2.787790 1.566279 -0.025690
H -0.768510 3.372146 0.191517
H 1.532476 1.925171 0.114963
H -2.983187 -0.810171 -0.675596
H -0.921136 -2.408041 0.982481
H -2.543534 -2.983245 0.295341
H 0.527062 -1.855952 -0.679020
H 3.871044 -0.237905 0.271297

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -456.112591512**

Comp_04Z_c04
B3LYP/6-31G* Geometry

N -0.622757 0.652070 0.108612
C -1.967453 0.804540 0.394273
C -2.615950 -0.389161 0.187602
C -1.637727 -1.314607 -0.253241
C -0.407895 -0.672525 -0.281575
C 0.213726 1.783030 -0.011796
C 1.298574 1.907025 -0.774069
C 0.855416 -1.341190 -0.580110
N 2.013702 -1.287427 -0.023098
O 2.057922 -0.381841 1.045003
H -2.348888 1.775001 0.678869
H -3.669962 -0.575537 0.340794
H -1.787235 -2.363893 -0.472562
H -0.145867 2.613483 0.589397
H 1.682658 1.104862 -1.392596

H 1.848827 2.841324 -0.763796
H 0.808292 -2.098711 -1.361575
H 2.980032 -0.456970 1.336338

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -456.105608325**

Comp_05E_c01
B3LYP/6-31G* Geometry

C 4.995620 -0.820786 0.000019
C 7.790455 -0.863912 0.000178
C 5.715689 0.386704 0.000257
C 5.683076 -2.041859 -0.000142
C 7.076807 -2.063569 -0.000060
C 7.105280 0.358074 0.000334
N 3.580533 -0.918771 -0.000085
N 2.975005 0.188142 0.000028
C 1.563736 0.094459 -0.000067
C -1.234472 0.140142 -0.000236
C 0.838528 -1.109326 -0.000193
C 0.874843 1.310605 -0.000021
C -0.522563 1.362656 -0.000102
C -0.549219 -1.085437 -0.000279
O -2.592566 0.249892 -0.000316
C -3.384662 -0.914505 -0.000284
C -1.259372 2.631612 -0.000051
C -4.846357 -0.480974 -0.000230
O -5.624789 -1.580455 0.000320
O -5.246531 0.656669 -0.000674
C -7.055792 -1.342301 0.000277
C -7.743435 -2.693642 0.000656
N -0.626609 3.747442 0.000236
O -1.520544 4.826088 0.000204
H 8.877128 -0.876601 0.000240
H 5.167450 1.322138 0.000377
H 5.101366 -2.958798 -0.000329
H 7.604579 -3.013325 -0.000178
H 7.663433 1.290781 0.000520
H 1.379733 -2.048669 -0.000223
H 1.442809 2.234333 0.000079
H -1.097517 -2.020771 -0.000378
H -3.196354 -1.534832 -0.887580
H -3.196247 -1.534889 0.886939
H -2.348433 2.604773 -0.000279
H -7.309585 -0.748953 -0.883626
H -7.309549 -0.748477 0.883872
H -7.470805 -3.273085 -0.887163
H -8.829888 -2.554569 0.000617
H -7.470806 -3.272596 0.888795
H -0.923355 5.590630 0.000454

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.90003372**

Comp_05E_c03

B3LYP/6-31G* Geometry

C -5.022128 -0.357265 0.000310
 C -7.776419 -0.833574 0.001156
 C -5.924102 0.715196 0.000894
 C -5.505790 -1.677313 0.000132
 C -6.876499 -1.907314 0.000551
 C -7.297670 0.477629 0.001329
 N -3.650357 0.002775 -0.000086
 N -2.848449 -0.971130 -0.000266
 C -1.479212 -0.616301 -0.000693
 C 1.279791 -0.147347 -0.001464
 C -0.577438 -1.687199 -0.001268
 C -0.987871 0.697419 -0.000456
 C 0.382689 0.954063 -0.000823
 C 0.795965 -1.459900 -0.001688
 O 2.603275 0.176481 -0.001910
 C 3.565877 -0.851336 -0.000913
 C 0.923121 2.319880 -0.000458
 C 4.944250 -0.200291 0.000464
 O 5.880017 -1.169587 -0.000140
 O 5.167649 0.984775 0.002019
 C 7.259027 -0.719876 0.001503
 C 8.140097 -1.954178 0.001370
 N 0.131606 3.329041 -0.000654
 O 0.854745 4.528472 0.000068
 H -8.846610 -1.022629 0.001475
 H -5.521989 1.723822 0.000994
 H -4.793554 -2.494834 -0.000332
 H -7.252009 -2.927397 0.000396
 H -7.992496 1.312962 0.001799
 H -0.973741 -2.697816 -0.001419
 H -1.686442 1.525422 0.000074
 H 1.477156 -2.302628 -0.002245
 H 3.473863 -1.493423 0.886236
 H 3.475610 -1.493601 -0.888096
 H 2.003944 2.455661 0.000110
 H 7.420808 -0.095991 0.885953
 H 7.422451 -0.094659 -0.881709
 H 7.955055 -2.567812 0.888730
 H 9.193922 -1.655640 0.002542
 H 7.956656 -2.566481 -0.887242
 H 0.150163 5.195358 -0.000178

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89993203

Comp_05E_c06**B3LYP/6-31G* Geometry**

C 5.015398 -0.728843 0.032518
 C 7.809212 -0.680264 0.102987
 C 5.694348 0.501251 0.082230
 C 5.743135 -1.926220 0.018147
 C 7.136387 -1.902275 0.053549
 C 7.083706 0.518129 0.117087
 N 3.604831 -0.873405 -0.006604

N 2.962277 0.212204 0.011126
 C 1.555376 0.071303 -0.028723
 C -1.241977 0.022726 -0.100736
 C 0.872391 -1.155525 -0.086698
 C 0.825161 1.262800 -0.007384
 C -0.572826 1.267855 -0.042305
 C -0.514907 -1.178315 -0.122426
 O -2.602706 0.086411 -0.132182
 C -3.353324 -1.103393 -0.197592
 C -1.352423 2.510752 -0.019974
 C -4.828706 -0.721384 -0.232555
 O -5.563492 -1.851213 -0.270537
 O -5.265261 0.403065 -0.233613
 C -7.005710 -1.686857 -0.313015
 C -7.584653 -1.522764 1.083447
 N -0.758749 3.646275 0.040192
 O -1.688945 4.693853 0.050890
 H 8.895368 -0.657238 0.130442
 H 5.115344 1.417910 0.092421
 H 5.192608 -2.861391 -0.020894
 H 7.695466 -2.833878 0.042273
 H 7.610169 1.468310 0.155524
 H 1.445433 -2.075653 -0.103014
 H 1.360666 2.204654 0.037477
 H -1.030152 -2.131181 -0.166793
 H -3.115637 -1.685827 -1.098691
 H -3.172296 -1.747773 0.673786
 H -2.439413 2.447863 -0.054794
 H -7.363852 -2.600032 -0.793795
 H -7.239621 -0.826930 -0.945108
 H -7.310135 -2.368716 1.721996
 H -8.678134 -1.475689 1.026503
 H -7.225958 -0.598000 1.543937
 H -1.118667 5.477266 0.097926

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89925671

Comp_05E_c07**B3LYP/6-31G* Geometry**

C -5.014320 -0.269529 0.048904
 C -7.781947 -0.655333 0.112085
 C -5.880166 0.831858 0.080589
 C -5.541061 -1.573011 0.049107
 C -6.918216 -1.757950 0.080710
 C -7.260368 0.639469 0.111864
 N -3.631968 0.045903 0.019152
 N -2.862297 -0.953109 -0.015207
 C -1.482670 -0.642310 -0.043601
 C 1.289228 -0.262128 -0.105971
 C -0.616592 -1.741315 -0.089817
 C -0.948888 0.654673 -0.028425
 C 0.428852 0.867166 -0.058744
 C 0.763005 -1.558255 -0.121501
 O 2.622151 0.019134 -0.133131

C 3.550145 -1.038418 -0.191576
 C 1.013261 2.214635 -0.043944
 C 4.948628 -0.432684 -0.217300
 O 5.848388 -1.435535 -0.270272
 O 5.206997 0.745367 -0.198607
 C 7.248757 -1.052488 -0.300425
 C 7.794829 -0.848617 1.103929
 N 0.255491 3.248402 0.000981
 O 1.017322 4.423650 0.006523
 H -8.857473 -0.809250 0.136684
 H -5.444987 1.826660 0.079883
 H -4.856416 -2.413402 0.024623
 H -7.327057 -2.765131 0.081124
 H -7.927102 1.497048 0.136110
 H -1.045617 -2.738419 -0.100836
 H -1.619901 1.504388 0.007223
 H 1.416093 -2.422204 -0.157484
 H 3.466178 -1.702200 0.680258
 H 3.410422 -1.652138 -1.092377
 H 2.097519 2.315835 -0.071897
 H 7.349308 -0.146914 -0.903150
 H 7.741919 -1.884487 -0.808364
 H 7.301893 -0.002980 1.591942
 H 8.869139 -0.637319 1.055476
 H 7.648448 -1.746096 1.713673
 H 0.335315 5.112735 0.041230

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89917174**

Comp_05E_c09

B3LYP/6-31G* Geometry

C 4.483743 -0.992002 -0.022875
 C 7.233191 -1.422926 0.239685
 C 5.337061 0.084660 0.275655
 C 5.016084 -2.277729 -0.187201
 C 6.387077 -2.492935 -0.056359
 C 6.703176 -0.136672 0.404812
 N 3.077464 -0.890780 -0.179347
 N 2.612579 0.272730 -0.030291
 C 1.211032 0.377602 -0.184679
 C -1.543800 0.809468 -0.448421
 C 0.350938 -0.696589 -0.472778
 C 0.676192 1.657609 -0.025383
 C -0.695870 1.901384 -0.152699
 C -1.012737 -0.480923 -0.601100
 O -2.869999 1.110536 -0.588969
 C -3.790227 0.110682 -0.960487
 C -1.262489 3.244125 0.010009
 C -4.172621 -0.803557 0.204458
 O -5.054510 -1.725282 -0.227229
 O -3.760501 -0.707386 1.334796
 C -5.543151 -2.656253 0.773677
 C -6.521570 -3.590084 0.088328
 N -0.502220 4.252226 0.235015

O -1.259369 5.426039 0.359318
 H 8.302647 -1.586373 0.342624
 H 4.908116 1.072677 0.399788
 H 4.333444 -3.090424 -0.416803
 H 6.794031 -3.492195 -0.184742
 H 7.364184 0.694775 0.635696
 H 0.770374 -1.689841 -0.585182
 H 1.344963 2.480545 0.201138
 H -1.662191 -1.324133 -0.805218
 H -4.688395 0.639843 -1.292900
 H -3.432200 -0.490096 -1.805831
 H -2.341683 3.369484 -0.062427
 H -6.011849 -2.084567 1.580589
 H -4.687644 -3.190970 1.197776
 H -7.363789 -3.033536 -0.334825
 H -6.914540 -4.310350 0.813962
 H -6.033872 -4.146029 -0.718727
 H -0.577478 6.095543 0.526268

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89992935**

Comp_05E_c11

B3LYP/6-31G* Geometry

C 4.397469 -0.838297 -0.045210
 C 7.154465 -1.195954 0.246083
 C 5.210283 0.247317 0.325221
 C 4.973738 -2.096356 -0.266024
 C 6.348569 -2.274907 -0.121137
 C 6.580414 0.062501 0.468354
 N 2.991589 -0.773022 -0.222786
 N 2.487809 0.367514 -0.029200
 C 1.086456 0.436392 -0.204451
 C -1.675588 0.795876 -0.500449
 C 0.265302 -0.649814 -0.553990
 C 0.509388 1.691584 -0.000538
 C -0.867117 1.899075 -0.142741
 C -1.102136 -0.470273 -0.698105
 O -3.007630 1.062039 -0.653979
 C -3.890377 0.041393 -1.058527
 C -1.477832 3.215652 0.067523
 C -4.239003 -0.922806 0.076385
 O -5.025603 -1.904327 -0.407662
 O -3.883935 -0.805274 1.224138
 C -5.497391 -2.892829 0.547384
 C -4.479995 -4.006721 0.736576
 N -0.752041 4.236614 0.342782
 O -1.546830 5.380119 0.506767
 H 8.226726 -1.331020 0.360368
 H 4.747623 1.213468 0.492719
 H 4.321783 -2.916884 -0.550404
 H 6.789797 -3.252708 -0.293892
 H 7.210122 0.900869 0.754940
 H 0.717426 -1.623868 -0.702075
 H 1.148279 2.523704 0.273664

H -1.720645 -1.322874 -0.953775
H -4.808200 0.548297 -1.371864
H -3.512533 -0.517107 -1.923555
H -2.559595 3.310331 -0.012764
H -6.426517 -3.264345 0.109188
H -5.716025 -2.387970 1.491335
H -4.233070 -4.476735 -0.221004
H -4.892985 -4.775361 1.399732
H -3.563505 -3.620061 1.191101
H -0.888062 6.063068 0.708479

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89921578

Comp_05E_c12
B3LYP/6-31G* Geometry
C 5.043074 -0.405174 0.000111
C 7.808195 0.001610 0.000050
C 5.559478 0.902427 -0.000261
C 5.917738 -1.499978 0.000425
C 7.296803 -1.297227 0.000414
C 6.935560 1.097641 -0.000293
N 3.662355 -0.729739 0.000128
N 2.885831 0.264633 0.000126
C 1.508257 -0.057000 0.000083
C -1.260868 -0.467456 -0.000014
C 0.987778 -1.362466 0.000047
C 0.631177 1.030941 0.000081
C -0.756117 0.854347 0.000024
C -0.385288 -1.565139 0.000004
O -2.619274 -0.580894 -0.000064
C -3.210444 -1.863644 -0.000256
C -1.689058 1.986167 0.000025
C -4.731282 -1.770566 -0.000456
O -5.193113 -0.517142 -0.000053
O -5.414585 -2.771556 -0.000876
C -6.638222 -0.377333 -0.000092
C -6.949629 1.106391 0.001719
N -1.252022 3.192021 -0.000640
O -2.316035 4.105363 -0.000416
H 8.882774 0.163705 0.000018
H 4.868008 1.737555 -0.000525
H 5.490968 -2.498472 0.000684
H 7.970454 -2.149719 0.000671
H 7.336469 2.107942 -0.000593
H 1.674335 -2.201440 0.000064
H 1.041537 2.034686 0.000138
H -0.772868 -2.577566 -0.000017
H -2.916904 -2.441676 -0.886945
H -2.917164 -2.441819 0.886436
H -2.758700 1.780446 0.000534
H -7.035769 -0.887009 0.882949
H -7.035464 -0.884724 -0.884599
H -6.535073 1.592929 0.890105
H -8.034955 1.254785 0.001264

H -6.534017 1.595272 -0.884888
H -1.855632 4.959285 -0.000993
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89957605

Comp_05E_c13
B3LYP/6-31G* Geometry
C 4.530964 -0.895526 0.000913
C 7.285377 -1.234526 0.335940
C 5.330598 0.195775 0.383124
C 5.119036 -2.149874 -0.209703
C 6.492576 -2.319118 -0.042985
C 6.699512 0.020248 0.547969
N 3.127612 -0.839851 -0.198603
N 2.613102 0.297258 -0.013167
C 1.214170 0.356484 -0.209778
C -1.545470 0.696746 -0.547579
C 0.405646 -0.735646 -0.570397
C 0.625612 1.607825 -0.015677
C -0.750039 1.805756 -0.178832
C -0.960599 -0.565625 -0.735094
O -2.876992 0.954130 -0.720923
C -3.746788 -0.067826 -1.149162
C -1.372561 3.118420 0.020872
C -4.121193 -1.034587 -0.024856
O -4.931328 -1.991296 -0.520031
O -3.755262 -0.944612 1.122009
C -5.422049 -2.982619 0.422292
C -6.679013 -2.497253 1.126555
N -0.658424 4.143910 0.309476
O -1.463498 5.282328 0.459196
H 8.356575 -1.362353 0.467285
H 4.858918 1.158920 0.542555
H 4.477123 -2.974974 -0.503532
H 6.942963 -3.294099 -0.207875
H 7.319016 0.863027 0.843727
H 0.866264 -1.706954 -0.709965
H 1.254620 2.444547 0.267235
H -1.569689 -1.423128 -0.996524
H -4.657595 0.436531 -1.485976
H -3.345296 -0.624680 -2.004699
H -2.453283 3.206442 -0.078790
H -4.625989 -3.207633 1.135856
H -5.618504 -3.862666 -0.194344
H -6.461192 -1.625372 1.750003
H -7.070202 -3.291022 1.773092
H -7.454916 -2.231480 0.401293
H -0.812864 5.969343 0.673102
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89924211

Comp_05E_c16
B3LYP/6-31G* Geometry

C 5.043453 -0.475930 0.048591
 C 7.818415 -0.151015 0.120317
 C 5.597602 0.815811 0.078842
 C 5.885561 -1.595956 0.054645
 C 7.269525 -1.434123 0.090209
 C 6.978404 0.970204 0.114521
 N 3.654378 -0.760116 0.012307
 N 2.906917 0.256222 0.001630
 C 1.521081 -0.025742 -0.032531
 C -1.257920 -0.356369 -0.098746
 C 0.963550 -1.315736 -0.048090
 C 0.675777 1.086917 -0.050486
 C -0.715647 0.950443 -0.084050
 C -0.414356 -1.478755 -0.080689
 O -2.618644 -0.431090 -0.130510
 C -3.245503 -1.696426 -0.142943
 C -1.615266 2.108778 -0.103895
 C -4.762958 -1.561865 -0.179131
 O -5.184739 -0.294995 -0.240192
 O -5.470406 -2.546204 -0.162683
 C -6.623084 -0.091421 -0.280954
 C -7.211290 -0.053792 1.120442
 N -1.143430 3.301379 -0.089812
 O -2.179880 4.245396 -0.113497
 H 8.896942 -0.020631 0.148339
 H 4.931110 1.670985 0.074009
 H 5.429803 -2.581272 0.031055
 H 7.917806 -2.306046 0.094634
 H 7.408572 1.968122 0.138161
 H 1.625454 -2.174158 -0.033947
 H 1.114824 2.078378 -0.038294
 H -0.830523 -2.479724 -0.091772
 H -2.948077 -2.284103 -1.022262
 H -2.989327 -2.281357 0.750574
 H -2.690109 1.934344 -0.131069
 H -7.071497 -0.885408 -0.882488
 H -6.738742 0.866150 -0.793155
 H -7.101693 -1.024131 1.613099
 H -8.279766 0.183760 1.065143
 H -6.719606 0.712185 1.728536
 H -1.694927 5.085525 -0.100698

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89877350**

Comp_05E_c17

B3LYP/6-31G* Geometry

C -4.330565 -0.533017 -0.095187
 C -7.091966 -0.647154 0.321150
 C -5.010406 0.589003 0.410271
 C -5.041080 -1.704675 -0.388512
 C -6.418246 -1.761862 -0.180871
 C -6.383683 0.525368 0.614930
 N -2.935655 -0.588721 -0.345799
 N -2.307774 0.472006 -0.076505

C -0.916841 0.418989 -0.327646
 C 1.849402 0.532920 -0.753699
 C -0.233316 -0.699283 -0.835686
 C -0.201824 1.582419 -0.034226
 C 1.180187 1.666221 -0.236482
 C 1.137052 -0.642033 -1.045458
 O 3.194407 0.673016 -0.948705
 C 3.938439 -0.408762 -1.474274
 C 1.936851 2.883713 0.073042
 C 4.170628 -1.578658 -0.515330
 O 4.057873 -1.211764 0.766587
 O 4.472060 -2.682828 -0.914694
 C 4.287442 -2.242509 1.765140
 C 3.020516 -3.038411 2.035108
 N 1.341397 3.926931 0.522716
 O 2.258883 4.961958 0.750881
 H -8.165646 -0.687515 0.484225
 H -4.444917 1.487329 0.631274
 H -4.490211 -2.555413 -0.778276
 H -6.964122 -2.672863 -0.410269
 H -6.911011 1.391855 1.005561
 H -0.792492 -1.601033 -1.057905
 H -0.735707 2.439805 0.360382
 H 1.647584 -1.516180 -1.433951
 H 3.498121 -0.805142 -2.395401
 H 4.917685 0.011456 -1.725065
 H 3.014400 2.884877 -0.083841
 H 4.609848 -1.686035 2.647833
 H 5.100511 -2.886140 1.421128
 H 2.197102 -2.374826 2.316863
 H 3.195590 -3.741225 2.857621
 H 2.726798 -3.612704 1.151874
 H 1.689382 5.675575 1.078878

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89873463**

Comp_05E_c19

B3LYP/6-31G* Geometry

C 4.359932 -0.331212 0.036696
 C 7.047075 -1.058862 0.285408
 C 5.303445 0.597773 0.495567
 C 4.767831 -1.633939 -0.299755
 C 6.105559 -1.989316 -0.173513
 C 6.643601 0.235063 0.619393
 N 3.027824 0.147749 -0.047403
 N 2.188394 -0.694890 -0.467963
 C 0.858299 -0.220594 -0.550439
 C -1.836579 0.502903 -0.793240
 C -0.084860 -1.140787 -1.024197
 C 0.439945 1.068901 -0.193924
 C -0.897454 1.449863 -0.306227
 C -1.425129 -0.786996 -1.147160
 O -3.125687 0.944708 -0.890921
 C -4.123207 0.067723 -1.376792

C -1.354008 2.794067 0.067539
 C -4.536326 -1.054926 -0.421911
 O -4.280600 -0.750721 0.855849
 O -5.078141 -2.064891 -0.817037
 C -4.654642 -1.740893 1.851970
 C -3.565938 -2.788149 2.023441
 N -0.521403 3.673271 0.489748
 O -1.178231 4.874134 0.790610
 H 8.090977 -1.345583 0.380750
 H 4.959497 1.596256 0.748063
 H 4.024556 -2.339758 -0.653296
 H 6.422707 -2.996110 -0.432991
 H 7.370921 0.959402 0.975576
 H 0.252794 -2.136844 -1.292973
 H 1.168712 1.779887 0.176289
 H -2.135301 -1.519610 -1.512782
 H -5.001913 0.698115 -1.546499
 H -3.843958 -0.385171 -2.334091
 H -2.413435 3.030535 -0.017989
 H -5.603614 -2.193260 1.554391
 H -4.798062 -1.155592 2.762740
 H -3.452941 -3.383188 1.112874
 H -3.832464 -3.464488 2.843581
 H -2.607106 -2.317250 2.261437
 H -0.449064 5.440213 1.089095

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89858406**

Comp_05E_c21

B3LYP/6-31G* Geometry

C 4.459169 -0.669878 0.008573
 C 7.209907 -0.840308 0.473556
 C 5.158571 0.448203 0.495713
 C 5.144899 -1.865955 -0.242075
 C 6.516741 -1.951177 -0.010158
 C 6.526416 0.356572 0.724698
 N 3.067500 -0.697982 -0.263808
 N 2.461956 0.384393 -0.032224
 C 1.074322 0.359007 -0.305149
 C -1.680341 0.530076 -0.781759
 C 0.371148 -0.755338 -0.794593
 C 0.384349 1.547374 -0.054973
 C -0.991524 1.660032 -0.283410
 C -0.993629 -0.669894 -1.029482
 O -3.018462 0.697625 -1.002713
 C -3.773327 -0.372107 -1.537182
 C -1.721872 2.904406 -0.021334
 C -4.048334 -1.531559 -0.577428
 O -3.978717 -1.154949 0.704849
 O -4.333185 -2.640174 -0.977310
 C -4.245691 -2.178384 1.701315
 C -5.735104 -2.293771 1.983601
 N -1.108524 3.943512 0.413567
 O -2.002937 5.007868 0.594196

H 8.279514 -0.902587 0.655436
 H 4.612140 1.365619 0.683718
 H 4.579340 -2.713081 -0.618431
 H 7.043372 -2.881056 -0.206430
 H 7.068805 1.220015 1.101203
 H 0.910675 -1.676675 -0.982239
 H 0.933306 2.401693 0.325342
 H -1.519871 -1.542179 -1.400924
 H -4.737997 0.066815 -1.811648
 H -3.320907 -0.784523 -2.445349
 H -2.795541 2.929488 -0.201262
 H -3.691922 -1.842149 2.580395
 H -3.830953 -3.125311 1.347950
 H -6.149629 -1.328238 2.290797
 H -5.902060 -3.012984 2.793520
 H -6.270835 -2.645913 1.097513
 H -1.421754 5.714846 0.916010

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89883676**

Comp_05E_c22

B3LYP/6-31G* Geometry

C -4.792433 -0.277423 0.269139
 C -7.486195 -0.895367 0.678986
 C -5.639688 0.643656 0.899533
 C -5.299853 -1.516903 -0.158504
 C -6.640777 -1.817812 0.048567
 C -6.983571 0.335563 1.104005
 N -3.446932 0.142801 0.114697
 N -2.692855 -0.692373 -0.454441
 C -1.349303 -0.271024 -0.610791
 C 1.347986 0.369601 -1.010932
 C -0.490141 -1.186072 -1.231640
 C -0.849456 0.972151 -0.202170
 C 0.493736 1.320044 -0.390130
 C 0.848871 -0.864285 -1.430160
 O 2.656832 0.672670 -1.300733
 C 3.606523 0.530857 -0.262683
 C 0.887230 2.665586 0.039798
 C 4.211793 -0.871503 -0.226907
 O 5.184472 -0.910535 0.706512
 O 3.886537 -1.810550 -0.916440
 C 5.861564 -2.181303 0.868223
 C 6.920336 -2.000981 1.939167
 N 2.089353 3.114299 0.030186
 O 2.111024 4.437775 0.500671
 H -8.533408 -1.139394 0.836355
 H -5.219953 1.592808 1.218842
 H -4.629814 -2.217238 -0.644442
 H -7.035555 -2.775285 -0.281203
 H -7.636527 1.053106 1.593033
 H -0.891948 -2.143771 -1.547672
 H -1.534036 1.674357 0.262320
 H 1.540508 -1.556360 -1.895655

H 4.402168 1.257045 -0.450274
H 3.184523 0.766482 0.720646
H 0.081096 3.315050 0.391601
H 6.293261 -2.472610 -0.094427
H 5.121320 -2.939430 1.143127
H 7.646107 -1.235384 1.646908
H 7.456625 -2.943789 2.092251
H 6.468527 -1.703128 2.890721
H 3.049514 4.670860 0.423700

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89280625

Comp_05E_c23

B3LYP/6-31G* Geometry

C 4.785270 -0.593565 0.051530
C 7.507615 -0.787744 0.649774
C 5.516935 -1.719979 -0.347901
C 5.423553 0.442266 0.755954
C 6.777914 0.339275 1.050275
C 6.875059 -1.816858 -0.049702
N 3.413028 -0.603648 -0.306040
N 2.763981 0.415714 0.054414
C 1.393711 0.401142 -0.304243
C -1.337015 0.596722 -0.895150
C 0.750771 -0.633860 -1.004858
C 0.660874 1.525299 0.081325
C -0.708478 1.657532 -0.200732
C -0.601780 -0.526858 -1.294179
O -2.653722 0.674795 -1.280416
C -3.638727 0.364491 -0.314156
C -1.348668 2.908496 0.214337
C -3.989729 -1.122412 -0.309859
O -5.009736 -1.334124 0.546743
O -3.452090 -1.987872 -0.961682
C -5.461583 -2.705131 0.672384
C -6.615048 -2.717039 1.657058
N -2.603074 3.157624 0.107565
O -2.878517 4.448232 0.589180
H 8.566283 -0.859525 0.884395
H 4.997374 -2.504038 -0.890384
H 4.841910 1.306304 1.057110
H 7.273677 1.138777 1.594703
H 7.438014 -2.692080 -0.361877
H 1.324152 -1.503311 -1.305537
H 1.186350 2.316788 0.608366
H -1.135052 -1.311077 -1.819086
H -3.338942 0.666775 0.695361
H -4.533063 0.940466 -0.567016
H -0.690959 3.670916 0.640717
H -4.622177 -3.319980 1.012484
H -5.759053 -3.067388 -0.316666
H -6.298331 -2.344599 2.636500
H -6.985701 -3.740385 1.780871
H -7.440468 -2.092563 1.300615

H -3.833079 4.528178 0.436130
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89297730

Comp_05E_c24

B3LYP/6-31G* Geometry

C -5.113277 -0.006251 0.232694
C -7.880101 -0.151565 0.590198
C -5.850348 1.152433 0.511910
C -5.768505 -1.246133 0.131663
C -7.145054 -1.311227 0.310794
C -7.230792 1.080053 0.690264
N -3.717938 0.186405 0.072026
N -3.062917 -0.861552 -0.178431
C -1.668852 -0.666472 -0.339397
C 1.108209 -0.491235 -0.686650
C -0.919114 -1.816859 -0.611791
C -1.019975 0.572676 -0.257094
C 0.365215 0.690791 -0.422420
C 0.457955 -1.722562 -0.785563
O 2.457354 -0.464351 -0.931069
C 3.289615 -0.485228 0.216989
C 0.920754 2.045994 -0.356069
C 4.735452 -0.591972 -0.240925
O 5.539312 -0.552331 0.845274
O 5.120658 -0.702145 -1.378569
C 6.958251 -0.664669 0.582994
C 7.675087 -0.616647 1.918851
N 2.174746 2.315870 -0.356678
O 2.371068 3.703004 -0.291272
H -8.956258 -0.212279 0.728481
H -5.317371 2.095705 0.583661
H -5.182439 -2.132114 -0.085287
H -7.654212 -2.268319 0.233235
H -7.798039 1.981063 0.906350
H -1.434792 -2.769250 -0.685011
H -1.621381 1.454790 -0.063238
H 1.057423 -2.598051 -1.014340
H 3.173697 0.428372 0.810168
H 3.056991 -1.348241 0.857495
H 0.198686 2.865057 -0.302348
H 7.259414 0.155866 -0.076222
H 7.143930 -1.602128 0.048963
H 7.472820 0.325245 2.438911
H 8.756254 -0.698780 1.762776
H 7.356720 -1.441625 2.564204
H 3.337063 3.779465 -0.339823

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1122.89236080

Comp_05E_c25

B3LYP/6-31G* Geometry

C -5.196472 -0.474168 0.107449

C -7.948935 -0.261251 0.535853
 C -5.750491 0.755071 0.505923
 C -6.026820 -1.588506 -0.073103
 C -7.400102 -1.482252 0.140338
 C -7.120447 0.854008 0.717397
 N -3.818312 -0.698601 -0.138272
 N -3.079723 0.311022 0.021186
 C -1.703906 0.080653 -0.225185
 C 1.059504 -0.130203 -0.648773
 C -1.148710 -1.146413 -0.625479
 C -0.869212 1.187523 -0.056377
 C 0.518812 1.117664 -0.256778
 C 0.219690 -1.236371 -0.834168
 O 2.390290 -0.292601 -0.937050
 C 3.234041 -0.533905 0.176900
 C 1.273725 2.362374 -0.090790
 C 4.648437 -0.758656 -0.333188
 O 5.463624 -0.967422 0.724902
 O 5.003032 -0.758839 -1.485948
 C 6.854936 -1.211980 0.409979
 C 7.581323 -1.464717 1.717409
 N 2.554006 2.440924 -0.113730
 O 2.960571 3.771269 0.063604
 H -9.019120 -0.174419 0.703411
 H -5.093093 1.606609 0.640722
 H -5.570874 -2.524565 -0.381123
 H -8.039914 -2.348789 -0.001320
 H -7.551310 1.803112 1.025338
 H -1.800700 -2.000797 -0.766616
 H -1.328772 2.127242 0.236912
 H 0.676171 -2.166281 -1.159902
 H 3.240778 0.318598 0.864824
 H 2.910218 -1.426409 0.731492
 H 0.686349 3.272159 0.059774
 H 7.253059 -0.341063 -0.120846
 H 6.916881 -2.068708 -0.268568
 H 7.502603 -0.599545 2.383580
 H 8.642448 -1.653744 1.521728
 H 7.165707 -2.335984 2.233640
 H 3.925406 3.706673 -0.015819

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89248825**

Comp_05E_c27

B3LYP/6-31G* Geometry

C 5.196463 -0.474186 0.107489
 C 7.948920 -0.261349 0.535954
 C 5.750446 0.754921 0.506393
 C 6.026825 -1.588459 -0.073379
 C 7.400116 -1.482231 0.140029
 C 7.120400 0.853817 0.717908
 N 3.818277 -0.698612 -0.138187
 N 3.079769 0.311131 0.020772
 C 1.703928 0.080738 -0.225521

C -1.059499 -0.130125 -0.648940
 C 1.148723 -1.146320 -0.625810
 C 0.869245 1.187604 -0.056642
 C -0.518795 1.117720 -0.256922
 C -0.219689 -1.236287 -0.834416
 O -2.390304 -0.292433 -0.937189
 C -3.233922 -0.534231 0.176747
 C -1.273769 2.362373 -0.090738
 C -4.648498 -0.758145 -0.333209
 O -5.463484 -0.967753 0.724867
 O -5.003379 -0.757075 -1.485882
 C -6.854946 -1.211625 0.410035
 C -7.580940 -1.466224 1.717324
 N -2.554069 2.440756 -0.113139
 O -2.960737 3.771052 0.064296
 H 9.019099 -0.174562 0.703574
 H 5.093034 1.606401 0.641495
 H 5.570894 -2.524444 -0.381646
 H 8.039951 -2.348702 -0.001931
 H 7.551225 1.802813 1.026239
 H 1.800713 -2.000691 -0.767036
 H 1.328819 2.127320 0.236629
 H -0.676155 -2.166189 -1.160194
 H -2.910280 -1.427199 0.730695
 H -3.240268 0.317822 0.865240
 H -0.686441 3.272234 0.059550
 H -6.917249 -2.067299 -0.269798
 H -7.253103 -0.339822 -0.119311
 H -7.165291 -2.338340 2.232096
 H -8.642160 -1.654785 1.521713
 H -7.501861 -0.602079 2.384785
 H -3.925594 3.706327 -0.014769

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89248871**

Comp_05E_c28

B3LYP/6-31G* Geometry

C -5.115519 0.061177 0.159254
 C -7.894120 -0.008654 0.440868
 C -5.835581 1.248494 0.347755
 C -5.793824 -1.169485 0.111454
 C -7.176051 -1.196958 0.252471
 C -7.221886 1.213771 0.488136
 N -3.712323 0.216339 0.029716
 N -3.073642 -0.857138 -0.142832
 C -1.671516 -0.700042 -0.271659
 C 1.118023 -0.601632 -0.541070
 C -0.939984 -1.878701 -0.459544
 C -0.997613 0.527890 -0.234615
 C 0.394296 0.608037 -0.362518
 C 0.443415 -1.822556 -0.595329
 O 2.474322 -0.616796 -0.743615
 C 3.270641 -0.594993 0.429845
 C 0.977791 1.952983 -0.348440

C 4.723942 -0.789194 0.028388
 O 5.492224 -0.698586 1.138550
 O 5.134336 -1.002231 -1.085863
 C 6.917596 -0.882661 0.955640
 C 7.599621 0.422107 0.573763
 N 2.236844 2.196840 -0.322731
 O 2.461224 3.581395 -0.321976
 H -8.974879 -0.040048 0.549878
 H -5.285075 2.183837 0.380274
 H -5.220633 -2.078006 -0.035300
 H -7.702942 -2.146880 0.215980
 H -7.775778 2.136959 0.633789
 H -1.474412 -2.822749 -0.498182
 H -1.584578 1.431385 -0.105796
 H 1.029688 -2.721316 -0.758685
 H 3.174603 0.359568 0.958450
 H 2.983941 -1.404191 1.116875
 H 0.272806 2.788449 -0.359630
 H 7.077692 -1.650607 0.194881
 H 7.268373 -1.250878 1.922910
 H 7.249608 0.767943 -0.403068
 H 8.683858 0.271707 0.516325
 H 7.399620 1.198914 1.319178
 H 3.429728 3.635874 -0.340098

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89154561**

Comp_05Z_c01

B3LYP/6-31G* Geometry

C -4.939183 -0.395675 -0.000033
 C -7.683496 -0.927716 0.000086
 C -5.862824 0.658156 0.000001
 C -5.396127 -1.725184 -0.000043
 C -6.761936 -1.982898 0.000011
 C -7.231330 0.392881 0.000084
 N -3.574870 -0.007987 -0.000148
 N -2.753996 -0.965766 0.000143
 C -1.391232 -0.586978 0.000057
 C 1.353601 -0.067329 -0.000138
 C -0.473735 -1.640614 -0.000015
 C -0.928668 0.740123 0.000072
 C 0.439151 1.030094 -0.000013
 C 0.895422 -1.386797 -0.000128
 O 2.673752 0.266879 -0.000246
 C 3.649127 -0.748609 -0.000130
 C 1.015204 2.383084 0.000062
 C 5.018336 -0.078156 -0.000026
 O 5.967469 -1.033865 0.000319
 O 5.224595 1.110122 -0.000260
 C 7.340355 -0.565137 0.000318
 C 8.238160 -1.787287 -0.000064
 N 0.484184 3.555363 0.000078
 O -0.918038 3.554471 0.000000
 H -8.749634 -1.138444 0.000119

H -5.481068 1.674658 -0.000029
 H -4.667602 -2.528225 -0.000094
 H -7.116688 -3.010401 -0.000017
 H -7.942917 1.214003 0.000134
 H -0.851190 -2.658547 0.000008
 H -1.652542 1.540179 0.000151
 H 1.592461 -2.216333 -0.000203
 H 3.566389 -1.391599 0.887130
 H 3.566558 -1.391608 -0.887406
 H 2.099931 2.435923 0.000077
 H 7.494262 0.061302 0.884357
 H 7.494118 0.061780 -0.883401
 H 8.062353 -2.402914 0.887778
 H 9.287799 -1.474357 -0.000028
 H 8.062264 -2.402420 -0.888231
 H -1.118899 4.503116 0.000026

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89711710**

Comp_05Z_c02

B3LYP/6-31G* Geometry

C -4.892698 -0.897843 0.000042
 C -7.685915 -1.004761 0.000122
 C -5.640193 0.292833 0.000262
 C -5.552123 -2.134279 -0.000109
 C -6.945006 -2.187774 -0.000082
 C -7.028776 0.232524 0.000301
 N -3.475647 -0.963255 -0.000027
 N -2.895802 0.157304 0.000027
 C -1.482416 0.096660 -0.000064
 C 1.308340 0.211425 -0.000199
 C -0.732082 -1.087937 -0.000263
 C -0.827493 1.334372 0.000055
 C 0.571516 1.428436 -0.000013
 C 0.655076 -1.029018 -0.000329
 O 2.663884 0.340486 -0.000245
 C 3.478564 -0.808058 -0.000238
 C 1.336375 2.682889 0.000135
 C 4.930679 -0.342835 -0.000091
 O 5.733082 -1.424486 0.000435
 O 5.305242 0.803622 -0.000455
 C 7.158683 -1.154896 0.000420
 C 7.875755 -2.490817 0.000199
 N 0.981805 3.919980 0.000129
 O -0.407145 4.122906 -0.000068
 H -8.772018 -1.042325 0.000143
 H -5.113304 1.240447 0.000398
 H -4.949679 -3.037742 -0.000263
 H -7.450939 -3.149356 -0.000211
 H -7.608062 1.152269 0.000466
 H -1.250173 -2.040373 -0.000375
 H -1.430146 2.230196 0.000201
 H 1.226430 -1.950302 -0.000481
 H 3.302809 -1.431812 0.887070

H 3.302993 -1.431652 -0.887705
H 2.417305 2.577332 0.000259
H 7.399222 -0.556046 0.884301
H 7.399170 -0.555750 -0.883267
H 7.615907 -3.075959 0.888099
H 8.958881 -2.327892 0.000242
H 7.615931 -3.075651 -0.887911
H -0.467040 5.090674 -0.000091
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89711214**

Comp_05Z_c03
B3LYP/6-31G* Geometry
C 4.579896 -0.490204 0.156364
C 7.237451 -1.255758 0.553533
C 5.525393 0.445441 0.596830
C 4.970144 -1.818718 -0.086947
C 6.293701 -2.192788 0.112734
C 6.851255 0.063709 0.795095
N 3.263239 0.010411 -0.009659
N 2.420113 -0.839222 -0.404258
C 1.102671 -0.340703 -0.571610
C -1.544896 0.420219 -0.965040
C 0.157247 -1.278102 -1.006914
C 0.721108 0.988506 -0.338923
C -0.605515 1.395965 -0.537387
C -1.167025 -0.899175 -1.203272
O -2.854573 0.797920 -1.209585
C -3.738962 0.777265 -0.104141
C -1.077944 2.781544 -0.396694
C -4.418428 -0.579109 0.089464
O -5.266639 -0.494333 1.133675
O -4.237024 -1.568207 -0.582010
C -6.023692 -1.688607 1.462609
C -7.297073 -1.777844 0.636307
N -0.574628 3.819344 0.172216
O 0.653277 3.581773 0.804892
H 8.270189 -1.557507 0.706627
H 5.194303 1.463926 0.775842
H 4.225154 -2.528838 -0.427983
H 6.598110 -3.219258 -0.074717
H 7.580710 0.792847 1.136713
H 0.482064 -2.299285 -1.181252
H 1.469314 1.696526 -0.015587
H -1.924554 -1.603204 -1.526224
H -3.236255 1.061484 0.829002
H -4.517539 1.522339 -0.299380
H -2.034669 3.001056 -0.863637
H -6.240605 -1.582682 2.528058
H -5.384598 -2.560799 1.306344
H -7.909800 -0.879888 0.766141
H -7.886037 -2.645245 0.955725
H -7.061142 -1.896547 -0.425056
H 0.861981 4.454263 1.173469

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89105393**

Comp_05Z_c04
B3LYP/6-31G* Geometry
C -4.931652 -0.312132 0.047494
C -7.690963 -0.755229 0.110585
C -5.820290 0.770989 0.076650
C -5.431393 -1.626162 0.050297
C -6.804447 -1.839639 0.081825
C -7.196252 0.550054 0.107842
N -3.555980 0.031630 0.017428
N -2.766484 -0.951658 -0.015275
C -1.392654 -0.616313 -0.043956
C 1.366620 -0.184056 -0.106420
C -0.509915 -1.698310 -0.088215
C -0.887670 0.695155 -0.030481
C 0.488288 0.941585 -0.060884
C 0.866225 -1.488072 -0.119983
O 2.696445 0.108268 -0.134117
C 3.638154 -0.937005 -0.191227
C 1.107578 2.275255 -0.050786
C 5.027754 -0.310891 -0.218404
O 5.941943 -1.300345 -0.268333
O 5.268433 0.871053 -0.203114
C 7.336848 -0.897412 -0.299188
C 7.879937 -0.684324 1.104917
N 0.615129 3.463575 -0.010684
O -0.785736 3.507200 0.032542
H -8.763079 -0.931337 0.135143
H -5.405763 1.774565 0.074003
H -4.729473 -2.452248 0.027845
H -7.192216 -2.855131 0.084213
H -7.880637 1.393695 0.130100
H -0.919836 -2.703558 -0.097651
H -1.585323 1.517443 0.003731
H 1.535816 -2.339177 -0.154568
H 3.563693 -1.600194 0.681766
H 3.506559 -1.553630 -1.091152
H 2.192955 2.293310 -0.082760
H 7.424383 0.008766 -0.903022
H 7.841622 -1.722947 -0.806239
H 7.375219 0.154831 1.592091
H 8.951161 -0.457998 1.056153
H 7.746231 -1.583099 1.715642
H -0.955657 4.461524 0.058216

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89631021**

Comp_05Z_c05
B3LYP/6-31G* Geometry
C 4.931656 -0.312142 0.047538
C 7.690959 -0.755348 0.110253

C 5.820349 0.770945 0.076222
 C 5.431336 -1.626194 0.050728
 C 6.804384 -1.839727 0.082079
 C 7.196309 0.549955 0.107160
 N 3.555987 0.031655 0.017749
 N 2.766492 -0.951609 -0.015561
 C 1.392655 -0.616259 -0.044066
 C -1.366632 -0.184004 -0.106168
 C 0.509908 -1.698254 -0.088103
 C 0.887676 0.695213 -0.030682
 C -0.488282 0.941633 -0.060913
 C -0.866242 -1.488021 -0.119657
 O -2.696460 0.108335 -0.133680
 C -3.638175 -0.936939 -0.190768
 C -1.107546 2.275321 -0.051009
 C -5.027761 -0.310822 -0.218119
 O -5.941914 -1.300268 -0.269036
 O -5.268481 0.871102 -0.202097
 C -7.336794 -0.897341 -0.299824
 C -7.880066 -0.684698 1.104284
 N -0.615049 3.463614 -0.010749
 O 0.785798 3.507172 0.032954
 H 8.763071 -0.931500 0.134696
 H 5.405873 1.774542 0.073386
 H 4.729371 -2.452255 0.028720
 H 7.192104 -2.855238 0.084826
 H 7.880738 1.393572 0.128997
 H 0.919820 -2.703506 -0.097521
 H 1.585340 1.517501 0.003326
 H -1.535830 -2.339135 -0.154022
 H -3.506502 -1.553714 -1.090566
 H -3.563812 -1.599974 0.682361
 H -2.192917 2.293410 -0.083191
 H -7.841522 -1.722719 -0.807176
 H -7.424324 0.009021 -0.903392
 H -7.746458 -1.583672 1.714739
 H -8.951283 -0.458356 1.055433
 H -7.375417 0.154297 1.591799
 H 0.955778 4.461486 0.058647

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89631042**

Comp_05Z_c08

B3LYP/6-31G* Geometry

C -4.511337 -0.697686 0.064539
 C -7.112912 -1.709190 0.218803
 C -5.582026 0.151428 0.374842
 C -4.748154 -2.063610 -0.169201
 C -6.044030 -2.560142 -0.091035
 C -6.879289 -0.352782 0.451540
 N -3.237910 -0.075308 0.013434
 N -2.282693 -0.849112 -0.269621
 C -1.009795 -0.235149 -0.321826
 C 1.595875 0.766611 -0.476000

C 0.057338 -1.083567 -0.629955
 C -0.767125 1.127546 -0.085319
 C 0.526341 1.654895 -0.154483
 C 1.355729 -0.589559 -0.706167
 O 2.833749 1.339255 -0.564184
 C 3.952559 0.556531 -0.910925
 C 0.868240 3.060728 0.104416
 C 4.454845 -0.302937 0.250557
 O 5.467880 -1.079744 -0.178542
 O 4.026098 -0.274662 1.378309
 C 6.090540 -1.924302 0.824599
 C 7.193172 -2.708361 0.140182
 N 0.152767 4.114176 0.288787
 O -1.229989 3.891340 0.219982
 H -8.122908 -2.106029 0.278042
 H -5.369057 1.201476 0.551058
 H -3.907955 -2.706205 -0.407446
 H -6.228530 -3.616105 -0.271422
 H -7.705583 0.310403 0.692511
 H -0.148663 -2.135083 -0.804470
 H -1.601509 1.767843 0.155974
 H 2.168175 -1.269313 -0.932941
 H 3.764802 -0.070115 -1.791112
 H 4.740847 1.267333 -1.177371
 H 1.928436 3.287468 0.156324
 H 5.323730 -2.576274 1.254153
 H 6.472813 -1.286227 1.627432
 H 6.789906 -3.331725 -0.664197
 H 7.687201 -3.361741 0.867327
 H 7.945482 -2.037342 -0.286413
 H -1.584081 4.781091 0.372432

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89683014**

Comp_05Z_c11

B3LYP/6-31G* Geometry

C 4.359451 -1.095839 -0.036685
 C 7.091662 -1.628592 0.219854
 C 5.251620 -0.053341 0.269359
 C 4.844627 -2.398639 -0.211988
 C 6.206936 -2.664657 -0.083985
 C 6.608907 -0.325263 0.395493
 N 2.957599 -0.942565 -0.190876
 N 2.534369 0.234787 -0.027449
 C 1.137147 0.391418 -0.180207
 C -1.595030 0.926429 -0.436151
 C 0.242950 -0.645842 -0.484270
 C 0.653561 1.691783 -0.001348
 C -0.711029 1.994525 -0.122233
 C -1.112235 -0.377871 -0.609143
 O -2.911953 1.264118 -0.575619
 C -3.862148 0.292966 -0.948364
 C -1.291732 3.330022 0.065383
 C -4.261853 -0.619733 0.212121

O -5.151271 -1.530319 -0.227240
O -3.857168 -0.529085 1.345535
C -5.660689 -2.454794 0.769529
C -6.645788 -3.375406 0.075934
N -0.773077 4.489961 0.269557
O 0.629694 4.494864 0.317215
H 8.154534 -1.831685 0.320415
H 4.858787 0.948584 0.401487
H 4.132732 -3.184084 -0.447512
H 6.577233 -3.676994 -0.220691
H 7.299900 0.479785 0.632113
H 0.626428 -1.651658 -0.613474
H 1.361247 2.471728 0.236488
H -1.791306 -1.193459 -0.827882
H -4.747489 0.850782 -1.268302
H -3.528086 -0.309118 -1.802200
H -2.375349 3.382120 0.030349
H -6.128254 -1.876914 1.572663
H -4.815867 -3.000926 1.200396
H -7.477351 -2.807780 -0.353532
H -7.053775 -4.090824 0.798062
H -6.158998 -3.937309 -0.727529
H 0.820816 5.432845 0.471614

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89692834**

Comp_05Z_c13

B3LYP/6-31G* Geometry

C 4.849659 -0.041552 -0.000053
C 7.642882 -0.145290 0.000259
C 5.600308 1.141729 -0.000071
C 5.505336 -1.285214 0.000060
C 6.894522 -1.329643 0.000215
C 6.993227 1.090220 0.000123
N 3.442241 0.132779 -0.000277
N 2.776764 -0.938713 0.000434
C 1.372125 -0.770441 0.000245
C -1.420203 -0.671626 -0.000060
C 0.623801 -1.950371 0.000630
C 0.714704 0.471547 -0.000235
C -0.681229 0.550907 -0.000376
C -0.768022 -1.906765 0.000461
O -2.776483 -0.541123 -0.000276
C -3.587773 -1.697120 -0.000066
C -1.454148 1.801102 -0.000897
C -5.067174 -1.332397 -0.000521
O -5.296152 -0.016245 0.000794
O -5.919316 -2.194099 -0.001774
C -6.692485 0.381671 0.000534
C -6.731128 1.897246 0.001568
N -1.110211 3.041293 -0.000880
O 0.275167 3.255984 -0.000256
H 8.728726 -0.189829 0.000367
H 5.066596 2.087325 -0.000217

H 4.909097 -2.190830 0.000023
H 7.403147 -2.290303 0.000278
H 7.570186 2.010911 0.000139
H 1.150591 -2.899646 0.001054
H 1.309755 1.371625 -0.000498
H -1.331544 -2.832199 0.000737
H -3.401556 -2.318152 -0.886563
H -3.401912 -2.317492 0.886996
H -2.533987 1.687502 -0.001357
H -7.175287 -0.047412 0.883919
H -7.174636 -0.046204 -0.883787
H -6.235146 2.301218 0.889617
H -7.771781 2.239176 0.001486
H -6.234603 2.302442 -0.885618
H 0.328654 4.224201 -0.000315

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89659458**

Comp_05Z_c15

B3LYP/6-31G* Geometry

C -4.408650 -1.001297 -0.018518
C -7.149278 -1.442415 0.311622
C -5.245201 0.053761 0.385747
C -4.953160 -2.270830 -0.253624
C -6.319754 -2.491021 -0.089389
C -6.606982 -0.172528 0.548088
N -3.008244 -0.893072 -0.217694
N -2.533161 0.257170 -0.009842
C -1.136999 0.368808 -0.205863
C 1.603667 0.813058 -0.534212
C -0.294691 -0.685565 -0.588893
C -0.597395 1.640438 0.014761
C 0.772956 1.897358 -0.140991
C 1.065003 -0.462938 -0.749272
O 2.927132 1.108129 -0.705877
C 3.828265 0.113383 -1.133938
C 1.411676 3.199205 0.090009
C 4.214643 -0.855078 -0.014954
O 5.026361 -1.806085 -0.518076
O 3.857298 -0.768601 1.134830
C 5.532120 -2.794787 0.419310
C 6.792006 -2.301612 1.112782
N 0.944425 4.369707 0.350034
O -0.456162 4.429178 0.420683
H -8.215208 -1.609967 0.441157
H -4.806823 1.029357 0.563656
H -4.283338 -3.067135 -0.564153
H -6.736225 -3.477625 -0.273251
H -7.254975 0.642223 0.860895
H -0.721241 -1.669045 -0.750886
H -1.265696 2.433963 0.313881
H 1.703607 -1.292003 -1.030692
H 3.452966 -0.443063 -2.001175
H 4.729516 0.646086 -1.452570

H 2.495822 3.208390 0.037740
H 5.728876 -3.673030 -0.199761
H 4.743756 -3.025456 1.139545
H 7.559805 -2.030411 0.380936
H 7.193988 -3.093205 1.755345
H 6.574077 -1.431591 1.738802
H -0.606429 5.367264 0.614577
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89618913**

Comp_05Z_c17
B3LYP/6-31G* Geometry
C 4.543502 -0.600630 0.106981
C 7.178950 -1.509325 0.315575
C 4.845844 -1.945531 -0.169262
C 5.566136 0.279266 0.486039
C 6.880248 -0.173662 0.590121
C 6.158309 -2.390859 -0.063763
N 3.247286 -0.029458 0.035369
N 2.334285 -0.831210 -0.303553
C 1.039150 -0.267633 -0.375731
C -1.599949 0.632845 -0.577445
C 0.017285 -1.147841 -0.742662
C 0.733891 1.075737 -0.104195
C -0.577674 1.552705 -0.196264
C -1.297594 -0.704386 -0.842413
O -2.857607 1.157586 -0.683662
C -3.932486 0.345997 -1.096303
C -0.984327 2.934719 0.094818
C -4.444951 -0.568066 0.017701
O -5.442414 -1.333739 -0.467566
O -4.028332 -0.587464 1.150496
C -6.084666 -2.239277 0.470204
C -7.183903 -1.537045 1.251240
N -0.318955 4.008304 0.340700
O 1.073168 3.841773 0.318487
H 8.202268 -1.866362 0.395769
H 4.042178 -2.612418 -0.460848
H 5.302902 1.312047 0.693589
H 7.668993 0.513131 0.884779
H 6.393577 -3.430494 -0.276965
H 0.271241 -2.184112 -0.943241
H 1.534228 1.740446 0.182132
H -2.074719 -1.409030 -1.112655
H -4.736993 1.034595 -1.371977
H -3.688539 -0.246122 -1.986695
H -2.053884 3.118517 0.113473
H -5.321153 -2.648747 1.135883
H -6.483434 -3.036880 -0.160713
H -6.765477 -0.750747 1.885825
H -7.697973 -2.259348 1.895520
H -7.922115 -1.094019 0.574863
H 1.385472 4.738767 0.513773
Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89609139**

Comp_05Z_c21
B3LYP/6-31G* Geometry
C 4.944508 -0.496162 0.000071
C 7.718818 -0.156737 0.000119
C 5.492571 0.798506 -0.000242
C 5.792401 -1.611826 0.000395
C 7.175968 -1.442761 0.000424
C 6.873024 0.960127 -0.000216
N 3.556375 -0.787400 0.000061
N 2.803757 0.225168 -0.000055
C 1.418602 -0.063601 -0.000078
C -1.354883 -0.403347 -0.000173
C 0.869648 -1.353983 -0.000099
C 0.571890 1.051243 -0.000101
C -0.824018 0.916831 -0.000139
C -0.508588 -1.521101 -0.000149
O -2.714162 -0.497890 -0.000245
C -3.327121 -1.770361 -0.000143
C -1.780261 2.031445 -0.000157
C -4.846147 -1.651117 -0.000108
O -5.287300 -0.390152 0.000051
O -5.545961 -2.640543 -0.000203
C -6.730170 -0.227233 0.000117
C -7.018015 1.261180 0.000691
N -1.632979 3.310066 -0.000076
O -0.296134 3.736303 0.000040
H 8.797020 -0.020764 0.000135
H 4.821580 1.650174 -0.000501
H 5.341405 -2.599620 0.000620
H 7.828669 -2.311408 0.000681
H 7.298408 1.960387 -0.000465
H 1.534932 -2.210077 -0.000084
H 1.021323 2.032931 -0.000083
H -0.921275 -2.523378 -0.000177
H -3.043764 -2.353200 -0.886856
H -3.043703 -2.353080 0.886632
H -2.829415 1.751469 -0.000236
H -7.135472 -0.729738 0.883714
H -7.135465 -0.729037 -0.883885
H -6.595691 1.741803 0.888671
H -8.100835 1.426739 0.000561
H -6.595370 1.742529 -0.886743
H -0.393325 4.701067 0.000079
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89661665**

Comp_05Z_c22
B3LYP/6-31G* Geometry
C 4.272768 -0.959260 -0.064911
C 7.013578 -1.429828 0.219615
C 5.127302 0.086890 0.324645

C 4.799540 -2.234673 -0.308461
 C 6.166210 -2.469575 -0.166879
 C 6.489077 -0.154041 0.464340
 N 2.870521 -0.835985 -0.240951
 N 2.411085 0.318965 -0.024203
 C 1.013260 0.445729 -0.197995
 C -1.727149 0.920154 -0.484016
 C 0.154012 -0.598773 -0.570074
 C 0.490703 1.722682 0.033119
 C -0.878952 1.994572 -0.101178
 C -1.205537 -0.361185 -0.709563
 O -3.049584 1.229444 -0.635785
 C -3.967486 0.241126 -1.043168
 C -1.500235 3.302521 0.142817
 C -4.335205 -0.724869 0.084339
 O -5.132343 -1.692871 -0.409082
 O -3.986042 -0.616971 1.234825
 C -5.625562 -2.677718 0.539176
 C -4.625873 -3.806971 0.731560
 N -1.016192 4.467537 0.396601
 O 0.385943 4.512150 0.442733
 H 8.079668 -1.608804 0.331299
 H 4.702528 1.067263 0.509183
 H 4.116083 -3.023784 -0.607440
 H 6.568906 -3.460675 -0.357130
 H 7.150993 0.653811 0.765659
 H 0.567707 -1.586242 -0.740988
 H 1.171895 2.508485 0.323434
 H -1.856992 -1.182310 -0.984998
 H -4.871899 0.781141 -1.339919
 H -3.616614 -0.317261 -1.919234
 H -2.584982 3.322983 0.109470
 H -6.556842 -3.033919 0.092949
 H -5.843480 -2.172894 1.483300
 H -4.379383 -4.277567 -0.225842
 H -5.054565 -4.571558 1.389414
 H -3.706894 -3.435252 1.193463
 H 0.549477 5.448251 0.635514

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89615987**

Comp_05Z_c23
B3LYP/6-31G* Geometry
 C 4.873968 -0.097803 0.065695
 C 7.661516 -0.277048 0.165896
 C 5.656969 1.064319 0.061072
 C 5.494184 -1.358312 0.120976
 C 6.880772 -1.440297 0.170697
 C 7.047082 0.975159 0.110995
 N 3.472796 0.114687 0.012914
 N 2.777937 -0.938004 0.014437
 C 1.379309 -0.731837 -0.036360
 C -1.407921 -0.557947 -0.128669
 C 0.599219 -1.890961 -0.037982

C 0.756623 0.527067 -0.082482
 C -0.635900 0.644012 -0.129147
 C -0.790120 -1.809950 -0.084349
 O -2.759562 -0.391300 -0.174287
 C -3.601134 -1.525062 -0.157614
 C -1.373600 1.914496 -0.175127
 C -5.070980 -1.124410 -0.183759
 O -5.264511 0.198308 -0.183252
 O -5.940151 -1.969258 -0.202580
 C -6.645641 0.651113 -0.199827
 C -7.216298 0.720833 1.207609
 N -0.995152 3.144349 -0.199320
 O 0.395487 3.320769 -0.179514
 H 8.745057 -0.350938 0.204983
 H 5.150132 2.023618 0.017881
 H 4.873231 -2.247140 0.124067
 H 7.362012 -2.414016 0.213715
 H 7.649253 1.879554 0.107125
 H 1.099456 -2.853846 -0.002650
 H 1.375858 1.410633 -0.080146
 H -1.378128 -2.719989 -0.086406
 H -3.421869 -2.171977 -1.026725
 H -3.441258 -2.128796 0.746048
 H -2.456001 1.830535 -0.193200
 H -7.226145 -0.022256 -0.834574
 H -6.593371 1.638168 -0.664156
 H -7.275033 -0.277078 1.651256
 H -8.227769 1.141469 1.174564
 H -6.598828 1.359633 1.847112
 H 0.475947 4.286813 -0.203785

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89577195**

Comp_05Z_c29
B3LYP/6-31G* Geometry
 C 4.943503 -0.565485 0.051744
 C 7.725575 -0.307146 0.123135
 C 5.528615 0.712675 0.074901
 C 5.758459 -1.705339 0.064610
 C 7.145910 -1.576799 0.100096
 C 6.912758 0.833867 0.110443
 N 3.547932 -0.816354 0.015946
 N 2.825185 0.217578 0.000404
 C 1.432630 -0.030954 -0.033682
 C -1.348738 -0.289745 -0.101361
 C 0.846532 -1.304837 -0.043864
 C 0.618989 1.107993 -0.057260
 C -0.779802 1.014462 -0.091945
 C -0.535595 -1.431623 -0.077268
 O -2.709839 -0.344851 -0.134436
 C -3.359001 -1.598962 -0.142192
 C -1.702670 2.156541 -0.119850
 C -4.873775 -1.437441 -0.180602
 O -5.273840 -0.163379 -0.239961

O -5.598046 -2.409415 -0.166277
 C -6.708839 0.063984 -0.282091
 C -7.298778 0.105544 1.118429
 N -1.517898 3.430281 -0.116336
 O -0.169668 3.817081 -0.077813
 H 8.806921 -0.202556 0.150953
 H 4.882897 1.583604 0.064740
 H 5.279054 -2.679490 0.046273
 H 7.772957 -2.464079 0.109860
 H 7.366890 1.821249 0.128558
 H 1.486230 -2.180012 -0.025096
 H 1.097049 2.076028 -0.048508
 H -0.977187 -2.421488 -0.084262
 H -3.071280 -2.195385 -1.018654
 H -3.114194 -2.184116 0.754245
 H -2.759131 1.907358 -0.149815
 H -7.168928 -0.720230 -0.887585
 H -6.807903 1.025237 -0.790839
 H -7.205665 -0.868369 1.607352
 H -8.363197 0.360422 1.062198
 H -6.796041 0.861096 1.730527
 H -0.238502 4.784275 -0.081592

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89581129**

Comp_05Z_c33
B3LYP/6-31G* Geometry
 C 4.280191 -0.694755 -0.055852
 C 7.028697 -0.886592 0.414754
 C 4.984324 0.412774 0.448260
 C 4.960159 -1.891052 -0.320640
 C 6.330836 -1.986949 -0.085916
 C 6.350980 0.310524 0.679959
 N 2.889109 -0.711404 -0.332460
 N 2.288695 0.370777 -0.087287
 C 0.901326 0.356787 -0.364272
 C -1.846570 0.551731 -0.841806
 C 0.196684 -0.744355 -0.872163
 C 0.221534 1.549652 -0.094376
 C -1.156864 1.680988 -0.320654
 C -1.167663 -0.646238 -1.107763
 O -3.183345 0.717962 -1.067834
 C -3.940453 -0.350923 -1.602316
 C -1.939698 2.893293 -0.050461
 C -4.206369 -1.513311 -0.643439
 O -4.129524 -1.142338 0.639026
 O -4.495125 -2.621994 -1.038813
 C -4.384800 -2.182338 1.619280
 C -4.223372 -1.560141 2.992269
 N -1.621511 4.066154 0.373300
 O -0.252235 4.236386 0.627489
 H 8.097394 -0.957289 0.598888
 H 4.442273 1.330553 0.646879
 H 4.391199 -2.729952 -0.710084

H 6.852911 -2.917010 -0.293242
 H 6.896955 1.165872 1.069565
 H 0.731394 -1.665501 -1.074745
 H 0.786853 2.381040 0.299294
 H -1.697862 -1.508916 -1.495224
 H -4.906874 0.088886 -1.868657
 H -3.493390 -0.758202 -2.515247
 H -3.006640 2.815353 -0.234204
 H -3.677821 -2.999911 1.448209
 H -5.393759 -2.573181 1.454868
 H -3.210199 -1.169274 3.127445
 H -4.408701 -2.315727 3.763371
 H -4.932687 -0.739081 3.136013
 H -0.216911 5.158967 0.923878

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89664649**

Comp_05Z_c36
B3LYP/6-31G* Geometry
 C -4.222698 -0.680626 -0.121521
 C -6.979191 -0.918080 0.275882
 C -4.951305 0.401199 0.403183
 C -4.882285 -1.874423 -0.443079
 C -6.256982 -1.992990 -0.245128
 C -6.321799 0.276317 0.598321
 N -2.825414 -0.672866 -0.365207
 N -2.244524 0.409039 -0.075620
 C -0.850957 0.419215 -0.319450
 C 1.904520 0.660851 -0.728065
 C -0.119774 -0.660979 -0.834792
 C -0.193689 1.614250 -0.006698
 C 1.187587 1.768742 -0.197957
 C 1.248261 -0.539809 -1.035771
 O 3.243205 0.850407 -0.920719
 C 4.028229 -0.195259 -1.460139
 C 1.947400 2.984622 0.118221
 C 4.307929 -1.365897 -0.514804
 O 4.193711 -1.014516 0.771269
 O 4.643587 -2.455244 -0.927199
 C 4.466815 -2.045455 1.758690
 C 3.229186 -2.884150 2.034648
 N 1.602388 4.145150 0.554672
 O 0.224149 4.294303 0.771031
 H -8.051074 -1.006508 0.431652
 H -4.424751 1.317328 0.646150
 H -4.294527 -2.693259 -0.847036
 H -6.763228 -2.920880 -0.496706
 H -6.886669 1.111741 1.003884
 H -0.637271 -1.584025 -1.070704
 H -0.779088 2.429065 0.392248
 H 1.799100 -1.386329 -1.429994
 H 3.601965 -0.597185 -2.385186
 H 4.989540 0.266730 -1.706769
 H 3.020109 2.922808 -0.035597

H 4.780233 -1.486103 2.642803
H 5.296624 -2.659565 1.400967
H 2.388033 -2.250388 2.332211
H 3.436340 -3.588702 2.848158
H 2.944121 -3.459291 1.149127
H 0.168686 5.210543 1.083574
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89571183**

Comp_05Z_c45
B3LYP/6-31G* Geometry
C 4.402453 -0.458231 0.121398
C 7.061868 -1.261923 0.429492
C 5.365247 0.448772 0.584009
C 4.776997 -1.777384 -0.188721
C 6.101036 -2.170536 -0.033040
C 6.691515 0.048282 0.737387
N 3.086960 0.059181 0.006514
N 2.230503 -0.763934 -0.417726
C 0.915711 -0.254479 -0.531313
C -1.748562 0.539462 -0.828758
C -0.041402 -1.155025 -1.006077
C 0.533305 1.055923 -0.200928
C -0.792624 1.479981 -0.338629
C -1.369176 -0.764776 -1.156100
O -3.027406 1.002488 -0.957541
C -4.032527 0.139215 -1.452334
C -1.278772 2.825737 -0.004219
C -4.479939 -0.969096 -0.496937
O -4.256771 -0.653229 0.784137
O -5.010013 -1.983914 -0.895984
C -4.662883 -1.632414 1.778109
C -6.123325 -1.452679 2.160346
N -0.689189 3.892521 0.408943
O 0.696415 3.759754 0.573654
H 8.094786 -1.578251 0.548087
H 5.046827 1.460628 0.815877
H 4.019219 -2.465948 -0.545502
H 6.392235 -3.190166 -0.272098
H 7.433829 0.755862 1.096374
H 0.271857 -2.164465 -1.254052
H 1.285376 1.736606 0.166906
H -2.093536 -1.483282 -1.521507
H -4.896405 0.784786 -1.640500
H -3.746433 -0.326355 -2.401404
H -2.346683 2.982988 -0.117506
H -3.996988 -1.443546 2.622727
H -4.473875 -2.631937 1.379633
H -6.311367 -0.433871 2.514069
H -6.381890 -2.149482 2.965763
H -6.774951 -1.659568 1.306677
H 0.948756 4.645861 0.876108
Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89578890**

Comp_05Z_c47
B3LYP/6-31G* Geometry
C -4.347778 -0.794299 -0.015465
C -7.091699 -1.071359 0.439241
C -5.087492 0.288551 0.491228
C -4.990009 -2.009045 -0.290304
C -6.358445 -2.147355 -0.063806
C -6.451634 0.143946 0.715039
N -2.955362 -0.767619 -0.284740
N -2.390357 0.332847 -0.036788
C -1.001638 0.362050 -0.305546
C 1.741465 0.642694 -0.766967
C -0.258866 -0.718323 -0.803617
C -0.362137 1.577359 -0.037318
C 1.012608 1.751825 -0.256264
C 1.103122 -0.577778 -1.030994
O 3.073849 0.850509 -0.985085
C 3.864277 -0.190740 -1.524802
C 1.754164 2.990243 0.011991
C 4.173898 -1.347743 -0.572637
O 4.087457 -0.983156 0.711977
O 4.496729 -2.443091 -0.980003
C 4.383781 -2.004662 1.702274
C 5.874845 -2.072323 1.991091
N 1.393891 4.157467 0.417138
O 0.016086 4.288541 0.647945
H -8.158728 -1.175194 0.617286
H -4.574341 1.221018 0.697995
H -4.393883 -2.828235 -0.681072
H -6.851225 -3.091479 -0.279107
H -7.025061 0.980153 1.106754
H -0.762439 -1.657188 -1.004584
H -0.956263 2.392005 0.348838
H 1.663293 -1.425352 -1.409612
H 3.428237 -0.609949 -2.437636
H 4.814929 0.281597 -1.792530
H 2.825595 2.943007 -0.155328
H 4.002540 -2.962113 1.339731
H 3.814892 -1.693665 2.580979
H 6.426297 -2.399990 1.105248
H 6.061806 -2.791428 2.796711
H 6.255483 -1.095789 2.307247
H -0.052070 5.213076 0.932265
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89581821**

Comp_05Z_c50
B3LYP/6-31G* Geometry
C 4.305914 -0.660698 -0.050422
C 7.049666 -0.856542 0.438870
C 4.979191 -1.867822 -0.280611

C 5.013584 0.455629 0.428631
 C 6.378285 0.351302 0.669859
 C 6.348089 -1.965636 -0.036671
 N 2.915972 -0.676402 -0.332914
 N 2.322019 0.416092 -0.124790
 C 0.932815 0.398896 -0.407035
 C -1.804093 0.590205 -0.888146
 C 0.226183 -0.718810 -0.884325
 C 0.266643 1.607571 -0.186817
 C -1.111099 1.736427 -0.433437
 C -1.136711 -0.616873 -1.120271
 O -3.152878 0.658199 -1.181164
 C -4.052815 0.651143 -0.080841
 C -1.854025 3.001328 -0.335267
 C -4.485042 -0.723939 0.429020
 O -4.085157 -1.737986 -0.352462
 O -5.161122 -0.833989 1.429188
 C -4.494017 -3.069851 0.060239
 C -3.531925 -3.652097 1.083774
 N -1.608628 4.106094 0.275116
 O -0.420596 4.089511 1.018690
 H 8.116943 -0.928738 0.630384
 H 4.406804 -2.713046 -0.650777
 H 4.475999 1.381262 0.601067
 H 6.927672 1.212839 1.040354
 H 6.865793 -2.903656 -0.216955
 H 0.761232 -1.646178 -1.054998
 H 0.840510 2.454138 0.162523
 H -1.716307 -1.459410 -1.479241
 H -3.655840 1.206655 0.776155
 H -4.960489 1.164201 -0.416033
 H -2.788820 3.043267 -0.889357
 H -4.494354 -3.645612 -0.868077
 H -5.510847 -3.014390 0.455729
 H -2.507403 -3.660631 0.697983
 H -3.820720 -4.683513 1.316193
 H -3.556463 -3.072199 2.010417
 H -0.415070 4.977258 1.409438

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.88999351**

Comp_05Z_c52

B3LYP/6-31G* Geometry

C 4.309881 -0.398768 0.064622
 C 6.982412 -1.159753 0.367208
 C 5.257743 0.521734 0.531407
 C 4.706068 -1.709907 -0.252469
 C 6.036528 -2.081841 -0.099440
 C 6.590583 0.142539 0.681995
 N 2.985822 0.097108 -0.046771
 N 2.143344 -0.737444 -0.476648
 C 0.820055 -0.249560 -0.586343
 C -1.857281 0.501712 -0.878348
 C -0.121355 -1.161896 -1.069967

C 0.415170 1.050974 -0.243997
 C -0.917723 1.453729 -0.378675
 C -1.455459 -0.792836 -1.217499
 O -3.143764 0.943635 -1.003167
 C -4.134831 0.066470 -1.502872
 C -1.426512 2.788478 -0.033976
 C -4.556075 -1.058951 -0.555437
 O -4.328493 -0.756484 0.727077
 O -5.075494 -2.078218 -0.955935
 C -4.710812 -1.766914 1.696924
 C -4.316561 -1.252259 3.067270
 N -0.857423 3.857241 0.402245
 O 0.526979 3.740183 0.587608
 H 8.020517 -1.459481 0.483598
 H 4.922698 1.526961 0.768628
 H 3.959661 -2.409177 -0.612381
 H 6.344504 -3.095251 -0.343833
 H 7.321286 0.860494 1.044182
 H 0.209251 -2.163486 -1.327120
 H 1.155345 1.741053 0.130359
 H -2.167258 -1.519838 -1.590705
 H -5.011107 0.697632 -1.681849
 H -3.843322 -0.384376 -2.457407
 H -2.494631 2.933272 -0.161058
 H -4.201856 -2.701391 1.441809
 H -5.788280 -1.939050 1.610840
 H -3.237650 -1.078021 3.123400
 H -4.588295 -1.989983 3.830021
 H -4.830592 -0.313558 3.296548
 H 0.762724 4.625244 0.906099

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89661575**

Comp_05Z_c53

B3LYP/6-31G* Geometry

C 4.397447 -0.825398 -0.004106
 C 7.143600 -1.084953 0.439774
 C 5.020677 -2.072112 -0.148306
 C 5.156697 0.298595 0.365476
 C 6.522293 0.162454 0.584670
 C 6.390759 -2.201736 0.073119
 N 3.001349 -0.811128 -0.254396
 N 2.452192 0.316161 -0.123039
 C 1.056630 0.328410 -0.372950
 C -1.682001 0.582588 -0.810491
 C 0.299310 -0.797240 -0.740943
 C 0.439546 1.575163 -0.237965
 C -0.938495 1.734941 -0.464146
 C -1.064359 -0.663730 -0.955923
 O -3.034690 0.679108 -1.078585
 C -3.904660 0.766022 0.042306
 C -1.635694 3.029040 -0.448012
 C -4.344643 -0.561490 0.659778
 O -4.046979 -1.629149 -0.096134

O -4.939506 -0.594229 1.715485
 C -4.476649 -2.919907 0.414188
 C -5.909402 -3.222013 0.004609
 N -1.335722 4.169580 0.064394
 O -0.126252 4.171016 0.772681
 H 8.212018 -1.181849 0.613186
 H 4.409017 -2.922363 -0.434682
 H 4.657429 1.255018 0.472576
 H 7.111562 1.029879 0.870477
 H 6.869496 -3.170450 -0.040085
 H 0.796378 -1.755011 -0.845424
 H 1.051484 2.424965 0.029367
 H -1.681663 -1.510593 -1.232773
 H -3.477481 1.373314 0.847962
 H -4.811934 1.270017 -0.308246
 H -2.585555 3.059297 -0.976499
 H -4.362845 -2.921486 1.500577
 H -3.773129 -3.629048 -0.027961
 H -6.601057 -2.513457 0.468791
 H -6.181958 -4.231801 0.332126
 H -6.023273 -3.170614 -1.082998
 H -0.080128 5.086136 1.090854

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.89013447**

Comp_05Z_c54
B3LYP/6-31G* Geometry
 C 5.154717 -0.090107 0.041760
 C 7.918466 -0.428019 0.286189
 C 6.010800 1.017016 -0.031400
 C 5.689426 -1.375376 0.239018
 C 7.064641 -1.536335 0.359798
 C 7.389062 0.848677 0.090524
 N 3.773704 0.200343 -0.095016
 N 3.012135 -0.803818 -0.028711
 C 1.635141 -0.516452 -0.163707
 C -1.132984 -0.169012 -0.430290
 C 0.774368 -1.617361 -0.111399
 C 1.092967 0.768583 -0.341091
 C -0.280059 0.965343 -0.445634
 C -0.601067 -1.449981 -0.252102
 O -2.455606 0.063136 -0.655717
 C -3.408014 -0.862635 -0.186592
 C -0.812905 2.336725 -0.625514
 C -4.720851 -0.126775 0.077482
 O -5.741429 -0.993012 -0.017177
 O -4.841416 1.041018 0.376821
 C -7.058500 -0.470839 0.303089
 C -8.049657 -1.606518 0.141366
 N -1.781127 2.906282 -0.008037
 O -2.260456 2.117272 1.049264
 H 8.992494 -0.563517 0.381740
 H 5.569837 1.997540 -0.183620
 H 5.012679 -2.220698 0.293755

H 7.479854 -2.529211 0.512573
 H 8.047978 1.710672 0.033286
 H 1.205003 -2.604978 0.021749
 H 1.769588 1.616321 -0.368167
 H -1.250895 -2.318621 -0.252315
 H -3.584384 -1.670353 -0.907475
 H -3.089028 -1.316612 0.762512
 H -0.335273 2.969412 -1.373493
 H -7.270946 0.364621 -0.370462
 H -7.037610 -0.079752 1.325041
 H -8.046400 -1.986350 -0.885126
 H -9.058818 -1.249651 0.373291
 H -7.813378 -2.433914 0.817927
 H -3.225751 2.246498 1.006604

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.88987201**

Comp_05Z_c55
B3LYP/6-31G* Geometry
 C 5.128792 -0.578657 0.077156
 C 7.915402 -0.531687 0.291304
 C 5.812188 0.650047 0.070259
 C 5.848703 -1.775482 0.192019
 C 7.238303 -1.752343 0.298427
 C 7.197828 0.666172 0.177371
 N 3.721731 -0.722758 -0.023936
 N 3.085869 0.361534 -0.135912
 C 1.683280 0.220124 -0.238657
 C -1.109212 0.181618 -0.472157
 C 0.994391 -1.002812 -0.251909
 C 0.956388 1.413498 -0.336914
 C -0.436302 1.423580 -0.423290
 C -0.388387 -1.018929 -0.375731
 O -2.454905 0.220152 -0.680053
 C -3.251466 -0.853093 -0.233764
 C -1.158748 2.712938 -0.519349
 C -4.657015 -0.334488 0.067039
 O -5.534043 -1.344273 -0.044335
 O -4.951263 0.791333 0.404395
 C -6.909991 -1.041364 0.308914
 C -7.712827 -2.316924 0.145462
 N -2.196086 3.099838 0.127117
 O -2.554546 2.187859 1.131420
 H 8.998709 -0.509197 0.374554
 H 5.239647 1.566496 -0.018503
 H 5.294851 -2.709486 0.195390
 H 7.791177 -2.683473 0.387077
 H 7.727616 1.615258 0.172794
 H 1.560036 -1.925195 -0.183384
 H 1.507369 2.349552 -0.316043
 H -0.909665 -1.969479 -0.427414
 H -3.315587 -1.654414 -0.980014
 H -2.854748 -1.284161 0.696350
 H -0.779655 3.452701 -1.224508

H -7.265134 -0.240283 -0.346113
H -6.930042 -0.666469 1.336866
H -7.670958 -2.677115 -0.887255
H -8.760654 -2.127504 0.401849
H -7.334797 -3.105830 0.803369
H -3.528658 2.184546 1.095617
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1122.88971059**

Comp_06E_c01
B3LYP/6-31G* Geometry

C -2.807983 2.366265 -0.453264
C -2.686191 0.918572 -0.038823
C -2.081851 0.025462 -0.837677
C -1.867079 -1.447812 -0.614303
C -0.406800 -1.895762 -0.881728
C 0.633077 -1.253621 0.010165
C 1.628930 -0.522357 -0.534908
C 2.704027 0.148570 0.171067
N 3.580081 0.807700 -0.502642
C -3.300310 0.604407 1.304347
O 4.533325 1.380849 0.357351
C 0.471186 -1.501243 1.488950
H -2.356738 2.550947 -1.433125
H -2.319550 3.028264 0.275718
H -3.860971 2.678826 -0.499043
H -1.688357 0.394972 -1.786872
H -2.509556 -2.018802 -1.302196
H -2.168833 -1.748169 0.394403
H -0.363320 -2.988526 -0.753116
H -0.160136 -1.694837 -1.931590
H 1.660228 -0.401403 -1.616160
H 2.780241 0.106311 1.258973
H -3.175186 -0.437949 1.607284
H -2.864698 1.239606 2.088168
H -4.377972 0.820571 1.296506
H 5.120872 1.839755 -0.263046
H -0.416075 -0.983478 1.876425
H 0.322276 -2.571523 1.685666
H 1.328585 -1.170143 2.078737

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.111729546**

Comp_06E_c02
B3LYP/6-31G* Geometry

C -3.013773 -2.261636 0.622948
C -2.984614 -0.822824 0.162312
C -1.923000 -0.043419 0.422746
C -1.703471 1.396467 0.045729
C -0.431261 1.616459 -0.820661
C 0.876252 1.285915 -0.132619
C 1.603416 0.223167 -0.541534
C 2.871683 -0.227779 -0.000235

N 3.435757 -1.265738 -0.510528
C -4.223354 -0.385601 -0.581718
O 4.647960 -1.540006 0.145665
C 1.279589 2.214076 0.986378
H -2.099342 -2.538798 1.156557
H -3.131987 -2.947131 -0.228299
H -3.867478 -2.447383 1.290282
H -1.094970 -0.497723 0.968157
H -1.621205 2.006046 0.958181
H -2.559225 1.798123 -0.506178
H -0.525974 1.020512 -1.735459
H -0.413257 2.673750 -1.125784
H 1.227753 -0.381146 -1.365120
H 3.353291 0.295258 0.827712
H -4.183534 0.650926 -0.924363
H -4.391369 -1.023863 -1.460400
H -5.114270 -0.493801 0.052771
H 4.964165 -2.326624 -0.325520
H 2.247708 1.967956 1.427308
H 1.329949 3.249896 0.623534
H 0.536957 2.205256 1.794927

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.111450264**

Comp_06E_c03
B3LYP/6-31G* Geometry

C 5.019596 -1.132654 0.185897
C 3.831596 -0.255631 -0.134205
C 2.598842 -0.778695 -0.225290
C 1.298047 -0.081365 -0.520260
C 0.307962 -0.172516 0.672260
C -1.052662 0.425436 0.388155
C -2.130066 -0.381026 0.272203
C -3.494686 0.020728 -0.012584
N -4.408920 -0.881405 -0.091201
C 4.172180 1.201392 -0.334109
O -5.655350 -0.296172 -0.372718
C -1.094143 1.926936 0.246632
H 4.730998 -2.179657 0.321635
H 5.523524 -0.796785 1.103311
H 5.771845 -1.088318 -0.614440
H 2.500049 -1.852331 -0.051558
H 0.821803 -0.552267 -1.392665
H 1.461774 0.967539 -0.785778
H 0.194528 -1.226236 0.954677
H 0.763746 0.336816 1.533957
H -1.997445 -1.454038 0.399564
H -3.757283 1.069384 -0.162552
H 3.303367 1.825595 -0.555351
H 4.659752 1.610163 0.561922
H 4.889645 1.322151 -1.157799
H -6.242801 -1.067297 -0.405083
H -2.104674 2.323567 0.128696
H -0.647072 2.405312 1.128578

H -0.506517 2.259988 -0.619153
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.112235120**

Comp_06E_c04
B3LYP/6-31G* Geometry
C 5.064159 -0.294887 -0.538549
C 3.679550 -0.437725 0.049044
C 2.799109 0.572984 -0.020868
C 1.385225 0.627272 0.491545
C 0.356763 0.812377 -0.656520
C -1.076316 0.926551 -0.183618
C -1.938485 -0.089068 -0.407308
C -3.333190 -0.153505 -0.013623
N -4.018542 -1.202032 -0.308254
C 3.413818 -1.774908 0.697078
O -5.339199 -1.073451 0.155260
C -1.435169 2.209304 0.524359
H 5.215114 0.687721 -0.996610
H 5.249776 -1.060219 -1.305483
H 5.837176 -0.433818 0.230579
H 3.127463 1.485145 -0.523942
H 1.294069 1.469455 1.192789
H 1.123411 -0.273155 1.056284
H 0.628222 1.716302 -1.222969
H 0.453918 -0.032192 -1.348146
H -1.582987 -0.969778 -0.939435
H -3.808438 0.667652 0.525855
H 2.403487 -1.869510 1.101341
H 3.564462 -2.590046 -0.024299
H 4.122047 -1.954649 1.518042
H -5.738705 -1.911571 -0.125283
H -2.484106 2.261724 0.823183
H -0.826787 2.346166 1.427790
H -1.227510 3.072233 -0.123228

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.112308885**

Comp_06E_c05
B3LYP/6-31G* Geometry
C -3.992172 -1.095099 0.889973
C -2.923095 -0.686965 -0.096977
C -2.514708 0.590283 -0.174331
C -1.500515 1.204119 -1.101130
C -0.338987 1.959582 -0.393294
C 0.651683 1.069461 0.330294
C 1.772242 0.671048 -0.311096
C 2.813142 -0.195650 0.206886
N 3.821829 -0.479823 -0.540154
C -2.400779 -1.816638 -0.950852
O 4.714176 -1.328058 0.139777
C 0.295120 0.688874 1.744198
H -4.344883 -0.247662 1.486403

H -3.622030 -1.866919 1.579567
H -4.859413 -1.531736 0.374616
H -2.985609 1.304144 0.505810
H -2.015812 1.940845 -1.736726
H -1.070116 0.460224 -1.778787
H 0.190716 2.540366 -1.157797
H -0.769635 2.685584 0.311104
H 1.945782 1.018825 -1.328520
H 2.755046 -0.608764 1.215393
H -1.600630 -1.514803 -1.630142
H -2.015712 -2.630190 -0.320728
H -3.209855 -2.250563 -1.555157
H 5.413892 -1.460871 -0.518591
H 1.024620 0.025498 2.214182
H 0.209902 1.589413 2.368361
H -0.684056 0.195746 1.771843

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.110628806**

Comp_06E_c06
B3LYP/6-31G* Geometry
C -5.058938 -0.081394 -0.353753
C -3.630771 -0.445420 -0.020792
C -2.608365 0.123714 -0.677953
C -1.130182 -0.099298 -0.495719
C -0.409073 1.187175 -0.054880
C 1.096357 1.127815 0.107159
C 1.801405 -0.003025 -0.108790
C 3.237867 -0.167211 0.018978
N 3.757945 -1.318508 -0.225164
C -3.491401 -1.474288 1.074989
O 5.151965 -1.276757 -0.047941
C 1.707727 2.441340 0.530579
H -5.115769 0.666817 -1.150651
H -5.581386 0.318534 0.526886
H -5.628027 -0.965021 -0.675965
H -2.858653 0.856319 -1.448332
H -0.699941 -0.436793 -1.450241
H -0.934411 -0.895409 0.229496
H -0.644213 1.992214 -0.769913
H -0.846095 1.528092 0.896782
H 1.282451 -0.908116 -0.411673
H 3.881453 0.662397 0.316142
H -2.453735 -1.714247 1.317573
H -3.979607 -1.125969 1.995818
H -3.994879 -2.409859 0.793846
H 5.414015 -2.186400 -0.259141
H 2.790560 2.399042 0.663011
H 1.491320 3.223029 -0.210561
H 1.267827 2.782531 1.477677

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.112021662**

Comp_06E_c07**B3LYP/6-31G* Geometry**

C -3.732351 1.886805 -0.261170
 C -3.239331 0.460241 -0.328012
 C -1.956541 0.189854 -0.620348
 C -1.290194 -1.155190 -0.741690
 C -0.355247 -1.534029 0.443923
 C 0.775252 -0.553135 0.694160
 C 1.917830 -0.657106 -0.018937
 C 3.081206 0.203984 0.069011
 N 4.097537 -0.034527 -0.683639
 C -4.298385 -0.578486 -0.048198
 O 5.114602 0.908031 -0.450121
 C 0.517259 0.486875 1.754614
 H -2.933244 2.606008 -0.466805
 H -4.151288 2.116464 0.728831
 H -4.540147 2.060131 -0.986291
 H -1.297750 1.040707 -0.799296
 H -0.686289 -1.166642 -1.659469
 H -2.031983 -1.954382 -0.848994
 H -0.965415 -1.630565 1.351077
 H 0.061609 -2.526538 0.231508
 H 2.010749 -1.463162 -0.745730
 H 3.107874 1.047361 0.761191
 H -3.926538 -1.604175 -0.104459
 H -4.726320 -0.432818 0.953508
 H -5.132945 -0.482558 -0.756754
 H 5.806604 0.621110 -1.066165
 H 1.305752 1.238868 1.833142
 H -0.431538 1.003355 1.563634
 H 0.414299 0.005402 2.737397

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -521.109917973

Comp_06E_c08**B3LYP/6-31G* Geometry**

C -3.187763 -1.440446 1.336057
 C -2.603650 -0.698385 0.157177
 C -2.122718 0.546070 0.299765
 C -1.529118 1.453284 -0.749532
 C -0.327626 2.279646 -0.254162
 C 0.979474 1.566809 0.030564
 C 1.145866 0.243898 -0.178611
 C 2.360354 -0.520158 0.038847
 N 2.356876 -1.782412 -0.211476
 C -2.623081 -1.471383 -1.139312
 O 3.619290 -2.340722 0.058793
 C 2.059494 2.487176 0.545963
 H -3.156104 -0.842480 2.252359
 H -2.643068 -2.376796 1.522320
 H -4.233976 -1.721865 1.149331
 H -2.179472 0.991814 1.295215
 H -2.296603 2.175887 -1.067706
 H -1.251200 0.899388 -1.652769

H -0.120299 3.070082 -0.992948
 H -0.625899 2.825048 0.656174
 H 0.309534 -0.349045 -0.534365
 H 3.272616 -0.047875 0.407007
 H -2.172476 -0.929438 -1.974217
 H -2.091041 -2.426513 -1.029914
 H -3.654740 -1.721700 -1.424247
 H 3.484149 -3.274183 -0.167040
 H 3.011884 1.986444 0.730002
 H 2.242719 3.304030 -0.165708
 H 1.744134 2.960790 1.485959

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -521.110480831

Comp_06E_c09**B3LYP/6-31G* Geometry**

C 3.378039 -1.870339 1.070390
 C 3.086513 -0.723941 0.129811
 C 1.820451 -0.362920 -0.133353
 C 1.333337 0.748323 -1.027422
 C 0.436380 1.773765 -0.302927
 C -0.951475 1.344110 0.136332
 C -1.535684 0.207281 -0.298129
 C -2.864377 -0.269037 0.040004
 N -3.275431 -1.379246 -0.464114
 C 4.318658 -0.074095 -0.452248
 O -4.577931 -1.668804 -0.021400
 C -1.611857 2.330681 1.068404
 H 2.461023 -2.315725 1.468614
 H 3.992907 -1.539608 1.919578
 H 3.949048 -2.662383 0.565167
 H 1.031680 -0.928269 0.362813
 H 0.783592 0.329481 -1.883155
 H 2.177245 1.294630 -1.459922
 H 0.976965 2.144470 0.580679
 H 0.315458 2.656450 -0.952271
 H -0.994537 -0.451340 -0.971681
 H -3.516933 0.292294 0.710561
 H 4.098470 0.765975 -1.114886
 H 4.977222 0.292069 0.347798
 H 4.906626 -0.804970 -1.025005
 H -4.763771 -2.511258 -0.464653
 H -2.646646 2.081948 1.311459
 H -1.052266 2.401017 2.011275
 H -1.604532 3.337407 0.628457

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -521.110025988

Comp_06E_c12**B3LYP/6-31G* Geometry**

C -5.121867 0.118410 0.337747
 C -3.728775 -0.240008 -0.124392
 C -2.736486 0.662336 -0.071860

C -1.294618 0.499523 -0.470594
 C -0.335760 0.628045 0.743189
 C 1.124366 0.544938 0.362186
 C 1.867459 -0.505063 0.780111
 C 3.272582 -0.796642 0.526520
 N 3.993728 -0.182178 -0.345228
 C -3.586620 -1.654509 -0.632065
 O 5.309455 -0.684117 -0.324387
 C 1.664039 1.663344 -0.491391
 H -5.181292 1.150837 0.696419
 H -5.452156 -0.543852 1.150652
 H -5.852223 -0.001801 -0.474985
 H -2.982237 1.649894 0.324661
 H -1.036268 1.273842 -1.207337
 H -1.115047 -0.463226 -0.959992
 H -0.527202 1.594826 1.233742
 H -0.585492 -0.151385 1.472274
 H 1.380774 -1.246365 1.411886
 H 3.729142 -1.598719 1.113664
 H -2.570855 -1.903060 -0.947732
 H -3.882913 -2.374478 0.143541
 H -4.255898 -1.828762 -1.486224
 H 5.733975 -0.177675 -1.034376
 H 2.710837 1.874688 -0.257703
 H 1.641050 1.396161 -1.556655
 H 1.068142 2.575028 -0.366855

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.107646775**

Comp_06E_c14
B3LYP/6-31G* Geometry
 C 2.960148 -2.042043 -0.889970
 C 2.588849 -0.843624 -0.048193
 C 2.222216 0.310660 -0.625840
 C 1.821071 1.608819 0.021328
 C 0.434821 2.120682 -0.453916
 C -0.726179 1.246022 -0.038968
 C -1.477535 0.632568 -0.980740
 C -2.630607 -0.243383 -0.814434
 N -2.992801 -0.763038 0.306259
 C 2.677341 -1.079674 1.440178
 O -4.157671 -1.535068 0.126620
 C -0.971148 1.115919 1.441383
 H 2.886053 -1.828378 -1.960892
 H 2.306906 -2.897738 -0.668144
 H 3.987122 -2.372673 -0.678961
 H 2.204617 0.334878 -1.717720
 H 2.558677 2.383890 -0.236862
 H 1.830218 1.534536 1.113460
 H 0.288196 3.128725 -0.037097
 H 0.451082 2.228888 -1.545607
 H -1.220898 0.810698 -2.023635
 H -3.211734 -0.475751 -1.711643
 H 2.388816 -0.210972 2.036585

H 2.034619 -1.920254 1.736579
 H 3.701126 -1.357441 1.727946
 H -4.303934 -1.895539 1.015100
 H -0.453826 0.235766 1.847068
 H -0.598089 1.994912 1.980468
 H -2.031834 0.972579 1.661606

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.106856337**

Comp_06E_c15
B3LYP/6-31G* Geometry
 C -3.252813 2.186636 -0.291795
 C -3.093072 0.690916 -0.147926
 C -1.905011 0.106421 -0.369234
 C -1.545960 -1.351846 -0.275344
 C -0.365526 -1.629018 0.696571
 C 0.954685 -1.038211 0.255270
 C 1.546266 -0.076317 0.999827
 C 2.804480 0.622493 0.770037
 N 3.464625 0.582268 -0.334484
 C -4.359115 -0.032751 0.242708
 O 4.644266 1.343059 -0.220105
 C 1.539051 -1.582615 -1.023106
 H -2.314751 2.671947 -0.578835
 H -3.597151 2.640649 0.648375
 H -4.009735 2.433713 -1.049866
 H -1.075011 0.757401 -0.647157
 H -1.272427 -1.727693 -1.272865
 H -2.401563 -1.952480 0.049253
 H -0.632241 -1.257199 1.692604
 H -0.250285 -2.720506 0.778589
 H 1.045118 0.229135 1.916667
 H 3.196184 1.226511 1.593584
 H -4.224633 -1.109411 0.369818
 H -4.761161 0.369513 1.183103
 H -5.140221 0.118285 -0.515746
 H 5.025461 1.266592 -1.108729
 H 1.268990 -0.953849 -1.882512
 H 2.631649 -1.593321 -0.990773
 H 1.167362 -2.593882 -1.225326

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.106799463**

Comp_06E_c17
B3LYP/6-31G* Geometry
 C 5.106510 -0.716169 0.021306
 C 3.793290 0.009227 -0.158308
 C 2.651374 -0.674408 -0.332471
 C 1.254776 -0.145058 -0.516740
 C 0.306359 -0.592879 0.627673
 C -1.116804 -0.119257 0.442339
 C -2.097678 -1.018332 0.200103
 C -3.519715 -0.791305 -0.023876

N -4.042234 0.363669 -0.248363
C 3.906467 1.514259 -0.126981
O -5.437594 0.242260 -0.395858
C -1.347894 1.367376 0.527900
H 4.981177 -1.803154 -0.007149
H 5.576136 -0.452627 0.979640
H 5.824586 -0.436055 -0.762501
H 2.719484 -1.764413 -0.331340
H 0.842838 -0.522539 -1.464271
H 1.247557 0.946913 -0.590651
H 0.333454 -1.686917 0.704200
H 0.704050 -0.198196 1.574059
H -1.821709 -2.071479 0.180661
H -4.172895 -1.668606 -0.008416
H 2.948818 2.025734 -0.247793
H 4.348745 1.848556 0.821891
H 4.577752 1.868518 -0.921787
H -5.703480 1.153569 -0.594879
H -1.325236 1.830107 -0.468329
H -2.332994 1.596022 0.942790
H -0.572006 1.850082 1.133603

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.107513791**

Comp_07Z_c01
B3LYP/6-31G* Geometry

C 2.774717 2.349618 -0.031267
C 2.640592 0.845455 0.013923
C 1.889194 0.197870 -0.889927
C 1.632513 -1.279936 -1.019916
C 0.128463 -1.620002 -1.187503
C -0.750729 -1.214516 -0.024946
C -1.763317 -0.340864 -0.220109
C -2.689078 0.137986 0.791953
N -3.666998 0.963626 0.638806
C 3.417537 0.186149 1.128094
C -0.414159 -1.851101 1.300098
O -3.785320 1.404118 -0.694667
H 2.202421 2.786535 -0.855433
H 3.825378 2.651318 -0.148133
H 2.423549 2.805887 0.905082
H 1.388284 0.805578 -1.646268
H 2.046925 -1.835256 -0.172443
H 2.149692 -1.663974 -1.912599
H -0.242300 -1.147847 -2.105292
H 0.045200 -2.707630 -1.336948
H -1.921113 0.057612 -1.217426
H -2.594530 -0.200059 1.821229
H 3.289562 -0.898416 1.166276
H 4.492473 0.389177 1.021700
H 3.121943 0.596943 2.103522
H 0.537004 -1.463933 1.688484
H -1.174291 -1.685304 2.066085
H -0.287611 -2.935698 1.183402

H -4.545435 2.002786 -0.637942
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.111106691**

Comp_07Z_c02
B3LYP/6-31G* Geometry

C 2.967432 -2.036720 0.897767
C 2.868927 -0.693804 0.212120
C 1.813042 0.106895 0.426948
C 1.530414 1.461960 -0.162821
C 0.196151 1.517690 -0.959695
C -1.051757 1.288453 -0.133780
C -1.781268 0.163923 -0.311751
C -2.997586 -0.193526 0.398321
N -3.709488 -1.258429 0.254434
C 4.035405 -0.372491 -0.690659
C -1.392182 2.383892 0.846172
O -3.177868 -2.124429 -0.721027
H 2.103654 -2.232141 1.540732
H 3.874341 -2.100873 1.515850
H 3.035376 -2.851564 0.163040
H 1.041097 -0.260644 1.104065
H 2.334601 1.779134 -0.834193
H 1.495616 2.212793 0.640639
H 0.129784 2.509811 -1.431477
H 0.243446 0.780067 -1.768502
H -1.447767 -0.557696 -1.050842
H -3.406555 0.474318 1.152894
H 3.946407 0.594052 -1.191959
H 4.975524 -0.368111 -0.121319
H 4.148066 -1.143617 -1.465525
H -2.327323 2.213981 1.382964
H -0.598827 2.504170 1.595548
H -1.474313 3.347598 0.325330
H -3.815237 -2.854474 -0.705798

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.110722401**

Comp_07Z_c03
B3LYP/6-31G* Geometry

C -4.808160 -1.307897 0.247729
C -3.687865 -0.354942 -0.098378
C -2.423372 -0.793254 -0.200931
C -1.178915 -0.011970 -0.526819
C -0.167447 -0.013294 0.651622
C 1.144657 0.670531 0.333753
C 2.267949 -0.068321 0.192117
C 3.592907 0.434419 -0.128006
N 4.679477 -0.243773 -0.272314
C -4.130729 1.072639 -0.310397
C 1.081127 2.170816 0.190349
O 4.472243 -1.624411 -0.083234
H -4.445813 -2.330726 0.390766

H -5.571675 -1.324940 -0.542892
H -5.322526 -0.996961 1.168140
H -2.248275 -1.855019 -0.015425
H -1.420437 1.017746 -0.807527
H -0.683538 -0.463866 -1.398472
H -0.643939 0.479065 1.511776
H 0.023472 -1.051436 0.948806
H 2.201134 -1.143787 0.325529
H 3.751457 1.500051 -0.276058
H -3.309409 1.753234 -0.546132
H -4.862218 1.134074 -1.128249
H -4.637541 1.456366 0.586033
H 2.054962 2.634801 0.022615
H 0.429228 2.459226 -0.644611
H 0.646256 2.620327 1.093301
H 5.363663 -1.978826 -0.221758

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.111557513**

Comp_07Z_c04

B3LYP/6-31G* Geometry

C -4.883845 -0.367180 -0.568265
C -3.508218 -0.428440 0.053510
C -2.652833 0.597855 -0.075559
C -1.251838 0.727773 0.458247
C -0.203538 0.855904 -0.680248
C 1.211065 1.058327 -0.181429
C 2.094081 0.036178 -0.239323
C 3.473348 0.065261 0.215733
N 4.335645 -0.892144 0.180183
C -3.221028 -1.706222 0.803940
C 1.520433 2.431371 0.360743
O 3.798325 -2.069408 -0.377078
H -5.050038 0.573401 -1.102895
H -5.668372 -0.467448 0.195218
H -5.034953 -1.193353 -1.277422
H -2.993887 1.461017 -0.651367
H -0.978364 -0.121640 1.091922
H -1.196390 1.620978 1.097441
H -0.254360 -0.045817 -1.300641
H -0.490579 1.700646 -1.324293
H 1.765979 -0.908221 -0.663034
H 3.886483 0.974052 0.647064
H -2.217141 -1.742704 1.232795
H -3.941062 -1.844550 1.622665
H -3.335343 -2.576071 0.142284
H 2.542329 2.536257 0.730146
H 1.365535 3.189550 -0.419233
H 0.842419 2.691630 1.183841
H 4.555864 -2.672428 -0.333235

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.111640163**

Comp_07Z_c05

B3LYP/6-31G* Geometry

C -4.046348 0.690869 0.848024
C -2.841318 0.625506 -0.061578
C -2.375922 -0.556709 -0.497557
C -1.225022 -0.833614 -1.426913
C -0.104078 -1.734299 -0.832418
C 0.720054 -1.076450 0.256860
C 1.846151 -0.408234 -0.081081
C 2.729427 0.300721 0.827767
N 3.801803 0.954348 0.536857
C -2.255399 1.970570 -0.416333
C 0.192844 -1.222383 1.660551
O 4.077247 0.931363 -0.845884
H -4.440822 -0.303873 1.078747
H -4.854743 1.278507 0.390389
H -3.801154 1.189342 1.796457
H -2.901926 -1.452809 -0.159766
H -0.769754 0.092067 -1.792251
H -1.615500 -1.357330 -2.312915
H -0.559830 -2.657850 -0.448697
H 0.556634 -2.026426 -1.657207
H 2.140187 -0.382280 -1.126451
H 2.513997 0.317937 1.893590
H -1.360481 1.904152 -1.038445
H -2.993511 2.585867 -0.949864
H -1.989863 2.526245 0.493449
H 0.791305 -0.701491 2.410954
H -0.835316 -0.845304 1.719615
H 0.153478 -2.284440 1.940069
H 4.894372 1.450475 -0.892543

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.110041839**

Comp_07Z_c06

B3LYP/6-31G* Geometry

C 4.874853 -0.051583 -0.379105
C 3.449423 -0.384312 -0.004233
C 2.421264 0.158959 -0.674181
C 0.944393 -0.041459 -0.458357
C 0.236812 1.277838 -0.100988
C -1.266706 1.240623 0.084426
C -1.978996 0.099235 -0.039406
C -3.417661 -0.031209 0.121877
N -4.126502 -1.102057 0.012950
C 3.319773 -1.353099 1.146140
C -1.861409 2.587168 0.418410
O -3.339957 -2.229243 -0.298543
H 4.924521 0.654227 -1.214260
H 5.430637 -0.955969 -0.664939
H 5.415737 0.387872 0.471032
H 2.665392 0.846964 -1.486573
H 0.753268 -0.782897 0.323622
H 0.499653 -0.442799 -1.380915

H 0.687681 1.683683 0.818229
H 0.466232 2.028804 -0.874312
H -1.464062 -0.822964 -0.280935
H -4.023608 0.838858 0.362685
H 2.284399 -1.570175 1.418187
H 3.809851 -2.306970 0.905773
H 3.827157 -0.962190 2.039128
H -2.942945 2.567852 0.563826
H -1.407686 2.989802 1.334252
H -1.643222 3.310831 -0.378797
H -4.008308 -2.929552 -0.345817

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.111451418**

Comp_07Z_c07

B3LYP/6-31G* Geometry

C 3.856315 1.310527 -1.051030
C 3.198494 0.081311 -0.469043
C 1.883572 -0.137841 -0.633998
C 1.063656 -1.300932 -0.140759
C 0.152934 -0.992781 1.084593
C -0.857532 0.115125 0.854441
C -2.043987 -0.176670 0.275528
C -3.101646 0.768532 -0.035377
N -4.242502 0.524586 -0.583758
C 4.137890 -0.833879 0.278334
C -0.433093 1.488103 1.309612
O -4.403075 -0.843070 -0.885838
H 3.139590 1.946063 -1.580665
H 4.652737 1.035474 -1.757032
H 4.333619 1.914906 -0.266691
H 1.322078 0.608500 -1.197613
H 1.704456 -2.147824 0.128388
H 0.416614 -1.647758 -0.957834
H -0.374374 -1.918941 1.344491
H 0.793341 -0.736468 1.938287
H -2.251779 -1.209150 0.009053
H -2.975482 1.822709 0.200362
H 3.648181 -1.723210 0.681895
H 4.956908 -1.166690 -0.374506
H 4.609059 -0.302251 1.116871
H -1.123892 2.282571 1.019055
H -0.339117 1.508231 2.404570
H 0.558874 1.732547 0.910813
H -5.288318 -0.855228 -1.280233

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.109347776**

Comp_07Z_c08

B3LYP/6-31G* Geometry

C -3.250229 0.421318 1.388779
C -2.426884 0.046923 0.178851
C -1.792960 -1.134121 0.122928

C -0.921080 -1.691599 -0.973259
C 0.434004 -2.227837 -0.469473
C 1.471035 -1.236342 0.022041
C 1.315475 0.098619 -0.110924
C 2.261042 1.115701 0.316001
N 2.146856 2.394562 0.202666
C -2.375756 1.107982 -0.894067
C 2.678341 -1.898088 0.640825
O 0.938941 2.768616 -0.425103
H -3.239538 -0.364808 2.150492
H -4.296552 0.615565 1.113412
H -2.873489 1.345634 1.849172
H -1.910514 -1.803752 0.978035
H -0.758936 -0.964063 -1.774851
H -1.440109 -2.542289 -1.440863
H 0.247205 -2.953626 0.338217
H 0.898303 -2.822265 -1.272813
H 0.410148 0.481279 -0.562670
H 3.192639 0.830726 0.798998
H -1.905562 0.766003 -1.819229
H -3.387690 1.454630 -1.143671
H -1.814260 1.984425 -0.542119
H 3.466270 -1.199119 0.926975
H 2.387947 -2.462438 1.537668
H 3.115085 -2.627121 -0.055340
H 1.011619 3.735013 -0.429473

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.109382415**

Comp_07Z_c09

B3LYP/6-31G* Geometry

C -3.325570 -1.534398 1.276347
C -2.946813 -0.554856 0.189678
C -1.656308 -0.296158 -0.075273
C -1.085423 0.644710 -1.104814
C -0.192475 1.749886 -0.502635
C 1.154020 1.360726 0.080063
C 1.727223 0.159264 -0.149963
C 3.023214 -0.275736 0.343978
N 3.595947 -1.414164 0.151472
C -4.125372 0.058286 -0.527481
C 1.782389 2.460270 0.901149
O 2.808282 -2.277343 -0.636408
H -2.445349 -1.956320 1.771324
H -3.919012 -2.366214 0.870773
H -3.950322 -1.054124 2.043038
H -0.912949 -0.817967 0.527265
H -1.885880 1.136610 -1.666164
H -0.507308 0.078372 -1.849479
H -0.003506 2.511637 -1.276951
H -0.765558 2.274509 0.276203
H 1.203083 -0.572323 -0.753423
H 3.628529 0.389929 0.954342
H -3.842010 0.778521 -1.298488

H -4.734256 -0.721068 -1.006810
H -4.786873 0.571633 0.184379
H 2.805770 2.247863 1.215630
H 1.794865 3.400855 0.333996
H 1.185447 2.651070 1.803593
H 3.368128 -3.067048 -0.684573
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.109419652**

Comp_07Z_c10
B3LYP/6-31G* Geometry
C 2.965672 2.072855 0.021593
C 2.797366 0.572490 -0.042503
C 1.605787 0.031906 -0.342480
C 1.239829 -1.424038 -0.450532
C 0.081759 -1.834966 0.501095
C -1.215269 -1.106010 0.227094
C -1.732229 -0.272869 1.150608
C -2.947750 0.544231 1.045749
N -3.326602 1.365335 0.131994
C 4.058439 -0.205253 0.247892
C -1.870143 -1.386290 -1.101321
O -2.403622 1.470676 -0.925961
H 2.029351 2.597653 -0.191759
H 3.722191 2.418616 -0.697492
H 3.315596 2.390211 1.014369
H 0.777748 0.717752 -0.525832
H 2.097617 -2.070649 -0.239567
H 0.937432 -1.648721 -1.484354
H -0.080232 -2.917149 0.386600
H 0.397570 -1.661474 1.536311
H -1.235693 -0.205795 2.119527
H -3.641220 0.526099 1.888319
H 4.456242 0.058391 1.237891
H 3.918643 -1.288458 0.221440
H 4.845014 0.047414 -0.477201
H -2.927968 -1.115054 -1.100576
H -1.393008 -0.814582 -1.906743
H -1.779830 -2.450487 -1.354356
H -2.825030 2.141157 -1.486016
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.103194783**

Comp_07Z_c11
B3LYP/6-31G* Geometry
C -3.482414 -1.663870 -0.482358
C -2.778831 -0.464156 0.108008
C -2.203949 0.451671 -0.686547
C -1.467232 1.706888 -0.305395
C -0.011890 1.749723 -0.847481
C 0.931422 0.755528 -0.203381
C 1.305516 -0.350580 -0.874195
C 2.191553 -1.431511 -0.424144

N 3.365636 -1.403640 0.098301
C -2.798461 -0.413560 1.616465
C 1.378062 1.074989 1.199305
O 3.867688 -0.097481 0.251199
H -3.447343 -1.661674 -1.576419
H -4.537780 -1.695484 -0.176311
H -3.029772 -2.601276 -0.129132
H -2.266752 0.283450 -1.764119
H -1.462926 1.856427 0.778953
H -1.996608 2.573745 -0.728829
H -0.036422 1.587993 -1.932241
H 0.380108 2.764841 -0.689144
H 0.860756 -0.528511 -1.854185
H 1.850446 -2.453904 -0.596715
H -2.282045 0.455836 2.029616
H -3.831961 -0.398092 1.990017
H -2.330152 -1.313568 2.038547
H 1.741100 0.192099 1.728901
H 2.198736 1.803692 1.181917
H 0.559351 1.518631 1.778820
H 4.747647 -0.269609 0.620958
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -521.102902996**

Comp_07Z_c12
B3LYP/6-31G* Geometry
C -4.931530 -0.189732 0.200774
C -3.515605 0.252627 -0.085809
C -2.534345 -0.649760 -0.242356
C -1.074240 -0.413010 -0.519495
C -0.175605 -0.888244 0.652903
C 1.302138 -0.708090 0.383626
C 2.021456 0.150834 1.132400
C 3.450900 0.469163 1.028015
N 4.175555 0.795900 0.017559
C -3.337632 1.748892 -0.176779
C 1.890857 -1.550050 -0.718873
O 3.447276 0.859052 -1.184656
H -5.016483 -1.279547 0.258114
H -5.622680 0.164406 -0.577299
H -5.293261 0.230183 1.150160
H -2.806419 -1.703003 -0.143720
H -0.863849 0.642829 -0.717348
H -0.788927 -0.960997 -1.428924
H -0.464895 -0.342714 1.558530
H -0.386518 -1.951814 0.841876
H 1.523671 0.641322 1.970117
H 4.021326 0.494387 1.958256
H -2.306380 2.052627 -0.369896
H -3.966317 2.166248 -0.975833
H -3.661523 2.233188 0.755064
H 1.702951 -1.102419 -1.702309
H 2.973240 -1.653731 -0.618429
H 1.438927 -2.550169 -0.718458

H 4.131685 1.139705 -1.812008
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -521.104064280

Comp_07Z_c13

B3LYP/6-31G* Geometry

C -4.904867 -0.719594 -0.278607
C -3.591739 0.022501 -0.189197
C -2.436353 -0.590773 -0.490310
C -1.037959 -0.035196 -0.456664
C -0.155927 -0.742729 0.606068
C 1.282072 -0.272677 0.596972
C 2.269337 -1.130535 0.273316
C 3.712312 -0.868758 0.200869
N 4.376414 0.062375 -0.386215
C -3.719433 1.461042 0.250213
C 1.518436 1.162997 0.989708
O 3.555060 0.972261 -1.076764
H -4.768004 -1.756110 -0.602683
H -5.589464 -0.230048 -0.985827
H -5.420004 -0.731839 0.692428
H -2.493353 -1.639619 -0.789370
H -1.041309 1.043252 -0.270584
H -0.565128 -0.178318 -1.439144
H -0.600181 -0.559276 1.595197
H -0.196868 -1.825987 0.437399
H 2.004689 -2.174177 0.097477
H 4.372245 -1.599981 0.671151
H -4.213672 1.522723 1.229811
H -2.760422 1.978283 0.326621
H -4.350677 2.026081 -0.449893
H 2.546906 1.333671 1.314490
H 1.333642 1.838497 0.145482
H 0.838860 1.453095 1.801194
H 4.212088 1.567385 -1.470351

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -521.103971953

Comp_08E_c01

B3LYP/6-31G* Geometry

C -2.280397 0.560916 1.053514
C -4.329042 0.038699 -0.750477
C -2.870748 -0.708321 0.989404
C -2.732545 1.592784 0.209075
C -3.758720 1.304458 -0.689087
C -3.900811 -0.998997 0.087645
Br -2.255791 -2.067796 2.175505
Br -5.738623 -0.330960 -1.996205
O -4.421667 -2.244642 0.072453
O -1.279356 0.848758 1.921221
C -2.137304 2.989411 0.307479
C -0.790005 3.135470 -0.363615
N -0.571227 3.148309 -1.628611

O -1.734649 3.000622 -2.376703
C 0.431447 3.337074 0.502124
N 1.628154 3.175646 -0.106324
C 2.898149 3.447798 0.558924
O 0.311346 3.636410 1.694945
C 3.360106 2.340394 1.536634
O 2.555593 2.289726 2.697313
C 3.426551 0.984940 0.841916
C 3.496131 -1.486503 -0.549994
C 4.544000 0.618216 0.085683
C 2.344608 0.105528 0.910336
C 2.389454 -1.098659 0.221131
C 4.577238 -0.593240 -0.597651
Br 0.886936 -2.292181 0.311693
Br 6.118329 -1.063690 -1.614196
O 3.565686 -2.653436 -1.227740
H -4.113792 2.080961 -1.356358
H -5.123414 -2.271995 -0.605021
H -1.111170 0.063632 2.476552
H -2.006369 3.272081 1.354616
H -2.829801 3.697322 -0.160143
H -1.410282 3.043318 -3.290914
H 1.615960 2.911994 -1.082158
H 2.810727 4.387532 1.116554
H 3.651384 3.583683 -0.222176
H 4.381538 2.616260 1.843329
H 1.748322 2.824500 2.548697
H 5.407977 1.274039 0.027729
H 1.478542 0.366582 1.506019
H 2.737832 -3.144978 -1.070250

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4110739

Comp_08E_c02

B3LYP/6-31G* Geometry

C 2.120128 0.112710 -0.493853
C 4.777013 0.131064 0.330269
C 2.791034 -1.087011 -0.220932
C 2.792297 1.342221 -0.350133
C 4.119972 1.327373 0.067104
C 4.129903 -1.102663 0.192546
Br 1.862993 -2.739204 -0.410075
Br 6.607698 0.133967 0.901630
O 4.721248 -2.292394 0.437904
O 0.828589 0.166081 -0.895717
C 2.091823 2.646172 -0.688932
C 0.870421 2.958438 0.144730
N 0.844827 3.160252 1.412252
O 2.098458 3.041920 2.000464
C -0.450225 3.155946 -0.561505
N -1.547456 3.215234 0.226413
C -2.855839 3.682888 -0.230101
O -0.481396 3.277598 -1.791910
C -3.599175 2.761180 -1.232503

O -3.097054 2.883524 -2.542032
 C -3.640563 1.314125 -0.744806
 C -3.654349 -1.363492 0.200321
 C -2.818718 0.346920 -1.326295
 C -4.484289 0.935752 0.302809
 C -4.482590 -0.377332 0.758266
 C -2.824912 -0.959759 -0.855476
 Br -5.645779 -0.895104 2.195697
 Br -1.659887 -2.244364 -1.653010
 O -3.623849 -2.647797 0.618692
 H 4.651485 2.264263 0.194153
 H 5.642314 -2.121379 0.710314
 H 0.454339 -0.732940 -0.985291
 H 1.769750 2.648713 -1.733996
 H 2.808740 3.465395 -0.558640
 H 1.916090 3.222703 2.936879
 H -1.378860 3.131073 1.220366
 H -2.754440 4.667301 -0.704740
 H -3.466967 3.803507 0.668686
 H -4.632568 3.136520 -1.263223
 H -2.129514 3.044202 -2.477810
 H -2.178282 0.621374 -2.155554
 H -5.153255 1.655388 0.765634
 H -4.265864 -2.748487 1.345855

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4113259

Comp_08E_c03

B3LYP/6-31G* Geometry

C -2.230414 0.730844 1.005405
 C -4.377616 -0.305256 -0.451062
 C -2.600697 -0.612496 1.123111
 C -2.942557 1.574106 0.135661
 C -4.007492 1.029944 -0.581363
 C -3.675605 -1.160463 0.407149
 Br -1.591076 -1.749544 2.291846
 Br -5.844496 -0.988948 -1.452813
 O -4.047949 -2.455303 0.507603
 O -1.190446 1.276080 1.686726
 C -2.541464 3.034815 -0.009274
 C -1.216964 3.205857 -0.719497
 N -1.011884 3.065178 -1.978828
 O -2.174600 2.739181 -2.672576
 C -0.004658 3.567815 0.102824
 N 1.197897 3.244019 -0.431775
 C 2.440892 3.499531 0.279963
 O -0.127553 4.110125 1.205114
 C 2.785163 2.417800 1.334799
 O 1.745162 2.266021 2.285611
 C 3.086455 1.072556 0.691384
 C 3.642501 -1.400862 -0.586098
 C 2.065332 0.144959 0.471405
 C 4.383206 0.753307 0.276266
 C 4.654797 -0.456864 -0.353365

C 2.350703 -1.060953 -0.154597
 Br 6.434113 -0.859961 -0.897920
 Br 0.944610 -2.337821 -0.441363
 O 3.948921 -2.567175 -1.193939
 H -4.560060 1.661806 -1.267672
 H -3.459302 -2.901402 1.142753
 H -0.787114 0.622828 2.285876
 H -2.445571 3.506383 0.972254
 H -3.316323 3.558799 -0.576814
 H -1.869637 2.689541 -3.593006
 H 1.204221 2.762767 -1.320284
 H 2.345958 4.466917 0.784056
 H 3.251681 3.574494 -0.450445
 H 3.704854 2.767649 1.834412
 H 1.127600 3.019783 2.202963
 H 1.058875 0.368335 0.798779
 H 5.201066 1.446348 0.449620
 H 3.133616 -3.098298 -1.264115

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4068443

Comp_08E_c04

B3LYP/6-31G* Geometry

C -2.236137 0.696042 0.996439
 C -4.421676 -0.307060 -0.424809
 C -2.614574 -0.645477 1.108692
 C -2.961249 1.554707 0.153181
 C -4.045523 1.027040 -0.546817
 C -3.707649 -1.177260 0.408087
 Br -1.594810 -1.801776 2.247726
 Br -5.914222 -0.968291 -1.403953
 O -4.087398 -2.470321 0.501257
 O -1.177723 1.226301 1.661952
 C -2.555468 3.015001 0.019217
 C -1.236852 3.189919 -0.700340
 N -1.040191 3.051625 -1.961341
 O -2.207026 2.725360 -2.647221
 C -0.019765 3.554456 0.112818
 N 1.180252 3.243155 -0.435200
 C 2.428091 3.515189 0.261296
 O -0.135112 4.090099 1.219308
 C 2.800292 2.441875 1.315224
 O 1.774656 2.277254 2.278545
 C 3.115025 1.098394 0.674418
 C 3.676824 -1.380879 -0.590652
 C 4.419400 0.778228 0.291662
 C 2.097428 0.170604 0.427603
 C 2.373969 -1.041145 -0.192452
 C 4.682248 -0.437032 -0.330946
 Br 0.959007 -2.279340 -0.499506
 Br 6.477907 -0.878486 -0.846417
 O 3.900450 -2.572698 -1.185189
 H -4.608580 1.670951 -1.213177
 H -3.479832 -2.931284 1.107452

H -0.762639 0.558898 2.237172
H -2.449829 3.476797 1.004443
H -3.333521 3.547374 -0.536210
H -1.906998 2.669202 -3.568884
H 1.181385 2.767928 -1.327006
H 2.327092 4.482375 0.764786
H 3.229060 3.599110 -0.479088
H 3.720619 2.807979 1.802395
H 1.141739 3.018750 2.198549
H 5.237746 1.465545 0.483607
H 1.085152 0.398544 0.733734
H 4.853241 -2.642930 -1.381665

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4067228

Comp_08E_c05

B3LYP/6-31G* Geometry

C 0.682833 0.015381 2.223033
C 2.792572 0.200461 0.379149
C 1.205814 -1.125276 1.596132
C 1.240993 1.274329 1.913799
C 2.289128 1.340447 0.990440
C 2.244794 -1.058158 0.658935
Br 0.434164 -2.829224 1.961315
Br 4.213107 0.345049 -0.880670
O 2.702927 -2.146848 -0.003919
O -0.316278 -0.152895 3.113770
C 0.706997 2.551546 2.548707
C -0.308251 3.225013 1.652731
N -0.094918 4.208924 0.857179
O 1.216184 4.676067 0.900626
C -1.705369 2.653712 1.621706
N -2.541688 3.140934 0.682767
C -3.829736 2.539838 0.391729
O -2.039456 1.776199 2.431612
C -3.864311 1.893520 -1.006328
O -3.679892 2.975930 -1.918087
C -2.831562 0.792190 -1.196098
C -0.884579 -1.255010 -1.470588
C -1.584590 1.070299 -1.762046
C -3.103652 -0.517963 -0.784312
C -2.148636 -1.519335 -0.916677
C -0.641474 0.058493 -1.900785
Br -2.547434 -3.285819 -0.341251
Br 1.062595 0.437280 -2.681187
O 0.012605 -2.256487 -1.576225
H 2.717836 2.305509 0.742383
H 2.202188 -2.921231 0.322019
H -0.957521 0.596882 3.033433
H 1.528067 3.247411 2.730270
H 0.235145 2.326478 3.509267
H 1.202928 5.410595 0.265785
H -2.172092 3.834827 0.044425
H -4.612810 3.305735 0.431158

H -4.026205 1.794718 1.163854
H -4.870460 1.459999 -1.126245
H -3.658307 2.610116 -2.816873
H -1.348939 2.073119 -2.098076
H -4.066687 -0.769912 -0.350552
H 0.863427 -1.890899 -1.887080

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4244994

Comp_08E_c06

B3LYP/6-31G* Geometry

C -0.645133 -0.019743 2.244726
C -2.714967 -0.528397 0.415796
C -1.318331 1.025858 1.595749
C -1.033668 -1.348219 1.970688
C -2.065952 -1.575710 1.054769
C -2.340185 0.798616 0.664655
Br -0.793305 2.826543 1.931266
Br -4.113558 -0.889730 -0.824677
O -2.944723 1.800018 -0.016925
O 0.327652 0.300728 3.124615
C -0.339032 -2.526948 2.639132
C 0.747945 -3.092100 1.753702
N 0.660431 -4.122756 0.994239
O -0.576004 -4.758346 1.070908
C 2.058195 -2.345098 1.686521
N 2.932780 -2.742759 0.738474
C 4.114598 -1.980829 0.385426
O 2.292600 -1.418433 2.475101
C 4.024262 -1.465332 -1.069923
O 3.849320 -2.575797 -1.953554
C 2.869924 -0.502659 -1.275329
C 0.696434 1.301789 -1.532477
C 2.981626 0.822550 -0.840906
C 1.671755 -0.920189 -1.857992
C 0.614232 -0.025971 -1.979853
C 1.918078 1.707870 -0.971976
Br -1.038923 -0.599871 -2.751895
Br 2.111068 3.503584 -0.380906
O -0.316301 2.189141 -1.625698
H -2.366161 -2.594755 0.835465
H -2.541142 2.641041 0.276873
H 1.061540 -0.358812 3.058648
H -1.064176 -3.315301 2.848923
H 0.105072 -2.214166 3.588148
H -0.473257 -5.501847 0.455014
H 2.620568 -3.461858 0.096479
H 5.009750 -2.611450 0.486851
H 4.203482 -1.155638 1.094835
H 4.966967 -0.942717 -1.294360
H 4.682426 -3.071239 -1.978982
H 3.903430 1.181530 -0.393642
H 1.567778 -1.932712 -2.226384
H -1.112636 1.726677 -1.951232

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4226327

Comp_08E_c07
B3LYP/6-31G* Geometry

C 2.015292 0.131595 -0.561274
C 4.649654 0.146224 0.330213
C 2.671060 -1.067155 -0.251288
C 2.690810 1.359239 -0.421449
C 4.007439 1.341913 0.030229
C 3.998209 -1.085923 0.196838
Br 1.733761 -2.715466 -0.441268
Br 6.464829 0.146597 0.947580
O 4.574162 -2.275251 0.476556
O 0.733950 0.181691 -0.996836
C 2.004524 2.661817 -0.794662
C 0.799850 3.014169 0.047717
N 0.802101 3.271823 1.305339
O 2.068443 3.179466 1.870602
C -0.536526 3.178892 -0.638221
N -1.615263 3.263055 0.171253
C -2.946306 3.674457 -0.273452
O -0.592800 3.251198 -1.871669
C -3.673762 2.699136 -1.236360
O -3.219934 2.827422 -2.563534
C -3.620561 1.260001 -0.725006
C -3.449157 -1.393835 0.270334
C -4.291679 0.884560 0.444400
C -2.880144 0.298260 -1.409916
C -2.802775 -0.993884 -0.907379
C -4.207022 -0.414396 0.932189
Br -1.754764 -2.307401 -1.843768
Br -5.133228 -0.887169 2.527930
O -3.382134 -2.642938 0.781324
H 4.541155 2.277529 0.156382
H 5.488762 -2.106396 0.771481
H 0.369156 -0.720563 -1.080222
H 1.667083 2.634014 -1.834317
H 2.734005 3.474603 -0.700123
H 1.906629 3.402807 2.801629
H -1.425475 3.214213 1.163680
H -2.888834 4.647908 -0.776829
H -3.543884 3.799983 0.633461
H -4.725393 3.020292 -1.243259
H -2.251880 2.995392 -2.528042
H -4.896064 1.604094 0.989192
H -2.376476 0.566557 -2.330150
H -2.804522 -3.177333 0.205358

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4115124

Comp_08E_c08
B3LYP/6-31G* Geometry

C -0.724237 0.112423 2.123952
C -2.824067 -0.489095 0.385970
C -1.428800 1.132166 1.463273
C -1.111476 -1.232479 1.925797
C -2.153603 -1.511472 1.038385
C -2.484924 0.856902 0.587396
Br -0.879911 2.938825 1.687311
Br -4.209400 -0.893324 -0.873272
O -3.106351 1.881191 -0.033346
O 0.284677 0.467391 2.946015
C -0.411710 -2.374589 2.651041
C 0.656176 -3.015792 1.794523
N 0.535582 -4.082238 1.091217
O -0.722154 -4.671079 1.195996
C 1.991734 -2.319796 1.697316
N 2.888133 -2.842228 0.834981
C 4.127491 -2.170315 0.492586
O 2.227449 -1.322547 2.394977
C 4.104494 -1.593463 -0.935917
O 4.012470 -2.727573 -1.795712
C 2.976603 -0.597007 -1.157260
C 0.831530 1.239134 -1.445878
C 3.117628 0.730606 -0.742620
C 1.766511 -0.995017 -1.733786
C 0.718771 -0.091478 -1.878202
C 2.064446 1.624496 -0.890148
Br -0.926365 -0.673887 -2.640169
Br 2.284866 3.439236 -0.336046
O -0.216611 2.071371 -1.605911
H -2.439620 -2.541777 0.857147
H -3.744874 1.506158 -0.668402
H 1.003655 -0.210396 2.900579
H -1.142211 -3.139189 2.922574
H 0.050390 -2.007483 3.571553
H -0.641824 -5.450076 0.621994
H 2.585449 -3.626852 0.270739
H 4.959941 -2.879495 0.561518
H 4.279849 -1.373037 1.221318
H 5.068821 -1.079960 -1.083227
H 3.955952 -2.406851 -2.710112
H 4.046632 1.077493 -0.300737
H 1.634079 -2.019322 -2.061852
H -0.139125 2.820924 -0.985051

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4232150

Comp_08E_c100
B3LYP/6-31G* Geometry

C 0.760530 -0.059113 -2.047383
C 2.952943 0.226616 -0.317064
C 1.363028 -1.170737 -1.440305
C 1.315549 1.216661 -1.817920
C 2.395377 1.334682 -0.936506
C 2.457536 -1.060294 -0.572206

Br	0.635890	-2.911167	-1.758446	N	-0.344886	1.665072	3.288050
Br	4.371863	0.446182	0.930755	O	0.231960	0.891189	4.286260
O	3.033242	-2.119767	0.029429	C	-0.082378	2.950928	1.330109
O	-0.305201	-0.266383	-2.851196	N	-1.421540	2.986142	1.242198
C	0.764902	2.453640	-2.514770	C	-2.148587	3.648754	0.160956
C	-0.175249	3.232742	-1.626328	O	0.660656	3.531597	0.514166
N	0.108106	4.281413	-0.942976	C	-2.118189	2.884921	-1.187551
O	1.423848	4.706343	-1.105482	O	-0.865099	2.996720	-1.832161
C	-1.583098	2.711586	-1.464664	C	-2.533000	1.428718	-0.999273
N	-2.366916	3.364377	-0.579119	C	-3.304506	-1.252092	-0.487482
C	-3.685117	2.899717	-0.190820	C	-3.882088	1.082266	-0.872468
O	-1.970455	1.737886	-2.124184	C	-1.568117	0.425829	-0.886043
C	-3.692631	2.219710	1.196089	C	-1.957260	-0.882152	-0.625580
O	-5.062944	1.904379	1.419634	C	-4.260103	-0.233115	-0.624288
C	-2.789852	1.001177	1.269813	Br	-0.623229	-2.243856	-0.397215
C	-1.077042	-1.254876	1.345090	Br	-6.106759	-0.669968	-0.464068
C	-1.534578	1.073726	1.881352	O	-3.712398	-2.514681	-0.235418
C	-3.191280	-0.209858	0.695345	H	1.838628	-0.781206	2.596913
C	-2.345276	-1.308673	0.741062	H	3.653646	-2.778949	-1.026251
C	-0.689045	-0.031226	1.912239	H	2.368732	3.127541	0.195309
Br	-2.888833	-2.964482	-0.052108	H	2.502857	2.890413	2.297334
Br	1.034372	0.110060	2.702197	H	2.291421	1.586802	3.466412
O	-0.237079	-2.307522	1.412955	H	-0.533836	0.616031	4.816581
H	2.806839	2.317140	-0.730442	H	-1.927335	2.417153	1.909636
H	2.526859	-2.917245	-0.214715	H	-1.726257	4.647952	0.011183
H	-0.939770	0.484672	-2.743825	H	-3.182393	3.763203	0.497105
H	0.229972	2.162716	-3.423008	H	-2.864689	3.376046	-1.829977
H	1.588851	3.107938	-2.805917	H	-0.199435	3.298769	-1.185907
H	1.468722	5.491739	-0.536400	H	-4.656788	1.836837	-0.974868
H	-1.938385	4.143355	-0.094081	H	-0.520588	0.669714	-1.017123
H	-4.026191	2.190699	-0.946735	H	-2.922628	-3.086231	-0.192792
H	-4.384285	3.742335	-0.166910	Number of Imaginary Frequencies= 0			
H	-3.339885	2.955279	1.939374	SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4169559			
H	-5.119865	1.405618	2.250003	Comp_08E_c106			
H	-1.199512	2.000235	2.337303	B3LYP/6-31G* Geometry			
H	-4.161718	-0.291516	0.218685	C	1.109342	-0.891423	2.053987
H	-0.596611	-3.026609	0.860015	C	1.767729	1.558434	0.911878
Number of Imaginary Frequencies= 0				C	2.239013	-0.769561	1.228275
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4229854				C	0.325683	0.250128	2.340993
Comp_08E_c103				C	0.657536	1.466007	1.738235
B3LYP/6-31G* Geometry				C	2.594975	0.455195	0.650499
C	3.025759	1.335167	0.205789	Br	3.279589	-2.301978	0.833592
C	2.755121	-1.380745	0.755375	Br	2.183693	3.221388	0.039765
C	3.506667	0.374885	-0.698839	O	3.690673	0.514280	-0.133810
C	2.445098	0.919684	1.424878	O	0.827560	-2.104306	2.573609
C	2.300975	-0.447190	1.674075	C	-0.845761	0.175902	3.313694
C	3.380350	-0.996541	-0.441025	C	-2.179722	0.077504	2.610668
Br	4.312410	0.935716	-2.319810	N	-3.008158	1.035642	2.403983
Br	2.509440	-3.254622	1.084042	O	-2.590373	2.251547	2.938924
O	3.842099	-1.879069	-1.351807	C	-2.562656	-1.252091	2.008652
O	3.167947	2.642012	-0.112269	N	-3.716822	-1.297409	1.307170
C	2.002761	1.933543	2.472495	C	-4.000937	-2.367628	0.367269
C	0.508684	2.150614	2.460765	O	-1.828252	-2.238473	2.155407

C -3.961789 -1.867492 -1.090818
 O -5.110732 -1.030965 -1.226556
 C -2.672888 -1.131187 -1.429731
 C -0.240013 0.242295 -1.934212
 C -1.511959 -1.831691 -1.777952
 C -2.610010 0.261082 -1.332209
 C -1.414159 0.922820 -1.581873
 C -0.318211 -1.159763 -2.017783
 Br -1.335016 2.829096 -1.404765
 Br 1.256699 -2.137965 -2.422064
 O 0.933762 0.851200 -2.197444
 H 0.046659 2.343220 1.921922
 H 3.755329 1.414631 -0.501464
 H -0.153712 -2.224802 2.578282
 H -0.854734 1.066587 3.944902
 H -0.725971 -0.694372 3.965060
 H -3.313334 2.851680 2.694449
 H -4.224339 -0.426137 1.208905
 H -4.995635 -2.785619 0.557293
 H -3.255394 -3.147874 0.527229
 H -4.055547 -2.753910 -1.738342
 H -5.112726 -0.669516 -2.127531
 H -1.523397 -2.914904 -1.851190
 H -3.490059 0.829283 -1.056131
 H 0.865775 1.797742 -1.968386

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4226932**

Comp_08E_c108

B3LYP/6-31G* Geometry

C 2.711408 0.452551 -0.825647
 C 0.668539 -1.177236 -1.780910
 C 2.596401 -0.878815 -0.400245
 C 1.787465 0.974783 -1.749960
 C 0.777406 0.135314 -2.221062
 C 1.565646 -1.710801 -0.846724
 Br 3.865096 -1.554109 0.855116
 Br -0.752953 -2.293736 -2.404223
 O 1.470591 -2.967651 -0.350830
 O 3.691398 1.270572 -0.371583
 C 1.877710 2.426269 -2.198751
 C 1.119344 3.363452 -1.282299
 N 1.608425 4.275240 -0.524111
 O 2.994758 4.379258 -0.590579
 C -0.391281 3.248442 -1.275518
 N -1.025466 3.867147 -0.241682
 C -2.458012 3.798585 -0.046252
 O -0.969513 2.624030 -2.161053
 C -2.847750 3.050540 1.247243
 O -4.264840 3.165553 1.310534
 C -2.374897 1.606911 1.275859
 C -1.456870 -1.076890 1.271760
 C -1.167655 1.270056 1.892079
 C -3.126801 0.592979 0.670239

C -2.678461 -0.722609 0.676546
 C -0.724544 -0.046738 1.881648
 Br -3.731220 -2.081143 -0.137800
 Br 0.938277 -0.504174 2.713227
 O -1.054521 -2.366297 1.247583
 H 0.043622 0.530719 -2.912075
 H 0.682151 -3.383149 -0.752726
 H 4.243944 0.767418 0.255678
 H 1.434730 2.512700 -3.195501
 H 2.919104 2.745974 -2.246593
 H 3.180033 5.114024 0.015769
 H -0.445139 4.408920 0.385661
 H -2.881997 3.283682 -0.910361
 H -2.892198 4.804489 0.002448
 H -2.382341 3.579076 2.097536
 H -4.567762 2.674382 2.090606
 H -0.566123 2.028984 2.381628
 H -4.071339 0.833960 0.195466
 H -0.158256 -2.421691 1.631178

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4158535**

Comp_08E_c109

B3LYP/6-31G* Geometry

C -3.268608 -0.922180 0.603154
 C -3.466418 1.841672 0.369080
 C -2.733002 -0.078549 1.584324
 C -3.889761 -0.371567 -0.534034
 C -3.975091 1.015514 -0.627142
 C -2.821319 1.315741 1.495574
 Br -1.820554 -0.862327 3.071570
 Br -3.601899 3.745814 0.218531
 O -2.284389 2.067399 2.480216
 O -3.199084 -2.273673 0.688845
 C -4.409184 -1.275258 -1.633789
 C -3.346113 -2.194449 -2.202937
 N -3.513046 -3.407158 -2.579421
 O -4.840399 -3.837611 -2.437566
 C -1.951653 -1.636138 -2.369806
 N -0.940990 -2.472150 -2.002329
 C 0.412405 -1.971826 -1.837494
 O -1.780911 -0.491575 -2.781493
 C 0.580075 -1.187702 -0.520914
 O 0.260458 -2.100453 0.528402
 C 1.981817 -0.614316 -0.390421
 C 4.609834 0.437394 -0.228462
 C 2.302620 0.609389 -0.989475
 C 2.979058 -1.313019 0.293552
 C 4.262149 -0.785278 0.366413
 C 3.591663 1.122981 -0.910793
 Br 5.634322 -1.736661 1.314665
 Br 3.993718 2.794122 -1.728202
 O 5.846873 0.975689 -0.170729
 H -4.432588 1.463502 -1.502327

H -2.426354 3.006742 2.255781
H -2.679089 -2.512519 1.478651
H -4.810470 -0.654815 -2.443725
H -5.228466 -1.903339 -1.271927
H -4.792961 -4.753407 -2.754393
H -1.202771 -3.300026 -1.485652
H 0.647293 -1.320593 -2.681805
H 1.104375 -2.819872 -1.846087
H -0.142903 -0.361057 -0.540966
H 0.070263 -1.585925 1.330820
H 1.542428 1.173519 -1.521403
H 2.743136 -2.254982 0.774753
H 6.419605 0.372093 0.338428

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4058311**

Comp_08E_c11

B3LYP/6-31G* Geometry

C -0.745149 -0.120461 -2.068879
C -2.941782 0.144169 -0.339197
C -1.312880 -1.232931 -1.429618
C -1.328528 1.146544 -1.858748
C -2.410010 1.253674 -0.977962
C -2.410250 -1.133510 -0.564187
Br -0.525539 -2.956898 -1.691207
Br -4.363077 0.354421 0.907828
O -2.954487 -2.194598 0.063927
O 0.314038 -0.324194 -2.880612
C -0.799347 2.389410 -2.561974
C 0.163832 3.161177 -1.690231
N -0.110852 4.180116 -0.960163
O -1.441168 4.579284 -1.051779
C 1.587428 2.667742 -1.608816
N 2.398034 3.299114 -0.734894
C 3.728701 2.822733 -0.411167
O 1.966326 1.731035 -2.327818
C 3.796450 2.189582 0.991483
O 3.489754 3.249141 1.894606
C 2.871045 0.992538 1.154377
C 1.128982 -1.233744 1.379214
C 3.266566 -0.265893 0.690900
C 1.603044 1.129068 1.729082
C 0.749842 0.035410 1.842371
C 2.403967 -1.348222 0.800320
Br -0.979433 0.253700 2.601793
Br 2.940088 -3.064775 0.144600
O 0.275313 -2.268696 1.516573
H -2.841500 2.230113 -0.785779
H -2.428599 -2.983297 -0.167001
H 0.923882 0.453701 -2.830511
H -1.632270 3.044939 -2.823501
H -0.287924 2.109377 -3.486942
H -1.477713 5.343271 -0.453632
H 1.981236 4.014779 -0.152027

H 4.433046 3.661597 -0.441897
H 4.013339 2.094299 -1.171726
H 4.836971 1.854463 1.134788
H 3.482485 2.884920 2.794246
H 4.243016 -0.409003 0.238472
H 1.272192 2.097039 2.087015
H 0.640524 -3.035981 1.037415

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4247258**

Comp_08E_c10

B3LYP/6-31G* Geometry

C 1.442273 -1.449024 1.628271
C 1.566572 1.315477 1.332818
C 2.455699 -0.859740 0.855917
C 0.515920 -0.627824 2.309628
C 0.580874 0.755786 2.131871
C 2.537140 0.529286 0.692282
Br 3.718020 -1.960776 -0.028106
Br 1.611419 3.217343 1.057049
O 3.523756 1.039971 -0.072105
O 1.402622 -2.796814 1.718042
C -0.530226 -1.227567 3.240950
C -1.893959 -1.290784 2.596124
N -2.881429 -0.499630 2.809523
O -2.613274 0.471717 3.771165
C -2.115019 -2.331957 1.526053
N -3.280678 -2.260174 0.845350
C -3.476133 -2.920274 -0.431502
O -1.251615 -3.188754 1.295426
C -3.747642 -1.876271 -1.538574
O -4.950081 -1.167089 -1.232533
C -2.621472 -0.863699 -1.658295
C -0.463200 0.971861 -1.775773
C -1.364994 -1.262554 -2.128963
C -2.798476 0.459745 -1.251206
C -1.731205 1.348575 -1.312661
C -0.306078 -0.363576 -2.184538
Br -1.968064 3.155500 -0.714626
Br 1.402231 -0.945073 -2.770256
O 0.591208 1.810625 -1.850529
H -0.141018 1.397018 2.626636
H 3.381463 2.000845 -0.151994
H 0.456885 -3.079695 1.688379
H -0.603732 -0.627022 4.149448
H -0.227548 -2.237473 3.531483
H -3.445698 0.970072 3.808130
H -3.889318 -1.480119 1.067113
H -4.326108 -3.616068 -0.379309
H -2.580375 -3.508053 -0.643074
H -3.855964 -2.416460 -2.492223
H -5.690805 -1.786602 -1.318840
H -1.191859 -2.285763 -2.447753
H -3.763057 0.794472 -0.893115

H 0.364322 2.646708 -1.401254
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4211528

Comp_08E_c112

B3LYP/6-31G* Geometry

C 2.780760 0.441109 -0.801941
C 0.740533 -1.228177 -1.679950
C 2.682526 -0.876447 -0.336364
C 1.841439 0.930829 -1.728963
C 0.823263 0.076184 -2.150851
C 1.664566 -1.738369 -0.758385
Br 3.948993 -1.493944 0.948685
Br -0.680400 -2.372597 -2.269919
O 1.627259 -2.993009 -0.265968
O 3.756723 1.282377 -0.382721
C 1.929467 2.364062 -2.230290
C 1.281673 3.349207 -1.282136
N 1.855509 4.284007 -0.616936
O 3.228372 4.366260 -0.829498
C -0.222013 3.266201 -1.125123
N -0.736972 3.918620 -0.046310
C -2.155543 3.964816 0.237029
O -0.898407 2.642975 -1.939088
C -2.546924 3.152632 1.488840
O -3.934865 3.424663 1.665835
C -2.262482 1.666144 1.360749
C -1.727322 -1.105767 1.111415
C -3.117111 0.845739 0.616346
C -1.143591 1.093415 1.971714
C -0.877213 -0.266556 1.845553
C -2.844234 -0.509727 0.502839
Br 0.668627 -1.009260 2.667505
Br -4.009584 -1.638146 -0.518529
O -1.449230 -2.426241 1.027411
H 0.070539 0.448252 -2.834890
H 0.786994 -3.402277 -0.543514
H 4.316760 0.803990 0.257559
H 1.402497 2.432632 -3.186776
H 2.970648 2.652580 -2.380179
H 3.482996 5.117598 -0.270535
H -0.085513 4.460086 0.506914
H -2.680310 3.568376 -0.634478
H -2.479497 5.000515 0.392960
H -1.966960 3.540310 2.343680
H -4.248586 2.887308 2.410292
H -3.993272 1.266023 0.135676
H -0.465681 1.706977 2.556512
H -2.133194 -2.840585 0.467854

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4160038

Comp_08E_c113

B3LYP/6-31G* Geometry

C 0.654015 1.770695 1.448648
C 2.096157 -0.639142 1.517205
C 1.802176 1.581009 0.666600
C 0.236377 0.727208 2.298820
C 0.964227 -0.467763 2.300213
C 2.546724 0.393370 0.682788
Br 2.354094 2.964350 -0.536651
Br 3.038935 -2.289435 1.547276
O 3.653541 0.203676 -0.060828
O 0.033900 2.970006 1.352845
C -0.981510 0.873173 3.206048
C -2.282303 0.632416 2.474286
N -3.076138 1.519351 2.001134
O -2.630827 2.835455 2.264160
C -2.650435 -0.815426 2.196478
N -3.757295 -1.016517 1.434052
C -3.995459 -2.280622 0.762618
O -1.943240 -1.714770 2.640471
C -3.890397 -2.141995 -0.769387
O -5.022863 -1.358915 -1.149855
C -2.581441 -1.509669 -1.220355
C -0.112313 -0.298412 -1.924165
C -1.423098 -2.279617 -1.375197
C -2.498808 -0.129194 -1.420884
C -1.285172 0.453719 -1.763832
C -0.212374 -1.685219 -1.714343
Br -1.175880 2.352964 -1.983932
Br 1.355791 -2.744706 -1.859429
O 1.080009 0.230428 -2.267146
H 0.622188 -1.288279 2.919498
H 3.787446 0.992634 -0.618501
H -0.866574 2.941661 1.735843
H -1.005522 1.859127 3.679121
H -0.911250 0.121513 3.995046
H -3.283487 3.381167 1.795634
H -4.239156 -0.196587 1.087025
H -4.996654 -2.658631 0.999548
H -3.255587 -2.990379 1.136947
H -3.968484 -3.156477 -1.192091
H -4.976991 -1.214756 -2.108765
H -1.450376 -3.353451 -1.217066
H -3.378324 0.492660 -1.304888
H 1.021513 1.204675 -2.238357

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4187437

Comp_08E_c117

B3LYP/6-31G* Geometry

C 0.735489 -0.096678 -2.104202
C 2.865820 0.377362 -0.365213
C 1.403007 -1.160385 -1.476348
C 1.183504 1.225113 -1.883591
C 2.239044 1.441427 -0.994525

C 2.473405 -0.949104 -0.599549
 Br 0.787341 -2.937589 -1.752052
 Br 4.271878 0.693115 0.895980
 O 3.057673 -2.012769 -0.010809
 O -0.299585 -0.384898 -2.921238
 C 0.541922 2.405690 -2.600668
 C -0.464264 3.121870 -1.730656
 N -0.269731 4.201586 -1.065081
 O 1.010927 4.725437 -1.225476
 C -1.828390 2.493894 -1.568738
 N -2.671745 3.101242 -0.705522
 C -3.944647 2.530031 -0.306543
 O -2.129176 1.478657 -2.209701
 C -3.905242 1.918666 1.112095
 O -5.234052 1.455803 1.326779
 C -2.865744 0.822427 1.257805
 C -0.871529 -1.187688 1.420083
 C -1.637013 1.081405 1.872054
 C -3.105099 -0.455989 0.742504
 C -2.126977 -1.437047 0.836344
 C -0.657478 0.096740 1.945448
 Br -2.476737 -3.187831 0.155148
 Br 1.025624 0.495564 2.741810
 O 0.109625 -2.104977 1.521987
 H 2.572905 2.454311 -0.796297
 H 3.718949 -1.681187 0.625117
 H -0.993888 0.311736 -2.821159
 H 0.038932 2.060152 -3.508007
 H 1.313338 3.119565 -2.895723
 H 0.986212 5.525327 -0.675710
 H -2.312134 3.922171 -0.233945
 H -4.202801 1.755092 -1.029812
 H -4.723867 3.299320 -0.331643
 H -3.657869 2.724412 1.824882
 H -5.251391 0.992159 2.178974
 H -1.428030 2.060887 2.290951
 H -4.056472 -0.684710 0.275322
 H -0.035422 -2.817569 0.870105

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4216140**

Comp_08E_c119

B3LYP/6-31G* Geometry

C 0.634109 0.138179 -2.140631
 C 2.602423 -0.940954 -0.484608
 C 1.546362 0.969867 -1.473501
 C 0.759743 -1.263381 -2.019103
 C 1.738767 -1.782733 -1.168857
 C 2.542051 0.453257 -0.635338
 Br 1.391108 2.855802 -1.653680
 Br 3.907872 -1.662927 0.715248
 O 3.376142 1.306452 -0.008131
 O -0.321924 0.711538 -2.904383
 C -0.135545 -2.203679 -2.815766

C -1.254171 -2.775575 -1.979065
 N -1.305541 -3.952647 -1.469590
 O -0.200808 -4.739997 -1.783380
 C -2.414428 -1.870423 -1.637371
 N -3.335159 -2.377617 -0.786909
 C -4.398397 -1.590423 -0.182107
 O -2.487833 -0.733020 -2.117689
 C -4.079484 -1.231323 1.291597
 O -3.959714 -2.422492 2.059915
 C -2.868401 -0.310293 1.417252
 C -0.582898 1.379442 1.510332
 C -2.901142 0.969002 0.851147
 C -1.696811 -0.720990 2.056884
 C -0.573625 0.100747 2.085021
 C -1.786783 1.794685 0.913571
 Br 1.036008 -0.538970 2.876593
 Br -1.872200 3.546458 0.157239
 O 0.531052 2.134748 1.575952
 H 1.829235 -2.857192 -1.047546
 H 3.943099 0.790062 0.594781
 H -1.161411 0.205020 -2.783910
 H 0.458011 -3.030597 -3.210033
 H -0.568207 -1.667345 -3.665019
 H -0.403613 -5.581269 -1.342970
 H -3.196895 -3.339017 -0.501466
 H -5.326081 -2.171755 -0.202656
 H -4.532249 -0.694427 -0.790835
 H -4.963614 -0.726692 1.699419
 H -3.139162 -2.864526 1.788644
 H -3.793846 1.334218 0.354170
 H -1.641717 -1.683080 2.552162
 H 0.497832 2.835503 0.896731

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4180803**

Comp_08E_c12

B3LYP/6-31G* Geometry

C 1.764220 -1.555771 -1.136216
 C -0.839096 -0.981495 -2.012152
 C 0.660972 -2.274952 -0.656121
 C 1.548770 -0.508659 -2.055839
 C 0.241234 -0.244344 -2.474578
 C -0.650151 -2.001618 -1.069205
 Br 0.929313 -3.670364 0.614298
 Br -2.590992 -0.604416 -2.647195
 O -1.721722 -2.675009 -0.599094
 O 2.980438 -1.922969 -0.669781
 C 2.695343 0.351950 -2.572401
 C 3.282509 1.206469 -1.475025
 N 4.385680 1.013957 -0.851280
 O 5.063905 -0.136996 -1.310045
 C 2.467225 2.402435 -1.016281
 N 2.748715 2.842062 0.226984
 C 2.128280 3.982177 0.904020

O 1.600867 2.867787 -1.761990
 C 0.578677 4.038529 0.908646
 O 0.080523 4.643493 -0.267781
 C -0.117609 2.709067 1.211726
 C -1.501870 0.277174 1.710971
 C 0.466404 1.689746 1.971797
 C -1.415921 2.514850 0.728169
 C -2.089073 1.330629 0.992568
 C -0.208019 0.494375 2.203009
 Br -3.879888 1.085635 0.363100
 Br 0.655987 -0.904879 3.162882
 O -2.111636 -0.907034 1.937261
 H 0.062618 0.565072 -3.173540
 H -1.409308 -3.282676 0.099180
 H 3.702532 -1.388309 -1.053837
 H 2.301167 1.029588 -3.333506
 H 3.486311 -0.247537 -3.032878
 H 5.840305 -0.176910 -0.727329
 H 3.505822 2.361629 0.695773
 H 2.467416 4.923058 0.454737
 H 2.500901 3.954298 1.932061
 H 0.328903 4.750040 1.708236
 H 0.424259 4.104709 -1.012470
 H 1.463651 1.796379 2.381940
 H -1.885877 3.292334 0.138435
 H -2.944534 -0.920508 1.428225

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4183847**

Comp_08E_c121

B3LYP/6-31G* Geometry

C -2.365017 0.119538 -0.519107
 C -5.041867 0.218278 0.229172
 C -3.099119 -1.059776 -0.333705
 C -2.984708 1.370540 -0.333277
 C -4.324169 1.394322 0.044691
 C -4.448446 -1.035583 0.043798
 Br -2.256230 -2.748563 -0.607385
 Br -6.885711 0.277389 0.753096
 O -5.100666 -2.207852 0.207400
 O -1.060006 0.127448 -0.882546
 C -2.224432 2.659022 -0.588948
 C -0.977909 2.868015 0.239900
 N -0.914715 2.949815 1.518453
 O -2.156976 2.794902 2.130193
 C 0.321772 3.123288 -0.495037
 N 1.446408 3.127324 0.267997
 C 2.724329 3.594015 -0.241570
 O 0.327382 3.331491 -1.706729
 C 3.385807 2.654981 -1.273219
 O 4.615533 3.306824 -1.587885
 C 3.600348 1.243418 -0.754753
 C 3.965694 -1.383613 0.249566
 C 4.774837 0.902764 -0.078008

C 2.614179 0.266625 -0.931576
 C 2.796647 -1.017965 -0.434385
 C 4.941865 -0.387533 0.408359
 Br 1.429598 -2.327779 -0.678944
 Br 6.556410 -0.863610 1.332191
 O 4.098136 -2.647393 0.706516
 H -4.816786 2.347122 0.205818
 H -6.020528 -2.007960 0.463825
 H -0.702357 -0.781804 -0.899977
 H -2.902641 3.499123 -0.396571
 H -1.912446 2.721114 -1.635794
 H -1.943271 2.881160 3.073266
 H 1.321635 2.991816 1.261892
 H 3.404075 3.713069 0.606995
 H 2.604842 4.569965 -0.725328
 H 2.727673 2.617977 -2.149757
 H 5.010874 2.842637 -2.342232
 H 5.555595 1.643325 0.053857
 H 1.697561 0.511608 -1.458033
 H 4.965453 -2.724832 1.146396

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4061125**

Comp_08E_c124

B3LYP/6-31G* Geometry

C -2.283286 0.089985 -0.431181
 C -4.986706 0.186859 0.209037
 C -2.994714 -1.085065 -0.156072
 C -2.935858 1.336293 -0.383071
 C -4.289025 1.359552 -0.057222
 C -4.357714 -1.062961 0.166921
 Br -2.087210 -2.761690 -0.218891
 Br -6.850185 0.245389 0.656754
 O -4.986665 -2.231688 0.420509
 O -0.965915 0.096121 -0.748055
 C -2.188129 2.613114 -0.720593
 C -0.986206 2.912910 0.145570
 N -0.991580 3.116155 1.412214
 O -2.263990 3.008418 1.969776
 C 0.349990 3.111426 -0.540799
 N 1.432339 3.167012 0.277856
 C 2.732261 3.639577 -0.170847
 O 0.414007 3.232318 -1.763146
 C 3.440963 2.729788 -1.195750
 O 4.706123 3.364529 -1.383939
 C 3.586650 1.289464 -0.737474
 C 3.850230 -1.394043 0.142200
 C 2.661212 0.323259 -1.139194
 C 4.646117 0.907735 0.093947
 C 4.772192 -0.406602 0.526449
 C 2.805250 -0.987193 -0.700751
 Br 6.225685 -0.896147 1.655211
 Br 1.541164 -2.321875 -1.268908
 O 4.012539 -2.659919 0.583975

H -4.808997 2.309885 -0.002968
H -5.919712 -2.034040 0.626296
H -0.613445 -0.814484 -0.737903
H -2.887816 3.453009 -0.634131
H -1.827561 2.588812 -1.753292
H -2.102089 3.191982 2.909268
H 1.244949 3.114522 1.270099
H 3.375237 3.729236 0.709370
H 2.642734 4.632103 -0.628602
H 2.851938 2.750168 -2.119994
H 5.164057 2.901209 -2.102604
H 1.830722 0.594470 -1.783000
H 5.384580 1.643621 0.392295
H 3.281037 -3.204170 0.238877

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4056664

Comp_08E_c125

B3LYP/6-31G* Geometry

C -5.306715 -1.057325 0.590113
C -4.415793 1.476391 -0.142852
C -6.181067 -0.127689 0.007439
C -3.959103 -0.709894 0.800339
C -3.535811 0.568181 0.430938
C -5.759619 1.150823 -0.372308
Br -8.003923 -0.626671 -0.267182
Br -3.817894 3.227836 -0.644186
O -6.654184 1.995886 -0.928657
O -5.723806 -2.286821 0.976972
C -2.987000 -1.698837 1.429093
C -1.892637 -2.135253 0.481893
N -1.969791 -3.072357 -0.392438
O -3.210591 -3.694340 -0.408927
C -0.574288 -1.397471 0.527448
N 0.436940 -1.926720 -0.219438
C 1.690472 -1.205068 -0.419541
O -0.443131 -0.384915 1.213094
C 2.673284 -1.428791 0.752488
O 2.909256 -2.818686 0.933681
C 3.993350 -0.739270 0.481535
C 6.421859 0.599946 -0.106128
C 5.079834 -1.447989 -0.036418
C 4.126837 0.635226 0.707457
C 5.317037 1.291313 0.415371
C 6.264019 -0.778358 -0.317220
Br 5.468271 3.161371 0.735681
Br 7.765577 -1.748724 -1.018582
O 7.561807 1.274239 -0.369390
H -2.502408 0.850709 0.603226
H -6.194915 2.834786 -1.123423
H -6.674130 -2.368121 0.771504
H -3.534470 -2.582627 1.761279
H -2.505368 -1.232135 2.292678
H -3.109242 -4.363612 -1.105230

H 0.182025 -2.680250 -0.845460
H 1.483085 -0.135825 -0.530753
H 2.147715 -1.574555 -1.341923
H 2.218770 -0.995525 1.655280
H 2.034033 -3.230816 1.020898
H 5.000345 -2.515544 -0.199011
H 3.301306 1.205385 1.122406
H 8.219381 0.639735 -0.710967

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4040140

Comp_08E_c128

B3LYP/6-31G* Geometry

C -3.887488 -0.741081 -0.825866
C -5.335522 1.297633 0.456649
C -5.175136 -0.967970 -0.316799
C -3.332641 0.550636 -0.707954
C -4.069147 1.543977 -0.053558
C -5.921008 0.029741 0.325225
Br -5.955977 -2.703735 -0.484300
Br -6.299815 2.689041 1.329257
O -7.157271 -0.181405 0.822621
O -3.265064 -1.767364 -1.443300
C -1.978141 0.887748 -1.317854
C -0.828885 0.733905 -0.347522
N -0.330260 1.652010 0.399419
O -0.949145 2.882238 0.240783
C -0.178850 -0.615911 -0.213209
N 0.865529 -0.719117 0.625950
C 1.527779 -1.989129 0.896031
O -0.606211 -1.588362 -0.866964
C 2.611086 -2.362706 -0.142781
O 2.077023 -2.417195 -1.451420
C 3.783916 -1.393799 -0.113286
C 5.935403 0.450071 0.012502
C 4.732057 -1.464740 0.913580
C 3.918795 -0.402550 -1.086640
C 4.977855 0.494045 -1.012358
C 5.783810 -0.558473 0.977783
Br 5.172862 1.853948 -2.353241
Br 7.055787 -0.686176 2.387741
O 6.973544 1.307464 0.108537
H -3.644133 2.536398 0.048989
H -7.401917 -1.108871 0.639567
H -2.286001 -1.680468 -1.358550
H -1.988930 1.923099 -1.666005
H -1.787512 0.247118 -2.183652
H -0.462600 3.454041 0.857075
H 1.181214 0.132386 1.072949
H 0.759732 -2.769689 0.906497
H 1.970193 -1.936299 1.894581
H 2.981279 -3.357873 0.158912
H 1.106135 -2.485581 -1.395069
H 4.665164 -2.238535 1.672908

H 3.209806 -0.356050 -1.903450
H 6.934389 1.920943 -0.649084
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4125759**

Comp_08E_c13
B3LYP/6-31G* Geometry
C 0.698669 0.139040 -2.140756
C 2.751006 -0.672720 -0.431875
C 1.487373 1.082529 -1.462572
C 0.979355 -1.236550 -1.980607
C 1.999317 -1.621198 -1.106897
C 2.521302 0.700989 -0.599864
Br 1.092779 2.932724 -1.647476
Br 4.111439 -1.217861 0.800592
O 3.228913 1.655982 0.038204
O -0.285903 0.592433 -2.944908
C 0.189978 -2.298376 -2.735029
C -0.914583 -2.884863 -1.887150
N -0.866802 -3.979049 -1.218492
O 0.342066 -4.656281 -1.357373
C -2.193156 -2.094202 -1.749049
N -3.111477 -2.581637 -0.887073
C -4.272742 -1.825589 -0.460597
O -2.365642 -1.062349 -2.412597
C -4.143493 -1.391947 1.018898
O -3.979478 -2.550908 1.838542
C -2.960441 -0.468699 1.241632
C -0.717753 1.249924 1.498064
C -1.778719 -0.923778 1.832443
C -3.026785 0.855972 0.801522
C -1.928038 1.694851 0.939550
C -0.681000 -0.077719 1.952756
Br -2.053767 3.511458 0.361461
Br 0.935963 -0.740155 2.711661
O 0.378877 2.022250 1.637637
H 2.204675 -2.675215 -0.955166
H 3.832521 1.215686 0.665422
H -1.055890 -0.026110 -2.905652
H 0.858293 -3.106182 -3.039710
H -0.250834 -1.867037 -3.637926
H 0.212708 -5.440914 -0.800329
H -2.830560 -3.377614 -0.326298
H -5.175554 -2.441800 -0.576268
H -4.368025 -0.960920 -1.120146
H -5.068802 -0.859846 1.290176
H -4.831724 -3.011012 1.878860
H -1.712636 -1.940540 2.197858
H -3.932626 1.247321 0.349091
H 0.329535 2.778195 1.021874

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4215530**

Comp_08E_c131
B3LYP/6-31G* Geometry
C 2.321931 0.483855 1.002706
C 4.647572 0.020375 -0.442528
C 2.910659 -0.787238 0.986230
C 2.908961 1.545310 0.290016
C 4.073053 1.285612 -0.430549
C 4.081506 -1.047714 0.264940
Br 2.090499 -2.193542 1.976668
Br 6.249938 -0.309019 -1.443209
O 4.597536 -2.295597 0.287374
O 1.187293 0.742696 1.702768
C 2.301606 2.937879 0.332484
C 0.997625 3.068379 -0.421381
N 0.846038 2.978652 -1.692499
O 2.045564 2.739411 -2.360713
C -0.254199 3.400618 0.362886
N -1.428145 3.207541 -0.295577
C -2.708209 3.497457 0.319018
O -0.186215 3.826880 1.512779
C -3.184791 2.421742 1.329965
O -4.434294 2.831194 1.880284
C -3.370718 1.063911 0.688125
C -3.660780 -1.459751 -0.575838
C -4.615901 0.660618 0.198012
C -2.279116 0.199950 0.548961
C -2.421858 -1.034820 -0.073765
C -4.742128 -0.578277 -0.418096
Br -0.907437 -2.180779 -0.220669
Br -6.452712 -1.143463 -1.084504
O -3.757294 -2.670046 -1.167944
H 4.534675 2.084196 -0.999977
H 5.402925 -2.300074 -0.263401
H 0.924636 -0.071715 2.173628
H 3.021492 3.642794 -0.098186
H 2.102846 3.239558 1.364292
H 1.768425 2.700491 -3.290294
H -1.382615 2.838445 -1.234999
H -3.461067 3.601717 -0.467682
H -2.627851 4.453260 0.850599
H -2.419713 2.342725 2.114127
H -4.283115 3.653340 2.371882
H -5.479606 1.303612 0.315462
H -1.303907 0.485387 0.928330
H -4.684421 -2.802748 -1.440758

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4057051**

Comp_08E_c133
B3LYP/6-31G* Geometry
C -5.310744 -1.021359 0.613585
C -4.395104 1.481937 -0.189791
C -6.173892 -0.103087 -0.002926
C -3.961813 -0.678159 0.822447

C -3.526216 0.584910 0.417514
 C -5.739849 1.159959 -0.418637
 Br -7.998632 -0.596296 -0.275108
 Br -3.779027 3.211855 -0.741558
 O -6.623957 1.994341 -1.006941
 O -5.739842 -2.235415 1.034307
 C -3.000845 -1.655781 1.485319
 C -1.903046 -2.123825 0.557473
 N -1.979607 -3.085624 -0.289680
 O -3.222602 -3.703176 -0.294709
 C -0.582065 -1.390039 0.588145
 N 0.427626 -1.938214 -0.146630
 C 1.682716 -1.224075 -0.362129
 O -0.448139 -0.362540 1.251019
 C 2.670831 -1.433419 0.808105
 O 2.908981 -2.820517 1.005765
 C 3.988381 -0.746290 0.520214
 C 6.411482 0.577636 -0.121450
 C 5.046382 -1.441198 -0.075387
 C 4.145209 0.613494 0.800691
 C 5.336692 1.251810 0.478442
 C 6.233527 -0.789276 -0.386841
 Br 5.556769 3.118601 0.865355
 Br 7.659675 -1.760626 -1.192252
 O 7.582053 1.169423 -0.442156
 H -2.491839 0.864696 0.588188
 H -6.156836 2.823161 -1.224667
 H -6.689121 -2.316348 0.823918
 H -3.556262 -2.526857 1.837206
 H -2.522320 -1.168976 2.339515
 H -3.119598 -4.393933 -0.969479
 H 0.171771 -2.706239 -0.754391
 H 1.477521 -0.155849 -0.486471
 H 2.134505 -1.606890 -1.281785
 H 2.220424 -0.988307 1.707279
 H 2.034643 -3.232946 1.101173
 H 4.944105 -2.500044 -0.278711
 H 3.346891 1.176802 1.273713
 H 7.530650 2.108523 -0.183542
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4039595**

Comp_08E_c134
B3LYP/6-31G* Geometry
 C -1.549720 0.056612 -1.033931
 C -4.236583 -0.088136 -0.350898
 C -2.114953 -1.155522 -0.617085
 C -2.345065 1.214284 -1.128212
 C -3.688483 1.117906 -0.773949
 C -3.465444 -1.254034 -0.263357
 Br -0.998734 -2.696483 -0.529853
 Br -6.090694 -0.194625 0.132152
 O -3.949598 -2.450236 0.138513
 O -0.243793 0.167111 -1.370109

C -1.749033 2.514587 -1.641903
 C -0.759181 3.163788 -0.702075
 N -1.040433 3.717403 0.420420
 O -2.402836 3.663014 0.719012
 C 0.694481 3.232743 -1.128787
 N 1.564342 3.638722 -0.163665
 C 2.991897 3.704454 -0.376337
 O 1.024384 2.947764 -2.275075
 C 3.772874 2.882658 0.664234
 O 3.464416 3.481710 1.923261
 C 3.446371 1.398317 0.639440
 C 2.796904 -1.362624 0.547117
 C 4.190188 0.522326 -0.155642
 C 2.384427 0.884306 1.391395
 C 2.067781 -0.468465 1.346924
 C 3.860453 -0.826741 -0.197099
 Br 0.622551 -1.128201 2.390799
 Br 4.886217 -2.028865 -1.284325
 O 2.456353 -2.670418 0.533493
 H -4.316694 2.000228 -0.822727
 H -4.896777 -2.338067 0.343490
 H 0.177707 -0.707936 -1.275475
 H -2.565296 3.222120 -1.823951
 H -1.221419 2.343038 -2.583967
 H -2.450899 4.118642 1.574718
 H 1.188295 3.892840 0.740162
 H 3.344144 4.742601 -0.311750
 H 3.187827 3.334172 -1.384714
 H 4.843253 3.009967 0.433438
 H 3.894304 2.958297 2.618341
 H 5.025805 0.884633 -0.746359
 H 1.800642 1.543524 2.021981
 H 3.071972 -3.141157 -0.059336
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4099966**

Comp_08E_c135
B3LYP/6-31G* Geometry
 C 3.083382 1.304930 0.145431
 C 2.776435 -1.406149 0.701854
 C 3.515721 0.336608 -0.774610
 C 2.534675 0.899191 1.382039
 C 2.371428 -0.464901 1.634956
 C 3.368917 -1.032417 -0.514458
 Br 4.278732 0.883538 -2.421243
 Br 2.501382 -3.273560 1.037188
 O 3.780751 -1.922910 -1.441038
 O 3.238827 2.610447 -0.176330
 C 2.139387 1.919866 2.441521
 C 0.647613 2.148263 2.473770
 N -0.185435 1.672233 3.327175
 O 0.415539 0.901526 4.313649
 C 0.029595 2.945391 1.355513
 N -1.312089 2.975659 1.298593

C -2.065468 3.651342 0.244822
 O 0.750925 3.528077 0.522338
 C -2.087678 2.895958 -1.108023
 O -0.844170 2.968927 -1.775827
 C -2.543931 1.451903 -0.925158
 C -3.375878 -1.215798 -0.434771
 C -3.902808 1.135924 -0.862916
 C -1.607169 0.426938 -0.758431
 C -2.014587 -0.877740 -0.506336
 C -4.298720 -0.175690 -0.624675
 Br -0.702066 -2.228423 -0.220143
 Br -6.167508 -0.610339 -0.552459
 O -3.728622 -2.497253 -0.193378
 H 1.930222 -0.790890 2.570887
 H 3.566488 -2.817915 -1.117675
 H 2.454775 3.107231 0.149906
 H 2.642180 2.871572 2.247328
 H 2.456203 1.572917 3.426720
 H -0.337412 0.625068 4.861267
 H -1.800147 2.407927 1.980019
 H -1.634592 4.645693 0.086580
 H -3.087046 3.777870 0.613024
 H -2.833066 3.415733 -1.729652
 H -0.163432 3.286015 -1.153039
 H -4.659145 1.901719 -1.007967
 H -0.550570 0.651141 -0.844618
 H -4.702211 -2.554106 -0.198642

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4156785**

Comp_08E_c138

B3LYP/6-31G* Geometry

C -3.917879 -1.531658 0.085035
 C -4.666868 1.163131 0.267485
 C -5.248740 -1.128358 -0.096270
 C -2.942845 -0.557711 0.357156
 C -3.344321 0.777628 0.449759
 C -5.654858 0.210641 -0.014743
 Br -6.580664 -2.467817 -0.466111
 Br -5.153454 2.997936 0.402501
 O -6.932493 0.613483 -0.189781
 O -3.536234 -2.832306 0.023808
 C -1.485558 -0.949172 0.560329
 C -0.570375 -0.385446 -0.502555
 N -0.349193 -0.891724 -1.661526
 O -1.058039 -2.062513 -1.882262
 C 0.165647 0.898247 -0.207327
 N 1.068640 1.302301 -1.123757
 C 1.750484 2.594620 -1.081663
 O -0.077070 1.521091 0.837403
 C 2.797102 2.764913 0.048773
 O 2.192326 3.050607 1.290271
 C 3.757617 1.576609 0.117994
 C 5.516243 -0.649063 0.230265

C 4.598318 1.268292 -0.958282
 C 3.809651 0.775799 1.258261
 C 4.673370 -0.312320 1.299331
 C 5.456834 0.176716 -0.903579
 Br 4.743525 -1.417120 2.868611
 Br 6.581622 -0.216003 -2.390401
 O 6.363751 -1.701215 0.241587
 H -2.599870 1.533269 0.677911
 H -7.487631 -0.166163 -0.369138
 H -4.315397 -3.384129 -0.165120
 H -1.397248 -2.037020 0.552696
 H -1.140267 -0.572303 1.526703
 H -0.776767 -2.321575 -2.775023
 H 1.190617 0.699020 -1.926804
 H 1.009956 3.395877 -0.971287
 H 2.235449 2.718117 -2.053456
 H 3.380717 3.658370 -0.217904
 H 1.330504 2.581451 1.319284
 H 4.600746 1.883224 -1.853647
 H 3.186324 1.021274 2.109279
 H 6.279860 -2.148697 1.104441

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4054426**

Comp_08E_c14

B3LYP/6-31G* Geometry

C 1.449167 0.281514 -0.493091
 C 4.195923 -0.219452 -0.466480
 C 1.946198 -0.984350 -0.165077
 C 2.341199 1.320939 -0.804499
 C 3.706767 1.045167 -0.780844
 C 3.320948 -1.264649 -0.145722
 Br 0.697122 -2.365647 0.299553
 Br 6.073366 -0.535028 -0.453265
 O 3.822674 -2.479382 0.168930
 O 0.125335 0.574838 -0.521333
 C 1.803832 2.702062 -1.145418
 C 0.996867 3.306775 -0.019283
 N 1.465828 3.748583 1.090799
 O 2.851697 3.626931 1.166839
 C -0.497798 3.442304 -0.188210
 N -1.213077 3.443290 0.959863
 C -2.645271 3.717002 1.066915
 O -0.984630 3.532503 -1.319679
 C -3.591923 2.853591 0.192640
 O -3.702564 3.360935 -1.118018
 C -3.285079 1.351634 0.209681
 C -2.830950 -1.456018 0.175499
 C -3.494374 0.609795 -0.956268
 C -2.844442 0.679293 1.355174
 C -2.616810 -0.694608 1.335296
 C -3.270839 -0.760638 -0.961583
 Br -1.977546 -1.570410 2.900464
 Br -3.559274 -1.773250 -2.565487

O -2.602071 -2.789673 0.201186
H 4.412700 1.837440 -1.004587
H 3.082145 -3.080051 0.368917
H -0.400685 -0.197840 -0.247237
H 1.155047 2.661814 -2.025060
H 2.647981 3.362091 -1.368915
H 3.055334 4.019826 2.030903
H -0.664125 3.428688 1.809484
H -2.859593 4.761206 0.806429
H -2.897888 3.584982 2.123110
H -4.589336 2.994657 0.633441
H -2.779453 3.460669 -1.446314
H -3.827215 1.119292 -1.851918
H -2.664540 1.212195 2.281970
H -2.802014 -3.147723 -0.684864

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4107653

Comp_08E_c141

B3LYP/6-31G* Geometry

C 2.349263 1.599015 0.608105
C 1.109994 -0.584234 1.816105
C 2.755662 0.288567 0.317563
C 1.291286 1.816221 1.510518
C 0.698527 0.708673 2.115034
C 2.133746 -0.824853 0.891131
Br 4.174600 0.024179 -0.928925
Br 0.247763 -2.087061 2.624555
O 2.535911 -2.064459 0.523471
O 2.946468 2.677266 0.050889
C 0.781002 3.224156 1.780998
C -0.718690 3.287908 1.636018
N -1.584704 3.329504 2.580970
O -1.009939 3.308806 3.856453
C -1.269968 3.253057 0.224283
N -2.617184 3.088108 0.120158
C -3.287301 2.980664 -1.159104
O -0.509518 3.353017 -0.734036
C -3.806677 1.564468 -1.475583
O -4.337915 1.681156 -2.796975
C -2.764565 0.464156 -1.369318
C -0.875812 -1.646663 -1.179854
C -3.043145 -0.690352 -0.631014
C -1.534821 0.551874 -2.034919
C -0.619531 -0.484679 -1.930401
C -2.120941 -1.729438 -0.543554
Br 1.082190 -0.353147 -2.796905
Br -2.548685 -3.287576 0.461125
O 0.005291 -2.662583 -1.053890
H -0.109171 0.856678 2.823727
H 1.963739 -2.710566 0.981416
H 3.604152 2.366274 -0.598920
H 1.222166 3.902655 1.048907
H 1.061774 3.556967 2.783961

H -1.784970 3.372308 4.437478
H -3.139088 3.026948 0.984502
H -2.574420 3.285473 -1.926948
H -4.137484 3.670814 -1.203084
H -4.614420 1.323951 -0.763320
H -4.617546 0.796927 -3.081258
H -3.991219 -0.790074 -0.111121
H -1.275136 1.434051 -2.607177
H 0.838932 -2.406396 -1.494160

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4147194

Comp_08E_c142

B3LYP/6-31G* Geometry

C 2.560951 -0.165728 1.522278
C 3.257625 0.487190 -1.099086
C 2.879258 -1.169702 0.595195
C 2.606076 1.188977 1.125204
C 2.947695 1.491568 -0.195686
C 3.228735 -0.865357 -0.725242
Br 2.773332 -2.990694 1.112373
Br 3.729474 0.919909 -2.905584
O 3.509533 -1.874847 -1.574063
O 2.235427 -0.569434 2.770651
C 2.283526 2.318830 2.096904
C 0.795651 2.483206 2.302739
N 0.098934 2.069883 3.296166
O 0.885156 1.421424 4.267553
C 0.019020 3.160724 1.193000
N -1.323222 3.035672 1.238251
C -2.213549 3.625037 0.241601
O 0.623546 3.767243 0.301216
C -2.261068 2.863935 -1.106794
O -1.067875 3.025618 -1.847422
C -2.598338 1.391853 -0.896653
C -3.205939 -1.324648 -0.350103
C -3.926130 0.974698 -0.782036
C -1.580974 0.442649 -0.754223
C -1.876896 -0.886510 -0.474700
C -4.211320 -0.360317 -0.516662
Br -0.457424 -2.128849 -0.218032
Br -6.038342 -0.935805 -0.371495
O -3.451674 -2.625836 -0.082796
H 2.960849 2.526246 -0.518022
H 3.705808 -1.489659 -2.448751
H 1.888053 0.164173 3.313750
H 2.656750 3.254672 1.674870
H 2.771814 2.169294 3.064226
H 0.226981 1.109656 4.910622
H -1.707125 2.457169 1.973635
H -1.892564 4.655170 0.051569
H -3.214118 3.655813 0.681318
H -3.080437 3.324433 -1.680938
H -0.381739 3.412158 -1.268888

H -4.743468 1.679157 -0.906245
H -0.548361 0.745955 -0.880239
H -4.417679 -2.754540 -0.047499
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4148708

Comp_08E_c144
B3LYP/6-31G* Geometry
C -2.716387 0.459151 -0.870813
C -0.760327 -1.397455 -1.567151
C -2.744488 -0.839721 -0.342319
C -1.702903 0.818731 -1.786433
C -0.721330 -0.121600 -2.107400
C -1.774378 -1.790475 -0.680861
Br -4.070453 -1.305038 0.929871
Br 0.612786 -2.666000 -2.004271
O -1.849227 -3.020890 -0.135130
O -3.693262 1.306447 -0.473553
C -1.648868 2.208577 -2.410492
C -0.951001 3.202826 -1.512148
N -1.497318 4.047939 -0.719756
O -2.908479 3.999770 -0.776149
C 0.568019 3.172691 -1.519164
N 1.175133 3.867983 -0.525703
C 2.605587 3.826287 -0.304648
O 1.161252 2.540115 -2.389215
C 2.969727 3.146409 1.027994
O 2.379865 3.964053 2.037280
C 2.515882 1.696999 1.112817
C 1.655770 -1.003163 1.220545
C 3.304858 0.680711 0.566066
C 1.297774 1.354183 1.708932
C 0.876610 0.029266 1.764298
C 2.870954 -0.637163 0.619194
Br -0.796168 -0.400607 2.557606
Br 3.945058 -2.026870 -0.146002
O 1.218743 -2.277644 1.304188
H 0.086166 0.160400 -2.773230
H -1.057139 -3.519898 -0.406766
H -3.464635 2.235702 -0.674896
H -2.650023 2.571448 -2.658802
H -1.069843 2.152557 -3.334572
H -3.175382 4.634133 -0.091050
H 0.590624 4.325265 0.162067
H 3.009424 4.845743 -0.285580
H 3.050391 3.287364 -1.143022
H 4.068913 3.176403 1.107417
H 2.548424 3.547923 2.897800
H 4.256342 0.908889 0.095692
H 0.669859 2.126754 2.136839
H 1.855235 -2.848447 0.834330
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4195687

Comp_08E_c146
B3LYP/6-31G* Geometry
C -3.895712 -0.746487 -0.832246
C -5.326929 1.274238 0.496961
C -5.176848 -0.980262 -0.309937
C -3.339088 0.543441 -0.703292
C -4.066995 1.527510 -0.025757
C -5.914305 0.008366 0.355400
Br -5.960301 -2.713583 -0.491707
Br -6.280027 2.653790 1.400294
O -7.144249 -0.209792 0.865582
O -3.281658 -1.764268 -1.471596
C -1.992184 0.889188 -1.324918
C -0.831033 0.718967 -0.371800
N -0.319026 1.625869 0.379745
O -0.936552 2.859444 0.246592
C -0.182490 -0.633869 -0.265314
N 0.867066 -0.752829 0.566204
C 1.540927 -2.024408 0.792093
O -0.614635 -1.594331 -0.933083
C 2.625403 -2.351830 -0.262644
O 2.091177 -2.342683 -1.572014
C 3.796610 -1.384489 -0.188891
C 5.925790 0.477432 0.028171
C 3.877659 -0.287186 -1.051339
C 4.791614 -1.556814 0.777043
C 5.828095 -0.636772 0.876728
C 4.921328 0.624726 -0.941362
Br 7.194965 -0.877312 2.201425
Br 5.001804 2.111041 -2.128073
O 6.920116 1.387926 0.098086
H -3.640322 2.518331 0.085291
H -7.391364 -1.134507 0.672284
H -2.301356 -1.677221 -1.401479
H -2.006178 1.929979 -1.656244
H -1.812882 0.262687 -2.203388
H -0.432296 3.424551 0.854800
H 1.191554 0.091914 1.019795
H 0.779035 -2.810721 0.776066
H 1.985488 -2.003484 1.791028
H 2.995659 -3.359566 -0.005625
H 1.123823 -2.450610 -1.519477
H 3.129252 -0.163664 -1.823865
H 4.771669 -2.409241 1.449620
H 7.531550 1.121637 0.809787
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4124023

Comp_08E_c147
B3LYP/6-31G* Geometry
C 3.954236 0.723155 0.865958
C 6.054727 -0.652054 -0.396139
C 4.945143 1.405771 0.144294

C 4.044735 -0.680155 0.976499
 C 5.092600 -1.341611 0.327001
 C 6.005384 0.746604 -0.492463
 Br 4.855416 3.308452 -0.001181
 Br 7.464869 -1.601398 -1.254631
 O 6.960036 1.394098 -1.191899
 O 2.987022 1.457074 1.456179
 C 3.059491 -1.470877 1.827699
 C 1.883478 -2.010743 1.045405
 N 1.807854 -3.160141 0.476898
 O 2.945927 -3.932344 0.649894
 C 0.662077 -1.144411 0.889329
 N -0.401205 -1.687175 0.275572
 C -1.613803 -0.952589 -0.098224
 O 0.662210 0.018946 1.339920
 C -2.530780 -0.564970 1.092110
 O -2.049217 0.568050 1.780470
 C -3.934599 -0.266557 0.587585
 C -6.528465 0.266296 -0.425624
 C -4.819091 -1.310030 0.293988
 C -4.351799 1.049506 0.380951
 C -5.626009 1.295361 -0.115111
 C -6.089050 -1.048950 -0.206171
 Br -6.210187 3.102352 -0.393708
 Br -7.267080 -2.493345 -0.593200
 O -7.771427 0.476993 -0.907621
 H 5.161298 -2.421255 0.399029
 H 6.768241 2.350703 -1.150215
 H 2.155299 0.934139 1.534651
 H 2.677668 -0.843530 2.638305
 H 3.578710 -2.318864 2.280533
 H 2.734812 -4.747803 0.166142
 H -0.280672 -2.640182 -0.045674
 H -2.159319 -1.598314 -0.789863
 H -1.338037 -0.036230 -0.633491
 H -2.581688 -1.441910 1.761238
 H -1.071802 0.543610 1.764217
 H -4.528127 -2.342702 0.463341
 H -3.685875 1.866619 0.628229
 H -7.908729 1.439803 -0.986618

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4121793**

Comp_08E_c15

B3LYP/6-31G* Geometry

C 2.126886 -0.071638 1.011674
 C 4.634420 0.077400 -0.171482
 C 2.631745 -1.148287 0.275088
 C 2.873468 1.113697 1.132504
 C 4.128555 1.164331 0.532714
 C 3.895239 -1.101427 -0.326764
 Br 1.541157 -2.694646 0.060335
 Br 6.368621 0.167829 -0.982389
 O 4.327666 -2.178715 -1.016909

O 0.910151 -0.101671 1.615334
 C 2.330528 2.288370 1.917692
 C 0.964490 2.798209 1.506680
 N 0.102076 3.316654 2.303709
 O 0.533181 3.361470 3.626942
 C 0.545870 2.771991 0.057887
 N -0.778907 2.903152 -0.184154
 C -1.315421 3.002533 -1.535395
 O 1.384014 2.635624 -0.840481
 C -1.478854 1.641480 -2.251420
 O -0.234197 1.021492 -2.499789
 C -2.403384 0.716119 -1.465853
 C -4.124918 -0.903405 0.104475
 C -3.777537 0.974197 -1.404920
 C -1.891086 -0.372204 -0.758721
 C -2.746960 -1.148950 0.012711
 C -4.620952 0.181210 -0.636047
 Br -2.042214 -2.626235 1.027343
 Br -6.485802 0.563577 -0.576516
 O -4.976308 -1.642792 0.848766
 H 4.722015 2.069420 0.605674
 H 5.207491 -1.969988 -1.383307
 H 0.496979 -0.975318 1.474968
 H 3.041621 3.121140 1.843810
 H 2.261936 2.035991 2.980948
 H -0.230791 3.746310 4.085809
 H -1.390729 2.988433 0.615765
 H -0.643866 3.631181 -2.130961
 H -2.284642 3.505208 -1.473514
 H -1.960713 1.864631 -3.218125
 H 0.478413 1.567801 -2.108844
 H -4.207990 1.799501 -1.965002
 H -0.836694 -0.607623 -0.833787
 H -4.465444 -2.348687 1.286822

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4081023**

Comp_08E_c16

B3LYP/6-31G* Geometry

C -2.738395 -0.094639 -0.883659
 C -0.365457 -1.236848 -1.784909
 C -2.342850 -1.368281 -0.449812
 C -1.927705 0.619382 -1.786489
 C -0.747915 0.021261 -2.231531
 C -1.145021 -1.954505 -0.868768
 Br -3.453867 -2.301130 0.790299
 Br 1.282525 -2.012448 -2.367385
 O -0.791256 -3.160912 -0.366049
 O -3.885594 0.485017 -0.456702
 C -2.305941 2.027412 -2.226210
 C -1.686338 3.079607 -1.330429
 N -2.285729 3.842302 -0.491152
 O -3.664300 3.652913 -0.447462
 C -0.188638 3.277963 -1.437042

N 0.393819 3.928950 -0.395506
 C 1.825630 4.070486 -0.256850
 O 0.428265 2.860504 -2.415363
 C 2.325133 3.488795 1.085145
 O 1.643322 4.128081 2.168293
 C 2.099428 1.994642 1.202035
 C 1.659257 -0.805612 1.301472
 C 3.028480 1.101585 0.658496
 C 0.952935 1.481941 1.813441
 C 0.749905 0.108311 1.856130
 C 2.814284 -0.271231 0.711478
 Br -0.830285 -0.598251 2.676368
 Br 4.110669 -1.455568 -0.018962
 O 1.483053 -2.145372 1.324471
 H -0.102904 0.570138 -2.906742
 H 0.090670 -3.383506 -0.724014
 H -4.325459 -0.126409 0.163400
 H -3.389062 2.150315 -2.224648
 H -1.927729 2.195066 -3.239000
 H -3.945517 4.312204 0.206860
 H -0.200691 4.213531 0.372102
 H 2.113471 5.132737 -0.306112
 H 2.290594 3.562994 -1.105490
 H 3.406965 3.685696 1.146400
 H 1.900326 5.063517 2.167863
 H 3.935662 1.468743 0.188599
 H 0.231117 2.148885 2.267070
 H 0.600757 -2.337235 1.696591

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4161048**

Comp_08E_c17

B3LYP/6-31G* Geometry

C -2.751131 -0.159244 -0.860515
 C -0.353778 -1.239301 -1.772769
 C -2.324062 -1.425398 -0.434155
 C -1.961134 0.577993 -1.762885
 C -0.768800 0.010191 -2.214304
 C -1.112903 -1.979672 -0.857845
 Br -3.405871 -2.388173 0.809070
 Br 1.314842 -1.969142 -2.357283
 O -0.725123 -3.177437 -0.357890
 O -3.909336 0.391834 -0.425600
 C -2.376179 1.977394 -2.197121
 C -1.784760 3.046598 -1.301654
 N -2.407164 3.803302 -0.474075
 O -3.781955 3.585683 -0.439054
 C -0.290758 3.274942 -1.399304
 N 0.273233 3.954865 -0.367355
 C 1.701019 4.155402 -0.250245
 O 0.340498 2.848439 -2.365323
 C 2.272983 3.543378 1.041649
 O 1.628188 4.245810 2.104941
 C 2.079609 2.038660 1.146624

C 1.697261 -0.770554 1.275977
 C 0.935819 1.505846 1.747836
 C 3.034069 1.158320 0.624375
 C 2.845816 -0.217682 0.687649
 C 0.762166 0.128921 1.810701
 Br 4.167166 -1.384515 -0.025011
 Br -0.805101 -0.600241 2.634632
 O 1.552766 -2.112893 1.317031
 H -0.139250 0.578021 -2.888107
 H 0.154992 -3.382013 -0.730928
 H -4.333403 -0.233209 0.191843
 H -3.462182 2.071597 -2.194385
 H -2.004240 2.156724 -3.210250
 H -4.081972 4.248365 0.203426
 H -0.334106 4.287068 0.370130
 H 1.935941 5.227458 -0.244378
 H 2.165932 3.701590 -1.127605
 H 3.353826 3.759327 1.042317
 H 1.930603 3.861825 2.943435
 H 0.185554 2.163440 2.170101
 H 3.938232 1.540767 0.160552
 H 0.669570 -2.321957 1.677637

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4180400**

Comp_08E_c18

B3LYP/6-31G* Geometry

C 2.040675 0.120898 -0.557391
 C 4.692318 0.101567 0.344826
 C 2.694397 -1.079495 -0.250709
 C 2.732074 1.335956 -0.405418
 C 4.048798 1.298217 0.048819
 C 4.023473 -1.119031 0.200276
 Br 1.751876 -2.741149 -0.437097
 Br 6.494809 0.113298 0.957579
 O 4.669331 -2.267463 0.498817
 O 0.759650 0.192477 -0.994000
 C 2.060776 2.650180 -0.766379
 C 0.864732 3.008257 0.085643
 N 0.878265 3.261161 1.344551
 O 2.148311 3.158790 1.898115
 C -0.476303 3.185051 -0.586576
 N -1.549385 3.256189 -0.233593
 C -2.877035 3.700122 -0.189479
 O -0.544127 3.277187 -1.817928
 C -3.629697 2.764178 -1.171981
 O -3.178000 2.910080 -2.496985
 C -3.613421 1.312251 -0.694673
 C -3.516012 -1.375643 0.218064
 C -4.358076 0.912965 0.418651
 C -2.837050 0.360453 -1.357541
 C -2.788909 -0.950623 -0.902005
 C -4.302547 -0.404489 0.857616
 Br -1.689534 -2.214978 -1.819800

Br -5.328307 -0.950449 2.385648
 O -3.433375 -2.663447 0.618684
 H 4.590132 2.228658 0.181346
 H 4.064953 -3.014976 0.338673
 H 0.370528 -0.695151 -1.111574
 H 1.718909 2.635790 -1.804792
 H 2.800892 3.452558 -0.666929
 H 1.998178 3.382110 2.831078
 H -1.346524 3.204676 1.223431
 H -2.808723 4.685791 -0.667528
 H -3.465933 3.810549 0.725322
 H -4.673288 3.110813 -1.165891
 H -2.207334 3.064072 -2.463061
 H -4.991311 1.619769 0.946981
 H -2.275471 0.652364 -2.236245
 H -4.010201 -2.779650 1.396503
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4101403**

Comp_08E_c19
B3LYP/6-31G* Geometry
 C 2.147237 -0.130472 0.980604
 C 4.635350 0.070860 -0.237589
 C 2.654917 -1.189557 0.219662
 C 2.885272 1.059567 1.115862
 C 4.129449 1.137365 0.496739
 C 3.908822 -1.114616 -0.400240
 Br 1.591980 -2.753019 0.001897
 Br 6.354726 0.198734 -1.075758
 O 4.345674 -2.174225 -1.115037
 O 0.939523 -0.178444 1.599144
 C 2.355227 2.207710 1.949193
 C 0.971446 2.714181 1.600612
 N 0.111046 3.155948 2.444599
 O 0.558513 3.115856 3.762135
 C 0.530882 2.781501 0.159924
 N -0.798178 2.928116 -0.052309
 C -1.359109 3.101085 -1.385564
 O 1.354766 2.703464 -0.758153
 C -1.532677 1.780698 -2.173262
 O -0.291346 1.175663 -2.468844
 C -2.443886 0.814082 -1.424174
 C -4.125144 -0.884096 0.106084
 C -3.830211 0.987309 -1.441429
 C -1.904281 -0.223952 -0.659774
 C -2.731363 -1.043266 0.098556
 C -4.644594 0.148296 -0.690186
 Br -1.964900 -2.420854 1.176985
 Br -6.550271 0.380718 -0.721798
 O -4.885956 -1.711395 0.856117
 H 4.714610 2.046931 0.580164
 H 5.217749 -1.947377 -1.488924
 H 0.512843 -1.044710 1.447234
 H 3.054404 3.049956 1.869349

H 2.328351 1.926632 3.006790
 H -0.209448 3.443934 4.256893
 H -1.396029 2.956018 0.762153
 H -0.699007 3.763494 -1.957017
 H -2.328432 3.596685 -1.279365
 H -2.029387 2.055436 -3.119011
 H 0.427830 1.708269 -2.071139
 H -4.284468 1.769755 -2.042434
 H -0.835008 -0.390920 -0.680402
 H -5.821271 -1.465341 0.730272
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4089736**

Comp_08E_c22
B3LYP/6-31G* Geometry
 C -0.705853 -0.125744 -2.089420
 C -2.894972 0.289728 -0.379130
 C -1.340324 -1.194354 -1.438352
 C -1.219700 1.174506 -1.904855
 C -2.299167 1.356600 -1.033608
 C -2.434708 -1.019298 -0.580882
 Br -0.656745 -2.964993 -1.675145
 Br -4.317588 0.597619 0.845375
 O -3.043348 -2.037758 0.058023
 O 0.347034 -0.401467 -2.889532
 C -0.618680 2.373365 -2.626050
 C 0.374259 3.106783 -1.755539
 N 0.145300 4.149766 -1.043736
 O -1.160308 4.617875 -1.159608
 C 1.768275 2.538999 -1.647029
 N 2.592449 3.136597 -0.759687
 C 3.872370 2.578791 -0.371031
 O 2.112692 1.582519 -2.355626
 C 3.832528 2.041886 1.079540
 O 3.445610 3.094844 1.964249
 C 2.857869 0.890282 1.239231
 C 1.027876 -1.266070 1.420641
 C 1.602687 1.067350 1.828581
 C 3.198633 -0.371003 0.743077
 C 2.295611 -1.421462 0.837960
 C 0.704384 0.007727 1.912691
 Br 2.765959 -3.145491 0.150811
 Br -1.018742 0.282440 2.669158
 O 0.129403 -2.266948 1.532770
 H -2.677688 2.358445 -0.862160
 H -2.556146 -2.857389 -0.148481
 H 0.998063 0.341527 -2.849353
 H -1.412661 3.067267 -2.908794
 H -0.113316 2.049094 -3.539831
 H -1.165952 5.387654 -0.567877
 H 2.180160 3.844856 -0.163722
 H 4.647845 3.354243 -0.445120
 H 4.118765 1.785465 -1.079403
 H 4.845071 1.686836 1.327885

H 4.189789 3.711814 2.037033
H 1.324461 2.034115 2.228375
H 4.164692 -0.545139 0.279529
H 0.466513 -3.039498 1.041768
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4227032

Comp_08E_c24
B3LYP/6-31G* Geometry
C 3.712465 -0.007068 -0.731034
C 6.321122 -0.287546 0.181143
C 4.646438 1.019706 -0.915999
C 4.090227 -1.198464 -0.084115
C 5.401640 -1.313410 0.369808
C 5.967759 0.902781 -0.467459
Br 4.094607 2.613949 -1.805836
Br 8.121166 -0.469662 0.814945
O 6.820142 1.928806 -0.676774
O 2.428819 0.092277 -1.152489
C 3.088415 -2.329072 0.081097
C 1.945167 -2.005434 1.014720
N 2.028268 -1.867855 2.288370
O 3.325724 -2.039297 2.760987
C 0.553123 -1.883647 0.439599
N -0.372721 -1.308308 1.240683
C -1.807266 -1.303418 0.951772
O 0.312153 -2.304306 -0.696508
C -2.231430 -0.348653 -0.194992
O -1.938137 -0.884575 -1.464916
C -3.726913 -0.078381 -0.112649
C -6.521943 0.352476 0.110707
C -4.225623 0.892741 0.759149
C -4.628796 -0.824323 -0.877364
C -5.997752 -0.611180 -0.765120
C -5.596616 1.092841 0.862378
Br -7.201507 -1.642437 -1.820749
Br -6.279132 2.429648 2.060362
O -7.859730 0.525396 0.186529
H 5.710686 -2.216163 0.884737
H 7.688834 1.681414 -0.307641
H 2.310886 0.947461 -1.607748
H 3.614303 -3.206518 0.472313
H 2.648321 -2.593025 -0.884251
H 3.222902 -1.927892 3.720031
H -0.058498 -1.056349 2.168777
H -2.307454 -1.007932 1.877391
H -2.141634 -2.316293 0.693657
H -1.697067 0.604643 -0.033876
H -1.121015 -1.422869 -1.386782
H -3.552793 1.502641 1.354481
H -4.246802 -1.558914 -1.575250
H -8.041032 1.234410 0.831052
Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4063859

Comp_08E_c26
B3LYP/6-31G* Geometry
C 0.994628 -0.640150 2.173767
C 1.773358 1.678116 0.787947
C 2.117929 -0.633009 1.334212
C 0.268809 0.557446 2.339766
C 0.667893 1.694279 1.628148
C 2.524762 0.505793 0.628195
Br 3.119576 -2.241308 1.094688
Br 2.266329 3.242364 -0.170651
O 3.583249 0.498542 -0.218069
O 0.674288 -1.789612 2.806601
C -0.921379 0.628194 3.288647
C -2.239648 0.500099 2.560518
N -3.022991 1.458838 2.222545
O -2.574458 2.708813 2.635556
C -2.658192 -0.872500 2.096455
N -3.788868 -0.951807 1.361835
C -4.107751 -2.122431 0.564477
O -1.973277 -1.865897 2.380463
C -3.999984 -1.832747 -0.945886
O -5.091116 -0.959611 -1.234295
C -2.659281 -1.229136 -1.342632
C -0.141317 -0.073220 -1.963659
C -2.509026 0.158542 -1.442809
C -1.540995 -2.040661 -1.556367
C -0.311830 -1.464020 -1.855840
C -1.276012 0.723054 -1.745382
Br 1.226535 -2.568879 -2.122315
Br -1.097404 2.613838 -1.828757
O 1.027470 0.524061 -2.263067
H 0.101807 2.613280 1.735645
H 4.023301 -0.369436 -0.129659
H -0.311776 -1.874216 2.819532
H -0.911351 1.582131 3.819228
H -0.849725 -0.170440 4.032550
H -3.255124 3.307176 2.287128
H -4.256588 -0.079243 1.146605
H -5.130116 -2.456013 0.774080
H -3.413734 -2.912283 0.855107
H -4.132715 -2.794973 -1.466611
H -5.038641 -0.713234 -2.171833
H -3.359046 0.808526 -1.272606
H -1.615771 -3.121296 -1.482891
H 1.745197 -0.135995 -2.245564
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4231830

Comp_08E_c28
B3LYP/6-31G* Geometry
C -3.612717 -0.760687 -0.502876

C -5.134926 1.450532 0.210775
 C -4.939992 -0.913694 -0.083850
 C -3.035775 0.520892 -0.569691
 C -3.816910 1.613380 -0.201615
 C -5.729415 0.184128 0.279516
 Br -5.684084 -2.668811 -0.010293
 Br -6.191300 2.970091 0.709659
 O -7.002778 -0.030766 0.674426
 O -2.835603 -1.813618 -0.854879
 C -1.610071 0.694504 -1.064114
 C -0.562596 0.057563 -0.180552
 N -0.247623 0.430976 1.005976
 O -0.990459 1.523012 1.440374
 C 0.263199 -1.076563 -0.742154
 N 1.035741 -1.744686 0.141704
 C 1.843552 -2.911088 -0.203420
 O 0.221693 -1.335658 -1.950622
 C 3.057189 -2.645381 -1.130863
 O 2.670193 -2.521014 -2.481551
 C 3.897034 -1.462999 -0.645692
 C 5.434782 0.741999 0.266246
 C 4.547647 -1.502694 0.593389
 C 4.028493 -0.320514 -1.434348
 C 4.782473 0.752614 -0.975115
 C 5.297605 -0.421168 1.040284
 Br 4.963595 2.327112 -2.060492
 Br 6.165879 -0.509531 2.734342
 O 6.173555 1.770438 0.738035
 H -3.389022 2.609453 -0.232057
 H -7.403246 0.832842 0.888827
 H -3.365320 -2.630514 -0.787718
 H -1.395201 1.766607 -1.133647
 H -1.495511 0.257609 -2.059888
 H -0.626236 1.693753 2.324198
 H 1.053764 -1.383803 1.086413
 H 1.209075 -3.656734 -0.696896
 H 2.188006 -3.338937 0.741876
 H 3.681254 -3.549669 -1.074099
 H 1.776502 -2.114022 -2.500420
 H 4.485147 -2.384959 1.223858
 H 3.552969 -0.289744 -2.406923
 H 6.167638 2.479882 0.068350
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4072768**

Comp_08E_c29
B3LYP/6-31G* Geometry
 C -4.002149 0.698772 -0.121576
 C -6.499881 -0.503470 -0.298379
 C -5.103253 1.239556 0.553455
 C -4.151539 -0.462805 -0.901394
 C -5.411989 -1.050685 -0.969848
 C -6.373251 0.654660 0.479171
 Br -4.856095 2.817214 1.597259

Br -8.226875 -1.326920 -0.414652
 O -7.394395 1.226537 1.152688
 O -2.767065 1.252704 -0.057850
 C -2.970002 -1.026230 -1.672163
 C -1.824169 -1.496123 -0.806608
 N -1.846693 -2.496104 -0.002779
 O -3.077254 -3.144246 0.012573
 C -0.492655 -0.789474 -0.928332
 N 0.447465 -1.130480 -0.019137
 C 1.749192 -0.476126 0.106095
 O -0.307277 0.028823 -1.835864
 C 2.732055 -0.734935 -1.067512
 O 2.432801 0.064026 -2.189306
 C 4.157068 -0.435080 -0.625450
 C 6.785993 0.140987 0.270066
 C 4.876197 -1.362759 0.135756
 C 4.758797 0.783010 -0.946764
 C 6.046964 1.050936 -0.501221
 C 6.163228 -1.078956 0.576779
 Br 6.883922 2.722031 -0.944933
 Br 7.114608 -2.367921 1.607258
 O 8.039544 0.375959 0.714637
 H -5.548326 -1.954216 -1.553872
 H -8.198070 0.696891 0.992367
 H -2.813234 2.059439 0.489495
 H -2.565426 -0.272916 -2.353814
 H -3.319209 -1.875643 -2.269784
 H -2.932828 -3.867691 0.643908
 H 0.179580 -1.834948 0.655608
 H 2.185863 -0.839795 1.039422
 H 1.611807 0.608671 0.197902
 H 2.665741 -1.809399 -1.315183
 H 1.456674 0.152799 -2.241918
 H 4.439719 -2.325547 0.384990
 H 4.220888 1.497411 -1.557197
 H 8.312334 1.258778 0.401364
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4065001**

Comp_08E_c30
B3LYP/6-31G* Geometry
 C 2.118003 -0.116658 0.964848
 C 4.646994 0.060309 -0.216794
 C 2.642234 -1.174545 0.214634
 C 2.863704 1.065391 1.102840
 C 4.121278 1.125820 0.506137
 C 3.908908 -1.115956 -0.387456
 Br 1.579931 -2.751658 -0.033972
 Br 6.375981 0.201265 -0.999563
 O 4.431690 -2.129478 -1.111869
 O 0.899134 -0.151299 1.566309
 C 2.328952 2.225573 1.915911
 C 0.957356 2.746155 1.540041
 N 0.104387 3.236905 2.364688

O 0.549973 3.237265 3.683617
 C 0.518413 2.769962 0.097215
 N -0.808735 2.928991 -0.120502
 C -1.366619 3.078490 -1.458144
 O 1.339936 2.646885 -0.817628
 C -1.547934 1.744526 -2.221334
 O -0.310305 1.135692 -2.523724
 C -2.449631 0.790050 -1.444920
 C -4.104278 -0.888143 0.136372
 C -3.835971 0.963886 -1.439349
 C -1.897381 -0.238924 -0.677939
 C -2.711172 -1.047384 0.105273
 C -4.637413 0.134620 -0.663580
 Br -1.925601 -2.411115 1.190512
 Br -6.542813 0.367326 -0.663274
 O -4.851056 -1.705832 0.910359
 H 4.711010 2.031667 0.598743
 H 3.782262 -2.854892 -1.147286
 H 0.460238 -1.012488 1.432008
 H 3.039127 3.059316 1.844181
 H 2.279055 1.954790 2.975603
 H -0.209575 3.603960 4.164068
 H -1.403745 3.004695 0.692995
 H -0.703641 3.725795 -2.043627
 H -2.333369 3.581006 -1.361765
 H -2.055261 2.002278 -3.165950
 H 0.412036 1.659739 -2.118934
 H -4.300616 1.739402 -2.041389
 H -0.828589 -0.404745 -0.716809
 H -5.788558 -1.460323 0.800210
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4075592**

Comp_08E_c31
B3LYP/6-31G* Geometry
 C -2.564873 1.358925 0.600655
 C -0.815335 -0.411910 1.850299
 C -2.769136 -0.026419 0.528713
 C -1.454727 1.864598 1.302095
 C -0.603975 0.958550 1.934590
 C -1.891052 -0.937704 1.123556
 Br -4.256995 -0.682483 -0.467906
 Br 0.407373 -1.633984 2.666602
 O -2.109292 -2.263858 0.960399
 O -3.405978 2.241660 0.012769
 C -1.170481 3.360421 1.323081
 C 0.285371 3.629523 1.039999
 N 1.200942 3.903602 1.895275
 O 0.726130 3.943072 3.211060
 C 0.735390 3.510732 -0.402165
 N 2.079680 3.422250 -0.591379
 C 2.666129 3.143830 -1.883600
 O -0.091829 3.483436 -1.309732
 C 3.409625 1.795053 -1.902771

O 4.462864 1.827228 -0.931514
 C 2.535620 0.584234 -1.603769
 C 0.976602 -1.739694 -1.112886
 C 3.045383 -0.479929 -0.850967
 C 1.239146 0.476915 -2.119121
 C 0.490735 -0.668202 -1.877915
 C 2.279763 -1.615706 -0.612698
 Br -1.284555 -0.811987 -2.580266
 Br 3.010769 -3.040398 0.417444
 O 0.259712 -2.855371 -0.848599
 H 0.249683 1.327994 2.492004
 H -1.367872 -2.742250 1.380323
 H -4.077784 1.742234 -0.488136
 H -1.441036 3.798417 2.288039
 H -1.761256 3.840151 0.540786
 H 1.521023 4.185077 3.712963
 H 2.668843 3.358070 0.228804
 H 3.388052 3.930735 -2.147126
 H 1.864563 3.181446 -2.623715
 H 3.843995 1.674372 -2.909541
 H 5.175805 2.377725 -1.290112
 H 4.045283 -0.415690 -0.442515
 H 0.784417 1.282052 -2.683340
 H -0.636748 -2.740109 -1.218934
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4155942**

Comp_08E_c32
B3LYP/6-31G* Geometry
 C -0.572388 -2.314822 1.010410
 C -1.692979 0.133519 1.764377
 C -1.749685 -1.839852 0.416985
 C 0.049863 -1.550304 2.012764
 C -0.531914 -0.332692 2.370863
 C -2.324991 -0.609675 0.761259
 Br -2.608884 -2.912707 -0.922793
 Br -2.428051 1.812776 2.280712
 O -3.442702 -0.121929 0.173352
 O -0.008137 -3.498108 0.665739
 C 1.321116 -2.048341 2.685655
 C 2.578699 -1.695044 1.920494
 N 3.386558 -2.502413 1.336802
 O 3.026214 -3.841579 1.450180
 C 2.959939 -0.231537 1.861546
 N 3.941626 0.093750 0.977833
 C 4.295675 1.465574 0.686737
 O 2.395313 0.584443 2.587646
 C 3.956658 1.867522 -0.761123
 O 4.816387 1.078896 -1.583266
 C 2.488472 1.671334 -1.106422
 C -0.263694 1.250066 -1.650165
 C 1.545143 2.653732 -0.791046
 C 2.048590 0.485694 -1.703767
 C 0.699577 0.283637 -1.970607

C 0.199495 2.437853 -1.060140
 Br 0.129264 -1.349452 -2.766666
 Br -1.094295 3.777529 -0.627878
 O -1.563545 1.006617 -1.923591
 H -0.045472 0.278653 3.120817
 H -3.684871 -0.714375 -0.561351
 H -0.532704 -3.900686 -0.048930
 H 1.282399 -3.131069 2.812757
 H 1.395461 -1.580658 3.672010
 H 3.740063 -4.291205 0.970472
 H 4.336373 -0.650272 0.417652
 H 5.371542 1.620756 0.834075
 H 3.751027 2.095288 1.392907
 H 4.207528 2.936207 -0.863194
 H 4.607538 1.276114 -2.510429
 H 1.850386 3.587289 -0.328662
 H 2.763110 -0.288180 -1.957552
 H -2.104581 1.710950 -1.518554
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4150949**

Comp_08E_c33
B3LYP/6-31G* Geometry
 C -2.511326 0.828904 -0.915656
 C -0.954994 -1.401811 -1.582897
 C -2.771301 -0.431352 -0.361203
 C -1.466031 0.959399 -1.852643
 C -0.694007 -0.166681 -2.157277
 C -2.008749 -1.563531 -0.673743
 Br -4.153961 -0.617388 0.939608
 Br 0.163861 -2.894325 -1.979158
 O -2.232154 -2.776523 -0.129731
 O -3.307724 1.849735 -0.523809
 C -1.155472 2.295009 -2.519755
 C -0.276408 3.175439 -1.661434
 N -0.652075 4.129365 -0.893847
 O -2.050939 4.331042 -0.932636
 C 1.213832 2.876493 -1.680601
 N 1.960877 3.531653 -0.756836
 C 3.355962 3.218347 -0.522712
 O 1.663149 2.081209 -2.501403
 C 3.586448 2.583167 0.861621
 O 3.224125 3.594395 1.801327
 C 2.805966 1.294404 1.063949
 C 1.294918 -1.093840 1.318912
 C 3.319645 0.077766 0.606427
 C 1.543528 1.305986 1.666020
 C 0.806008 0.134008 1.791438
 C 2.574847 -1.087447 0.738583
 Br -0.926438 0.191386 2.578886
 Br 3.299450 -2.747671 0.126824
 O 0.537001 -2.199416 1.461386
 H 0.140842 -0.063052 -2.840759
 H -2.942130 -2.683619 0.534076

H -2.914531 2.717003 -0.750173
 H -2.073542 2.831463 -2.776257
 H -0.606701 2.100469 -3.443489
 H -2.188050 5.027041 -0.269434
 H 1.482532 4.133204 -0.098636
 H 3.958829 4.132398 -0.580738
 H 3.673511 2.536168 -1.313108
 H 4.664157 2.363000 0.934288
 H 3.305462 3.218125 2.692367
 H 4.300715 0.029250 0.144109
 H 1.126976 2.237316 2.031265
 H 0.863519 -2.895088 0.860423
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4194950**

Comp_08E_c37
B3LYP/6-31G* Geometry
 C 2.094683 -0.077526 0.982629
 C 4.647402 0.087777 -0.145799
 C 2.632873 -1.140386 0.250409
 C 2.835253 1.106420 1.124174
 C 4.106049 1.160154 0.555349
 C 3.911571 -1.088803 -0.325448
 Br 1.564274 -2.712159 -0.013800
 Br 6.393330 0.220444 -0.890271
 O 4.448427 -2.107230 -1.032452
 O 0.862805 -0.112682 1.559416
 C 2.274147 2.277560 1.901649
 C 0.919141 2.796652 1.465769
 N 0.057654 3.340876 2.246888
 O 0.480116 3.403406 3.572068
 C 0.508023 2.750218 0.014947
 N -0.812888 2.904315 -0.236512
 C -1.342621 2.993375 -1.591484
 O 1.346453 2.577176 -0.876434
 C -1.512726 1.626655 -2.295972
 O -0.270532 1.010235 -2.564250
 C -2.420579 0.704553 -1.486906
 C -4.099529 -0.908135 0.136825
 C -3.795358 0.952460 -1.403719
 C -1.887355 -0.370680 -0.776142
 C -2.721828 -1.143223 0.021842
 C -4.617953 0.162498 -0.609349
 Br -1.980930 -2.598728 1.045227
 Br -6.484225 0.529861 -0.520332
 O -4.931616 -1.643195 0.906856
 H 4.693671 2.067017 0.651283
 H 3.799110 -2.831524 -1.081993
 H 0.447242 -0.984371 1.427789
 H 2.989218 3.108664 1.850553
 H 2.180751 2.020550 2.962130
 H -0.280353 3.809489 4.018335
 H -1.424152 3.026903 0.559047
 H -0.666697 3.612098 -2.192683

H -2.309242 3.501798 -1.536795
H -2.010495 1.840201 -3.256314
H 0.443633 1.539861 -2.152091
H -4.242758 1.767517 -1.965483
H -0.832499 -0.596463 -0.869344
H -4.408881 -2.336776 1.349782

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4064564**

Comp_08E_c38

B3LYP/6-31G* Geometry

C 3.510351 -1.178021 0.395453
C 4.767040 1.262169 -0.030366
C 4.594041 -1.078934 -0.485351
C 3.050770 -0.038584 1.081532
C 3.691621 1.175466 0.847080
C 5.245830 0.138645 -0.716558
Br 5.190503 -2.649918 -1.389106
Br 5.638093 2.942469 -0.334652
O 6.285517 0.167990 -1.577916
O 2.863877 -2.346369 0.626867
C 1.890502 -0.154364 2.054474
C 0.559586 -0.363252 1.373845
N -0.135005 0.531060 0.767401
O 0.458518 1.784303 0.740590
C -0.163742 -1.679112 1.529392
N -1.057707 -1.973677 0.545993
C -2.100574 -2.968052 0.746597
O 0.020570 -2.386722 2.521746
C -3.289657 -2.434256 1.587299
O -2.874944 -2.071399 2.893077
C -3.925679 -1.230848 0.904374
C -4.880950 1.003309 -0.565808
C -4.930415 -1.390869 -0.052511
C -3.424829 0.053808 1.143320
C -3.876441 1.138092 0.404516
C -5.397334 -0.288013 -0.759903
Br -3.091915 2.858603 0.688027
Br -6.785462 -0.506248 -2.066521
O -5.295247 2.090246 -1.251484
H 3.340665 2.069008 1.350794
H 6.616798 1.084848 -1.621070
H 3.291119 -3.050300 0.103271
H 1.833571 0.765568 2.645633
H 2.042408 -0.995885 2.736002
H -0.275196 2.342219 0.423022
H -1.236010 -1.226294 -0.114054
H -1.651569 -3.826548 1.255691
H -2.457300 -3.303121 -0.232014
H -4.033531 -3.247169 1.638001
H -1.984269 -2.432240 3.055822
H -5.354447 -2.370154 -0.253399
H -2.666919 0.195686 1.901136
H -5.996001 1.813454 -1.871091

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4031821**

Comp_08E_c40

B3LYP/6-31G* Geometry

C -0.364196 0.108634 -2.287652
C -0.667112 2.414455 -0.750313
C 0.753523 0.876565 -1.927030
C -1.655017 0.543690 -1.920963
C -1.785845 1.693890 -1.139079
C 0.625012 2.029367 -1.141756
Br 2.482676 0.316756 -2.460991
Br -0.855828 3.968689 0.350728
O 1.739520 2.702904 -0.781075
O -0.165336 -1.023642 -3.004399
C -2.895957 -0.222512 -2.358609
C -3.445240 -1.048595 -1.222898
N -4.498509 -0.803544 -0.531451
O -5.181752 0.334794 -0.948134
C -2.646383 -2.250935 -0.776827
N -2.942550 -2.722655 0.444165
C -2.304137 -3.834742 1.153005
O -1.759766 -2.716857 -1.516795
C -0.756904 -3.907582 1.119693
O -0.297043 -4.573632 -0.040589
C -0.022421 -2.583584 1.347558
C 1.453770 -0.180455 1.709361
C -0.589728 -1.478889 1.992005
C 1.304858 -2.486961 0.912140
C 2.022739 -1.317019 1.112048
C 0.129585 -0.297524 2.151406
Br 3.853173 -1.211466 0.567426
Br -0.710007 1.219823 2.939341
O 2.108253 0.989405 1.869304
H -2.772060 2.028304 -0.834451
H 1.474188 3.411457 -0.164711
H -0.782777 -1.711946 -2.668410
H -2.654113 -0.879307 -3.199000
H -3.669069 0.472173 -2.691037
H -5.942659 0.361498 -0.345487
H -3.712082 -2.246732 0.900138
H -2.663210 -4.792823 0.759537
H -2.646410 -3.754770 2.189220
H -0.500036 -4.590346 1.941529
H -0.610052 -4.035320 -0.796498
H -1.607070 -1.505860 2.362649
H 1.764475 -3.329648 0.410153
H 2.967485 0.923051 1.410738

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4192150**

Comp_08E_c42

B3LYP/6-31G* Geometry

C 2.644178 0.334816 0.893682
 C 0.587854 -1.369011 1.701884
 C 2.557928 -0.972045 0.387740
 C 1.699275 0.775922 1.844905
 C 0.675671 -0.091929 2.232210
 C 1.519975 -1.832554 0.761690
 Br 3.830868 -1.568848 -0.885861
 Br -0.849741 -2.526689 2.204407
 O 1.434631 -3.052639 0.179397
 O 3.657955 1.106909 0.438647
 C 1.747522 2.184733 2.425016
 C 1.044377 3.172911 1.523042
 N 1.584984 3.959487 0.669095
 O 2.994711 3.852936 0.662637
 C -0.473832 3.189061 1.594467
 N -1.107029 3.859321 0.600412
 C -2.543061 3.801848 0.414462
 O -1.044781 2.600062 2.508834
 C -2.926343 3.167705 -0.935772
 O -2.388030 4.047943 -1.923170
 C -2.429929 1.739954 -1.103493
 C -1.471913 -0.922252 -1.330747
 C -3.191938 0.660484 -0.641927
 C -1.192179 1.479031 -1.697647
 C -0.734921 0.171641 -1.810644
 C -2.721305 -0.642963 -0.753103
 Br 0.965076 -0.180590 -2.611872
 Br -3.782896 -2.086060 -0.116737
 O -1.050611 -2.201665 -1.412051
 H -0.075283 0.253965 2.932663
 H 0.643696 -3.497962 0.541269
 H 3.488709 2.054101 0.614606
 H 2.775841 2.509238 2.605110
 H 1.217829 2.187376 3.379935
 H 3.254657 4.453086 -0.055151
 H -0.542550 4.295809 -0.117120
 H -2.967990 4.812583 0.444538
 H -2.956330 3.223405 1.242592
 H -4.027339 3.167803 -0.983845
 H -2.569047 3.664410 -2.796235
 H -4.163220 0.827743 -0.186376
 H -0.586233 2.293211 -2.077047
 H -0.133367 -2.212362 -1.748235
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4197852**

Comp_08E_c44
B3LYP/6-31G* Geometry
 C 1.266313 -1.292801 1.846106
 C 1.543578 1.446705 1.278867
 C 2.299951 -0.818779 1.026229
 C 0.384377 -0.359413 2.427340
 C 0.535849 0.997042 2.121884
 C 2.451108 0.538599 0.715630

Br 3.537531 -2.057269 0.266007
 Br 1.691170 3.296042 0.872549
 O 3.410990 0.990359 -0.128761
 O 1.171966 -2.624182 2.063249
 C -0.719418 -0.809131 3.375664
 C -2.058403 -0.875577 2.679823
 N -3.005091 -0.012659 2.756307
 O -2.721385 1.043103 3.616442
 C -2.296158 -2.017008 1.722203
 N -3.427121 -1.959871 0.985510
 C -3.620858 -2.759506 -0.208957
 O -1.475866 -2.940891 1.627139
 C -3.774487 -1.848170 -1.447985
 O -4.929926 -1.023752 -1.285364
 C -2.571945 -0.941065 -1.647340
 C -0.284749 0.720123 -1.905565
 C -1.343207 -1.482406 -2.035841
 C -2.653669 0.432835 -1.401388
 C -1.529975 1.242485 -1.523775
 C -0.230210 -0.659607 -2.162364
 Br -1.659939 3.099683 -1.132752
 Br 1.451384 -1.405470 -2.684064
 O 0.770233 1.550843 -2.009488
 H -0.150898 1.718580 2.551829
 H 3.983097 0.231092 -0.355430
 H 0.213893 -2.869094 2.047056
 H -0.796285 -0.111116 4.211239
 H -0.480150 -1.795626 3.782703
 H -3.514092 1.598923 3.542270
 H -3.995786 -1.126780 1.089837
 H -4.520850 -3.383695 -0.110417
 H -2.763061 -3.428475 -0.305002
 H -3.890835 -2.497972 -2.329774
 H -5.712242 -1.594344 -1.333665
 H -1.238797 -2.543510 -2.239462
 H -3.598438 0.873591 -1.111416
 H 1.588134 1.031812 -2.122293
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4212650**

Comp_08E_c45
B3LYP/6-31G* Geometry
 C 3.989744 0.685851 0.165542
 C 6.488524 -0.524133 0.250215
 C 5.081472 1.257041 -0.499656
 C 4.149528 -0.510196 0.889276
 C 5.410257 -1.101069 0.912240
 C 6.351719 0.668691 -0.471214
 Br 4.820793 2.882080 -1.464242
 Br 8.216076 -1.353407 0.301821
 O 7.363486 1.270330 -1.132838
 O 2.754265 1.241731 0.144716
 C 2.978243 -1.108133 1.649994
 C 1.827835 -1.551609 0.776572

N 1.847241 -2.525837 -0.058467
 O 3.078435 -3.172288 -0.099556
 C 0.496793 -0.848849 0.925474
 N -0.443794 -1.155526 0.004242
 C -1.742413 -0.491598 -0.102223
 O 0.312901 -0.064456 1.862356
 C -2.728622 -0.779797 1.062212
 O -2.429390 -0.013702 2.206223
 C -4.150453 -0.460235 0.624605
 C -6.767091 0.175621 -0.267573
 C -4.717343 0.787354 0.902432
 C -4.899131 -1.394908 -0.094711
 C -6.178764 -1.071301 -0.528684
 C -5.999324 1.096115 0.462897
 Br -7.209142 -2.360471 -1.511162
 Br -6.746911 2.802992 0.856565
 O -8.009663 0.518006 -0.672468
 H 5.554117 -2.030327 1.452402
 H 8.168844 0.733632 -1.008466
 H 2.793243 2.074185 -0.363249
 H 2.575988 -0.382645 2.362453
 H 3.337283 -1.977192 2.212294
 H 2.931589 -3.875898 -0.752342
 H -0.174995 -1.833359 -0.696818
 H -2.179950 -0.826145 -1.046057
 H -1.600110 0.594803 -0.162727
 H -2.667251 -1.861400 1.278556
 H -1.452901 0.065381 2.266426
 H -4.152980 1.505710 1.483964
 H -4.496746 -2.379778 -0.311944
 H -8.394914 -0.239242 -1.151145
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4061153**

Comp_08E_c46
B3LYP/6-31G* Geometry
 C 2.434568 -0.257256 1.559872
 C 3.400791 0.564268 -0.947911
 C 2.843386 -1.186985 0.593930
 C 2.526467 1.116751 1.258946
 C 3.001305 1.496816 -0.001541
 C 3.327473 -0.807549 -0.664885
 Br 2.696689 -3.054513 0.967457
 Br 4.049026 1.137768 -2.641235
 O 3.713476 -1.696536 -1.601541
 O 1.988324 -0.753666 2.736359
 C 2.127073 2.185542 2.270525
 C 0.628705 2.338944 2.388210
 N -0.128406 1.867779 3.308910
 O 0.595714 1.154284 4.284703
 C -0.076958 3.083003 1.272745
 N -1.422950 3.000240 1.254316
 C -2.247328 3.628880 0.224920
 O 0.587396 3.701078 0.433650

C -2.234896 2.893787 -1.138939
 O -1.011321 3.070101 -1.824121
 C -2.579033 1.418254 -0.963727
 C -3.216638 -1.299230 -0.462087
 C -3.909140 1.005277 -0.836898
 C -1.565616 0.463271 -0.857338
 C -1.889304 -0.862994 -0.600902
 C -4.221317 -0.328478 -0.594398
 Br -0.489672 -2.157656 -0.374427
 Br -6.044047 -0.858702 -0.436046
 O -3.561155 -2.581451 -0.213496
 H 3.052147 2.551087 -0.248433
 H 3.588146 -2.594312 -1.239229
 H 1.618479 -0.055941 3.312760
 H 2.523964 3.144530 1.929951
 H 2.549579 1.979980 3.258488
 H -0.101199 0.819190 4.873003
 H -1.856507 2.399907 1.943261
 H -1.898085 4.656161 0.074435
 H -3.268855 3.669785 0.612346
 H -3.027217 3.362733 -1.742600
 H -0.342266 3.415756 -1.201565
 H -4.719888 1.721770 -0.934215
 H -0.531892 0.759666 -0.990617
 H -2.743469 -3.112112 -0.168930
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4151295**

Comp_08E_c48
B3LYP/6-31G* Geometry
 C 2.639796 0.526710 0.997861
 C 0.703932 -1.336484 1.681630
 C 2.664101 -0.753969 0.438357
 C 1.631807 0.890354 1.902384
 C 0.671303 -0.064757 2.238654
 C 1.686048 -1.703915 0.751009
 Br 4.013878 -1.175278 -0.838219
 Br -0.643323 -2.617465 2.117755
 O 1.720000 -2.905114 0.131430
 O 3.575671 1.471270 0.675591
 C 1.533673 2.316862 2.415855
 C 0.707447 3.194026 1.493518
 N 1.112479 3.981509 0.561958
 O 2.452080 4.070140 0.282287
 C -0.793441 3.088742 1.659452
 N -1.532173 3.744473 0.725824
 C -2.944829 3.499341 0.540215
 O -1.275248 2.419999 2.573720
 C -3.235293 2.892714 -0.853295
 O -2.748675 3.770879 -1.870640
 C -2.585438 1.538037 -1.058929
 C -1.364934 -1.006292 -1.351775
 C -3.233609 0.376127 -0.628052
 C -1.324450 1.424033 -1.650961

C -0.738740 0.171555 -1.787590
C -2.636590 -0.871149 -0.775494
Br 0.997408 0.007371 -2.585449
Br -3.560277 -2.431284 -0.199959
O -0.815739 -2.236199 -1.471852
H -0.133837 0.212204 2.908938
H 0.941256 -3.415890 0.428690
H 4.166231 1.107057 -0.012412
H 2.527687 2.750564 2.561183
H 1.024877 2.311370 3.382402
H 2.914589 3.267194 0.613294
H -1.019218 4.207174 -0.015718
H -3.512432 4.437568 0.637469
H -3.272473 2.829600 1.338998
H -4.327083 2.773973 -0.939895
H -3.234763 4.607496 -1.798914
H -4.219212 0.431121 -0.176230
H -0.810280 2.304199 -2.015277
H 0.074138 -2.141961 -1.862799

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.413996**

Comp_08E_c50
B3LYP/6-31G* Geometry

C 0.263095 1.740783 1.572973
C 2.043279 -0.392726 1.629228
C 1.416945 1.751490 0.774588
C 0.004700 0.648827 2.423508
C 0.912883 -0.409225 2.436591
C 2.315706 0.680935 0.773768
Br 1.750698 3.258069 -0.339205
Br 3.273535 -1.861462 1.646197
O 3.387457 0.717243 -0.059457
O -0.626394 2.760633 1.563664
C -1.237691 0.632160 3.300969
C -2.486820 0.201267 2.561360
N -3.538783 0.901565 2.342651
O -3.479378 2.187829 2.867725
C -2.526447 -1.220898 2.048265
N -3.544075 -1.523634 1.197158
C -3.582556 -2.770969 0.465104
O -1.670547 -2.029465 2.403534
C -3.435720 -2.569156 -1.054834
O -4.643633 -1.934881 -1.472720
C -2.200905 -1.760861 -1.428282
C 0.111906 -0.219984 -2.014350
C -0.940194 -2.363050 -1.472814
C -2.296587 -0.388949 -1.680513
C -1.163286 0.362584 -1.967782
C 0.185036 -1.599532 -1.758086
Br -1.331871 2.234927 -2.269567
Br 1.911562 -2.424434 -1.794556
O 1.177323 0.554544 -2.300971
H 0.712488 -1.270991 3.060619

H 3.942024 -0.060842 0.144068
H -0.333479 3.417064 0.903277
H -1.411203 1.620469 3.729340
H -1.075478 -0.078919 4.117069
H -4.336145 2.561027 2.606029
H -4.188679 -0.783385 0.952401
H -4.530528 -3.293343 0.642908
H -2.767166 -3.388501 0.846639
H -3.358680 -3.572309 -1.505561
H -4.583049 -1.774188 -2.428120
H -0.824317 -3.424413 -1.276929
H -3.261832 0.101451 -1.640506
H 2.000069 0.069443 -2.102688

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4169458**

Comp_08E_c51
B3LYP/6-31G* Geometry

C 1.720602 -1.510682 1.531886
C 1.302408 1.245372 1.545935
C 2.515885 -0.656033 0.752316
C 0.677760 -0.972038 2.309395
C 0.498329 0.411831 2.312682
C 2.312226 0.726789 0.724987
Br 3.918125 -1.412368 -0.297233
Br 1.051497 3.140752 1.579796
O 3.084943 1.489533 -0.084846
O 1.931171 -2.845041 1.572868
C -0.254698 -1.878744 3.100022
C -1.682536 -1.732393 2.628696
N -2.606946 -1.033499 3.177050
O -2.179286 -0.361188 4.328373
C -2.058235 -2.450283 1.348639
N -3.306670 -2.203122 0.865286
C -3.736941 -2.725494 -0.414157
O -1.250247 -3.200381 0.807982
C -3.913803 -1.643341 -1.493668
O -5.087572 -0.919058 -1.132128
C -2.691722 -0.741281 -1.639218
C -0.402063 0.923153 -1.858595
C -2.743882 0.604805 -1.271073
C -1.484558 -1.255734 -2.124788
C -0.369526 -0.434436 -2.220657
C -1.624898 1.422921 -1.393060
Br 1.296501 -1.145707 -2.836727
Br -1.745357 3.257003 -0.900964
O 0.666913 1.746072 -1.938033
H -0.290307 0.842747 2.920222
H 2.782352 2.414037 0.006217
H 2.629809 -3.069478 0.930439
H -0.205949 -1.643732 4.166593
H 0.046136 -2.916163 2.949274
H -2.987217 0.092629 4.617591
H -3.879620 -1.526934 1.352854

H -4.694512 -3.248990 -0.308629
H -2.979442 -3.446223 -0.727272
H -4.081269 -2.173670 -2.446020
H -5.278725 -0.282370 -1.839186
H -3.660182 1.020835 -0.870247
H -1.397971 -2.299089 -2.409302
H 1.451902 1.217982 -2.179207
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4146842**

Comp_08E_c53
B3LYP/6-31G* Geometry
C 2.681584 0.447422 0.975610
C 0.672650 -1.328069 1.681880
C 2.653942 -0.840209 0.432172
C 1.689872 0.861990 1.876112
C 0.692434 -0.050043 2.224712
C 1.638142 -1.745868 0.755446
Br 3.979661 -1.328262 -0.846288
Br -0.731323 -2.544930 2.125067
O 1.620058 -2.953278 0.146246
O 3.652497 1.350321 0.639178
C 1.645763 2.298849 2.367965
C 0.843527 3.189989 1.436929
N 1.268931 3.946846 0.489451
O 2.609120 3.984057 0.199255
C -0.658873 3.134860 1.613751
N -1.386375 3.816768 0.692682
C -2.813667 3.634697 0.543205
O -1.151822 2.473389 2.528562
C -3.176098 2.976275 -0.802868
O -2.743587 3.905180 -1.796540
C -2.562688 1.597881 -1.001825
C -1.411838 -0.976881 -1.325439
C -3.247115 0.447322 -0.593844
C -1.299279 1.454205 -1.584604
C -0.748600 0.187957 -1.740830
C -2.682882 -0.813483 -0.752563
Br 0.981992 -0.014784 -2.540884
Br -3.648705 -2.355810 -0.199824
O -0.899988 -2.220047 -1.462616
H -0.101188 0.268368 2.890092
H 0.826349 -3.431908 0.457223
H 4.228362 0.953357 -0.042979
H 2.655422 2.699307 2.500223
H 1.143832 2.326123 3.337623
H 3.047546 3.175114 0.547353
H -0.874539 4.303403 -0.033476
H -3.326876 4.602880 0.588190
H -3.154797 3.017934 1.376898
H -4.273722 2.877142 -0.823402
H -2.911389 3.513689 -2.668593
H -4.234056 0.525337 -0.148077
H -0.749826 2.326505 -1.918038

H -0.001317 -2.148390 -1.837973
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4157550**

Comp_08E_c54
B3LYP/6-31G* Geometry
C -2.811592 0.904836 0.513198
C -0.692479 -0.327544 1.834626
C -2.712011 -0.491871 0.566039
C -1.825835 1.699404 1.127282
C -0.784762 1.058993 1.797443
C -1.644482 -1.135628 1.200505
Br -4.036545 -1.537634 -0.321002
Br 0.790671 -1.182524 2.687805
O -1.576484 -2.486366 1.159641
O -3.832712 1.531096 -0.117048
C -1.881778 3.215868 1.009014
C -0.518516 3.781795 0.708025
N 0.238801 4.447017 1.501276
O -0.320697 4.640140 2.766928
C 0.050010 3.493096 -0.667558
N 1.390633 3.688781 -0.797345
C 2.123988 3.404074 -2.017665
O -0.678765 3.076476 -1.563205
C 3.091644 2.212768 -1.863920
O 4.073002 2.527792 -0.872723
C 2.430939 0.862865 -1.581732
C 1.296169 -1.682914 -1.017477
C 3.123547 -0.087496 -0.819268
C 1.169865 0.519459 -2.083466
C 0.632848 -0.732114 -1.808640
C 2.563832 -1.328104 -0.537759
Br -1.098906 -1.197147 -2.481372
Br 3.520695 -2.568575 0.543000
O 0.775384 -2.890054 -0.702987
H -0.018520 1.651770 2.285583
H -0.736376 -2.759895 1.576629
H -4.389165 0.856572 -0.549755
H -2.273223 3.670962 1.922786
H -2.547002 3.473179 0.181856
H 0.351065 5.179062 3.214797
H 1.868476 4.113385 -0.013255
H 2.727031 4.277604 -2.289353
H 1.393496 3.238185 -2.811670
H 3.665057 2.144761 -2.797937
H 3.656098 2.380505 -0.007287
H 4.110884 0.144182 -0.437629
H 0.574039 1.224021 -2.649851
H -0.131083 -2.936668 -1.064203

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4144911**

Comp_08E_c56

B3LYP/6-31G* Geometry

C 0.286175 -0.260121 2.284229
 C 2.426889 -1.156456 0.757480
 C 1.225129 0.646580 1.770943
 C 0.417875 -1.636784 2.024209
 C 1.498605 -2.063375 1.254220
 C 2.304259 0.218505 0.991569
 Br 1.002407 2.499859 2.143937
 Br 3.917731 -1.761588 -0.281630
 O 3.163954 1.142884 0.493134
 O -0.766239 0.142280 3.034579
 C -0.606883 -2.619106 2.565578
 C -1.930333 -2.545676 1.835710
 N -3.072599 -2.238398 2.331142
 O -3.038261 -1.961821 3.694312
 C -1.926172 -2.902987 0.366235
 N -3.035432 -2.539945 -0.333558
 C -3.114472 -2.649556 -1.772380
 O -0.964209 -3.488152 -0.127113
 C -3.365636 -1.277283 -2.430549
 O -4.606740 -0.743532 -1.964201
 C -2.271174 -0.268896 -2.121479
 C -0.200788 1.577236 -1.514121
 C -0.953936 -0.524859 -2.514266
 C -2.547971 0.915072 -1.432790
 C -1.529663 1.814570 -1.134668
 C 0.049767 0.387013 -2.215636
 Br -1.934246 3.399370 -0.158328
 Br 1.851916 0.017871 -2.744434
 O 0.747763 2.483788 -1.202534
 H 1.601754 -3.116074 1.020039
 H 3.884024 0.660926 0.042281
 H -0.739343 1.115955 3.103325
 H -0.785802 -2.438916 3.627198
 H -0.213387 -3.633301 2.445434
 H -3.963959 -1.743573 3.887053
 H -3.748421 -2.012520 0.153889
 H -3.928630 -3.330848 -2.064994
 H -2.177764 -3.094246 -2.116077
 H -3.411031 -1.433295 -3.520988
 H -5.318473 -1.290480 -2.330133
 H -0.694319 -1.434351 -3.045647
 H -3.561687 1.132922 -1.123678
 H 1.629785 2.096435 -1.356004

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4152807

Comp_08E_c57**B3LYP/6-31G* Geometry**

C -2.432191 0.949729 -0.946356
 C -1.010589 -1.375949 -1.591411
 C -2.766687 -0.287377 -0.380086
 C -1.379465 1.009236 -1.882649
 C -0.675402 -0.163504 -2.175759

C -2.072605 -1.465680 -0.681791
 Br -4.166971 -0.381867 0.911274
 Br 0.012220 -2.937598 -1.978292
 O -2.370851 -2.658420 -0.129626
 O -3.170177 2.018628 -0.568468
 C -0.992206 2.316714 -2.565439
 C -0.069055 3.157815 -1.714612
 N -0.393369 4.139838 -0.958920
 O -1.778610 4.418052 -1.004137
 C 1.404156 2.782599 -1.727475
 N 2.171599 3.385632 -0.783371
 C 3.533586 2.978843 -0.506842
 O 1.823703 1.984086 -2.559680
 C 3.667334 2.420957 0.929166
 O 3.243729 3.414155 1.866373
 C 2.829083 1.175509 1.138071
 C 1.212962 -1.144892 1.355329
 C 3.283659 -0.053088 0.653076
 C 1.575038 1.235207 1.752492
 C 0.784077 0.095878 1.852269
 C 2.489598 -1.187009 0.771653
 Br -0.947003 0.219999 2.636234
 Br 3.141170 -2.866480 0.130435
 O 0.402789 -2.216501 1.476136
 H 0.163459 -0.116831 -2.860920
 H -3.070714 -2.516212 0.536226
 H -2.728156 2.859464 -0.803933
 H -1.877885 2.899946 -2.833491
 H -0.451146 2.080365 -3.484068
 H -1.879528 5.124920 -0.345933
 H 1.702595 3.963192 -0.096647
 H 4.213998 3.836157 -0.620588
 H 3.812612 2.229184 -1.250651
 H 4.727313 2.169862 1.091257
 H 3.892045 4.135067 1.847458
 H 4.257482 -0.138366 0.181024
 H 1.212896 2.173005 2.154204
 H 0.705409 -2.919863 0.871743

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4174928

Comp_08E_c58**B3LYP/6-31G* Geometry**

C -0.855031 0.127839 2.297972
 C -2.439443 -1.124483 0.354862
 C -1.689693 0.867949 1.447618
 C -0.779251 -1.267662 2.134313
 C -1.591285 -1.867278 1.168647
 C -2.480128 0.270662 0.457181
 Br -1.742891 2.775516 1.636156
 Br -3.557854 -2.003191 -0.910185
 O -3.261540 0.980169 -0.393924
 O -0.127938 0.703831 3.281088
 C 0.196631 -2.097232 2.958018

C 1.336731 -2.603243 2.101753
 N 1.419340 -3.750996 1.536224
 O 0.307756 -4.566524 1.783228
 C 2.494113 -1.655018 1.856579
 N 3.397436 -2.044285 0.914548
 C 4.481609 -1.180760 0.499178
 O 2.574042 -0.605911 2.487704
 C 4.332529 -0.669519 -0.945619
 O 4.513080 -1.815120 -1.776970
 C 3.002615 0.026171 -1.200488
 C 0.494941 1.295102 -1.591348
 C 2.795721 1.347821 -0.788701
 C 1.951698 -0.654859 -1.817708
 C 0.731241 -0.020310 -2.015835
 C 1.564511 1.965040 -0.975863
 Br -0.704792 -0.953366 -2.865802
 Br 1.303271 3.753908 -0.380258
 O -0.686122 1.932767 -1.749622
 H -1.550558 -2.943860 1.044292
 H -3.166858 1.926711 -0.178919
 H -0.192985 1.672152 3.205956
 H -0.316817 -2.952442 3.404598
 H 0.620673 -1.477428 3.748870
 H 0.540079 -5.384748 1.315527
 H 3.229057 -2.911264 0.421905
 H 5.437265 -1.714629 0.565803
 H 4.501378 -0.339320 1.194339
 H 5.149723 0.051538 -1.112401
 H 4.432408 -1.529868 -2.701292
 H 3.591934 1.905161 -0.305103
 H 2.084221 -1.680918 -2.139360
 H -1.336912 1.300529 -2.111864
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4138040**

Comp_08E_c59
B3LYP/6-31G* Geometry
 C -2.590357 0.469559 -0.924417
 C -0.639171 -1.365563 -1.706335
 C -2.583997 -0.833553 -0.401698
 C -1.616353 0.842038 -1.875990
 C -0.646125 -0.090866 -2.249568
 C -1.600282 -1.760375 -0.763704
 Br -3.900420 -1.340684 0.866407
 Br 0.714737 -2.621150 -2.204931
 O -1.595641 -2.978476 -0.172648
 O -3.561384 1.304505 -0.487376
 C -1.579936 2.242443 -2.477102
 C -0.830105 3.203103 -1.583823
 N -1.331675 4.030723 -0.744804
 O -2.745003 4.003224 -0.747420
 C 0.687283 3.139484 -1.644748
 N 1.343003 3.766463 -0.635533
 C 2.764989 3.610259 -0.409601

O 1.237189 2.536439 -2.561967
 C 3.042193 3.029433 0.996383
 O 2.452492 3.879938 1.984159
 C 2.478983 1.633232 1.174030
 C 1.399543 -0.982313 1.369940
 C 3.182271 0.528107 0.683366
 C 1.240181 1.424368 1.783914
 C 0.721571 0.138326 1.874609
 C 2.654203 -0.754098 0.784139
 Br -0.992580 -0.145942 2.673980
 Br 3.643606 -2.234938 0.117677
 O 0.916244 -2.241471 1.433416
 H 0.124903 0.198973 -2.953876
 H -0.827995 -3.472925 -0.520363
 H -3.338909 2.237643 -0.677715
 H -2.586552 2.621707 -2.672186
 H -1.042725 2.200886 -3.426947
 H -2.975849 4.622179 -0.035698
 H 0.788605 4.181003 0.103316
 H 3.273621 4.582373 -0.497908
 H 3.155365 2.958025 -1.194130
 H 4.134503 2.990261 1.128772
 H 2.939256 4.718838 1.982385
 H 4.153836 0.655313 0.215780
 H 0.687513 2.257519 2.198736
 H 0.007594 -2.211871 1.790863
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4179947**

Comp_08E_c60
B3LYP/6-31G* Geometry
 C 0.280364 -0.068949 2.304398
 C 2.388339 -1.139276 0.844973
 C 1.245234 0.768767 1.725599
 C 0.369701 -1.464351 2.145359
 C 1.435307 -1.978788 1.408548
 C 2.307034 0.252189 0.976698
 Br 1.083824 2.650121 1.967051
 Br 3.857230 -1.865529 -0.146876
 O 3.190432 1.110971 0.406745
 O -0.757196 0.419169 3.023760
 C -0.682560 -2.374412 2.756372
 C -1.997400 -2.333866 2.008445
 N -3.135842 -1.955423 2.461722
 O -3.106776 -1.558901 3.794924
 C -1.989456 -2.822084 0.577092
 N -3.086727 -2.504334 -0.162701
 C -3.151220 -2.731421 -1.588498
 O -1.035141 -3.466741 0.147141
 C -3.370454 -1.413961 -2.360644
 O -4.608747 -0.824244 -1.958765
 C -2.263553 -0.401891 -2.116178
 C -0.167365 1.446879 -1.616606
 C -2.524374 0.825971 -1.502104

C -0.949983 -0.700037 -2.490731
 C 0.066598 0.213699 -2.245909
 C -1.493340 1.726574 -1.255986
 Br 1.862951 -0.209314 -2.753267
 Br -1.874838 3.373562 -0.378192
 O 0.793695 2.356400 -1.356341
 H 1.506037 -3.048389 1.252408
 H 3.890719 0.574953 -0.013222
 H -0.701973 1.394046 3.019035
 H -0.866522 -2.101780 3.797139
 H -0.311600 -3.403587 2.725254
 H -4.028293 -1.301568 3.957052
 H -3.791851 -1.920170 0.268347
 H -3.973539 -3.421223 -1.834608
 H -2.218231 -3.217655 -1.882801
 H -3.402255 -1.657938 -3.435259
 H -5.324245 -1.392961 -2.281741
 H -3.535489 1.077780 -1.210765
 H -0.703993 -1.643202 -2.967260
 H 1.670985 1.947124 -1.476453
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4153128**

Comp_08E_c61
B3LYP/6-31G* Geometry

C -0.732940 -0.023507 -2.170444
 C -2.821482 -0.479675 -0.378856
 C -0.914061 -1.292101 -1.590198
 C -1.629107 1.021429 -1.850867
 C -2.666630 0.773762 -0.948729
 C -1.946131 -1.533318 -0.676777
 Br 0.306489 -2.681896 -1.994708
 Br -4.217126 -0.795553 0.896939
 O -2.032545 -2.752975 -0.086087
 O 0.286364 0.132317 -3.039366
 C -1.465271 2.415788 -2.440074
 C -0.709686 3.314311 -1.488041
 N -1.213175 4.174260 -0.680035
 O -2.602084 4.260069 -0.764845
 C 0.789991 3.151762 -1.418774
 N 1.421497 3.784337 -0.410020
 C 2.830020 3.597772 -0.119085
 O 1.381319 2.463694 -2.263513
 C 3.055367 2.880988 1.224757
 O 2.487993 3.746612 2.207124
 C 2.472461 1.476140 1.276659
 C 1.396037 -1.151786 1.323306
 C 3.188373 0.395903 0.745809
 C 1.214617 1.235532 1.834660
 C 0.702617 -0.057750 1.862659
 C 2.657225 -0.887452 0.759700
 Br -1.011088 -0.381294 2.653783
 Br 3.637158 -2.324281 -0.003088
 O 0.941131 -2.418318 1.338072

H -3.350423 1.573196 -0.684717
 H -2.841163 -2.760969 0.460702
 H 0.684547 1.030413 -2.928127
 H -2.444866 2.855646 -2.635329
 H -0.921263 2.365846 -3.386960
 H -2.811739 4.956707 -0.121897
 H 0.850697 4.295528 0.251831
 H 3.327151 4.573694 -0.072501
 H 3.262165 3.020760 -0.937867
 H 4.146893 2.812681 1.361727
 H 2.582032 3.318598 3.073143
 H 4.169383 0.549378 0.306295
 H 0.636867 2.051070 2.253565
 H -0.014529 -2.424851 1.532785
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4229958**

Comp_08E_c62
B3LYP/6-31G* Geometry

C -0.732630 -0.266592 -2.269326
 C -2.745529 -0.037032 -0.359225
 C -1.119587 -1.373811 -1.496186
 C -1.342703 0.984817 -2.052422
 C -2.358600 1.072564 -1.098864
 C -2.117498 -1.277650 -0.522486
 Br -0.235301 -3.036323 -1.776265
 Br -4.144420 0.100842 0.942600
 O -2.417919 -2.371664 0.223357
 O 0.209542 -0.363297 -3.230424
 C -0.864075 2.225713 -2.793736
 C -0.140190 3.163210 -1.853241
 N -0.641176 4.167191 -1.233010
 O -2.004217 4.355157 -1.505420
 C 1.327259 2.883248 -1.592319
 N 1.873332 3.525923 -0.523883
 C 3.238960 3.291199 -0.108133
 O 1.946622 2.114226 -2.320177
 C 3.345112 2.604508 1.264855
 O 2.851664 3.554734 2.207975
 C 2.602481 1.276758 1.335654
 C 1.202880 -1.193656 1.406956
 C 3.154267 0.121938 0.767806
 C 1.347655 1.189914 1.940749
 C 0.677358 -0.027908 1.981785
 C 2.464095 -1.083097 0.795822
 Br -1.036007 -0.136835 2.830892
 Br 3.219005 -2.624656 -0.025320
 O 0.584287 -2.391479 1.419941
 H -2.837742 2.029350 -0.922819
 H -3.182802 -2.143229 0.786037
 H 0.591252 -1.261041 -3.205418
 H -1.710583 2.753015 -3.240934
 H -0.164172 1.932855 -3.577051
 H -2.207987 5.159476 -1.001718

H 1.276812 4.126210 0.029390
H 3.784608 4.240954 -0.049063
H 3.702248 2.668730 -0.876012
H 4.417613 2.419292 1.441334
H 2.921301 3.161677 3.092732
H 4.125402 0.156322 0.284001
H 0.894251 2.070762 2.379390
H -0.345315 -2.278295 1.693445
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4150364**

Comp_08E_c63
B3LYP/6-31G* Geometry
C -3.208205 -0.339484 -0.516127
C -5.940703 -0.114700 0.025759
C -3.875586 -1.308939 0.238570
C -3.922213 0.766834 -1.011687
C -5.282290 0.856673 -0.723422
C -5.247077 -1.223292 0.525957
Br -2.880403 -2.807579 0.908544
Br -7.801795 0.061898 0.384973
O -5.910290 -2.148241 1.254026
O -1.888876 -0.392012 -0.809586
C -3.201699 1.825438 -1.834848
C -2.159531 2.571887 -1.032639
N -2.387388 3.494958 -0.170501
O -3.746595 3.776276 -0.043418
C -0.710688 2.198136 -1.224540
N 0.110902 2.438861 -0.173750
C 1.513450 2.048812 -0.198312
O -0.322315 1.673869 -2.272399
C 1.735159 0.555808 0.144666
O 1.026740 -0.300727 -0.737940
C 3.226743 0.239518 0.151200
C 6.016614 -0.273930 0.128167
C 4.021421 0.598341 1.243349
C 3.830406 -0.383907 -0.944104
C 5.197686 -0.633853 -0.953720
C 5.387318 0.344915 1.219513
Br 5.988522 -1.491515 -2.457712
Br 6.476231 0.833369 2.723116
O 7.339712 -0.539469 0.077238
H -5.845952 1.709857 -1.084440
H -5.285421 -2.848136 1.515951
H -1.434225 -1.126785 -0.361250
H -3.937706 2.540702 -2.213003
H -2.688123 1.366880 -2.684616
H -3.756552 4.502278 0.601016
H -0.296868 2.846055 0.656530
H 2.060363 2.675209 0.512062
H 1.910504 2.250409 -1.198515
H 1.342301 0.383349 1.158785
H 0.656845 0.231229 -1.472000
H 3.583797 1.066406 2.120218

H 3.218467 -0.694401 -1.782084
H 7.746713 -0.232941 0.908786
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4023018**

Comp_08E_c65
B3LYP/6-31G* Geometry
C -3.920442 -1.530073 0.085446
C -4.652856 1.149590 0.265776
C -5.255737 -1.135854 -0.087902
C -2.935169 -0.559711 0.347557
C -3.326427 0.777194 0.440032
C -5.650836 0.203387 -0.004989
Br -6.571012 -2.474934 -0.438506
Br -5.170785 2.991040 0.394842
O -6.953291 0.513043 -0.183013
O -3.544566 -2.829977 0.024890
C -1.479023 -0.960273 0.542285
C -0.566885 -0.418024 -0.534501
N -0.341450 -0.952045 -1.680331
O -1.041715 -2.132061 -1.872265
C 0.161142 0.877013 -0.272864
N 1.073130 1.254858 -1.191513
C 1.750801 2.549980 -1.183617
O -0.094527 1.532948 0.748841
C 2.784937 2.759656 -0.048159
O 2.165743 3.082322 1.177189
C 3.749078 1.578277 0.068492
C 5.517017 -0.633730 0.267993
C 4.606048 1.244114 -0.986948
C 3.789483 0.810626 1.231820
C 4.657853 -0.271362 1.315546
C 5.469306 0.159328 -0.889560
Br 4.711827 -1.331055 2.916078
Br 6.617038 -0.267801 -2.348947
O 6.369499 -1.680464 0.320591
H -2.578090 1.531813 0.658373
H -7.050148 1.479130 -0.083817
H -4.336061 -3.371400 -0.154976
H -1.401269 -2.048829 0.546715
H -1.122403 -0.575782 1.501627
H -0.759927 -2.411344 -2.758773
H 1.205250 0.626694 -1.973687
H 1.007069 3.352132 -1.106312
H 2.245654 2.644086 -2.153741
H 3.368095 3.646546 -0.336904
H 1.305980 2.609930 1.212254
H 4.618045 1.833710 -1.899082
H 3.153846 1.076995 2.067298
H 6.275914 -2.104416 1.194277
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4074196**

Comp_08E_c66**B3LYP/6-31G* Geometry**

C 2.559003 -0.131128 1.588361
 C 3.193204 0.638303 -0.997822
 C 2.924071 -1.086883 0.637405
 C 2.496725 1.228143 1.247723
 C 2.819128 1.593531 -0.060210
 C 3.244943 -0.725136 -0.675962
 Br 2.905506 -2.928270 1.122887
 Br 3.625018 1.151761 -2.789723
 O 3.572498 -1.695343 -1.552655
 O 2.245351 -0.479026 2.872153
 C 2.034186 2.254987 2.267365
 C 0.524991 2.330256 2.400866
 N -0.227115 1.829072 3.316205
 O 0.330631 1.055165 4.298177
 C -0.200458 3.073600 1.307423
 N -1.545988 2.992445 1.322262
 C -2.402434 3.596099 0.307164
 O 0.441762 3.676988 0.433289
 C -2.371393 2.881152 -1.069264
 O -1.184096 3.162024 -1.782519
 C -2.609362 1.381305 -0.914415
 C -3.049309 -1.386923 -0.473059
 C -3.902164 0.879446 -0.732246
 C -1.534749 0.489907 -0.893445
 C -1.762328 -0.861699 -0.666908
 C -4.117570 -0.477781 -0.518655
 Br -0.276838 -2.080231 -0.576724
 Br -5.891769 -1.129312 -0.283934
 O -3.301683 -2.696027 -0.254473
 H 2.749349 2.635148 -0.350786
 H 3.743509 -1.278481 -2.418792
 H 2.248670 -1.453321 2.946726
 H 2.370296 3.243063 1.943672
 H 2.481581 2.059571 3.247347
 H 1.167100 0.662704 3.960922
 H -1.950344 2.420003 2.053181
 H -2.105239 4.640553 0.159274
 H -3.421204 3.586711 0.703779
 H -3.207110 3.301484 -1.648974
 H -0.503866 3.463988 -1.145927
 H -4.759853 1.545450 -0.762096
 H -0.530521 0.856528 -1.069905
 H -2.452345 -3.175574 -0.263117

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4124010**

Comp_08E_c67**B3LYP/6-31G* Geometry**

C -0.906899 0.284166 2.195264
 C -2.497153 -1.107916 0.379437
 C -1.788713 0.959743 1.337966
 C -0.805978 -1.119232 2.120998

C -1.614701 -1.793276 1.203781
 C -2.599672 0.288805 0.417465
 Br -1.854610 2.868717 1.406010
 Br -3.599280 -2.055871 -0.865939
 O -3.430517 1.005259 -0.366612
 O -0.150863 0.936577 3.105753
 C 0.182198 -1.877908 2.997338
 C 1.293192 -2.498824 2.180954
 N 1.330436 -3.694370 1.719171
 O 0.189314 -4.442428 2.038628
 C 2.490265 -1.625709 1.859667
 N 3.374102 -2.134708 0.957287
 C 4.503550 -1.364291 0.483473
 O 2.619751 -0.533399 2.403452
 C 4.348537 -0.883784 -0.971443
 O 4.441871 -2.056972 -1.776618
 C 3.053337 -0.117898 -1.205714
 C 0.603578 1.273521 -1.549164
 C 1.960221 -0.731841 -1.822874
 C 2.919360 1.201330 -0.762380
 C 1.714824 1.871469 -0.931378
 C 0.764007 -0.044980 -1.998327
 Br 1.527600 3.669251 -0.297122
 Br -0.710710 -0.919130 -2.826227
 O -0.581874 1.890484 -1.734413
 H -1.545661 -2.873071 1.133366
 H -3.854028 0.392160 -0.996518
 H -0.276509 1.896314 2.988828
 H -0.333909 -2.669293 3.547915
 H 0.638460 -1.186037 3.706051
 H 0.390819 -5.307826 1.647834
 H 3.155632 -3.023463 0.527284
 H 5.418647 -1.965369 0.541264
 H 4.604668 -0.506054 1.150393
 H 5.201346 -0.215619 -1.177242
 H 4.357351 -1.790310 -2.706101
 H 2.037424 -1.759281 -2.158069
 H 3.744034 1.708751 -0.272052
 H -0.596213 2.722376 -1.225354

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4151871**

Comp_08E_c68**B3LYP/6-31G* Geometry**

C -2.843104 -0.067662 -0.844590
 C -0.479809 -1.270499 -1.677914
 C -2.488154 -1.344285 -0.389931
 C -1.997934 0.619010 -1.737480
 C -0.815677 -0.003781 -2.139244
 C -1.304231 -1.972830 -0.789265
 Br -3.621996 -2.218991 0.869941
 Br 1.171684 -2.084109 -2.216635
 O -1.022453 -3.199337 -0.304620
 O -3.982231 0.546812 -0.445026

C -2.350682 2.022447 -2.209139
 C -1.794853 3.086045 -1.286711
 N -2.450594 3.872443 -0.514105
 O -3.830314 3.696379 -0.573571
 C -0.294022 3.282153 -1.292017
 N 0.217548 3.946053 -0.222508
 C 1.632212 4.195035 -0.059972
 O 0.385904 2.854567 -2.223893
 C 2.209774 3.530338 1.202092
 O 1.510820 4.122465 2.295357
 C 2.104777 2.012582 1.196947
 C 1.913750 -0.816467 1.155713
 C 3.092080 1.244787 0.572216
 C 1.022392 1.357669 1.793747
 C 0.932021 -0.030701 1.776584
 C 2.984901 -0.139171 0.552278
 Br -0.555525 -0.893751 2.589259
 Br 4.332091 -1.190778 -0.313919
 O 1.797181 -2.163800 1.168969
 H -0.137669 0.527631 -2.796105
 H -0.106669 -3.420447 -0.555737
 H -4.447201 -0.045167 0.175944
 H -3.432361 2.140898 -2.277326
 H -1.910786 2.183862 -3.197748
 H -4.153610 4.372302 0.043255
 H -0.427924 4.274838 0.483189
 H 1.818774 5.273923 0.015458
 H 2.133145 3.815080 -0.952536
 H 3.277233 3.804270 1.240138
 H 1.825624 3.706795 3.113919
 H 3.946151 1.719260 0.098867
 H 0.244681 1.934164 2.280484
 H 2.571162 -2.534561 0.704299

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4175562**

Comp_08E_c69

B3LYP/6-31G* Geometry

C 0.697029 0.118503 -2.035186
 C 2.382222 -1.549707 -0.534482
 C 0.299270 -1.173559 -1.664905
 C 1.991580 0.552730 -1.691225
 C 2.807957 -0.291185 -0.929858
 C 1.116985 -2.026043 -0.909597
 Br -1.447392 -1.781830 -2.134656
 Br 3.493845 -2.630424 0.566406
 O 0.736576 -3.258268 -0.520990
 O -0.174345 0.885807 -2.734593
 C 2.497962 1.929265 -2.098737
 C 2.399690 2.882586 -0.934245
 N 3.362144 3.302462 -0.196219
 O 4.608826 2.828651 -0.593727
 C 1.020740 3.339819 -0.518775
 N 0.919374 3.791488 0.741392

C -0.262240 4.310857 1.438215
 O 0.072883 3.246984 -1.321738
 C -1.626010 3.643477 1.150349
 O -2.206135 4.136624 -0.041618
 C -1.659259 2.114224 1.212307
 C -1.886604 -0.717655 1.295308
 C -0.688204 1.331278 1.845230
 C -2.753289 1.467679 0.624090
 C -2.860201 0.087210 0.683244
 C -0.792718 -0.058140 1.871383
 Br -4.368771 -0.788598 -0.111130
 Br 0.599937 -1.094970 2.650210
 O -1.955417 -2.066436 1.343952
 H 3.795021 0.049290 -0.634439
 H -0.199768 -3.378859 -0.767810
 H -0.098333 1.814688 -2.419513
 H 1.911347 2.318241 -2.935603
 H 3.539375 1.869079 -2.418768
 H 5.211026 3.246525 0.043115
 H 1.804888 3.840165 1.232771
 H -0.392294 5.376235 1.213297
 H -0.034155 4.224382 2.505498
 H -2.278044 4.029025 1.946636
 H -1.601814 3.855815 -0.759922
 H 0.178878 1.782298 2.312237
 H -3.508910 2.052834 0.114285
 H -2.783039 -2.338520 0.903961

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4199514**

Comp_08E_c71

B3LYP/6-31G* Geometry

C -4.007009 0.718555 -0.152046
 C -6.504535 -0.533453 -0.272456
 C -5.117611 1.249951 0.514078
 C -4.149699 -0.463464 -0.896976
 C -5.404727 -1.069247 -0.934698
 C -6.383503 0.646894 0.470851
 Br -4.903076 2.870568 1.526073
 Br -8.193012 -1.405797 -0.369692
 O -7.467095 1.144783 1.105769
 O -2.777763 1.292479 -0.114666
 C -2.968765 -1.032732 -1.665284
 C -1.822360 -1.497129 -0.797326
 N -1.845018 -2.494062 0.010687
 O -3.073991 -3.143226 0.026158
 C -0.491776 -0.788547 -0.918084
 N 0.452050 -1.137821 -0.015596
 C 1.753210 -0.483262 0.113852
 O -0.310336 0.039303 -1.817775
 C 2.732292 -0.721621 -1.067391
 O 2.428472 0.096020 -2.174318
 C 4.158119 -0.427107 -0.624667
 C 6.787959 0.138308 0.275052

C 4.881374 -1.367211 0.117145
C 4.756253 0.798186 -0.924626
C 6.044889 1.060800 -0.477224
C 6.168891 -1.088758 0.560168
Br 6.876459 2.742215 -0.890975
Br 7.125823 -2.394808 1.563425
O 8.041900 0.367960 0.721218
H -5.530455 -1.989601 -1.494332
H -7.214532 1.964371 1.567095
H -2.820988 2.119100 0.397910
H -2.565121 -0.285215 -2.353633
H -3.320105 -1.886780 -2.254769
H -2.931999 -3.863836 0.661341
H 0.186933 -1.850129 0.652075
H 2.194309 -0.860605 1.039652
H 1.614922 0.599885 0.222918
H 2.666499 -1.791841 -1.332761
H 1.451683 0.177985 -2.226137
H 4.447766 -2.335525 0.349387
H 4.215348 1.522704 -1.520312
H 8.312226 1.256917 0.423577

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4046202**

Comp_08E_c73
B3LYP/6-31G* Geometry
C 2.457142 -0.180139 1.585977
C 3.293653 0.551502 -0.973575
C 2.844747 -1.154527 0.653206
C 2.505076 1.185034 1.227263
C 2.918057 1.526948 -0.063211
C 3.264537 -0.810654 -0.636732
Br 2.745704 -2.990589 1.119166
Br 3.857683 1.037831 -2.739021
O 3.607159 -1.793660 -1.494490
O 2.063977 -0.622093 2.801336
C 2.114080 2.284818 2.208447
C 0.615721 2.428418 2.342368
N -0.123715 1.982044 3.289408
O 0.620522 1.313521 4.279901
C -0.112398 3.127080 1.212511
N -1.456503 3.022582 1.209216
C -2.303414 3.617594 0.177644
O 0.534210 3.731075 0.348620
C -2.286732 2.865800 -1.177366
O -1.079686 3.075621 -1.882894
C -2.584625 1.382767 -0.981237
C -3.133742 -1.347228 -0.446152
C -3.899075 0.935826 -0.811869
C -1.543820 0.455388 -0.900361
C -1.822690 -0.878325 -0.628577
C -4.167464 -0.404146 -0.552078
Br -0.384935 -2.134885 -0.441956
Br -5.969644 -0.981767 -0.332467

O -3.436239 -2.636385 -0.180511
H 2.934199 2.570001 -0.357085
H 3.856813 -1.381696 -2.343132
H 1.682263 0.093391 3.346138
H 2.497214 3.235429 1.830763
H 2.553306 2.115748 3.195930
H -0.064619 0.984097 4.884984
H -1.873778 2.438159 1.921557
H -1.980411 4.650865 0.009847
H -3.321979 3.639352 0.574130
H -3.100137 3.304017 -1.775711
H -0.406413 3.421133 -1.264378
H -4.731402 1.629834 -0.888494
H -0.522843 0.778825 -1.065124
H -2.602853 -3.143740 -0.153316

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4157934**

Comp_08E_c75
B3LYP/6-31G* Geometry
C 3.898057 0.649057 -0.074221
C 6.447123 -0.416343 -0.360340
C 4.997065 1.250651 0.551136
C 4.075662 -0.504566 -0.860269
C 5.362060 -1.023160 -0.983518
C 6.292526 0.735589 0.421156
Br 4.710405 2.815643 1.604279
Br 8.208731 -1.148091 -0.550100
O 7.310108 1.364272 1.048287
O 2.638876 1.134855 0.045168
C 2.894293 -1.132560 -1.579571
C 1.814951 -1.668267 -0.667939
N 1.924525 -2.668757 0.127994
O 3.191132 -3.248241 0.087728
C 0.446090 -1.023617 -0.727895
N -0.440053 -1.418438 0.233177
C -1.746638 -0.785540 0.365483
O 0.162485 -0.221165 -1.610371
C -2.776344 -1.374822 -0.626049
O -2.880679 -2.781039 -0.444098
C -4.139233 -0.750499 -0.417690
C -6.648738 0.491497 0.029149
C -4.412931 0.520397 -0.935549
C -5.125988 -1.405115 0.322748
C -6.351626 -0.784812 0.530859
C -5.642056 1.129725 -0.712348
Br -7.717121 -1.685341 1.537076
Br -5.981652 2.859232 -1.431440
O -7.831177 1.116792 0.217002
H 5.521754 -1.919342 -1.572869
H 8.133069 0.877533 0.853635
H 2.665767 1.945490 0.587922
H 3.264460 -1.958156 -2.197585
H 2.414827 -0.400991 -2.236290

H 3.113532 -3.979367 0.721775
H -0.086445 -2.016705 0.967365
H -1.645201 0.291433 0.197210
H -2.100938 -0.951632 1.387025
H -2.426605 -1.144607 -1.642710
H -1.976368 -3.128264 -0.515402
H -3.667345 1.043260 -1.526621
H -4.938239 -2.396878 0.714636
H -8.407830 0.528576 0.739590
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4036322**

Comp_08E_c76
B3LYP/6-31G* Geometry
C 0.590279 0.016195 -2.233943
C 2.397294 -1.234682 -0.489792
C 1.573035 0.751485 -1.558004
C 0.547352 -1.382301 -2.060662
C 1.453501 -1.983122 -1.181477
C 2.472976 0.153756 -0.665447
Br 1.668520 2.636941 -1.803864
Br 3.605395 -2.093326 0.704379
O 3.376850 0.868328 0.046253
O -0.266634 0.675879 -3.046510
C -0.457110 -2.230835 -2.828891
C -1.638694 -2.621747 -1.973776
N -1.857257 -3.771778 -1.446909
O -0.886575 -4.718410 -1.760780
C -2.648879 -1.551102 -1.631478
N -3.611428 -1.900300 -0.747729
C -4.537800 -0.954090 -0.146100
O -2.572159 -0.425365 -2.137429
C -4.162819 -0.640088 1.324330
O -4.228736 -1.830613 2.100796
C -2.823345 0.082205 1.448786
C -0.314117 1.411776 1.563670
C -2.659902 1.364721 0.908649
C -1.729885 -0.515246 2.076188
C -0.502218 0.138295 2.117163
C -1.436679 2.019246 0.975402
Br 1.006630 -0.715472 2.924107
Br -1.263563 3.765702 0.247532
O 0.864929 2.068205 1.577725
H 1.424302 -3.058324 -1.037608
H 3.296725 1.802449 -0.232330
H -1.170112 0.304751 -2.898524
H 0.024918 -3.140989 -3.190258
H -0.818402 -1.674204 -3.698442
H -1.204850 -5.514063 -1.304210
H -3.613073 -2.867912 -0.450055
H -5.545378 -1.382817 -0.159895
H -4.531898 -0.052011 -0.760507
H -4.956425 -0.001390 1.730115
H -3.500743 -2.406395 1.816524

H -3.489360 1.870005 0.424391
H -1.821083 -1.480040 2.560485
H 1.552444 1.469936 1.929261
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4180872**

Comp_08E_c77
B3LYP/6-31G* Geometry
C 2.514319 -0.256011 1.511445
C 3.383465 0.508596 -1.048634
C 2.859337 -1.208254 0.543091
C 2.618947 1.111393 1.185082
C 3.045260 1.463402 -0.100721
C 3.292304 -0.857170 -0.742160
Br 2.687977 -3.065399 0.951168
Br 3.968977 1.042903 -2.777591
O 3.614790 -1.767832 -1.681677
O 2.115020 -0.725523 2.715483
C 2.279087 2.202373 2.194562
C 0.788580 2.376447 2.368534
N 0.062085 1.931688 3.326423
O 0.816015 1.230069 4.288295
C 0.047304 3.107282 1.267925
N -1.298366 3.008330 1.285122
C -2.155057 3.635881 0.282964
O 0.680439 3.729940 0.408794
C -2.196020 2.894570 -1.076319
O -0.980861 3.023158 -1.786304
C -2.582206 1.431117 -0.891845
C -3.282938 -1.271573 -0.387513
C -3.923911 1.050692 -0.820533
C -1.596442 0.452302 -0.727994
C -1.939725 -0.869036 -0.468056
C -4.255198 -0.277725 -0.576225
Br -0.563007 -2.153081 -0.177271
Br -6.100846 -0.802096 -0.492234
O -3.572703 -2.567541 -0.138708
H 3.106680 2.512643 -0.366197
H 3.468958 -2.656799 -1.305262
H 1.779716 -0.013126 3.294491
H 2.673945 3.150210 1.821847
H 2.738362 2.007069 3.168098
H 0.138004 0.908634 4.905499
H -1.707355 2.410217 1.990623
H -1.802937 4.659486 0.114740
H -3.162711 3.687425 0.704381
H -2.988083 3.386820 -1.662658
H -0.301734 3.405717 -1.197483
H -4.716711 1.779352 -0.962373
H -0.552327 0.726524 -0.821887
H -4.542589 -2.669610 -0.135814
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4145358**

Comp_08E_c78

B3LYP/6-31G* Geometry

C -2.773962 0.182991 -0.876436
C -0.551423 -1.338576 -1.678740
C -2.566302 -1.114927 -0.392287
C -1.854393 0.715162 -1.802579
C -0.753539 -0.059617 -2.180179
C -1.458586 -1.887013 -0.763092
Br -3.776495 -1.843886 0.891756
Br 0.987089 -2.328822 -2.191251
O -1.217193 -3.114940 -0.240192
O -3.863759 0.845480 -0.423022
C -2.010977 2.127174 -2.354219
C -1.436664 3.147642 -1.399049
N -2.078267 3.861380 -0.551227
O -3.473965 3.628616 -0.605644
C 0.075198 3.308107 -1.414097
N 0.610895 3.943739 -0.343761
C 2.040296 4.068599 -0.142061
O 0.723351 2.859027 -2.355496
C 2.505221 3.387080 1.157416
O 1.823220 4.078757 2.204108
C 2.251262 1.887834 1.190248
C 1.775149 -0.912178 1.190503
C 1.092288 1.365946 1.769708
C 3.171857 1.001836 0.617740
C 2.934646 -0.366933 0.611751
C 0.873895 -0.007511 1.772437
Br 4.192324 -1.538999 -0.197818
Br -0.713605 -0.711402 2.580007
O 1.603026 -2.247547 1.177588
H -0.026034 0.359481 -2.865815
H -1.982031 -3.354506 0.318692
H -3.787888 1.808508 -0.582668
H -3.057111 2.361693 -2.568617
H -1.444599 2.204073 -3.284580
H -3.814688 4.191794 0.108291
H -0.011710 4.262826 0.386990
H 2.319598 5.128074 -0.086394
H 2.532589 3.621960 -1.007727
H 3.591031 3.560854 1.231230
H 2.062002 3.657720 3.045387
H 0.365148 2.026784 2.226785
H 4.083833 1.375338 0.161949
H 0.674269 -2.460455 1.385991

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4195244

Comp_08E_c79

B3LYP/6-31G* Geometry

C -0.680256 -0.012974 -2.193771
C -2.814363 -0.250386 -0.413275
C -0.980098 -1.251338 -1.597807

C -1.482302 1.112306 -1.899552
C -2.544864 0.974012 -1.003087
C -2.035174 -1.383110 -0.688063
Br 0.102843 -2.754931 -1.983506
Br -4.251458 -0.423029 0.843726
O -2.237516 -2.580614 -0.080863
O 0.356438 0.038993 -3.055817
C -1.190015 2.475115 -2.512565
C -0.370416 3.321458 -1.566121
N -0.807422 4.235551 -0.778961
O -2.182126 4.440625 -0.885326
C 1.108806 3.031339 -1.472153
N 1.773569 3.623142 -0.458223
C 3.141496 3.298050 -0.106364
O 1.653602 2.288669 -2.300541
C 3.216108 2.655131 1.298414
O 2.602329 3.528367 2.250238
C 2.526165 1.305471 1.361643
C 1.250313 -1.229889 1.372651
C 3.150651 0.183965 0.803689
C 1.262508 1.155240 1.935298
C 0.650063 -0.093886 1.936988
C 2.525665 -1.056451 0.808244
Br -1.086781 -0.294929 2.719629
Br 3.395259 -2.553047 0.025617
O 0.693363 -2.455774 1.361474
H -3.157974 1.835178 -0.760736
H -3.047887 -2.505569 0.458231
H 0.831378 0.899196 -2.953794
H -2.124730 2.995376 -2.729177
H -0.640849 2.358922 -3.450694
H -2.339802 5.159268 -0.251861
H 1.223028 4.151015 0.208494
H 3.752362 4.212341 -0.114322
H 3.532297 2.625014 -0.872070
H 4.281375 2.517171 1.539829
H 3.195746 4.282279 2.389130
H 4.135044 0.266863 0.353215
H 0.766078 2.001464 2.392796
H -0.258736 -2.388052 1.561606

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4209208

Comp_08E_c80

B3LYP/6-31G* Geometry

C 3.539035 -1.375528 -0.206101
C 4.897850 1.049904 -0.229113
C 4.678253 -1.186948 0.587507
C 3.077299 -0.333464 -1.032371
C 3.770204 0.876791 -1.023124
C 5.381152 0.023461 0.593469
Br 5.280476 -2.626220 1.687016
Br 5.843410 2.717822 -0.233068
O 6.472472 0.140052 1.380169

O 2.847788 -2.539882 -0.217504
 C 1.847669 -0.537485 -1.900469
 C 0.559803 -0.272755 -1.157693
 N -0.408620 -1.087170 -0.938205
 O -0.220104 -2.369339 -1.419156
 C 0.251623 1.145244 -0.742652
 N -0.633369 1.278743 0.281171
 C -1.321504 2.535648 0.530592
 O 0.753773 2.101476 -1.342677
 C -2.512897 2.768537 -0.434818
 O -2.076070 2.827360 -1.782195
 C -3.542754 1.657107 -0.287080
 C -5.265630 -0.552465 0.175088
 C -4.570777 1.746554 0.653911
 C -3.400664 0.470531 -1.015533
 C -4.228770 -0.615265 -0.768321
 C -5.414690 0.661321 0.865222
 Br -3.934291 -2.252248 -1.710380
 Br -6.835287 0.788897 2.148747
 O -6.052502 -1.631505 0.372857
 H 3.410564 1.697838 -1.632623
 H 6.834644 1.038730 1.262587
 H 3.286462 -3.167280 0.387538
 H 1.820748 -1.554854 -2.293573
 H 1.890005 0.163171 -2.740736
 H -1.111945 -2.749179 -1.317687
 H -1.090598 0.420678 0.566950
 H -0.594110 3.344898 0.413661
 H -1.673136 2.543819 1.566662
 H -2.978083 3.724918 -0.142014
 H -1.111971 2.967167 -1.796811
 H -4.720683 2.656700 1.226586
 H -2.626422 0.397749 -1.766646
 H -6.716395 -1.406602 1.051296

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4029389

Comp_08E_c81

B3LYP/6-31G* Geometry

C 3.906551 0.675766 -0.059874
 C 6.450342 -0.394897 -0.371613
 C 5.006362 1.248772 0.590381
 C 4.080718 -0.450988 -0.884666
 C 5.364492 -0.973105 -1.020108
 C 6.299230 0.730483 0.448353
 Br 4.724631 2.778373 1.695702
 Br 8.208223 -1.131107 -0.577930
 O 7.317741 1.330975 1.101019
 O 2.649672 1.164884 0.071038
 C 2.898247 -1.046622 -1.629099
 C 1.816960 -1.614271 -0.739376
 N 1.923161 -2.645637 0.016652
 O 3.188004 -3.226868 -0.045556
 C 0.449161 -0.965643 -0.776030

N -0.434271 -1.388095 0.175121
 C -1.745990 -0.769865 0.322248
 O 0.164449 -0.136613 -1.633479
 C -2.772306 -1.346413 -0.680526
 O -2.861853 -2.757506 -0.532078
 C -4.140542 -0.741762 -0.451744
 C -6.660883 0.453765 0.056282
 C -4.461759 0.495392 -1.016185
 C -5.083186 -1.379463 0.361598
 C -6.318383 -0.791358 0.606533
 C -5.698824 1.072559 -0.756716
 Br -7.585369 -1.686083 1.711734
 Br -6.142176 2.771266 -1.532593
 O -7.872970 0.987058 0.322000
 H 5.521281 -1.849725 -1.638896
 H 8.138609 0.845970 0.893583
 H 2.679010 1.954424 0.643928
 H 3.266213 -1.848366 -2.279063
 H 2.421413 -0.288327 -2.256707
 H 3.107606 -3.982353 0.558919
 H -0.081442 -2.012836 0.887282
 H -1.653857 0.311159 0.176114
 H -2.097201 -0.959823 1.340708
 H -2.428188 -1.087432 -1.692246
 H -1.953869 -3.093734 -0.610639
 H -3.755978 1.008882 -1.661551
 H -4.853522 -2.348037 0.788304
 H -7.939657 1.841076 -0.144457

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4035529

Comp_08E_c84

B3LYP/6-31G* Geometry

C 5.350452 -1.140445 0.538247
 C 4.595319 1.465334 -0.086753
 C 6.261271 -0.247989 -0.046602
 C 4.034544 -0.718463 0.805581
 C 3.680261 0.594736 0.490481
 C 5.907689 1.065261 -0.373494
 Br 8.039563 -0.848389 -0.398317
 Br 4.091809 3.265569 -0.512035
 O 6.833941 1.870600 -0.936306
 O 5.702783 -2.404965 0.873008
 C 3.024545 -1.667348 1.436550
 C 1.871566 -1.997358 0.515976
 N 1.861417 -2.902848 -0.394632
 O 3.057965 -3.597731 -0.476577
 C 0.599535 -1.194662 0.642145
 N -0.453779 -1.615260 -0.090451
 C -1.695331 -0.857888 -0.260644
 O 0.565582 -0.209664 1.393893
 C -2.594689 -0.785528 1.002445
 O -2.128920 0.171212 1.926364
 C -4.015579 -0.419105 0.600679

C -6.630867 0.282622 -0.242934
C -4.439315 0.913297 0.618868
C -4.906955 -1.403838 0.168001
C -6.184830 -1.047977 -0.245341
C -5.721165 1.254077 0.203520
Br -7.411209 -2.403437 -0.833882
Br -6.270466 3.076973 0.237818
O -7.867030 0.659799 -0.635445
H 2.673987 0.937056 0.708421
H 6.422390 2.742101 -1.090399
H 6.639209 -2.537180 0.632952
H 2.607711 -1.208500 2.337040
H 3.525553 -2.596917 1.712003
H 2.893433 -4.232451 -1.192989
H -0.280307 -2.415139 -0.686232
H -2.241150 -1.345845 -1.071754
H -1.467987 0.168698 -0.574957
H -2.609106 -1.796231 1.447634
H -1.148515 0.163799 1.899244
H -3.763320 1.678094 0.980590
H -4.616840 -2.450119 0.159338
H -8.361183 -0.138001 -0.900628

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4058287**

Comp_08E_c88
B3LYP/6-31G* Geometry
C 0.698903 0.043142 -2.203456
C 2.811979 0.194549 -0.361272
C 1.227059 -1.109788 -1.605129
C 1.262190 1.294991 -1.877829
C 2.311131 1.345431 -0.954509
C 2.266991 -1.059374 -0.667646
Br 0.469397 -2.808321 -2.017075
Br 4.235860 0.314861 0.897202
O 2.729203 -2.161135 -0.029943
O -0.312016 -0.102061 -3.086452
C 0.740524 2.578883 -2.509059
C -0.236556 3.286093 -1.598421
N 0.010858 4.295068 -0.845055
O 1.321737 4.753132 -0.950121
C -1.635960 2.725757 -1.497229
N -2.436638 3.270242 -0.555362
C -3.733708 2.721537 -0.205634
O -2.001113 1.812688 -2.249063
C -3.736052 2.043747 1.182900
O -5.085007 1.629893 1.363414
C -2.746119 0.897626 1.299199
C -0.867753 -1.222261 1.452618
C -3.053316 -0.370220 0.788995
C -1.501823 1.094689 1.902398
C -0.585895 0.051194 1.971586
C -2.134006 -1.409112 0.871796
Br 1.123805 0.325729 2.781889

Br -2.583032 -3.122785 0.183381
O -0.002715 -2.256073 1.499086
H 2.745056 2.305215 -0.694650
H 2.233729 -2.929871 -0.376809
H -0.960059 0.633351 -2.953968
H 0.241289 2.353574 -3.455668
H 1.571894 3.254176 -2.718972
H 1.335325 5.508745 -0.340583
H -2.032561 4.017159 -0.003533
H -4.000988 1.991420 -0.970866
H -4.491479 3.512759 -0.203416
H -3.464064 2.806908 1.933162
H -5.133729 1.131617 2.194619
H -4.018953 -0.548100 0.328708
H -1.237846 2.059396 2.324298
H 0.855514 -1.938301 1.840461

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4222026**

Comp_08E_c89
B3LYP/6-31G* Geometry
C 3.996456 0.705846 0.196920
C 6.492749 -0.554124 0.224183
C 5.098438 1.265306 -0.460536
C 4.147658 -0.508501 0.886271
C 5.401803 -1.117283 0.878343
C 6.363440 0.658879 -0.463146
Br 4.872865 2.930677 -1.394056
Br 8.180162 -1.433475 0.255579
O 7.438677 1.183246 -1.090924
O 2.767834 1.281861 0.202483
C 2.976205 -1.109892 1.644870
C 1.825458 -1.549128 0.769526
N 1.844874 -2.521943 -0.067548
O 3.074088 -3.170152 -0.106851
C 0.495512 -0.843663 0.915549
N -0.448657 -1.160707 0.001233
C -1.746853 -0.496965 -0.110808
O 0.315541 -0.047263 1.843087
C -2.729052 -0.762898 1.062459
O -2.425175 0.024384 2.190679
C -4.151899 -0.449925 0.623685
C -6.770186 0.172221 -0.273307
C -4.904356 -1.397687 -0.074237
C -4.715846 0.804063 0.877841
C -5.998616 1.106059 0.435935
C -6.184794 -1.080783 -0.510810
Br -6.742141 2.821972 0.796732
Br -7.220208 -2.387844 -1.463699
O -8.013365 0.508506 -0.681338
H 5.533710 -2.061837 1.394497
H 7.181221 2.023531 -1.510422
H 2.805441 2.131993 -0.270539
H 2.574892 -0.388560 2.361856

H 3.336448 -1.982205 2.201126
H 2.929726 -3.871836 -0.762322
H -0.182637 -1.848336 -0.691398
H -2.188843 -0.847437 -1.046775
H -1.603943 0.588155 -0.190852
H -2.667951 -1.840332 1.298584
H -1.448108 0.097359 2.249588
H -4.504291 -2.387448 -0.272708
H -4.148661 1.533141 1.443070
H -8.401759 -0.257997 -1.142450
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4042614**

Comp_08E_c90
B3LYP/6-31G* Geometry

C 3.041591 1.324405 0.121873
C 2.792520 -1.402785 0.724439
C 3.461235 0.339703 -0.783266
C 2.530620 0.924567 1.373326
C 2.399669 -0.441741 1.643946
C 3.347328 -1.030357 -0.508623
Br 4.176854 0.861274 -2.474592
Br 2.541541 -3.249063 1.111144
O 3.724315 -1.989477 -1.378313
O 3.174918 2.624179 -0.233491
C 2.136059 1.952081 2.426042
C 0.641923 2.163990 2.473345
N -0.176300 1.682045 3.337796
O 0.443798 0.923868 4.320799
C 0.002584 2.951152 1.360391
N -1.339387 2.973209 1.322300
C -2.114974 3.647561 0.283213
O 0.708527 3.535397 0.514049
C -2.143309 2.907793 -1.078428
O -0.914511 3.023246 -1.768162
C -2.563663 1.451624 -0.907359
C -3.327621 -1.240528 -0.441207
C -1.602109 0.447008 -0.759087
C -3.914128 1.102902 -0.838303
C -4.276289 -0.220686 -0.612139
C -1.974579 -0.870503 -0.518990
Br -6.133905 -0.700759 -0.531097
Br -0.627774 -2.190117 -0.256855
O -3.648224 -2.532454 -0.211890
H 1.984234 -0.759589 2.594501
H 4.066355 -1.551704 -2.181413
H 2.395908 3.121135 0.106916
H 2.624604 2.908004 2.215966
H 2.468436 1.619178 3.410929
H -0.300176 0.634241 4.873913
H -1.813534 2.405634 2.013711
H -1.702305 4.650507 0.130143
H -3.133615 3.753459 0.665639
H -2.910395 3.418339 -1.680503

H -0.224977 3.316474 -1.143115
H -0.551474 0.696200 -0.849441
H -4.689916 1.851738 -0.968702
H -4.620160 -2.612276 -0.209196
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4168836**

Comp_08E_c95
B3LYP/6-31G* Geometry

C -0.593987 -0.101566 -2.115243
C -2.749546 0.567276 -0.447522
C -1.357327 -1.089912 -1.478474
C -0.970678 1.247555 -1.960085
C -2.037568 1.556652 -1.109870
C -2.436165 -0.787324 -0.636074
Br -0.896621 -2.927693 -1.735037
Br -4.156206 1.038847 0.742369
O -3.166228 -1.726700 -0.004394
O 0.454489 -0.484941 -2.879228
C -0.248583 2.354517 -2.716779
C 0.736927 3.088976 -1.841149
N 0.575932 4.243213 -1.302952
O -0.637859 4.840830 -1.628257
C 2.026484 2.385676 -1.489268
N 2.817895 3.010630 -0.588207
C 3.995388 2.405068 0.013427
O 2.313851 1.298512 -2.004699
C 3.706830 1.893476 1.447665
O 3.298413 2.980393 2.268603
C 2.723965 0.724533 1.470145
C 0.879081 -1.435005 1.425230
C 3.044660 -0.473459 0.821684
C 1.484213 0.822971 2.106223
C 0.572220 -0.228543 2.068293
C 2.140759 -1.526185 0.813299
Br -1.144241 -0.019948 2.857974
Br 2.592346 -3.157531 -0.079547
O -0.027482 -2.434813 1.426619
H -2.318686 2.594671 -0.965196
H -2.763996 -2.596830 -0.185855
H 1.191190 0.156970 -2.733494
H -0.974518 3.073492 -3.100931
H 0.286173 1.929462 -3.571049
H -0.595165 5.688458 -1.156487
H 2.508143 3.923783 -0.279520
H 4.788803 3.157432 0.069010
H 4.324702 1.596668 -0.641835
H 4.663772 1.568836 1.873940
H 2.418172 3.257675 1.966512
H 3.996213 -0.596034 0.315067
H 1.213449 1.716568 2.655672
H 0.288693 -3.141179 0.832563
Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4191625

Comp_08E_c98

B3LYP/6-31G* Geometry

C -2.731293 0.578284 -0.943479
C -0.858899 -1.370809 -1.538251
C -2.836522 -0.695255 -0.380352
C -1.676142 0.891713 -1.812702
C -0.739274 -0.103662 -2.094540
C -1.904046 -1.699160 -0.663629
Br -4.217656 -1.030627 0.886403
Br 0.457719 -2.711521 -1.912815
O -2.053851 -2.905408 -0.082977
O -3.634723 1.565730 -0.659913
C -1.519954 2.301729 -2.357063
C -0.699623 3.193759 -1.444153
N -1.111514 4.017059 -0.547092
O -2.453649 4.131759 -0.293941
C 0.801998 3.075454 -1.586454
N 1.533628 3.795542 -0.697727
C 2.956712 3.605710 -0.529934
O 1.290318 2.345544 -2.450478
C 3.300683 2.929396 0.812024
O 2.849802 3.838104 1.814165
C 2.691125 1.544350 0.972027
C 1.552923 -1.039798 1.240679
C 3.378579 0.416261 0.514975
C 1.430556 1.372094 1.556521
C 0.874854 0.103593 1.688259
C 2.809309 -0.843394 0.646515
Br -0.846587 -0.103633 2.476554
Br 3.749012 -2.389854 0.014503
O 0.986606 -2.256216 1.403426
H 0.107931 0.135072 -2.726958
H -1.276014 -3.448494 -0.309199
H -4.261962 1.234215 0.012295
H -2.498477 2.755206 -2.543552
H -0.985811 2.254919 -3.308618
H -2.923056 3.327044 -0.611292
H 1.022166 4.325505 -0.002261
H 3.470624 4.573982 -0.557000
H 3.308352 2.996870 -1.365106
H 4.398570 2.833707 0.848189
H 2.999481 3.430054 2.681886
H 4.357470 0.512841 0.055703
H 0.878991 2.233529 1.914298
H 1.597942 -2.923133 1.037851

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4160864

Comp_08E_c99

B3LYP/6-31G* Geometry

C -2.738744 0.211142 -0.907091

C -0.527454 -1.334217 -1.695684
C -2.543539 -1.085927 -0.415136
C -1.809410 0.732357 -1.830005
C -0.714238 -0.054054 -2.199968
C -1.442822 -1.870605 -0.780807
Br -3.773015 -1.804111 0.856373
Br 0.994783 -2.346193 -2.211708
O -1.219411 -3.102027 -0.259284
O -3.828343 0.881831 -0.465655
C -1.951427 2.142391 -2.390834
C -1.392496 3.165221 -1.429671
N -2.047302 3.885790 -0.597573
O -3.442911 3.658114 -0.678558
C 0.119347 3.326796 -1.417967
N 0.633176 3.928041 -0.316359
C 2.054853 4.026958 -0.060958
O 0.784322 2.916058 -2.364181
C 2.423417 3.367690 1.287580
O 1.639240 3.954977 2.330374
C 2.189172 1.869528 1.295051
C 1.762024 -0.935159 1.205504
C 3.109079 1.022100 0.667544
C 1.056799 1.309625 1.888913
C 0.860514 -0.066328 1.839395
C 2.899049 -0.350440 0.623292
Br -0.703575 -0.826750 2.642826
Br 4.164690 -1.469325 -0.247870
O 1.608531 -2.272115 1.144759
H 0.019240 0.354386 -2.885938
H -1.986602 -3.329763 0.301340
H -3.751363 1.842535 -0.637889
H -2.992508 2.379237 -2.626585
H -1.366999 2.213804 -3.310566
H -3.795104 4.222922 0.028450
H -0.001122 4.173139 0.433176
H 2.361462 5.083867 -0.033882
H 2.576053 3.550244 -0.894197
H 3.493530 3.556577 1.464717
H 1.952236 4.863342 2.461488
H 4.002692 1.425996 0.201546
H 0.341397 1.938303 2.403651
H 0.688896 -2.505327 1.370872

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4176282

Comp_08Z_c02

B3LYP/6-31G* Geometry

C -2.461833 1.012997 1.029630
C -3.307648 -0.615012 -1.063745
C -2.477966 -0.382720 1.165859
C -2.858485 1.602972 -0.185934
C -3.278490 0.765575 -1.219310
C -2.900975 -1.223797 0.131427
Br -1.867377 -1.138419 2.802111

Br -3.898258 -1.743617 -2.495921
 O -2.899477 -2.559753 0.332823
 O -2.065641 1.828250 2.032154
 C -2.772001 3.107495 -0.398000
 C -1.439738 3.495388 -1.015747
 N -1.417827 3.605432 -2.293088
 C -0.293149 3.703509 -0.043300
 N 0.930447 3.257482 -0.405650
 C 2.083154 3.434754 0.471662
 O -0.520899 4.215897 1.056551
 C 2.216881 2.338110 1.553567
 O 1.070749 2.273368 2.382322
 C 2.503885 0.970240 0.943587
 C 3.056718 -1.536924 -0.265893
 C 3.719937 0.737778 0.289510
 C 1.570301 -0.064414 1.010491
 C 1.853570 -1.286658 0.410572
 C 3.988664 -0.488151 -0.306361
 Br 0.564127 -2.707109 0.489423
 Br 5.652549 -0.762248 -1.192829
 O 3.353908 -2.713296 -0.859554
 O -0.142394 3.900085 -2.816613
 H -3.577560 1.200077 -2.167568
 H -3.213933 -2.988562 -0.485583
 H -1.747887 1.286155 2.779155
 H -2.879586 3.636135 0.551244
 H -3.568174 3.427173 -1.075652
 H 1.061346 2.944214 -1.357749
 H 1.988028 4.407820 0.965679
 H 2.982917 3.455098 -0.148696
 H 3.092331 2.627179 2.161112
 H 0.498986 3.044131 2.194755
 H 4.478948 1.513400 0.243344
 H 0.645653 0.081376 1.552742
 H 2.601230 -3.319045 -0.720761
 H -0.323966 3.959933 -3.767869
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4047629**

Comp_08Z_c03
B3LYP/6-31G* Geometry
 C 2.100386 0.097551 -0.507459
 C 4.740037 0.309293 0.335566
 C 2.836136 -1.046789 -0.181240
 C 2.694180 1.371411 -0.408388
 C 4.015809 1.454367 0.016630
 C 4.169442 -0.965585 0.245015
 Br 2.004273 -2.756454 -0.322915
 Br 6.561520 0.444772 0.918045
 O 4.826532 -2.107701 0.543491
 O 0.812159 0.058429 -0.922444
 C 1.891720 2.594765 -0.787367
 C 0.714208 2.881210 0.140269
 N 0.978357 2.824109 1.394568

C -0.593878 3.218227 -0.556496
 N -1.728287 3.241034 0.173439
 C -3.026253 3.622730 -0.382394
 O -0.576559 3.442499 -1.775108
 C -3.652850 2.619215 -1.386309
 O -3.092764 2.738035 -2.674578
 C -3.602773 1.188338 -0.850458
 C -3.441736 -1.443114 0.204923
 C -4.349294 0.815687 0.273607
 C -2.790630 0.234009 -1.461218
 C -2.721239 -1.047817 -0.930662
 C -4.268968 -0.471703 0.791435
 Br -1.581194 -2.356621 -1.762893
 Br -5.294819 -0.939200 2.326566
 O -3.382669 -2.680378 0.744536
 O -0.097835 3.108514 2.250375
 H 4.493162 2.424850 0.101108
 H 5.732668 -1.872569 0.818478
 H 0.499773 -0.865615 -0.974721
 H 1.485028 2.493281 -1.796149
 H 2.550096 3.471302 -0.799529
 H -1.652200 3.039870 1.161519
 H -2.934812 4.589337 -0.891599
 H -3.697503 3.752963 0.470579
 H -4.709438 2.910459 -1.480898
 H -2.157870 3.017878 -2.567261
 H -5.010083 1.528306 0.758739
 H -2.226863 0.500470 -2.346646
 H -2.753161 -3.211720 0.222680
 H 0.291699 2.961820 3.126619
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4055651**

Comp_08Z_c07
B3LYP/6-31G* Geometry
 C 2.196305 0.085214 -0.485179
 C 4.845931 0.260960 0.337097
 C 2.924614 -1.071152 -0.184281
 C 2.803799 1.351897 -0.370837
 C 4.129578 1.417562 0.043301
 C 4.262706 -1.006859 0.230967
 Br 2.079527 -2.771412 -0.341510
 Br 6.674051 0.370973 0.905662
 O 4.913138 -2.159034 0.505597
 O 0.904773 0.069384 -0.889205
 C 2.009434 2.587917 -0.724411
 C 0.827758 2.857000 0.202769
 N 1.082362 2.770492 1.457217
 C -0.473134 3.219909 -0.493076
 N -1.617070 3.207457 0.223313
 C -2.901418 3.640770 -0.326069
 O -0.443769 3.497811 -1.700100
 C -3.551323 2.685478 -1.360284
 O -2.946570 2.782240 -2.629544

C -3.600801 1.248160 -0.843590
 C -3.635416 -1.406490 0.163874
 C -2.735087 0.278707 -1.354590
 C -4.497706 0.882963 0.164170
 C -4.505273 -0.418514 0.651141
 C -2.753179 -1.017305 -0.853967
 Br -5.741556 -0.918159 2.032967
 Br -1.539092 -2.312940 -1.557452
 O -3.614072 -2.680045 0.613992
 O -0.000945 3.038164 2.311177
 H 4.616039 2.382496 0.139143
 H 5.823901 -1.935278 0.774449
 H 0.567317 -0.846643 -0.945634
 H 1.608477 2.513139 -1.737898
 H 2.671583 3.461616 -0.711677
 H -1.550276 2.975267 1.205234
 H -2.777504 4.618663 -0.806396
 H -3.574933 3.765232 0.526306
 H -4.587721 3.036982 -1.476896
 H -2.017683 3.072450 -2.501884
 H -2.055474 0.544039 -2.155261
 H -5.201464 1.603647 0.570344
 H -4.296809 -2.772958 1.304197
 H 0.383736 2.874060 3.186427

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4051693**

Comp_08Z_c10

B3LYP/6-31G* Geometry

C -1.917167 2.082903 -0.773766
 C -0.821633 -0.221744 -1.880918
 C -2.600457 0.861216 -0.710446
 C -0.657908 2.151121 -1.400340
 C -0.133477 0.983438 -1.951894
 C -2.070135 -0.315793 -1.252691
 Br -4.286744 0.798996 0.173945
 Br -0.051917 -1.807595 -2.629862
 O -2.781099 -1.456537 -1.151483
 O -2.429983 3.222698 -0.252276
 C 0.090285 3.474022 -1.475787
 C 1.574642 3.303386 -1.253608
 N 2.315924 3.451151 -2.292381
 C 1.988659 2.991063 0.177670
 N 3.114640 2.268639 0.358281
 C 3.701644 1.958739 1.664697
 O 1.250631 3.367803 1.094150
 C 2.796182 1.216593 2.683788
 O 1.989173 2.111120 3.414712
 C 1.998417 0.062291 2.069122
 C 0.481671 -2.095892 1.016797
 C 2.601143 -0.894428 1.245483
 C 0.639652 -0.073443 2.363572
 C -0.102298 -1.130253 1.847796
 C 1.847491 -1.944668 0.735653

Br -1.954479 -1.265234 2.257038
 Br 2.674727 -3.244222 -0.409291
 O -0.276967 -3.106126 0.526724
 O 3.695276 3.276887 -2.054572
 H 0.830621 1.010567 -2.447561
 H -2.201283 -2.204194 -1.386922
 H -3.271113 3.005741 0.192904
 H -0.301221 4.147630 -0.710792
 H -0.055856 3.946563 -2.453458
 H 3.689885 2.127715 -0.462230
 H 4.037209 2.879400 2.158332
 H 4.589411 1.356149 1.453154
 H 3.488658 0.792090 3.424517
 H 1.553674 2.691209 2.751760
 H 3.655515 -0.838607 0.995383
 H 0.165757 0.654383 3.009897
 H 0.300234 -3.678019 -0.013101
 H 4.072503 3.424692 -2.936043

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4130175**

Comp_08Z_c14

B3LYP/6-31G* Geometry

C -3.167987 -0.106855 -0.776184
 C -5.818289 -0.208087 0.044746
 C -3.727782 -1.310595 -0.334792
 C -3.942330 1.070501 -0.804106
 C -5.268482 0.995497 -0.386691
 C -5.062857 -1.387123 0.083850
 Br -2.636785 -2.871595 -0.301136
 Br -7.648852 -0.290244 0.608560
 O -5.546733 -2.577280 0.499255
 O -1.886960 0.005309 -1.187086
 C -3.327255 2.383752 -1.260871
 C -2.317438 2.943449 -0.267249
 N -2.804036 3.645049 0.688950
 C -0.858125 2.618427 -0.535342
 N -0.069254 2.367040 0.534306
 C 1.336705 2.001639 0.380129
 O -0.456220 2.532893 -1.699135
 C 1.545961 0.503531 0.060416
 O 0.978140 0.138070 -1.188175
 C 3.032008 0.168620 0.091697
 C 5.815357 -0.369273 0.177475
 C 3.767165 0.074830 -1.090832
 C 3.690585 -0.017335 1.311907
 C 5.055029 -0.277680 1.354048
 C 5.129949 -0.188695 -1.033996
 Br 5.915745 -0.528180 3.033987
 Br 6.144946 -0.325047 -2.657897
 O 7.137951 -0.628229 0.261668
 O -1.839265 4.108820 1.606413
 H -5.885100 1.888047 -0.393568
 H -6.481199 -2.453507 0.751179

H -1.391746 -0.827115 -1.070424
 H -4.124968 3.119635 -1.391461
 H -2.811932 2.257669 -2.217184
 H -0.434767 2.586729 1.451134
 H 1.850893 2.250324 1.312138
 H 1.777226 2.605444 -0.421154
 H 1.045255 -0.074594 0.853493
 H 0.533007 0.918237 -1.578525
 H 3.263677 0.187082 -2.043100
 H 3.139914 0.029901 2.246828
 H 7.499452 -0.666114 -0.643782
 H -2.382171 4.616650 2.229921
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.3982132**

Comp_08Z_c19
B3LYP/6-31G* Geometry
 C 2.155272 0.095298 -0.502602
 C 4.817244 0.247725 0.349423
 C 2.881019 -1.058763 -0.189298
 C 2.776364 1.352128 -0.383846
 C 4.100297 1.401460 0.043483
 C 4.218842 -1.011788 0.238229
 Br 2.032903 -2.774795 -0.340595
 Br 6.626502 0.375938 0.927235
 O 4.936414 -2.115888 0.542382
 O 0.865261 0.091173 -0.917480
 C 1.999648 2.598278 -0.743516
 C 0.820651 2.886770 0.181655
 N 1.082776 2.832523 1.436446
 C -0.485892 3.228220 -0.514564
 N -1.625368 3.225584 0.209466
 C -2.915245 3.644164 -0.338362
 O -0.465682 3.479760 -1.727462
 C -3.562899 2.675570 -1.361935
 O -2.974430 2.776648 -2.638107
 C -3.586217 1.239166 -0.839670
 C -3.570445 -1.414404 0.172730
 C -4.446275 0.869653 0.198450
 C -2.733131 0.274147 -1.378890
 C -2.727124 -1.020623 -0.875232
 C -4.429534 -0.430840 0.687692
 Br -1.531183 -2.311576 -1.621314
 Br -5.612965 -0.935418 2.112576
 O -3.524607 -2.686808 0.624439
 O 0.003951 3.116566 2.290707
 H 4.593033 2.363072 0.141262
 H 4.375337 -2.900314 0.403749
 H 0.512749 -0.816397 -0.990659
 H 1.599264 2.526726 -1.757390
 H 2.675183 3.461321 -0.730207
 H -1.549456 3.021970 1.197069
 H -2.802814 4.618873 -0.828022
 H -3.585533 3.770714 0.516217

H -4.605223 3.011697 -1.469481
 H -2.042374 3.061520 -2.518932
 H -5.140038 1.586530 0.627835
 H -2.082678 0.543081 -2.202191
 H -4.183500 -2.783032 1.337101
 H 0.397510 2.983698 3.167351
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4037681**

Comp_08Z_c20
B3LYP/6-31G* Geometry
 C -0.268919 -2.439351 1.060663
 C -1.576228 -0.093558 1.840384
 C -1.501675 -2.074433 0.503672
 C 0.316346 -1.614710 2.037798
 C -0.358614 -0.450357 2.409611
 C -2.173648 -0.898610 0.863823
 Br -2.307029 -3.230256 -0.799881
 Br -2.442628 1.516711 2.372938
 O -3.352757 -0.520513 0.316574
 O 0.384192 -3.574401 0.708367
 C 1.645578 -1.999848 2.666551
 C 2.851219 -1.558076 1.853779
 N 3.538636 -2.508507 1.332474
 C 3.082904 -0.054301 1.814475
 N 3.860045 0.443098 0.818331
 C 4.009324 1.866684 0.596644
 O 2.531023 0.650639 2.659188
 C 3.586637 2.275031 -0.825682
 O 4.508097 1.620754 -1.697370
 C 2.141605 1.925217 -1.144444
 C -0.561041 1.226252 -1.645613
 C 1.107895 2.802568 -0.804650
 C 1.816473 0.704723 -1.745299
 C 0.491050 0.366215 -1.990753
 C -0.212812 2.451720 -1.054083
 Br 0.079090 -1.311577 -2.790888
 Br -1.627317 3.653295 -0.596547
 O -1.833366 0.853008 -1.900826
 O 4.659270 -2.082331 0.591849
 H 0.095446 0.204611 3.143229
 H -3.562324 -1.133683 -0.411093
 H -0.128853 -4.032632 0.019168
 H 1.705311 -3.084419 2.781401
 H 1.716357 -1.536213 3.654389
 H 4.340285 -0.203023 0.205678
 H 5.056045 2.166192 0.734878
 H 3.398774 2.380508 1.340905
 H 3.709847 3.368390 -0.892455
 H 4.247330 1.817683 -2.611325
 H 1.323617 3.760511 -0.341668
 H 2.602305 0.010737 -2.018555
 H -2.436232 1.487578 -1.468877
 H 5.019029 -2.922690 0.268397

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4113002

Comp_08Z_c21
B3LYP/6-31G* Geometry

C -2.406426 1.674518 0.669959
C -0.815331 -0.281348 1.852944
C -2.767055 0.321215 0.611708
C -1.219330 2.053607 1.324669
C -0.448499 1.057225 1.921408
C -1.973936 -0.682737 1.176791
Br -4.357961 -0.163587 -0.321809
Br 0.291286 -1.633152 2.629732
O -2.350081 -1.975533 1.035472
O -3.167923 2.646967 0.115809
C -0.792221 3.513332 1.365499
C 0.688498 3.676532 1.104908
N 1.392397 4.014897 2.125147
C 1.120607 3.417127 -0.333813
N 2.421660 3.092374 -0.546540
C 2.931052 2.746033 -1.856827
O 0.277964 3.478653 -1.226792
C 3.507487 1.319274 -1.899353
O 4.578928 1.214377 -0.954439
C 2.500046 0.219469 -1.594170
C 0.681058 -1.906351 -1.103467
C 1.189739 0.279483 -2.081124
C 2.893145 -0.911976 -0.870454
C 2.000001 -1.950283 -0.631687
C 0.312996 -0.770748 -1.841018
Br 2.570345 -3.468418 0.365498
Br -1.480348 -0.685125 -2.506234
O -0.161988 -2.929718 -0.836656
O 2.770798 4.158105 1.867266
H 0.465918 1.327378 2.438076
H -1.654341 -2.534430 1.433581
H -3.913831 2.226552 -0.351692
H -1.018573 3.955957 2.341685
H -1.343442 4.064839 0.601627
H 3.054534 3.070223 0.242208
H 3.734668 3.442580 -2.137676
H 2.120946 2.882599 -2.574564
H 3.900853 1.158998 -2.917481
H 5.349766 1.663513 -1.333678
H 0.824717 1.143009 -2.623972
H 3.901980 -0.976016 -0.484259
H -1.046011 -2.696150 -1.180202
H 3.115588 4.390892 2.743416

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4111156

Comp_08Z_c23
B3LYP/6-31G* Geometry

C -2.850356 0.796017 -1.268854
C -4.763693 -0.856010 -0.053021
C -2.814098 -0.596112 -1.424372
C -3.850938 1.363760 -0.457781
C -4.797594 0.522393 0.130154
C -3.754913 -1.448290 -0.825696
Br -1.403510 -1.378547 -2.455185
Br -6.077455 -1.960291 0.770199
O -3.726482 -2.791601 -0.961463
O -1.978981 1.628467 -1.885324
C -3.807773 2.848396 -0.129341
C -2.931332 3.089764 1.084941
N -3.488158 3.482266 2.167924
C -1.443899 2.832909 0.928668
N -0.983600 1.686924 1.487686
C 0.426886 1.308254 1.433700
O -0.734288 3.589959 0.262549
C 0.836468 0.651999 0.096505
O 0.590728 1.532680 -1.002815
C 2.296683 0.223091 0.142731
C 5.014350 -0.566986 0.309720
C 3.285471 0.964552 -0.504835
C 2.670050 -0.917109 0.863498
C 4.002482 -1.302045 0.948569
C 4.613668 0.566170 -0.414812
Br 4.474829 -2.856845 1.938279
Br 5.975750 1.576767 -1.310894
O 6.295266 -0.978116 0.413074
O -2.561926 3.600296 3.223814
H -5.570364 0.946865 0.763282
H -2.972118 -3.027218 -1.532942
H -1.041777 1.327453 -1.801131
H -4.809323 3.221615 0.101516
H -3.406481 3.412776 -0.975942
H -1.616311 1.153091 2.067484
H 0.623984 0.616403 2.256228
H 1.039236 2.202647 1.596377
H 0.214549 -0.238845 -0.066037
H 0.364631 2.425209 -0.651856
H 3.011824 1.832374 -1.092003
H 1.920148 -1.525801 1.360194
H 6.856573 -0.362929 -0.095372
H -3.112053 3.956098 3.939638

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4009841

Comp_08Z_c24
B3LYP/6-31G* Geometry

C 2.210376 -0.144323 1.146953
C 4.564023 0.063203 -0.316682
C 2.641632 -1.197689 0.330756
C 2.957102 1.045853 1.214485
C 4.131766 1.124736 0.468765
C 3.824768 -1.122180 -0.412374

Br 1.553455 -2.756197 0.206542
 Br 6.188490 0.196508 -1.324884
 O 4.184235 -2.176959 -1.174839
 O 1.066535 -0.213177 1.875841
 C 2.521506 2.212742 2.081481
 C 1.084010 2.674331 1.912952
 N 0.442962 2.840378 3.012684
 C 0.624079 2.917902 0.489928
 N -0.704105 2.958612 0.240641
 C -1.215365 3.146900 -1.110476
 O 1.473951 3.030564 -0.402565
 C -1.274106 1.840329 -1.937190
 O 0.003761 1.252353 -2.078759
 C -2.242963 0.840326 -1.318371
 C -4.075321 -0.913211 -0.046071
 C -3.624005 1.038353 -1.428657
 C -1.775915 -0.253886 -0.588221
 C -2.687044 -1.097515 0.036085
 C -4.521663 0.179564 -0.805992
 Br -2.054169 -2.586477 1.079136
 Br -6.394281 0.479041 -0.979779
 O -4.980731 -1.717744 0.552235
 O -0.871293 3.315603 2.862355
 H 4.718098 2.036887 0.492505
 H 5.012684 -1.948128 -1.636735
 H 0.648795 -1.084865 1.736236
 H 3.178371 3.060444 1.854184
 H 2.648466 1.977192 3.144005
 H -1.340578 2.865877 1.020821
 H -0.564740 3.862868 -1.623541
 H -2.214786 3.585098 -1.038630
 H -1.664944 2.127152 -2.928932
 H 0.680412 1.885045 -1.767544
 H -4.015574 1.868599 -2.009427
 H -0.711828 -0.445101 -0.535117
 H -4.499189 -2.421269 1.026036
 H -1.188496 3.328906 3.778997
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4024229**

Comp_08Z_c25
B3LYP/6-31G* Geometry
 C 3.578728 -0.983875 0.539268
 C 5.278530 1.092296 -0.176149
 C 4.634417 -1.203961 -0.352291
 C 3.368522 0.294992 1.087363
 C 4.231503 1.321029 0.711358
 C 5.506141 -0.174090 -0.728800
 Br 4.884351 -2.954454 -1.068349
 Br 6.455436 2.519253 -0.677398
 O 6.505488 -0.451029 -1.593578
 O 2.720380 -1.966385 0.909467
 C 2.230474 0.528561 2.059777
 C 0.851810 0.431420 1.416822

N 0.540069 1.383982 0.615638
 C -0.037688 -0.702110 1.892772
 N -0.904768 -1.246647 1.007155
 C -1.830128 -2.301490 1.401470
 O 0.068222 -1.092973 3.060251
 C -3.105882 -1.778122 2.109222
 O -2.787498 -1.065475 3.289483
 C -3.914979 -0.891958 1.174373
 C -5.224534 0.728887 -0.752200
 C -3.655686 0.478846 1.112650
 C -4.849389 -1.440561 0.290088
 C -5.496981 -0.644525 -0.649265
 C -4.288641 1.253585 0.151755
 Br -6.770442 -1.421388 -1.832321
 Br -3.843638 3.120007 0.003472
 O -5.857027 1.463742 -1.692897
 O -0.736761 1.252276 0.041614
 H 4.087069 2.317134 1.115650
 H 7.010568 0.369900 -1.745747
 H 2.986690 -2.795671 0.469087
 H 2.341606 1.524422 2.499336
 H 2.260360 -0.198019 2.875806
 H -1.071750 -0.740434 0.147115
 H -1.297033 -2.977683 2.077051
 H -2.109395 -2.863832 0.505603
 H -3.708674 -2.669444 2.353938
 H -1.851152 -1.228697 3.514271
 H -2.954688 0.924291 1.805204
 H -5.083270 -2.500497 0.326763
 H -5.555016 2.387547 -1.613699
 H -0.861920 2.095223 -0.423089
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.3985074**

Comp_08Z_c26
B3LYP/6-31G* Geometry
 C -0.718888 -0.309344 2.370823
 C -1.693932 -2.088746 0.434817
 C -1.812319 0.022199 1.556469
 C -0.069928 -1.541176 2.170825
 C -0.585692 -2.412487 1.209496
 C -2.312107 -0.840471 0.572048
 Br -2.654641 1.729632 1.791176
 Br -2.389675 -3.347961 -0.811300
 O -3.349804 -0.515757 -0.238004
 O -0.274435 0.504987 3.353289
 C 1.173159 -1.919936 2.963087
 C 2.414418 -1.935122 2.087730
 N 2.805982 -3.103143 1.724236
 C 3.008088 -0.563468 1.785467
 N 3.878068 -0.453075 0.745540
 C 4.437232 0.828522 0.363397
 O 2.662933 0.389278 2.479637
 C 4.048367 1.256023 -1.062094

O 4.684460 0.320281 -1.931129
 C 2.543824 1.320219 -1.279879
 C -0.274252 1.403644 -1.596197
 C 1.806405 2.429505 -0.850363
 C 1.866830 0.258445 -1.882367
 C 0.487833 0.314677 -2.044186
 C 0.425181 2.465865 -1.001668
 Br -0.434832 -1.136366 -2.878390
 Br -0.551759 3.980356 -0.389573
 O -1.618544 1.476711 -1.717024
 O 3.945221 -3.111886 0.895930
 H -0.102565 -3.372370 1.057566
 H -3.643629 0.385926 -0.010017
 H -0.749153 1.353596 3.307864
 H 1.051455 -2.920336 3.388840
 H 1.326702 -1.204567 3.771740
 H 4.155440 -1.287425 0.246444
 H 5.532530 0.788363 0.411389
 H 4.081694 1.563486 1.087122
 H 4.471835 2.262539 -1.214418
 H 4.463205 0.561757 -2.844902
 H 2.303527 3.273760 -0.382800
 H 2.415402 -0.611958 -2.221787
 H -1.947590 0.622712 -2.059178
 H 4.070582 -4.059110 0.730728

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4087688**

Comp_08Z_c27

B3LYP/6-31G* Geometry

C 2.215081 -0.205816 1.106690
 C 4.523346 0.007303 -0.426927
 C 2.625535 -1.261512 0.281992
 C 2.967576 0.982597 1.159319
 C 4.117422 1.065559 0.376485
 C 3.785686 -1.180767 -0.497139
 Br 1.556868 -2.835388 0.204826
 Br 6.114372 0.146362 -1.487430
 O 4.127465 -2.235182 -1.268476
 O 1.090137 -0.266984 1.864258
 C 2.578246 2.136931 2.065575
 C 1.144929 2.627724 1.962439
 N 0.538841 2.752600 3.087145
 C 0.647671 2.946752 0.567561
 N -0.687965 3.003415 0.360181
 C -1.241190 3.252253 -0.964047
 O 1.472118 3.101703 -0.341834
 C -1.320392 1.984682 -1.849210
 O -0.046242 1.404079 -2.043923
 C -2.270574 0.953524 -1.256401
 C -4.052831 -0.876828 -0.021333
 C -1.791055 -0.048269 -0.406354
 C -3.643671 1.028014 -1.501172
 C -4.507651 0.125517 -0.891835

C -2.668921 -0.934548 0.204663
 Br -6.393690 0.222048 -1.236408
 Br -1.993935 -2.267922 1.393317
 O -4.864524 -1.767098 0.589831
 O -0.771578 3.254642 2.997627
 H 4.705644 1.976705 0.387316
 H 4.941492 -2.003418 -1.753827
 H 0.639241 -1.122898 1.724776
 H 3.240911 2.979257 1.835478
 H 2.738474 1.872669 3.116820
 H -1.299416 2.876875 1.155568
 H -0.608601 3.994023 -1.463148
 H -2.239894 3.681421 -0.842008
 H -1.735849 2.316971 -2.816526
 H 0.638916 2.029196 -1.735874
 H -0.725224 -0.134343 -0.242209
 H -4.047561 1.781792 -2.170456
 H -5.781222 -1.588705 0.308442
 H -1.063815 3.221873 3.922056

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4036379**

Comp_08Z_c28

B3LYP/6-31G* Geometry

C -0.507640 -0.469400 2.261120
 C -2.296239 -1.613791 0.422101
 C -1.533410 0.286235 1.672867
 C -0.380969 -1.830180 1.909625
 C -1.283691 -2.373846 0.990507
 C -2.428297 -0.255997 0.741631
 Br -1.686659 2.139480 2.091501
 Br -3.505823 -2.407064 -0.815987
 O -3.380462 0.483757 0.124601
 O 0.293276 0.143166 3.156963
 C 0.702195 -2.716265 2.508394
 C 1.919322 -2.835359 1.607669
 N 2.043694 -3.964670 1.007791
 C 2.807103 -1.606681 1.538602
 N 3.667225 -1.480234 0.509869
 C 4.449350 -0.275881 0.288923
 O 2.701485 -0.744619 2.425735
 C 4.146394 0.361736 -1.078537
 O 4.530041 -0.620232 -2.040337
 C 2.699474 0.801344 -1.239761
 C -0.012486 1.606105 -1.459248
 C 1.751440 -0.051308 -1.811242
 C 2.286316 2.062783 -0.795275
 C 0.957087 2.455807 -0.901422
 C 0.427548 0.356544 -1.923236
 Br 0.429232 4.173713 -0.285272
 Br -0.868187 -0.807069 -2.710741
 O -1.291514 2.026124 -1.540138
 O 3.150705 -4.056775 0.148460
 H -1.196190 -3.420055 0.715190

H -3.313526 1.396759 0.468911
H 1.208972 -0.221122 3.076700
H 0.307968 -3.724962 2.656054
H 1.012575 -2.333847 3.485169
H 3.743366 -2.239368 -0.155644
H 5.517632 -0.521317 0.320522
H 4.224353 0.420931 1.096770
H 4.795370 1.248793 -1.158518
H 4.314738 -0.276239 -2.922046
H 2.044661 -1.029465 -2.173774
H 3.000846 2.753111 -0.357145
H -1.849524 1.286269 -1.848998
H 3.063403 -4.954735 -0.207926

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4195403

Comp_08Z_c30

B3LYP/6-31G* Geometry

C -4.494527 1.109097 0.960248
C -5.076914 -1.119055 -0.605282
C -5.256327 1.233215 -0.210767
C -4.010115 -0.154633 1.348829
C -4.318179 -1.255681 0.550179
C -5.561705 0.130283 -1.016324
Br -5.894177 2.959350 -0.712910
Br -5.488617 -2.647618 -1.686132
O -6.298576 0.321551 -2.130844
O -4.211956 2.169855 1.750851
C -3.188907 -0.313415 2.619921
C -1.899616 -1.060171 2.378028
N -1.815935 -2.243113 2.867829
C -0.791630 -0.288588 1.675795
N -0.094141 -0.964953 0.723463
C 1.168515 -0.452552 0.203077
O -0.586307 0.880491 1.980417
C 2.316028 -0.662957 1.223586
O 2.367868 -2.026117 1.626838
C 3.649043 -0.276150 0.619833
C 6.097793 0.487787 -0.588336
C 4.003419 1.072969 0.507479
C 4.524392 -1.247521 0.129204
C 5.721329 -0.857762 -0.458467
C 5.203093 1.446280 -0.087115
Br 6.932928 -2.189198 -1.127020
Br 5.657118 3.289987 -0.218665
O 7.255088 0.893070 -1.154161
O -0.565381 -2.876442 2.616254
H -3.958882 -2.238371 0.837643
H -6.419171 -0.542421 -2.568041
H -4.581097 2.973928 1.339434
H -3.761382 -0.851228 3.383398
H -2.934742 0.673814 3.012095
H -0.237315 -1.965101 0.676953
H 1.048246 0.608924 -0.024917

H 1.397396 -0.989443 -0.721746
H 2.112792 -0.015532 2.089131
H 1.552544 -2.214041 2.122962
H 3.346937 1.846970 0.892970
H 4.275139 -2.296860 0.223417
H 7.751079 0.101253 -1.434550
H -0.674868 -3.719778 3.083431

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.3978440

Comp_08Z_c31

B3LYP/6-31G* Geometry

C 3.589010 -0.999434 0.531320
C 5.252860 1.111680 -0.166352
C 4.648169 -1.193352 -0.362401
C 3.357494 0.270623 1.091267
C 4.202645 1.314523 0.723598
C 5.502125 -0.145712 -0.730049
Br 4.927501 -2.933154 -1.094266
Br 6.404317 2.563244 -0.655889
O 6.506174 -0.397857 -1.597155
O 2.747957 -2.000043 0.892330
C 2.215397 0.478473 2.065495
C 0.840063 0.385339 1.416444
N 0.508033 1.372648 0.665876
C -0.031168 -0.783255 1.838497
N -0.899387 -1.294380 0.933207
C -1.822829 -2.364100 1.289457
O 0.082072 -1.226541 2.986563
C -3.095654 -1.871713 2.025623
O -2.773098 -1.211470 3.234253
C -3.910515 -0.946662 1.133723
C -5.217092 0.764961 -0.716158
C -4.869342 -1.455237 0.254444
C -3.632163 0.423558 1.105101
C -4.254630 1.251309 0.181352
C -5.509936 -0.606003 -0.641293
Br -3.756311 3.093241 0.095616
Br -6.835634 -1.302387 -1.841843
O -5.801217 1.612550 -1.590435
O -0.756176 1.235315 0.071887
H 4.040970 2.304483 1.136348
H 6.996709 0.433161 -1.742047
H 3.028836 -2.820426 0.444503
H 2.318876 1.467321 2.522168
H 2.248389 -0.263464 2.867425
H -1.077866 -0.746818 0.101232
H -1.286329 -3.067479 1.933814
H -2.107259 -2.889626 0.372963
H -3.696797 -2.773594 2.233818
H -1.833602 -1.377184 3.444148
H -5.122847 -2.511114 0.261051
H -2.912384 0.833732 1.799970
H -6.442190 1.107394 -2.124733

H -0.942890 2.117077 -0.290799
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.3981903

Comp_08Z_c34

B3LYP/6-31G* Geometry

C -4.945988 -1.053103 0.491798
C -4.410250 1.640946 0.052556
C -5.626935 -0.341822 -0.505249
C -3.985491 -0.400985 1.288280
C -3.730274 0.949496 1.047896
C -5.375788 1.013797 -0.746980
Br -6.933777 -1.253857 -1.555595
Br -4.048616 3.495992 -0.264352
O -6.065680 1.639989 -1.723551
O -5.181143 -2.365690 0.732237
C -3.250360 -1.164470 2.374954
C -1.992588 -1.844112 1.872709
N -1.942193 -3.119806 1.989365
C -0.874832 -0.920843 1.415657
N -0.141205 -1.332308 0.348902
C 1.121721 -0.693775 -0.000819
O -0.691902 0.141190 2.005920
C 2.257967 -1.162730 0.943454
O 2.322117 -2.583502 0.964707
C 3.594091 -0.616023 0.488412
C 6.047348 0.470377 -0.428561
C 3.928656 0.718217 0.745498
C 4.491713 -1.411771 -0.226813
C 5.690549 -0.865535 -0.667883
C 5.130392 1.250469 0.293357
Br 6.932491 -1.956836 -1.644725
Br 5.555255 3.068384 0.663746
O 7.205821 1.024956 -0.845587
O -0.717072 -3.688922 1.540210
H -2.978096 1.459565 1.639229
H -5.768025 2.569013 -1.756579
H -5.881434 -2.669998 0.124347
H -3.897206 -1.928943 2.810118
H -2.951194 -0.466217 3.163316
H -0.281938 -2.284972 0.039141
H 0.995295 0.389474 0.059286
H 1.367024 -0.965775 -1.031285
H 2.035155 -0.774838 1.948452
H 1.496917 -2.907116 1.364833
H 3.254222 1.353962 1.310768
H 4.258367 -2.451324 -0.419510
H 7.717543 0.342489 -1.318926
H -0.866937 -4.632397 1.710246

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.3986972

Comp_08Z_c36

B3LYP/6-31G* Geometry

C 2.445459 -0.147980 1.620519
C 3.419080 0.492660 -0.926713
C 2.829115 -1.144948 0.714057
C 2.561384 1.201566 1.244257
C 3.047727 1.490944 -0.032698
C 3.314585 -0.857990 -0.569381
Br 2.672487 -2.987210 1.239824
Br 4.074091 0.951508 -2.651967
O 3.681113 -1.808830 -1.454777
O 1.976665 -0.426575 2.862552
C 2.190439 2.305417 2.220612
C 0.695447 2.545881 2.343724
N 0.188931 2.266385 3.490622
C 0.021842 3.109176 1.106354
N -1.321950 3.034626 1.008698
C -2.058785 3.571412 -0.133994
O 0.731902 3.592807 0.212782
C -1.995013 2.698803 -1.411823
O -0.727301 2.755529 -2.031325
C -2.415795 1.263207 -1.113434
C -3.198608 -1.369815 -0.405468
C -3.767155 0.922991 -0.996044
C -1.452952 0.277402 -0.891639
C -1.849920 -1.005141 -0.537068
C -4.150733 -0.368498 -0.650644
Br -0.517737 -2.342081 -0.170734
Br -6.001091 -0.797902 -0.506115
O -3.611616 -2.610695 -0.064311
O -1.192087 2.500264 3.600198
H 3.126662 2.526614 -0.340855
H 3.538348 -2.684731 -1.053898
H 1.941321 -1.392680 2.978484
H 2.659782 3.236795 1.890590
H 2.561908 2.064453 3.219986
H -1.827954 2.630463 1.785418
H -1.666905 4.566516 -0.372874
H -3.099916 3.680883 0.181409
H -2.729258 3.132116 -2.109073
H -0.085502 3.141304 -1.400883
H -4.539307 1.664152 -1.181475
H -0.403507 0.518124 -1.012276
H -2.822629 -3.173354 0.046601
H -1.379255 2.200701 4.503702

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4071179

Comp_08Z_c37

B3LYP/6-31G* Geometry

C 3.861571 -1.503938 -0.122408
C 4.831094 1.091457 -0.363609
C 4.902990 -1.050205 0.698328
C 3.299994 -0.643969 -1.085957
C 3.800175 0.654376 -1.186902

C 5.408693 0.251103 0.597810
 Br 5.650736 -2.248567 1.982002
 Br 5.509317 2.877728 -0.520205
 O 6.412427 0.625640 1.419312
 O 3.366679 -2.761582 -0.033366
 C 2.176886 -1.134116 -1.982861
 C 0.803780 -0.967591 -1.361018
 N 0.148748 -2.047007 -1.127867
 C 0.323453 0.463110 -1.203104
 N -0.505921 0.750328 -0.173573
 C -1.049147 2.090772 0.011085
 O 0.728100 1.319657 -2.000223
 C -2.288372 2.382784 -0.873274
 O -1.987214 2.237671 -2.248631
 C -3.443131 1.465321 -0.503423
 C -5.433589 -0.360997 0.364566
 C -4.337516 1.809157 0.515036
 C -3.562705 0.212547 -1.109093
 C -4.528376 -0.676552 -0.660192
 C -5.318073 0.916440 0.935493
 Br -4.621214 -2.436264 -1.431300
 Br -6.525653 1.421420 2.317805
 O -6.384659 -1.207157 0.816267
 O -1.122274 -1.829351 -0.564263
 H 3.365000 1.334058 -1.910551
 H 6.641541 1.551908 1.214097
 H 3.862765 -3.240988 0.656944
 H 2.310599 -2.193377 -2.212104
 H 2.192418 -0.566570 -2.918134
 H -0.941960 -0.029355 0.302711
 H -0.256919 2.806118 -0.230141
 H -1.309679 2.212848 1.066424
 H -2.583902 3.422927 -0.653302
 H -1.017550 2.229525 -2.359449
 H -4.278072 2.783105 0.991662
 H -2.895259 -0.059540 -1.915355
 H -6.325645 -2.035561 0.305094
 H -1.515464 -2.716664 -0.554034

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4006328**

Comp_08Z_c38

B3LYP/6-31G* Geometry

C -2.863368 -0.246205 -0.899870
 C -0.404256 -1.261019 -1.706026
 C -2.414450 -1.489444 -0.436695
 C -2.066982 0.501263 -1.789111
 C -0.835313 -0.026562 -2.176942
 C -1.180330 -2.023395 -0.823019
 Br -3.493768 -2.452388 0.806455
 Br 1.308718 -1.946530 -2.229670
 O -0.808894 -3.223658 -0.332873
 O -4.052276 0.278841 -0.516326
 C -2.533979 1.864497 -2.270029

C -2.123437 2.979809 -1.324475
 N -3.079175 3.539280 -0.676374
 C -0.635178 3.300783 -1.317502
 N -0.121781 3.874057 -0.199554
 C 1.284831 4.195607 -0.071175
 O 0.042320 2.997494 -2.299480
 C 1.914314 3.578603 1.188863
 O 1.182506 4.122533 2.285457
 C 1.922243 2.057343 1.190411
 C 1.945560 -0.777473 1.164873
 C 2.969467 1.363146 0.577229
 C 0.888808 1.326321 1.785171
 C 0.903786 -0.064974 1.776502
 C 2.966937 -0.024999 0.564564
 Br -0.518648 -1.031050 2.588430
 Br 4.395230 -0.976355 -0.286535
 O 1.929800 -2.130057 1.182318
 O -2.667102 4.569113 0.195417
 H -0.198171 0.551515 -2.835797
 H 0.128575 -3.366625 -0.558946
 H -4.476284 -0.346080 0.101806
 H -3.622060 1.881235 -2.357794
 H -2.093866 2.072017 -3.249218
 H -0.760637 4.185442 0.520627
 H 1.416103 5.283956 -0.012004
 H 1.789160 3.832818 -0.968254
 H 2.959380 3.928842 1.218172
 H 1.530424 3.731545 3.102756
 H 3.788988 1.898105 0.107357
 H 0.067616 1.846297 2.263912
 H 2.738367 -2.443629 0.734615
 H -3.507283 4.838601 0.597766

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4138207**

Comp_08Z_c40

B3LYP/6-31G* Geometry

C -0.694013 -0.076993 -2.321991
 C -2.752559 0.048946 -0.448913
 C -1.090556 -1.221989 -1.610521
 C -1.321275 1.157050 -2.063796
 C -2.353669 1.193281 -1.126257
 C -2.115102 -1.179958 -0.660857
 Br -0.186006 -2.863612 -1.945995
 Br -4.187514 0.115229 0.818584
 O -2.434293 -2.313519 0.014668
 O 0.272724 -0.121261 -3.262655
 C -0.873226 2.435887 -2.757133
 C -0.188247 3.379060 -1.785527
 N -0.917042 4.338641 -1.342942
 C 1.273090 3.058443 -1.492584
 N 1.778819 3.453014 -0.293657
 C 3.145844 3.157626 0.086737
 O 1.915874 2.430202 -2.328687

C 3.242941 2.406631 1.424159
 O 2.745795 3.310597 2.409663
 C 2.502604 1.076395 1.429253
 C 1.113924 -1.400458 1.383221
 C 3.074789 -0.056987 0.839323
 C 1.233421 0.964981 1.999388
 C 0.569137 -0.256244 1.983726
 C 2.389580 -1.265162 0.808795
 Br -1.160777 -0.399194 2.792308
 Br 3.174602 -2.775232 -0.041594
 O 0.499491 -2.599712 1.342295
 O -0.266305 5.184281 -0.420016
 H -2.843591 2.138192 -0.915054
 H -3.211580 -2.114527 0.571486
 H 0.650528 -1.020850 -3.280540
 H -1.739484 2.953550 -3.179743
 H -0.173253 2.197003 -3.558467
 H 1.222538 4.058180 0.295423
 H 3.720888 4.087585 0.183994
 H 3.582986 2.562458 -0.716683
 H 4.314558 2.212430 1.595879
 H 2.803015 2.872238 3.273756
 H 4.059398 -0.003328 0.385051
 H 0.765703 1.828625 2.456717
 H -0.441319 -2.491952 1.576732
 H -0.959899 5.829382 -0.212262

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4101986**

Comp_08Z_c41

B3LYP/6-31G* Geometry

C -2.852514 0.769540 -1.280338
 C -4.767399 -0.846445 -0.018836
 C -2.821522 -0.626111 -1.402215
 C -3.848625 1.359891 -0.479749
 C -4.795881 0.536103 0.131554
 C -3.763448 -1.460428 -0.780664
 Br -1.416649 -1.437967 -2.418072
 Br -6.082481 -1.925884 0.834911
 O -3.740089 -2.806824 -0.884993
 O -1.980817 1.583716 -1.919648
 C -3.799691 2.851963 -0.187695
 C -2.918092 3.120570 1.017087
 N -3.469874 3.541377 2.091980
 C -1.431874 2.855810 0.861618
 N -0.973051 1.722837 1.448325
 C 0.435602 1.336971 1.397979
 O -0.722819 3.593049 0.173508
 C 0.836857 0.644844 0.076182
 O 0.589268 1.497728 -1.044088
 C 2.295496 0.212360 0.128303
 C 5.016871 -0.562371 0.308052
 C 3.298670 0.984452 -0.463614
 C 2.654464 -0.956892 0.804433

C 3.991419 -1.324897 0.889363
 C 4.632484 0.603164 -0.373925
 Br 4.483638 -2.930540 1.816420
 Br 5.974698 1.671871 -1.195279
 O 6.323322 -0.894853 0.367402
 O -2.539473 3.682635 3.141451
 H -5.564916 0.978377 0.756999
 H -2.991193 -3.057685 -1.457191
 H -1.043789 1.282723 -1.830566
 H -4.799332 3.233693 0.037503
 H -3.399809 3.394270 -1.049254
 H -1.605407 1.206772 2.044321
 H 0.633569 0.664935 2.236702
 H 1.052690 2.232384 1.535314
 H 0.211375 -0.247834 -0.059982
 H 0.370201 2.400396 -0.715830
 H 3.032116 1.876316 -1.017373
 H 1.899172 -1.591253 1.258777
 H 6.407010 -1.729183 0.865539
 H -3.085482 4.060024 3.849326

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4007097**

Comp_08Z_c42

B3LYP/6-31G* Geometry

C -0.886960 -0.019121 2.269856
 C -1.907393 -1.910659 0.492956
 C -1.965267 0.287033 1.425108
 C -0.296161 -1.295734 2.203129
 C -0.825015 -2.222909 1.304579
 C -2.500540 -0.641304 0.526417
 Br -2.711661 2.045529 1.489356
 Br -2.629330 -3.209706 -0.712569
 O -3.548481 -0.279212 -0.240851
 O -0.399131 0.870557 3.162367
 C 0.889059 -1.668217 3.083024
 C 2.134392 -1.963946 2.268004
 N 2.369670 -3.211579 2.071456
 C 2.918678 -0.734964 1.821358
 N 3.839300 -0.883989 0.831302
 C 4.597449 0.246044 0.332657
 O 2.680935 0.340801 2.365099
 C 4.243832 0.628759 -1.114777
 O 4.709027 -0.446709 -1.926408
 C 2.760037 0.909308 -1.308439
 C -0.020322 1.401094 -1.590303
 C 2.201793 2.106404 -0.849620
 C 1.923345 -0.033870 -1.910268
 C 0.562724 0.213645 -2.054799
 C 0.839362 2.335309 -0.988697
 Br -0.551622 -1.099860 -2.864578
 Br 0.076013 3.967707 -0.339072
 O -1.347110 1.587152 -1.747727
 O 3.515491 -3.483382 1.298735

H -0.376023 -3.208602 1.238615
H -3.733797 -1.007850 -0.862656
H -0.863404 1.719730 3.044123
H 0.649075 -2.562221 3.666990
H 1.109717 -0.847284 3.765609
H 4.000294 -1.804517 0.445982
H 5.669062 0.015618 0.364535
H 4.397885 1.086386 0.999308
H 4.811192 1.546503 -1.343489
H 4.516134 -0.228766 -2.852404
H 2.819990 2.860067 -0.372237
H 2.332794 -0.975100 -2.257210
H -1.626252 2.363984 -1.228209
H 3.511631 -4.452282 1.261100

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.4102178

Comp_08Z_c44

B3LYP/6-31G* Geometry

C -4.959213 -1.013600 0.530997
C -4.402489 1.658521 -0.005560
C -5.638369 -0.332103 -0.487862
C -3.990121 -0.341823 1.300369
C -3.724703 0.997097 1.011457
C -5.376420 1.011763 -0.778865
Br -6.958391 -1.268977 -1.498954
Br -4.026448 3.498235 -0.388979
O -6.064626 1.608701 -1.774786
O -5.204403 -2.314718 0.818569
C -3.256475 -1.072689 2.410347
C -1.999798 -1.768985 1.928643
N -1.954764 -3.041794 2.075598
C -0.877171 -0.861364 1.452350
N -0.142673 -1.301277 0.397821
C 1.124195 -0.677755 0.035662
O -0.691448 0.214024 2.017412
C 2.257714 -1.132904 0.990223
O 2.310676 -2.552952 1.047030
C 3.597021 -0.609565 0.517944
C 6.056528 0.417870 -0.448865
C 3.983075 0.698881 0.819673
C 4.444356 -1.401523 -0.264010
C 5.649912 -0.894962 -0.734772
C 5.189572 1.191909 0.337760
Br 6.785412 -1.998506 -1.792297
Br 5.721405 2.987673 0.754905
O 7.237124 0.866887 -0.926679
O -0.731474 -3.626167 1.642423
H -2.966378 1.521413 1.582169
H -5.759431 2.533407 -1.841702
H -5.909088 -2.634669 0.223927
H -3.904798 -1.822550 2.867974
H -2.956471 -0.351189 3.177142
H -0.288006 -2.259913 0.109224

H 1.004491 0.407345 0.073211
H 1.368143 -0.972618 -0.988866
H 2.040298 -0.717150 1.985229
H 1.479920 -2.860537 1.448617
H 3.353297 1.334881 1.433817
H 4.165622 -2.423389 -0.489328
H 7.357521 1.787663 -0.628235
H -0.884790 -4.564851 1.834611

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -11504.3986164

Comp_08Z_c46

B3LYP/6-31G* Geometry

C 3.863641 -1.484757 -0.155658
C 4.840899 1.113059 -0.328900
C 4.918506 -1.061035 0.664038
C 3.292255 -0.592677 -1.083750
C 3.796660 0.706164 -1.150909
C 5.428494 0.240732 0.597181
Br 5.678467 -2.301494 1.899877
Br 5.523650 2.901460 -0.437785
O 6.445567 0.585604 1.415563
O 3.364774 -2.742556 -0.099294
C 2.154522 -1.049709 -1.979713
C 0.790393 -0.893563 -1.335906
N 0.131733 -1.976890 -1.128240
C 0.313756 0.533605 -1.140878
N -0.528114 0.796822 -0.114120
C -1.090867 2.127209 0.082119
O 0.723315 1.409969 -1.914060
C -2.322672 2.417414 -0.814302
O -2.001399 2.300738 -2.187491
C -3.470431 1.478208 -0.476894
C -5.434456 -0.406065 0.328297
C -4.402463 1.806304 0.510181
C -3.545031 0.218498 -1.080303
C -4.490427 -0.708646 -0.664820
C -5.366526 0.878761 0.890006
Br -4.480679 -2.457870 -1.430262
Br -6.657555 1.333888 2.235367
O -6.340247 -1.339278 0.691803
O -1.122868 -1.771794 -0.531645
H 3.353999 1.409782 -1.846570
H 6.676001 1.516620 1.234873
H 3.866930 -3.245165 0.569704
H 2.278360 -2.102998 -2.239844
H 2.162943 -0.456531 -2.898989
H -0.966341 0.004674 0.339064
H -0.305497 2.856557 -0.138562
H -1.366840 2.231025 1.135604
H -2.635152 3.449674 -0.580157
H -1.030216 2.302067 -2.285104
H -4.384520 2.781652 0.987135
H -2.847428 -0.035771 -1.866357

H -6.913889 -0.957111 1.382031
H -1.560240 -2.635946 -0.605930
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4002079**

Comp_08Z_c47
B3LYP/6-31G* Geometry
C -0.692539 -0.153122 2.165271
C -2.541424 -1.326574 0.433054
C -1.671956 0.621891 1.522281
C -0.666967 -1.549514 1.950544
C -1.589815 -2.110733 1.065121
C -2.611530 0.057285 0.652481
Br -1.679406 2.506895 1.769128
Br -3.772984 -2.108765 -0.807035
O -3.517750 0.859514 0.056023
O 0.173931 0.472899 2.987184
C 0.316763 -2.458110 2.675002
C 1.522940 -2.826241 1.829247
N 1.503846 -4.021790 1.357625
C 2.564170 -1.735521 1.661785
N 3.523888 -1.887492 0.727813
C 4.481906 -0.841014 0.416020
O 2.500627 -0.733738 2.392001
C 4.278807 -0.270382 -0.999717
O 4.527862 -1.360818 -1.884044
C 2.904873 0.349016 -1.201658
C 0.312826 1.474370 -1.453442
C 1.860344 -0.383286 -1.774025
C 2.654214 1.656282 -0.774632
C 1.383271 2.201811 -0.904156
C 0.591904 0.173420 -1.900408
Br 1.066510 3.999305 -0.340962
Br -0.816822 -0.857780 -2.659999
O -0.935881 1.962135 -1.594688
O 2.599967 -4.360596 0.549986
H -1.567202 -3.178909 0.874406
H -4.024419 0.321655 -0.580860
H 1.049643 0.016900 2.941007
H -0.185422 -3.391317 2.943011
H 0.656826 -1.987007 3.601516
H 3.522581 -2.729339 0.165769
H 5.496706 -1.250839 0.476081
H 4.372084 -0.055049 1.163593
H 5.044084 0.511944 -1.132988
H 4.364575 -1.054797 -2.790568
H 2.032760 -1.398136 -2.112858
H 3.445519 2.257933 -0.338081
H -1.075796 2.691559 -0.961132
H 2.391748 -5.270142 0.285119
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4179757**

Comp_08Z_c48
B3LYP/6-31G* Geometry
C -4.819962 -0.686605 -0.465888
C -3.585768 1.770294 -0.049049
C -5.166674 0.111023 0.633323
C -3.839441 -0.243950 -1.374916
C -3.232218 0.991037 -1.143994
C -4.561411 1.351216 0.865878
Br -6.504552 -0.518339 1.841143
Br -2.742679 3.465463 0.251042
O -4.941037 2.070818 1.942988
O -5.405096 -1.886113 -0.699517
C -3.467860 -1.103100 -2.571531
C -2.390195 -2.125130 -2.254890
N -2.774756 -3.349893 -2.245969
C -0.996138 -1.550397 -2.048374
N -0.089227 -2.292655 -1.353185
C 1.293430 -1.839801 -1.213147
O -0.741296 -0.426268 -2.477331
C 1.452441 -0.828071 -0.055063
O 0.987058 -1.397027 1.161350
C 2.905272 -0.436476 0.112931
C 5.646867 0.248981 0.338701
C 3.485225 0.495127 -0.755431
C 3.698002 -1.024405 1.100985
C 5.039084 -0.676122 1.201090
C 4.830509 0.827304 -0.646111
Br 6.131410 -1.472666 2.564967
Br 5.589185 2.097682 -1.843442
O 6.947701 0.603986 0.413762
O -1.758943 -4.282738 -1.956600
H -2.461629 1.335254 -1.823765
H -4.422408 2.897706 1.951437
H -6.072945 -2.043203 -0.005398
H -3.097036 -0.459405 -3.373910
H -4.345721 -1.644756 -2.929579
H -0.315116 -3.265988 -1.192614
H 1.624709 -1.384841 -2.151799
H 1.912648 -2.717084 -1.005665
H 0.865407 0.065987 -0.309939
H 0.076611 -1.689889 0.993230
H 2.886287 0.975556 -1.523030
H 3.261147 -1.733895 1.792278
H 7.355384 0.114435 1.152541
H -2.241250 -5.123738 -1.983872
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4002161**

Comp_08Z_c49
B3LYP/6-31G* Geometry
C 2.190642 -0.182052 1.085331
C 4.549016 -0.011111 -0.412410
C 2.614638 -1.241144 0.272743
C 2.957833 0.993939 1.139076

C 4.126104 1.050541 0.378687
 C 3.792580 -1.186198 -0.486882
 Br 1.534305 -2.823118 0.168683
 Br 6.159266 0.128427 -1.416850
 O 4.215943 -2.199686 -1.273017
 O 1.051532 -0.223501 1.826534
 C 2.569224 2.165863 2.023285
 C 1.138019 2.660688 1.911016
 N 0.534800 2.814665 3.033719
 C 0.639068 2.950721 0.510222
 N -0.697060 3.011076 0.304317
 C -1.251208 3.241367 -1.023004
 O 1.461556 3.078501 -0.404689
 C -1.336207 1.961555 -1.889779
 O -0.063927 1.378027 -2.087103
 C -2.280371 0.937920 -1.274299
 C -4.043021 -0.881247 0.005556
 C -3.656647 1.006690 -1.502211
 C -1.788275 -0.052693 -0.418839
 C -2.656427 -0.932626 0.213799
 C -4.511026 0.109658 -0.871325
 Br -1.963199 -2.249474 1.413152
 Br -6.401183 0.197691 -1.192005
 O -4.844099 -1.765939 0.638195
 O -0.773181 3.322375 2.935312
 H 4.725353 1.954499 0.397000
 H 3.566451 -2.924294 -1.224762
 H 0.579082 -1.066822 1.694340
 H 3.234763 3.001168 1.776596
 H 2.729066 1.922790 3.079763
 H -1.307203 2.913831 1.104789
 H -0.617760 3.973537 -1.535171
 H -2.248453 3.675272 -0.905782
 H -1.759462 2.279575 -2.858407
 H 0.624187 2.002661 -1.783538
 H -4.070756 1.751744 -2.175002
 H -0.720142 -0.132229 -0.268267
 H -5.765319 -1.591961 0.368834
 H -1.061835 3.317184 3.861395
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4014048**

Comp_08Z_c51
B3LYP/6-31G* Geometry
 C 2.755123 -0.396090 0.899496
 C 0.260884 -1.244956 1.793402
 C 2.214822 -1.615578 0.467518
 C 2.034765 0.409379 1.802169
 C 0.789603 -0.041179 2.242001
 C 0.954716 -2.054559 0.884921
 Br 3.215014 -2.678902 -0.761467
 Br -1.472966 -1.815671 2.364896
 O 0.463745 -3.215167 0.388092
 O 3.963652 0.046073 0.475241

C 2.595039 1.749718 2.249176
 C 2.177063 2.887650 1.332694
 N 3.116559 3.405600 0.628752
 C 0.704784 3.269559 1.412832
 N 0.152536 3.883603 0.336166
 C -1.260991 4.195460 0.264509
 O 0.068665 2.967368 2.422605
 C -1.908832 3.647999 -1.018961
 O -1.224724 4.296214 -2.091719
 C -1.858201 2.132877 -1.134344
 C -1.746918 -0.698372 -1.281768
 C -2.892868 1.345046 -0.617847
 C -0.770673 1.497559 -1.740213
 C -0.730019 0.111062 -1.811990
 C -2.837403 -0.042334 -0.689512
 Br 0.759638 -0.759484 -2.641463
 Br -4.265635 -1.080400 0.015971
 O -1.730196 -2.048044 -1.330865
 O 2.699910 4.458052 -0.212415
 H 0.214331 0.579783 2.917944
 H -0.433260 -3.339295 0.756145
 H 4.333059 -0.614597 -0.140377
 H 3.685922 1.715648 2.265882
 H 2.230023 1.974721 3.255048
 H 0.760701 4.197866 -0.408968
 H -1.409771 5.283057 0.277320
 H -1.738235 3.769907 1.148678
 H -2.965284 3.961236 -0.996188
 H -1.574888 3.944367 -2.925713
 H -3.756564 1.809830 -0.152059
 H 0.038620 2.083502 -2.158783
 H -0.869837 -2.336362 -1.692239
 H 3.525966 4.696500 -0.660905
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4143737**

Comp_08Z_c52
B3LYP/6-31G* Geometry
 C -0.469353 -0.427498 2.293912
 C -2.092801 -1.810316 0.465466
 C -1.571374 0.190570 1.683789
 C -0.186015 -1.772830 1.978320
 C -1.007889 -2.436750 1.062522
 C -2.387139 -0.471446 0.756798
 Br -1.953310 2.016353 2.073317
 Br -3.192425 -2.768820 -0.757952
 O -3.417371 0.135779 0.122186
 O 0.251510 0.293176 3.178694
 C 0.979771 -2.515984 2.614613
 C 2.208380 -2.530734 1.723134
 N 2.459762 -3.658129 1.160899
 C 2.954848 -1.213851 1.614189
 N 3.789688 -1.029202 0.573095
 C 4.422265 0.244932 0.285524

O 2.762934 -0.343214 2.477278
 C 4.080796 0.717623 -1.146129
 O 4.468161 -0.288619 -2.084720
 C 2.602532 1.002181 -1.327448
 C -0.176423 1.526670 -1.529449
 C 2.064444 2.208183 -0.865541
 C 1.749367 0.064826 -1.913109
 C 0.389397 0.334939 -2.009182
 C 0.702489 2.466726 -0.969081
 Br -0.787946 -0.952792 -2.791418
 Br 0.007177 4.120584 -0.342292
 O -1.494200 1.810145 -1.595193
 O 3.575534 -3.656618 0.306281
 H -0.798684 -3.472437 0.814382
 H -3.454009 1.060955 0.437042
 H 1.202730 0.035011 3.109693
 H 0.696278 -3.556047 2.795235
 H 1.237634 -2.068521 3.578836
 H 3.910610 -1.786037 -0.089118
 H 5.513982 0.145986 0.378666
 H 4.086619 0.965078 1.033616
 H 4.643918 1.646232 -1.326604
 H 5.437125 -0.314475 -2.111998
 H 2.704054 2.963184 -0.418499
 H 2.143947 -0.864222 -2.304333
 H -1.971929 1.017684 -1.907731
 H 3.576892 -4.566089 -0.031254
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4175836**

Comp_08Z_c53
B3LYP/6-31G* Geometry
 C 4.963197 -1.110308 0.261162
 C 4.275109 1.583783 0.297558
 C 5.564924 -0.206185 -0.624718
 C 4.001459 -0.656081 1.184486
 C 3.671357 0.699569 1.183224
 C 5.236185 1.154087 -0.627821
 Br 6.871155 -0.856257 -1.855755
 Br 3.808854 3.442946 0.310011
 O 5.851231 1.971920 -1.508131
 O 5.279765 -2.427638 0.272669
 C 3.355078 -1.633632 2.151763
 C 2.144788 -2.338742 1.564116
 N 2.300089 -3.589336 1.317387
 C 0.905921 -1.476848 1.398460
 N -0.058813 -1.885106 0.548422
 C -1.215190 -1.063887 0.184271
 O 0.839619 -0.413356 2.032781
 C -2.279095 -0.888288 1.301583
 O -1.882120 0.065737 2.260154
 C -3.600331 -0.445315 0.689891
 C -6.018694 0.395129 -0.531271
 C -4.476604 -1.382565 0.137294

C -3.941796 0.909417 0.637581
 C -5.127186 1.318021 0.037929
 C -5.656989 -0.959075 -0.460932
 Br -5.566986 3.170053 -0.015168
 Br -6.862766 -2.249531 -1.214446
 O -7.160047 0.838106 -1.101942
 O 1.168046 -4.227139 0.775965
 H 2.919497 1.060819 1.874732
 H 5.507687 2.875309 -1.371456
 H 5.970131 -2.584127 -0.399235
 H 3.033518 -1.094479 3.046879
 H 4.074652 -2.401853 2.442198
 H 0.040770 -2.807945 0.145655
 H -1.670004 -1.545447 -0.684781
 H -0.872519 -0.067772 -0.120033
 H -2.427660 -1.879092 1.766841
 H -0.905051 0.030957 2.333314
 H -4.251921 -2.444190 0.177523
 H -3.280907 1.638365 1.089553
 H -7.657682 0.066830 -1.431266
 H 1.486830 -5.134195 0.647513
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4015568**

Comp_08Z_c55
B3LYP/6-31G* Geometry
 C -4.802250 -0.679966 -0.461986
 C -3.569596 1.776089 -0.035681
 C -5.131488 0.101814 0.653879
 C -3.840392 -0.221569 -1.383072
 C -3.233557 1.012606 -1.147121
 C -4.526449 1.341182 0.891607
 Br -6.444373 -0.548477 1.877710
 Br -2.727302 3.470597 0.270824
 O -4.888693 2.044962 1.984955
 O -5.386909 -1.878623 -0.700614
 C -3.486708 -1.063482 -2.597194
 C -2.405039 -2.089934 -2.310490
 N -2.787124 -3.315385 -2.321901
 C -1.010097 -1.517690 -2.103615
 N -0.103868 -2.265945 -1.414385
 C 1.277656 -1.813252 -1.263348
 O -0.755459 -0.390189 -2.523932
 C 1.428666 -0.808859 -0.097483
 O 0.948626 -1.382823 1.110497
 C 2.881447 -0.425104 0.088403
 C 5.626201 0.230656 0.361580
 C 3.456892 0.555489 -0.723842
 C 3.679780 -1.071867 1.037385
 C 5.024238 -0.746005 1.170163
 C 4.804245 0.864958 -0.582945
 Br 6.083263 -1.636518 2.478456
 Br 5.596341 2.212670 -1.696184
 O 6.936216 0.514782 0.526807

O -1.766115 -4.250642 -2.059989
H -2.476975 1.368725 -1.836421
H -4.372205 2.873120 1.995753
H -6.040505 -2.048194 0.004074
H -3.127243 -0.408154 -3.395387
H -4.369529 -1.600055 -2.950776
H -0.329791 -3.240830 -1.263148
H 1.614430 -1.351631 -2.196900
H 1.895979 -2.691706 -1.058308
H 0.848254 0.089158 -0.353696
H 0.041749 -1.679134 0.928977
H 2.860178 1.083719 -1.460907
H 3.240148 -1.819706 1.685310
H 7.179122 1.216656 -0.105426
H -2.246778 -5.092267 -2.096543

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4002548

Comp_08Z_c56

B3LYP/6-31G* Geometry

C -0.713515 0.118759 -2.129132
C -2.831715 0.736650 -0.390669
C -1.469313 -0.887334 -1.507970
C -1.058146 1.465111 -1.890794
C -2.105807 1.743762 -1.007085
C -2.534057 -0.610919 -0.640146
Br -1.004072 -2.717845 -1.808931
Br -4.215688 1.173126 0.839384
O -3.262707 -1.569456 -0.035004
O 0.290536 -0.254691 -2.950584
C -0.338332 2.615409 -2.580007
C 0.724294 3.251966 -1.703068
N 0.400774 4.389974 -1.200875
C 2.004423 2.454397 -1.543018
N 2.867494 2.796409 -0.566226
C 4.068868 2.031599 -0.283407
O 2.220171 1.508586 -2.317968
C 4.008610 1.339960 1.090275
O 3.910663 2.398501 2.039863
C 2.873260 0.334759 1.210989
C 0.747453 -1.533737 1.377307
C 3.031575 -0.963380 0.716730
C 1.649197 0.690617 1.786358
C 0.607489 -0.228026 1.871991
C 1.982721 -1.869250 0.798692
Br -1.050750 0.289398 2.642262
Br 2.200745 -3.643492 0.113762
O -0.284091 -2.396231 1.486098
O 1.366440 4.964985 -0.359886
H -2.362274 2.777617 -0.798680
H -2.877362 -2.434441 -0.269516
H 1.017575 0.412774 -2.894406
H -1.061590 3.395613 -2.830957
H 0.120703 2.275058 -3.512584

H 2.638502 3.582565 0.028851
H 4.933470 2.705357 -0.287494
H 4.190003 1.294212 -1.077317
H 4.965432 0.805814 1.211419
H 3.827187 2.003732 2.922625
H 3.968198 -1.275312 0.265057
H 1.504544 1.693295 2.171344
H -0.042716 -3.221648 1.025374
H 0.932114 5.783546 -0.073104

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4192871

Comp_08Z_c59

B3LYP/6-31G* Geometry

C -2.578285 1.462866 0.620833
C -0.717448 -0.210770 1.841161
C -2.765588 0.074771 0.642419
C -1.431242 2.023758 1.213503
C -0.523136 1.166175 1.832022
C -1.834790 -0.790181 1.227528
Br -4.304577 -0.656038 -0.213306
Br 0.577949 -1.374239 2.633560
O -2.050170 -2.124368 1.161862
O -3.471322 2.301125 0.044058
C -1.198812 3.525038 1.154096
C 0.244483 3.878271 0.871860
N 0.856052 4.490807 1.821496
C 0.749533 3.463543 -0.506510
N 2.094224 3.320998 -0.661895
C 2.698389 2.902429 -1.918089
O -0.069751 3.222172 -1.388696
C 3.395436 1.532447 -1.805862
O 4.430644 1.608586 -0.823472
C 2.469823 0.343389 -1.548602
C 0.846765 -1.938571 -1.059516
C 2.963912 -0.759219 -0.838711
C 1.157528 0.288114 -2.032314
C 0.380169 -0.839044 -1.796158
C 2.166411 -1.870249 -0.593590
Br -1.416898 -0.912471 -2.452874
Br 2.863631 -3.324004 0.417567
O 0.094907 -3.027089 -0.780951
O 2.194873 4.829532 1.535176
H 0.364078 1.575889 2.302979
H -1.273515 -2.576237 1.545209
H -4.172381 1.766240 -0.373390
H -1.487398 4.004788 2.095860
H -1.819396 3.942980 0.358161
H 2.688719 3.696168 0.065750
H 3.463203 3.632934 -2.204042
H 1.921807 2.907596 -2.684466
H 3.932169 1.369140 -2.749708
H 3.995145 1.565856 0.044538
H 3.982234 -0.747567 -0.468985

H 0.709705 1.123457 -2.555677
H -0.805720 -2.874972 -1.127298
H 2.473409 5.271167 2.352467
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4103231**

Comp_08Z_c62
B3LYP/6-31G* Geometry
C -2.745678 -0.390160 -0.923605
C -0.247436 -1.231318 -1.814341
C -2.200782 -1.606118 -0.487894
C -2.027472 0.416121 -1.827327
C -0.779975 -0.029868 -2.264840
C -0.939143 -2.041844 -0.904693
Br -3.200912 -2.673594 0.737210
Br 1.485957 -1.798817 -2.388382
O -0.447326 -3.202241 -0.409883
O -3.956811 0.048030 -0.502560
C -2.589759 1.755895 -2.272874
C -2.172649 2.885503 -1.346714
N -3.107632 3.387579 -0.625844
C -0.703248 3.277528 -1.431706
N -0.145899 3.852705 -0.336635
C 1.267750 4.150619 -0.244179
O -0.075254 3.020764 -2.458239
C 1.860111 3.636117 1.086187
O 1.129059 4.186503 2.185434
C 1.824583 2.125659 1.202833
C 1.744394 -0.707149 1.300453
C 2.856363 1.358599 0.652973
C 0.756105 1.471754 1.820410
C 0.729785 0.083709 1.862370
C 2.818663 -0.030480 0.704385
Br -0.742873 -0.817579 2.690509
Br 4.251022 -1.038350 -0.036557
O 1.738191 -2.058523 1.322103
O -2.687031 4.427878 0.231003
H -0.206350 0.591149 -2.942498
H 0.456013 -3.317482 -0.764928
H -4.322978 -0.611554 0.116266
H -3.680547 1.720685 -2.292249
H -2.221718 1.986793 -3.276238
H -0.746364 4.102046 0.438955
H 1.434921 5.238051 -0.306060
H 1.763926 3.693710 -1.103187
H 2.910629 3.964047 1.124686
H 1.264833 5.147127 2.179530
H 3.706908 1.839115 0.179367
H -0.042262 2.041446 2.278208
H 0.889360 -2.358281 1.700993
H -3.509720 4.646413 0.695757
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4125165**

Comp_08Z_c64
B3LYP/6-31G* Geometry
C -0.663521 -0.132261 2.188444
C -2.441772 -1.437858 0.476866
C -1.686824 0.574796 1.535902
C -0.560741 -1.528505 1.999517
C -1.448871 -2.156352 1.123260
C -2.592385 -0.057127 0.676112
Br -1.808818 2.458336 1.759766
Br -3.632610 -2.310513 -0.742290
O -3.546641 0.680563 0.072044
O 0.169214 0.555553 2.996926
C 0.470029 -2.366750 2.742827
C 1.690939 -2.687138 1.900105
N 1.735855 -3.891842 1.454427
C 2.669029 -1.544202 1.701042
N 3.614457 -1.661443 0.746912
C 4.493760 -0.569736 0.371303
O 2.569479 -0.538989 2.421260
C 4.245916 -0.133257 -1.091865
O 4.420002 -1.253972 -1.960285
C 2.851140 0.426514 -1.291641
C 0.217400 1.457055 -1.498361
C 2.554397 1.712906 -0.833945
C 1.834478 -0.332848 -1.876556
C 0.543612 0.176702 -1.972645
C 1.264186 2.215165 -0.947652
Br -0.835658 -0.897476 -2.728220
Br 0.891289 3.992923 -0.355537
O -1.052216 1.896942 -1.614556
O 2.845977 -4.188249 0.647229
H -1.366218 -3.224842 0.951837
H -4.017908 0.105821 -0.559781
H 1.068335 0.148641 2.957010
H 0.019234 -3.319357 3.033114
H 0.786140 -1.857119 3.657343
H 3.616650 -2.496969 0.174710
H 5.539728 -0.892004 0.476495
H 4.322730 0.254886 1.065064
H 4.981473 0.651538 -1.328110
H 5.367343 -1.455762 -2.001056
H 3.323690 2.335981 -0.388418
H 2.048782 -1.323611 -2.256589
H -1.206115 2.622181 -0.979686
H 2.675710 -5.108270 0.391254
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4161024**

Comp_08Z_c71
B3LYP/6-31G* Geometry
C -0.263345 -2.439260 1.061434
C -1.575386 -0.096128 1.841202
C -1.496846 -2.076877 0.504468

C 0.320271 -1.613442 2.038560
 C -0.357012 -0.450463 2.410409
 C -2.171153 -0.902395 0.864662
 Br -2.299787 -3.234251 -0.799144
 Br -2.445044 1.512340 2.373818
 O -3.351079 -0.526704 0.317407
 O 0.392060 -3.572999 0.709144
 C 1.650257 -1.995993 2.667283
 C 2.855037 -1.551897 1.854519
 N 3.544876 -2.501032 1.334070
 C 3.083287 -0.047641 1.814268
 N 3.858461 0.450951 0.817175
 C 4.004902 1.874805 0.595118
 O 2.530505 0.656456 2.659063
 C 3.581293 2.281905 -0.827278
 O 4.504003 1.629299 -1.698846
 C 2.136896 1.929054 -1.145838
 C -0.564367 1.224326 -1.646379
 C 1.101366 2.804074 -0.805502
 C 1.814264 0.708020 -1.746871
 C 0.489469 0.366687 -1.992009
 C -0.218618 2.450442 -1.054653
 Br 0.080986 -1.311873 -2.792348
 Br -1.635648 3.648755 -0.596368
 O -1.835993 0.848436 -1.901284
 O 4.664761 -2.072594 0.593574
 H 0.095674 0.205424 3.144053
 H -3.559450 -1.140429 -0.410139
 H -0.119832 -4.032012 0.019613
 H 1.712139 -3.080451 2.782045
 H 1.720139 -1.532347 3.655186
 H 4.340268 -0.194473 0.205017
 H 5.051035 2.176429 0.733176
 H 3.393361 2.387564 1.339293
 H 3.702215 3.375498 -0.894346
 H 4.244129 1.827313 -2.612815
 H 1.315154 3.762318 -0.342237
 H 2.601547 0.015887 -2.020608
 H -2.440046 1.481650 -1.468983
 H 5.026603 -2.912267 0.270669
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4113024**

Comp_08Z_c80
B3LYP/6-31G* Geometry
 C -3.343158 -0.865814 0.608467
 C -3.337282 1.899191 0.291182
 C -2.782285 -0.029957 1.583641
 C -3.885749 -0.307530 -0.565434
 C -3.867237 1.079539 -0.699055
 C -2.769969 1.363742 1.454211
 Br -1.968847 -0.827388 3.119911
 Br -3.333565 3.802999 0.082798
 O -2.214233 2.105504 2.435870

O -3.371200 -2.213550 0.739920
 C -4.431364 -1.188936 -1.674897
 C -3.449518 -2.242274 -2.153599
 N -3.915195 -3.422845 -2.320276
 C -2.034315 -1.748611 -2.397753
 N -1.035968 -2.525071 -1.905195
 C 0.315168 -2.018077 -1.750819
 O -1.854769 -0.659882 -2.938803
 C 0.471223 -1.196511 -0.455736
 O 0.151229 -2.082897 0.613815
 C 1.869580 -0.611962 -0.335348
 C 4.499405 0.437152 -0.190095
 C 2.179387 0.604428 -0.950561
 C 2.876132 -1.297179 0.352604
 C 4.164395 -0.780001 0.423829
 C 3.472186 1.106953 -0.873851
 Br 5.513075 -1.730934 1.373728
 Br 3.899313 2.780809 -1.710151
 O 5.762866 0.903260 -0.093932
 O -2.944738 -4.342175 -2.766414
 H -4.260715 1.531235 -1.603026
 H -2.289491 3.045713 2.184456
 H -2.899591 -2.458940 1.557821
 H -4.690920 -0.543516 -2.521631
 H -5.341755 -1.710590 -1.360667
 H -1.294512 -3.367343 -1.411086
 H 0.551758 -1.392566 -2.613648
 H 1.009981 -2.863483 -1.728614
 H -0.256824 -0.374532 -0.502460
 H -0.038616 -1.553278 1.406254
 H 1.418040 1.162171 -1.487342
 H 2.642526 -2.233961 0.845113
 H 5.814173 1.749927 -0.575637
 H -3.467906 -5.154364 -2.855585
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.4012388**

Comp_08Z_c82
B3LYP/6-31G* Geometry
 C 0.717042 -0.432893 2.366049
 C 1.565828 1.838385 0.983326
 C 1.892502 -0.459511 1.596562
 C -0.019798 0.767506 2.466767
 C 0.418397 1.889303 1.759530
 C 2.326647 0.663196 0.882163
 Br 2.904114 -2.061082 1.495137
 Br 2.160393 3.390285 0.033027
 O 3.439305 0.566912 0.117918
 O 0.348979 -1.561896 3.009674
 C -1.251238 0.875999 3.355071
 C -2.549981 0.794444 2.576242
 N -3.201379 1.898748 2.489814
 C -2.883072 -0.569092 2.000765
 N -3.794854 -0.644018 1.010819

C -4.030892 -1.856933 0.250351
O -2.294387 -1.567938 2.441373
C -3.831546 -1.597212 -1.259720
O -4.718273 -0.561508 -1.686034
C -2.409916 -1.178447 -1.587206
C 0.276140 -0.404133 -2.059182
C -1.381184 -2.123290 -1.538221
C -2.093462 0.147485 -1.894158
C -0.773847 0.523453 -2.122648
C -0.068593 -1.736120 -1.776429
Br -0.365788 2.341341 -2.507170
Br 1.335552 -3.029755 -1.721309
O 1.541848 0.011873 -2.274242
O -4.391146 1.827493 1.745778
H -0.141071 2.817056 1.823517
H 3.549687 1.416408 -0.350347
H -0.636005 -1.622914 2.994381
H -1.245349 1.839282 3.872146
H -1.236119 0.091591 4.117284
H -4.242134 0.210488 0.700607
H -5.057867 -2.212827 0.420309
H -3.347268 -2.623934 0.618576
H -4.059245 -2.536019 -1.788516
H -5.621087 -0.914298 -1.665215
H -1.590309 -3.164621 -1.314112
H -2.878576 0.889762 -1.957417
H 2.153686 -0.718844 -2.063353
H -4.702957 2.745815 1.767410

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4160631

Comp_08Z_c85

B3LYP/6-31G* Geometry

C 0.667696 -0.135187 -2.152472
C 2.732301 -0.955121 -0.433259
C 1.510796 0.794513 -1.524876
C 0.899766 -1.508802 -1.936690
C 1.922979 -1.888362 -1.062042
C 2.550762 0.416299 -0.665041
Br 1.210111 2.661067 -1.809858
Br 4.082066 -1.525637 0.779418
O 3.363579 1.300489 -0.054461
O -0.307587 0.332501 -2.961468
C 0.082593 -2.582737 -2.640185
C -1.019328 -3.143960 -1.761720
N -0.785376 -4.312539 -1.280792
C -2.226404 -2.244523 -1.571353
N -3.089016 -2.527044 -0.574838
C -4.199909 -1.663261 -0.222751
O -2.383413 -1.280755 -2.336964
C -4.030650 -1.089480 1.203053
O -3.869638 -2.160619 2.133875
C -2.834964 -0.162769 1.313210
C -0.599891 1.575926 1.413017

C -2.915604 1.125116 0.776860
C -1.636566 -0.575051 1.902421
C -0.539020 0.279505 1.946720
C -1.815530 1.970282 0.832522
Br 1.095482 -0.318783 2.710781
Br -1.935677 3.736032 0.102233
O 0.485997 2.374784 1.485528
O -1.785484 -4.821102 -0.435367
H 2.093042 -2.943136 -0.870826
H 3.048383 2.198425 -0.268873
H -1.087543 -0.271385 -2.908900
H 0.736518 -3.415015 -2.913273
H -0.355640 -2.187967 -3.561191
H -2.883258 -3.314308 0.027847
H -5.135497 -2.239053 -0.267935
H -4.256732 -0.866357 -0.966011
H -4.942276 -0.516603 1.434316
H -4.729676 -2.594403 2.243029
H -3.831442 1.479948 0.314547
H -1.559177 -1.564271 2.335319
H 0.289874 3.200460 1.004422
H -1.406986 -5.669720 -0.156773

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -11504.4173163

Comp_08Z_c86

B3LYP/6-31G* Geometry

C 3.857379 -1.506774 -0.140736
C 4.822835 1.113435 -0.347189
C 4.891016 -1.045236 0.684393
C 3.300169 -0.636958 -1.094171
C 3.798252 0.665259 -1.173987
C 5.395619 0.261091 0.605525
Br 5.655381 -2.249552 1.975248
Br 5.464058 2.897979 -0.505176
O 6.390753 0.722161 1.394083
O 3.367149 -2.769831 -0.068894
C 2.182160 -1.118439 -2.002509
C 0.806451 -0.955604 -1.385655
N 0.153934 -2.036199 -1.151180
C 0.320974 0.474178 -1.232607
N -0.501853 0.763653 -0.198282
C -1.048147 2.103419 -0.016873
O 0.716753 1.326886 -2.037516
C -2.294828 2.386494 -0.893587
O -2.003216 2.236516 -2.270404
C -3.442591 1.465123 -0.511519
C -5.416101 -0.369084 0.378398
C -4.327200 1.805534 0.516622
C -3.563771 0.211847 -1.115746
C -4.520949 -0.680982 -0.656182
C -5.299421 0.908876 0.947909
Br -4.614844 -2.441444 -1.426022
Br -6.493154 1.408803 2.344060

O -6.358609 -1.219219 0.840798
O -1.118235 -1.818928 -0.588990
H 3.363792 1.349577 -1.893848
H 6.675793 0.008655 1.992391
H 3.856552 -3.264570 0.611984
H 2.316001 -2.175485 -2.241683
H 2.203519 -0.541250 -2.931624
H -0.934342 -0.015112 0.282614
H -0.259919 2.819912 -0.267499
H -1.301275 2.230347 1.039697
H -2.593360 3.426239 -0.675910
H -1.034391 2.233667 -2.388598
H -4.266356 2.779721 0.992567
H -2.903684 -0.057411 -1.928975
H -6.302293 -2.047064 0.328459
H -1.512880 -2.705625 -0.582345
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -11504.3986129**

Comp_09E_c01
B3LYP/6-31G* Geometry
C -1.062403 0.037976 0.226062
C -0.275443 0.644264 -0.957412
C 1.209546 0.856915 -0.633676
C -0.395408 -1.293553 0.636251
C 1.098221 -1.120534 0.990468
C 1.833355 -0.427743 -0.124915
C -2.607238 -0.067737 -0.026639
C -3.307517 -0.588211 1.248000
C -3.183752 1.333152 -0.328989
C -2.951973 -1.008307 -1.199797
N 2.914970 -0.798926 -0.703032
O 3.427604 -2.003288 -0.170104
O 1.273084 1.880474 0.364578
C 2.571383 2.411688 0.561507
H -0.944154 0.732892 1.070231
H -0.685246 1.614926 -1.251900
H -0.336069 -0.017893 -1.831368
H 1.752798 1.182181 -1.533288
H -0.478290 -2.020573 -0.183000
H -0.901505 -1.734879 1.500810
H 1.562134 -2.083087 1.213401
H 1.180973 -0.494509 1.889930
H -3.050078 -1.628831 1.471062
H -3.043556 0.020021 2.122421
H -4.396790 -0.543185 1.129237
H -2.828447 1.734265 -1.283845
H -4.278173 1.289432 -0.384017
H -2.917987 2.050981 0.457087
H -2.598082 -2.030432 -1.024276
H -4.039104 -1.058173 -1.337188
H -2.521185 -0.660195 -2.145380
H 4.209088 -2.146255 -0.725881
H 3.285731 1.651445 0.906658

H 2.479231 3.190111 1.323664
H 2.965801 2.859291 -0.364091
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -636.863218734**

Comp_09E_c02
B3LYP/6-31G* Geometry
C 0.954105 -0.086001 -0.240245
C 0.162927 0.626577 0.879969
C -1.296023 0.911557 0.469119
C 0.224249 -1.395813 -0.613283
C -1.247414 -1.159846 -1.023512
C -1.966736 -0.371073 0.034936
C 2.480830 -0.267434 0.072343
C 3.190066 -0.903721 -1.143356
C 3.131831 1.112627 0.315010
C 2.727988 -1.153674 1.310626
N -3.048753 -0.672272 0.648867
O -3.595852 -1.897101 0.205370
O -1.364280 1.805919 -0.649418
C -1.233301 3.171125 -0.308104
H 0.904257 0.570614 -1.121761
H 0.640161 1.571007 1.161003
H 0.138198 0.006425 1.786376
H -1.856273 1.334234 1.314919
H 0.242103 -2.088107 0.239306
H 0.731351 -1.901985 -1.440865
H -1.757006 -2.107178 -1.208663
H -1.273575 -0.576692 -1.954213
H 2.876426 -1.938685 -1.313879
H 2.992585 -0.335774 -2.061415
H 4.275441 -0.915671 -0.987395
H 2.769184 1.589282 1.231641
H 4.219019 1.008472 0.414157
H 2.938591 1.796429 -0.521333
H 2.321366 -2.162966 1.181511
H 3.804682 -1.256536 1.493561
H 2.283336 -0.724899 2.215900
H -4.384270 -1.972545 0.764379
H -2.000094 3.479974 0.419680
H -1.371071 3.741194 -1.230893
H -0.243225 3.412823 0.107269
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -636.860636574**

Comp_09Z_c01
B3LYP/6-31G* Geometry
C -1.094238 0.057322 0.246396
C -0.158689 0.447332 -0.920332
C 1.313168 0.563279 -0.498926
C -0.597247 -1.267876 0.865757
C 0.873860 -1.174160 1.323083
C 1.757078 -0.715633 0.193623

C -2.616577 0.059941 -0.133962
C -3.465452 -0.247590 1.119170
C -3.025839 1.462607 -0.635979
C -2.954810 -0.974795 -1.226921
N 2.777893 -1.433765 -0.093520
O 3.528035 -0.907530 -1.175146
O 1.408276 1.666789 0.406909
C 2.740800 2.069368 0.673400
H -0.976869 0.835956 1.014238
H -0.445744 1.410704 -1.352378
H -0.217210 -0.301256 -1.721691
H 1.939451 0.754325 -1.377486
H -0.686294 -2.081673 0.133280
H -1.209038 -1.550073 1.728772
H 1.233897 -2.135252 1.702958
H 0.944172 -0.442807 2.140277
H -3.326327 -1.273637 1.475135
H -3.217771 0.432631 1.943890
H -4.531954 -0.124304 0.896044
H -2.556365 1.716907 -1.591753
H -4.111200 1.511317 -0.785504
H -2.753842 2.239363 0.089613
H -2.718876 -1.997547 -0.912004
H -4.026601 -0.943748 -1.458299
H -2.415659 -0.776832 -2.160205
H 4.240097 -1.560752 -1.251599
H 3.329508 1.269336 1.145114
H 2.680837 2.920235 1.357230
H 3.257722 2.380615 -0.246940

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -636.861199721

Comp_09Z_c02

B3LYP/6-31G* Geometry

C 1.001272 -0.056743 -0.266517
C 0.023067 0.469903 0.808384
C -1.425550 0.576216 0.287826
C 0.502638 -1.427862 -0.776333
C -0.950020 -1.362161 -1.297169
C -1.857468 -0.770475 -0.254060
C 2.504825 -0.043615 0.182445
C 3.399903 -0.533360 -0.977457
C 2.936439 1.400921 0.519570
C 2.759147 -0.936845 1.414190
N -2.863732 -1.461643 0.129734
O -3.619387 -0.815391 1.138115
O -1.532553 1.497225 -0.805736
C -1.649677 2.849243 -0.408440
H 0.935788 0.640966 -1.114867
H 0.334250 1.453595 1.175454
H 0.013444 -0.198649 1.680101
H -2.095089 0.887235 1.096760
H 0.551563 -2.169836 0.032367
H 1.142087 -1.797112 -1.584552

H -1.313238 -2.355162 -1.579315
H -0.983401 -0.723838 -2.190533
H 3.253464 -1.596226 -1.195052
H 3.202749 0.030207 -1.898318
H 4.458264 -0.396850 -0.725073
H 2.424298 1.793842 1.404018
H 4.012671 1.438314 0.726603
H 2.735286 2.081488 -0.317498
H 2.488689 -1.981725 1.224606
H 3.822569 -0.918015 1.682721
H 2.195871 -0.596812 2.290615
H -4.326303 -1.460395 1.292412
H -2.524782 3.004063 0.241505
H -1.778476 3.435520 -1.322349
H -0.755510 3.214881 0.118603

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -636.858767295

Comp_10E_c01

B3LYP/6-31G* Geometry

C -2.085998 0.421559 1.345244
C -1.643764 -1.823465 0.299369
C -3.404936 -0.278082 -0.709377
C -2.350315 -1.346691 -0.994084
C -2.780243 0.886823 0.066799
C -1.000451 -0.664360 1.113748
C 0.237198 -0.082946 0.341133
C 1.118864 -1.169339 -0.275276
C 0.718787 -2.448941 -0.415286
C -0.636356 -2.907661 -0.065623
C 2.415249 -0.661104 -0.881901
C 3.237264 0.222162 0.097544
C 2.362756 1.415524 0.514504
C 1.060205 0.935054 1.182732
C 4.487456 0.540592 -0.797951
C 4.747492 -0.794567 -1.562956
C 3.453948 -1.646731 -1.431778
O -0.963465 -4.083756 -0.156071
O -4.439249 -0.898374 0.097005
C -5.726326 -0.524890 -0.112551
C -6.645536 -1.259495 0.834544
O -6.080017 0.281592 -0.944574
O -3.801153 1.830834 0.452805
C -4.141535 2.771580 -0.472372
C -5.333540 3.567924 -0.008268
O -3.564400 2.914095 -1.526983
C -0.595678 -1.223440 2.497072
H -2.407791 -2.303433 0.920226
C 3.670529 -0.594091 1.336401
C 5.677275 1.121997 -0.062733
C 5.660986 2.576323 0.340279
N 6.665488 0.343163 0.189579
O 7.686584 1.017405 0.897263
H 4.164952 1.297123 -1.521533

O 2.011446 0.223700 -1.962550
H -0.133502 0.488275 -0.521252
H -2.851311 0.009944 2.014054
H -1.661545 1.291831 1.857183
H -3.863022 0.090772 -1.629087
H -2.823645 -2.205284 -1.481718
H -1.624347 -0.934153 -1.706435
H -2.087975 1.398322 -0.607923
H 1.366589 -3.203590 -0.853827
H 2.902368 2.057216 1.221917
H 2.131020 2.023534 -0.365833
H 1.307182 0.496568 2.153921
H 0.429070 1.805452 1.393791
H 5.607830 -1.317812 -1.143623
H 4.980980 -0.581152 -2.609930
H 3.600502 -2.481687 -0.739397
H 3.132855 -2.079298 -2.386541
H -7.682271 -1.031429 0.584986
H -6.471111 -2.338210 0.777165
H -6.438597 -0.948312 1.864358
H -5.404463 4.490679 -0.585760
H -6.231293 2.963892 -0.182581
H -5.272749 3.785615 1.061377
H 0.247883 -1.918791 2.429915
H -0.321302 -0.426713 3.195465
H -1.437605 -1.767490 2.939706
H 4.063720 0.075924 2.108697
H 2.839816 -1.156996 1.773033
H 4.466110 -1.305894 1.101949
H 5.626776 2.676622 1.432047
H 6.584550 3.067264 0.015124
H 4.804208 3.101022 -0.088356
H 8.366278 0.329613 0.968797
H 1.613465 -0.337934 -2.647421

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79798311

Comp_10E_c02

B3LYP/6-31G* Geometry

C -2.072653 0.676440 1.398637
C -1.749640 -1.633691 0.445831
C -3.448338 -0.050709 -0.606340
C -2.443038 -1.177013 -0.861564
C -2.757701 1.112451 0.104216
C -1.046162 -0.474616 1.209406
C 0.215663 0.014613 0.411146
C 1.027396 -1.130854 -0.193174
C 0.568518 -2.394972 -0.277084
C -0.796748 -2.778358 0.121332
C 2.328014 -0.698620 -0.847884
C 3.221108 0.161308 0.089082
C 2.417084 1.401757 0.512790
C 1.112441 0.993492 1.223315
C 4.455512 0.402967 -0.850990

C 4.631363 -0.959269 -1.590524
C 3.301307 -1.744030 -1.408945
O -1.174025 -3.942443 0.100055
O -4.506257 -0.521629 0.265781
C -5.600189 -1.064560 -0.328356
C -6.597100 -1.517439 0.712174
O -5.736504 -1.170894 -1.526377
O -3.711083 2.143395 0.451840
C -3.992931 3.065264 -0.503895
C -5.003510 4.065715 0.004447
O -3.494836 3.068563 -1.608365
C -0.663263 -0.994852 2.613873
H -2.529023 -2.051343 1.092313
C 3.655249 -0.654818 1.327939
C 5.691876 0.947616 -0.166809
C 5.757489 2.413644 0.185615
N 6.647653 0.129511 0.086040
O 7.719670 0.776168 0.742459
H 4.143542 1.155958 -1.582483
O 1.935786 0.184616 -1.934198
H -0.129319 0.591383 -0.457909
H -2.849557 0.340874 2.095146
H -1.594547 1.547832 1.859202
H -3.898785 0.282824 -1.542951
H -2.961150 -2.025955 -1.318541
H -1.705656 -0.824830 -1.594551
H -2.045017 1.545292 -0.603184
H 1.171237 -3.192633 -0.703429
H 3.007553 2.026418 1.194529
H 2.188976 2.008379 -0.369620
H 1.364610 0.546616 2.189267
H 0.533091 1.896173 1.447684
H 5.474978 -1.515084 -1.179048
H 4.850162 -0.781259 -2.647269
H 3.427299 -2.574099 -0.706653
H 2.931840 -2.175708 -2.346480
H -7.513776 -1.842139 0.218822
H -6.177625 -2.350051 1.287584
H -6.810990 -0.707397 1.416072
H -5.165644 4.834331 -0.751832
H -5.949339 3.558967 0.223971
H -4.653188 4.520830 0.936173
H 0.141572 -1.736858 2.573358
H -0.341634 -0.184562 3.275573
H -1.530020 -1.473501 3.083297
H 4.100658 0.007861 2.077854
H 2.814242 -1.174561 1.797003
H 4.411476 -1.404420 1.081166
H 5.780500 2.551782 1.273395
H 6.684749 2.851904 -0.199394
H 4.904687 2.960997 -0.222050
H 8.366125 0.057922 0.822346
H 1.491912 -0.369522 -2.596632

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79774632

Comp_10E_c03

B3LYP/6-31G* Geometry

C -2.150127 0.658995 1.105674
C -1.765325 -1.747384 0.484624
C -3.494957 -0.359901 -0.788060
C -2.476766 -1.499927 -0.868812
C -2.832811 0.903009 -0.240343
C -1.088931 -0.472386 1.065473
C 0.143701 -0.076062 0.178350
C 1.032834 -1.278229 -0.143531
C 0.597599 -2.550950 -0.046065
C -0.784114 -2.903936 0.320584
C 2.372220 -0.939499 -0.772200
C 3.148348 0.156365 0.007934
C 2.278657 1.422376 0.044164
C 0.928148 1.149245 0.733749
C 4.463097 0.229772 -0.848254
C 4.743564 -1.255856 -1.231597
C 3.421468 -2.037975 -0.992595
O -1.150708 -4.069028 0.406456
O -4.551420 -0.756971 0.119040
C -5.830241 -0.734460 -0.344162
C -6.788657 -1.121643 0.756794
O -6.142005 -0.449839 -1.477623
O -3.863474 1.909664 -0.107740
C -3.470095 3.202658 -0.216510
C -4.653222 4.131242 -0.083040
O -2.321529 3.547149 -0.396217
C -0.671151 -0.771168 2.523336
H -2.532334 -2.088652 1.188837
C 3.476733 -0.319845 1.440592
C 5.613115 0.970916 -0.198682
C 5.604214 2.479828 -0.178511
N 6.561052 0.275019 0.315085
O 7.546205 1.100158 0.904685
H 4.207587 0.780678 -1.759945
O 2.049465 -0.350206 -2.061960
H -0.231490 0.247299 -0.802935
H -2.926116 0.384126 1.829970
H -1.702841 1.594477 1.453845
H -3.947134 -0.161494 -1.761977
H -2.986537 -2.418005 -1.178849
H -1.748908 -1.260892 -1.655184
H -2.111190 1.266158 -0.977598
H 1.240461 -3.391998 -0.293084
H 2.790832 2.225652 0.588015
H 2.111759 1.777603 -0.977478
H 1.103893 1.019125 1.805918
H 0.295301 2.036912 0.628912
H 5.555975 -1.663009 -0.628154
H 5.060922 -1.315214 -2.276680
H 3.497722 -2.681580 -0.110548

H 3.155094 -2.686213 -1.835615
H -7.803992 -1.153092 0.360429
H -6.516272 -2.098122 1.169718
H -6.730921 -0.393344 1.572630
H -5.405987 3.892605 -0.841171
H -5.124238 3.999086 0.896763
H -4.320298 5.163267 -0.197259
H 0.142203 -1.501873 2.577487
H -0.349156 0.133271 3.048633
H -1.522614 -1.181955 3.077746
H 3.860936 0.516750 2.034366
H 2.597215 -0.716992 1.956289
H 4.247075 -1.095353 1.451288
H 5.487568 2.854413 0.845877
H 6.562758 2.866836 -0.540478
H 4.796728 2.882397 -0.793959
H 8.200906 0.448283 1.198847
H 1.681670 -1.064788 -2.606841

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79763049

Comp_10E_c05

B3LYP/6-31G* Geometry

C 2.073183 -0.451786 1.334916
C 1.679786 1.822864 0.332395
C 3.383728 0.244564 -0.725284
C 2.357381 1.348195 -0.977502
C 2.734847 -0.915019 0.038616
C 1.016073 0.668658 1.137586
C -0.248732 0.132214 0.376023
C -1.105960 1.249947 -0.218378
C -0.673164 2.520135 -0.346344
C 0.696872 2.938350 -0.004461
C -2.418602 0.782244 -0.822423
C -3.253129 -0.103053 0.148251
C -2.403545 -1.319762 0.547053
C -1.091343 -0.871313 1.216298
C -4.486233 -0.390212 -0.753987
C -4.768646 0.991504 -1.442911
C -3.444399 1.803798 -1.338494
O 1.053297 4.106989 -0.081039
O 4.446270 0.819748 0.078203
C 5.718729 0.412429 -0.155164
C 6.671209 1.099430 0.794835
O 6.037942 -0.387540 -1.007249
O 3.731571 -1.896901 0.392316
C 4.034318 -2.825429 -0.557844
C 5.206708 -3.667505 -0.125472
O 3.442691 -2.926060 -1.609276
C 0.647160 1.215847 2.535464
H 2.463647 2.273290 0.950655
C -3.642345 0.725779 1.398930
C -5.716434 -1.041362 -0.162518
C -6.921658 -1.230632 -1.053070

N	-5.675117	-1.459415	1.048871	C	2.431524	1.266888	0.596527
O	-6.893393	-2.078627	1.419860	C	1.099591	0.826160	1.233614
H	-4.143336	-1.068233	-1.546197	C	4.508453	0.371651	-0.725860
O	-2.039549	-0.079415	-1.930773	C	4.750259	-0.945609	-1.532069
H	0.094027	-0.439673	-0.497501	C	3.427897	-1.765551	-1.446377
H	2.859661	-0.073602	1.998739	O	-1.067944	-4.106544	-0.208945
H	1.630622	-1.317988	1.838231	O	-4.446325	-0.812963	0.065743
H	3.819326	-0.120687	-1.657226	C	-5.718841	-0.396547	-0.151480
H	2.849404	2.201229	-1.456359	C	-6.670478	-1.114980	0.775782
H	1.611511	0.968862	-1.687749	O	-6.038541	0.431706	-0.975840
H	2.017570	-1.392459	-0.634680	O	-3.720092	1.888838	0.466990
H	-1.304561	3.297874	-0.768465	C	-4.025848	2.847833	-0.451752
H	-2.968329	-1.954078	1.238217	C	-5.193474	3.678639	0.013836
H	-2.184226	-1.918778	-0.343029	O	-3.439947	2.979832	-1.502822
H	-1.326753	-0.430500	2.189413	C	-0.638207	-1.303389	2.492112
H	-0.477298	-1.755030	1.422617	H	-2.466277	-2.298823	0.882685
H	-5.585024	1.522354	-0.942251	C	3.627354	-0.822446	1.374499
H	-5.072344	0.853948	-2.484238	C	5.713901	0.953270	-0.014710
H	-3.551501	2.637166	-0.637909	C	6.698295	0.136620	0.785556
H	-3.137109	2.231438	-2.299610	N	5.840088	2.225417	-0.157981
H	7.697751	0.852296	0.522299	O	6.965219	2.714993	0.543173
H	6.522924	2.183205	0.768829	H	4.188479	1.143384	-1.428662
H	6.473194	0.765854	1.819426	O	2.040435	0.159392	-1.912984
H	5.244089	-4.577962	-0.725237	H	-0.092231	0.447323	-0.489084
H	6.120335	-3.086491	-0.295460	H	-2.847243	0.011814	2.008878
H	5.150339	-3.908731	0.939361	H	-1.614683	1.256711	1.883072
H	-0.174361	1.938977	2.491513	H	-3.822698	0.181975	-1.640314
H	0.355223	0.415789	3.222672	H	-2.861930	-2.149858	-1.518642
H	1.511639	1.724682	2.976707	H	-1.620186	-0.916054	-1.717324
H	-3.995527	0.063157	2.190560	H	-2.012540	1.413066	-0.584153
H	-2.797250	1.307677	1.780753	H	1.288414	-3.283603	-0.890552
H	-4.451220	1.431987	1.189469	H	2.998965	1.866856	1.318755
H	-7.245088	-2.276541	-1.033441	H	2.241534	1.906475	-0.270350
H	-7.767847	-0.636249	-0.688414	H	1.307287	0.369029	2.205082
H	-6.707740	-0.939213	-2.083923	H	0.496081	1.716573	1.441699
H	-6.708173	-2.350433	2.331808	H	5.584868	-1.527260	-1.129413
H	-1.603222	0.487899	-2.587112	H	5.007987	-0.706727	-2.567599
Number of Imaginary Frequencies= 0				H	3.544958	-2.635823	-0.793261
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79551955				H	3.103835	-2.143532	-2.422695
Comp_10E_c06				H	-7.696818	-0.850069	0.519737
B3LYP/6-31G* Geometry				H	-6.530153	-2.197795	0.703652
C	-2.062499	0.408767	1.353923	H	-6.463969	-0.825954	1.812097
C	-1.682869	-1.832928	0.275448	H	-5.230597	4.608646	-0.555140
C	-3.384943	-0.215471	-0.722668	H	-6.109696	3.106430	-0.171406
C	-2.364059	-1.314369	-1.015526	H	-5.131646	3.884081	1.085829
C	-2.728504	0.915978	0.076363	H	0.183886	-2.023906	2.421595
C	-1.010273	-0.707997	1.114793	H	-0.347123	-0.528056	3.207535
C	0.252785	-0.151978	0.364447	H	-1.501287	-1.828624	2.916291
C	1.101229	-1.254932	-0.271189	H	2.748688	-1.280068	1.838343
C	0.662934	-2.518505	-0.437622	H	4.307736	-1.638544	1.115977
C	-0.706709	-2.942072	-0.099955	H	4.121734	-0.210020	2.136235
C	2.413736	-0.770874	-0.861112	H	7.711608	0.294221	0.398932
C	3.256295	0.049216	0.154077	H	6.713757	0.471721	1.829049
				H	6.474296	-0.930269	0.763055
				H	6.942565	3.658153	0.319131

H 1.614056 -0.365695 -2.609633
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1554.79645826

Comp_10E_c07
B3LYP/6-31G* Geometry
C -2.055386 0.716602 1.380060
C -1.784450 -1.620716 0.478756
C -3.427345 -0.013282 -0.625889
C -2.451938 -1.172840 -0.845074
C -2.711793 1.144647 0.068299
C -1.058118 -0.465346 1.226899
C 0.225976 -0.025644 0.435612
C 1.012112 -1.204530 -0.138981
C 0.519227 -2.456959 -0.204986
C -0.859427 -2.796253 0.186284
C 2.329566 -0.820211 -0.789220
C 3.234490 0.042919 0.137345
C 2.457697 1.310057 0.529717
C 1.141554 0.943525 1.239479
C 4.455572 0.244233 -0.804051
C 4.649496 -1.167611 -1.460689
C 3.287108 -1.906041 -1.306646
O -1.267126 -3.950336 0.183166
O -4.508926 -0.434139 0.242984
C -5.609201 -0.961656 -0.352828
C -6.636462 -1.351190 0.683913
O -5.730576 -1.098587 -1.549422
O -3.638743 2.210498 0.381284
C -3.883120 3.116885 -0.599107
C -4.862720 4.163221 -0.123343
O -3.376296 3.077084 -1.698926
C -0.705774 -0.965873 2.646275
H -2.581079 -2.005407 1.124865
C 3.616947 -0.775952 1.396628
C 5.732749 0.846684 -0.262731
C 6.920766 0.951754 -1.189757
N 5.746435 1.294320 0.938711
O 7.004662 1.856727 1.263824
H 4.125639 0.917812 -1.605414
O 1.966221 0.033397 -1.908806
H -0.093695 0.544569 -0.447621
H -2.849736 0.416398 2.073103
H -1.559021 1.583698 1.828987
H -3.856840 0.312423 -1.575042
H -2.989182 -2.016582 -1.289409
H -1.697832 -0.857263 -1.577766
H -1.978269 1.541447 -0.639027
H 1.104362 -3.278947 -0.609367
H 3.071137 1.928942 1.192856
H 2.246899 1.900837 -0.367974
H 1.378521 0.502972 2.212146
H 0.581436 1.861961 1.448513
H 5.447519 -1.727840 -0.962423

H 4.936955 -1.073952 -2.511397
H 3.368250 -2.729409 -0.590852
H 2.933627 -2.336780 -2.250332
H -7.543383 -1.693776 0.184769
H -6.240205 -2.153139 1.316233
H -6.861272 -0.501334 1.335870
H -5.015260 4.902395 -0.910317
H -5.817400 3.691368 0.131971
H -4.487042 4.650102 0.782280
H 0.076274 -1.732701 2.629942
H -0.364739 -0.150938 3.292242
H -1.591513 -1.406670 3.117541
H 4.034332 -0.115577 2.158295
H 2.753773 -1.298661 1.820804
H 4.376047 -1.533451 1.179719
H 6.653721 0.686209 -2.215408
H 7.323917 1.969282 -1.173095
H 7.729461 0.290005 -0.856770
H 6.856763 2.161677 2.172102
H 1.483905 -0.525607 -2.539628
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1554.79523902

Comp_10E_c08
B3LYP/6-31G* Geometry
C -2.144072 0.693408 1.087500
C -1.800407 -1.732860 0.524943
C -3.465080 -0.334626 -0.819331
C -2.470474 -1.497414 -0.851357
C -2.789425 0.924443 -0.279328
C -1.108069 -0.462231 1.096877
C 0.155194 -0.110862 0.234871
C 1.018165 -1.340778 -0.053946
C 0.551509 -2.601154 0.058907
C -0.843726 -2.915018 0.409313
C 2.372158 -1.044571 -0.672695
C 3.164414 0.050019 0.097214
C 2.323653 1.335240 0.111759
C 0.963192 1.098154 0.793276
C 4.459158 0.089451 -0.762481
C 4.755766 -1.423296 -1.049973
C 3.403699 -2.171004 -0.854727
O -1.237791 -4.069409 0.516487
O -4.552814 -0.691331 0.067370
C -5.819347 -0.640211 -0.425825
C -6.813433 -0.982478 0.658312
O -6.097191 -0.364991 -1.570422
O -3.802168 1.953880 -0.190564
C -3.382654 3.236342 -0.325398
C -4.550750 4.189209 -0.237335
O -2.225080 3.555078 -0.492978
C -0.734050 -0.740851 2.570386
H -2.593080 -2.041377 1.215805
C 3.448692 -0.435448 1.540634

C	5.663717	0.867559	-0.281859	C	2.372243	-1.044488	-0.672753
C	6.916093	0.835401	-1.126119	C	3.164431	0.050192	0.097154
N	5.565684	1.565361	0.789316	C	2.323520	1.335332	0.111703
O	6.771354	2.254545	1.066136	C	0.963137	1.098101	0.793280
H	4.180403	0.539473	-1.724119	C	4.459159	0.089763	-0.762505
O	2.073439	-0.485210	-1.981925	C	4.755919	-1.422982	-1.049968
H	-0.188074	0.211678	-0.758363	C	3.403923	-2.170747	-0.854760
H	-2.943096	0.452149	1.798760	O	-1.237523	-4.069611	0.516231
H	-1.683770	1.626153	1.426039	O	-4.552754	-0.691696	0.067266
H	-3.887872	-0.145820	-1.808237	C	-5.819386	-0.639885	-0.425647
H	-2.991978	-2.410255	-1.157472	C	-6.813394	-0.981580	0.658733
H	-1.716883	-1.289214	-1.622143	O	-6.097374	-0.364369	-1.570147
H	-2.042928	1.258468	-1.005812	O	-3.802301	1.953491	-0.190580
H	1.177856	-3.461599	-0.162976	C	-3.382900	3.235993	-0.325504
H	2.863471	2.125411	0.643969	C	-4.551057	4.188770	-0.237307
H	2.170161	1.679621	-0.916046	O	-2.225359	3.554792	-0.493201
H	1.127143	0.967343	1.867286	C	-0.734017	-0.741070	2.570326
H	0.351437	1.999453	0.679888	H	-2.592921	-2.041679	1.215718
H	5.512205	-1.813136	-0.360927	C	3.448759	-0.435274	1.540588
H	5.147719	-1.561074	-2.061299	C	5.663636	0.867984	-0.281894
H	3.437408	-2.815751	0.028456	C	6.916050	0.835697	-1.126063
H	3.151988	-2.810986	-1.708020	N	5.565488	1.565703	0.789346
H	-7.819522	-0.995361	0.238034	O	6.771258	2.254492	1.066622
H	-6.576433	-1.957538	1.095657	H	4.180350	0.539673	-1.724191
H	-6.756324	-0.240446	1.461748	O	2.073341	-0.485199	-1.981950
H	-4.197215	5.211526	-0.374661	H	-0.188039	0.211572	-0.758398
H	-5.295525	3.942694	-1.000801	H	-2.943132	0.451834	1.798686
H	-5.039508	4.093086	0.737964	H	-1.683897	1.625926	1.426006
H	0.063396	-1.485613	2.659208	H	-3.887788	-0.146245	-1.808360
H	-0.406978	0.167178	3.085984	H	-2.991738	-2.410613	-1.157513
H	-1.607447	-1.124072	3.110299	H	-1.716741	-1.289456	-1.622229
H	3.801429	0.397992	2.149846	H	-2.042975	1.258260	-1.005875
H	2.554474	-0.857351	2.010400	H	1.178212	-3.461607	-0.162938
H	4.223833	-1.207209	1.571903	H	2.863277	2.125593	0.643832
H	6.745044	0.327339	-2.078184	H	2.169926	1.679645	-0.916111
H	7.267530	1.854190	-1.318456	H	1.127154	0.967235	1.867270
H	7.726196	0.320989	-0.595335	H	0.351291	1.999352	0.679989
H	6.539731	2.743505	1.870591	H	5.512309	-1.812784	-0.360849
H	1.663888	-1.198008	-2.498747	H	5.147995	-1.560658	-2.061259
Number of Imaginary Frequencies= 0				H	3.437698	-2.815450	0.028465
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79508479				H	3.152343	-2.810847	-1.708010
Comp_10E_c09				H	-7.819403	-0.995904	0.238319
B3LYP/6-31G* Geometry				H	-6.575586	-1.955726	1.097654
C	-2.144109	0.693142	1.087447	H	-6.757088	-0.238220	1.461015
C	-1.800257	-1.733082	0.524872	H	-4.197666	5.211114	-0.374756
C	-3.465019	-0.334973	-0.819432	H	-5.295945	3.942107	-1.000618
C	-2.470327	-1.497698	-0.851449	H	-5.039634	4.092640	0.738086
C	-2.789470	0.924159	-0.279416	H	0.063490	-1.485772	2.659132
C	-1.108023	-0.462423	1.096815	H	-0.407038	0.166963	3.085972
C	0.155212	-0.110970	0.234835	H	-1.607389	-1.124389	3.110211
C	1.018285	-1.340818	-0.053956	H	3.801205	0.398240	2.149883
C	0.551748	-2.601242	0.058917	H	2.554659	-0.857478	2.010291
C	-0.843499	-2.915199	0.409195	H	4.224154	-1.206786	1.571836
				H	6.743968	0.330815	-2.079639
				H	7.269789	1.854248	-1.315255

H 7.724919 0.317725 -0.596808
H 6.539399 2.743681 1.870878
H 1.664741 -1.198334 -2.499061
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79508587**

Comp_10E_c10
B3LYP/6-31G* Geometry
C -2.043944 0.665171 1.409727
C -1.788426 -1.638117 0.419973
C -3.426080 0.017236 -0.617978
C -2.457151 -1.138015 -0.884217
C -2.702399 1.144770 0.116880
C -1.053536 -0.515328 1.209085
C 0.230504 -0.052691 0.430170
C 1.006621 -1.214420 -0.192992
C 0.507347 -2.460835 -0.304193
C -0.871057 -2.807554 0.082210
C 2.323747 -0.808970 -0.830066
C 3.235493 -0.015158 0.145594
C 2.484758 1.249568 0.589652
C 1.150109 0.886051 1.268195
C 4.475610 0.228124 -0.775438
C 4.629081 -1.114412 -1.560932
C 3.269392 -1.864141 -1.425776
O -1.284453 -3.958759 0.040653
O -4.506706 -0.431012 0.238153
C -5.613835 -0.925800 -0.373232
C -6.637337 -1.353949 0.651887
O -5.742323 -1.011549 -1.573770
O -3.622254 2.202849 0.473070
C -3.869551 3.143678 -0.473859
C -4.841210 4.176997 0.044457
O -3.370754 3.139118 -1.577963
C -0.700984 -1.073049 2.607087
H -2.585536 -2.041286 1.053955
C 3.597016 -0.884913 1.370350
C 5.728807 0.762542 -0.111831
C 6.690168 -0.085223 0.684133
N 5.918309 2.021949 -0.292963
O 7.087218 2.467960 0.364462
H 4.173014 1.000793 -1.484674
O 1.968053 0.120488 -1.888701
H -0.089549 0.550052 -0.430550
H -2.837607 0.343548 2.093815
H -1.541775 1.512589 1.888754
H -3.857185 0.380765 -1.552470
H -3.000037 -1.961946 -1.357910
H -1.703756 -0.799213 -1.607123
H -1.968948 1.563671 -0.577661
H 1.085714 -3.268715 -0.745176
H 3.101166 1.830828 1.286633
H 2.303525 1.885234 -0.282083
H 1.360691 0.423826 2.236425

H 0.600658 1.808698 1.486120
H 5.443402 -1.730576 -1.167914
H 4.871764 -0.908502 -2.607120
H 3.360871 -2.729832 -0.762443
H 2.898881 -2.239753 -2.386404
H -7.557291 -1.647041 0.145067
H -6.251358 -2.201886 1.228282
H -6.835246 -0.541210 1.357444
H -4.994062 4.944605 -0.714749
H -5.797017 3.700911 0.287459
H -4.458673 4.629311 0.965002
H 0.080743 -1.839109 2.559747
H -0.361033 -0.285948 3.287280
H -1.586557 -1.533376 3.059406
H 4.138953 -0.285948 2.110110
H 2.709755 -1.293599 1.862743
H 4.231101 -1.736165 1.108062
H 7.701229 0.016047 0.273722
H 6.744071 0.267975 1.720402
H 6.414407 -1.140157 0.687660
H 7.110228 3.404167 0.113007
H 1.498187 -0.394512 -2.564609
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79624137**

Comp_10E_c11
B3LYP/6-31G* Geometry
C -2.156845 0.650913 1.109244
C -1.761949 -1.751498 0.478699
C -3.497256 -0.367640 -0.788877
C -2.472626 -1.501795 -0.874461
C -2.839019 0.895474 -0.237356
C -1.092397 -0.477136 1.068039
C 0.143244 -0.070025 0.187171
C 1.028368 -1.267257 -0.171104
C 0.600142 -2.540286 -0.072327
C -0.773743 -2.901862 0.313246
C 2.360475 -0.912374 -0.812977
C 3.152165 0.150339 0.009361
C 2.297639 1.423597 0.111500
C 0.936949 1.134876 0.778311
C 4.463157 0.243116 -0.847196
C 4.732459 -1.233179 -1.270875
C 3.398165 -2.007336 -1.077788
O -1.131856 -4.068157 0.413152
O -4.550973 -0.773462 0.117114
C -5.832917 -0.731619 -0.337635
C -6.786671 -1.142994 0.758491
O -6.149280 -0.416316 -1.461475
O -3.867080 1.903809 -0.102868
C -3.470774 3.195026 -0.219462
C -4.649156 4.128202 -0.080233
O -2.321820 3.534323 -0.409631
C -0.677246 -0.783774 2.524954

H	-2.527917	-2.098145	1.181192	C	0.670834	-2.511531	-0.360736
C	3.479441	-0.379968	1.423868	C	-0.690882	-2.940208	-0.000240
C	5.617248	0.964561	-0.183545	C	2.396358	-0.750869	-0.854516
C	5.619099	2.473091	-0.133339	C	3.253130	0.090192	0.144234
N	6.559851	0.253031	0.318364	C	2.421478	1.292978	0.620257
O	7.548622	1.060732	0.924835	C	1.103994	0.828527	1.271224
H	4.208006	0.815826	-1.746389	C	4.476010	0.403355	-0.761101
O	2.053209	-0.409533	-2.139060	C	4.739530	-0.956321	-1.498965
H	-0.252348	0.282391	-0.779198	C	3.405001	-1.755113	-1.423836
H	-2.932799	0.371396	1.831589	O	-1.038740	-4.112171	-0.058293
H	-1.714385	1.587710	1.460810	O	-4.445980	-0.824008	0.054576
H	-3.950617	-0.166631	-1.761736	C	-5.714915	-0.413409	-0.192815
H	-2.977954	-2.421180	-1.187588	C	-6.682048	-1.115552	0.730808
H	-1.745078	-1.259251	-1.659909	O	-6.020670	0.398522	-1.038554
H	-2.117920	1.260291	-0.974319	O	-3.737947	1.885078	0.408424
H	1.240218	-3.374878	-0.344327	C	-4.014570	2.841353	-0.522206
H	2.815911	2.192565	0.696624	C	-5.205362	3.663666	-0.103277
H	2.152306	1.867811	-0.883989	O	-3.388146	2.977749	-1.549348
H	1.112993	0.964712	1.843656	C	-0.658903	-1.239027	2.545686
H	0.310631	2.030493	0.706776	H	-2.468234	-2.281908	0.941906
H	5.532023	-1.665072	-0.667086	C	3.653311	-0.788789	1.356782
H	5.064629	-1.263756	-2.312188	C	5.713353	1.033126	-0.161859
H	3.458580	-2.691168	-0.226239	C	6.920594	1.224806	-1.048549
H	3.116604	-2.592943	-1.956759	N	5.674115	1.432888	1.056126
H	-7.805802	-1.146946	0.370802	O	6.896766	2.035599	1.438459
H	-6.524460	-2.137367	1.133779	H	4.129204	1.105423	-1.531686
H	-6.711270	-0.445303	1.599185	O	2.016782	0.036918	-2.013410
H	-4.313745	5.158735	-0.200288	H	-0.115859	0.465713	-0.448404
H	-5.408389	3.889427	-0.831830	H	-2.871024	0.053081	2.006067
H	-5.113304	4.000614	0.903441	H	-1.643387	1.300845	1.864134
H	0.144872	-1.504800	2.575820	H	-3.796641	0.132332	-1.663387
H	-0.371230	0.119150	3.062398	H	-2.832063	-2.192349	-1.469991
H	-1.526341	-1.211481	3.069707	H	-1.589890	-0.962955	-1.682145
H	3.874802	0.428115	2.049266	H	-2.015296	1.398905	-0.609587
H	2.597898	-0.789396	1.926352	H	1.298005	-3.278711	-0.806326
H	4.240927	-1.163342	1.400241	H	2.999327	1.883245	1.338293
H	5.512085	2.828981	0.898776	H	2.213903	1.975174	-0.218616
H	6.577838	2.860875	-0.494026	H	1.345999	0.341547	2.219381
H	4.811610	2.894340	-0.736602	H	0.499372	1.706427	1.525158
H	8.199854	0.399795	1.206341	H	5.551747	-1.511522	-1.017950
H	1.548521	0.413319	-2.053604	H	5.041895	-0.784267	-2.535103
Number of Imaginary Frequencies= 0							
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79464788							
Comp_10E_c12							
B3LYP/6-31G* Geometry							
C	-2.080884	0.437630	1.350425	H	-6.108901	3.081304	-0.316969
C	-1.679566	-1.828393	0.332214	H	-5.183403	3.874848	0.969207
C	-3.372814	-0.242373	-0.729651	H	0.166511	-1.957478	2.499663
C	-2.343258	-1.343388	-0.980788	H	-0.377456	-0.444448	3.243755
C	-2.734942	0.910660	0.053398	H	-1.523680	-1.757298	2.974719
C	-1.022091	-0.680793	1.150999	H	2.804640	-1.363847	1.740243
C	0.246529	-0.136728	0.399397	H	4.436565	-1.507092	1.098228
C	1.095337	-1.240153	-0.236600	H	4.044924	-0.164363	2.161672

H 7.258377 2.265510 -1.007506
H 7.758330 0.611468 -0.695946
H 6.703012 0.956538 -2.084762
H 6.715678 2.288905 2.356567
H 1.602856 0.860407 -1.713062
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79280546**

Comp_10E_c13

B3LYP/6-31G* Geometry

C -2.156943 0.650807 1.109317
C -1.761893 -1.751562 0.478799
C -3.497133 -0.367768 -0.788974
C -2.472431 -1.501862 -0.874445
C -2.839039 0.895366 -0.237304
C -1.092436 -0.477195 1.068205
C 0.143284 -0.070039 0.187477
C 1.028388 -1.267250 -0.170905
C 0.600236 -2.540297 -0.072064
C -0.773660 -2.901915 0.313411
C 2.360460 -0.912315 -0.812858
C 3.152213 0.150345 0.009481
C 2.297641 1.423550 0.111850
C 0.937089 1.134668 0.778854
C 4.463080 0.243238 -0.847254
C 4.732379 -1.233032 -1.271057
C 3.398147 -2.007255 -1.077801
O -1.131769 -4.068213 0.413262
O -4.550970 -0.773753 0.116798
C -5.832860 -0.731442 -0.338066
C -6.786871 -1.142773 0.757864
O -6.149021 -0.415775 -1.461853
O -3.867178 1.903617 -0.102775
C -3.471022 3.194866 -0.219368
C -4.649483 4.127916 -0.079907
O -2.322123 3.534308 -0.409604
C -0.677401 -0.783802 2.525163
H -2.527930 -2.098232 1.181203
C 3.479691 -0.380088 1.423906
C 5.617245 0.964683 -0.183716
C 5.619121 2.473215 -0.133525
N 6.559951 0.253164 0.318001
O 7.548866 1.060866 0.924267
H 4.207779 0.815995 -1.746379
O 2.053121 -0.409398 -2.138888
H -0.252216 0.282590 -0.778856
H -2.932935 0.371224 1.831599
H -1.714554 1.587625 1.460918
H -3.950334 -0.166726 -1.761905
H -2.977683 -2.421255 -1.187655
H -1.744779 -1.259269 -1.659785
H -2.117953 1.260292 -0.974230
H 1.240351 -3.374868 -0.344046
H 2.815967 2.192485 0.696971

H 2.152105 1.867841 -0.883578
H 1.113348 0.964165 1.844109
H 0.310781 2.030323 0.707709
H 5.532067 -1.664904 -0.667422
H 5.064337 -1.263541 -2.312438
H 3.458702 -2.691069 -0.226248
H 3.116502 -2.592873 -1.956733
H -7.805949 -1.146333 0.370010
H -6.525043 -2.137323 1.132945
H -6.711433 -0.445287 1.598719
H -4.314363 5.158420 -0.201023
H -5.409351 3.888383 -0.830611
H -5.112710 4.001025 0.904297
H 0.144795 -1.504737 2.576096
H -0.371528 0.119159 3.062625
H -1.526495 -1.211612 3.069832
H 3.875040 0.427972 2.049338
H 4.241260 -1.163374 1.400098
H 2.598240 -0.789664 1.926433
H 5.512804 2.829099 0.898661
H 6.577635 2.860982 -0.494835
H 4.811258 2.894482 -0.736274
H 8.200116 0.399916 1.205688
H 1.548304 0.413367 -2.053385

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79464813**

Comp_10E_c14

B3LYP/6-31G* Geometry

C -2.070418 0.404984 1.367151
C -1.675246 -1.827841 0.275947
C -3.369237 -0.210893 -0.729396
C -2.336957 -1.299251 -1.021159
C -2.732317 0.917712 0.089150
C -1.013388 -0.707213 1.128868
C 0.253013 -0.139564 0.392447
C 1.085570 -1.221780 -0.292676
C 0.667598 -2.490145 -0.454593
C -0.689906 -2.931498 -0.089811
C 2.376618 -0.705210 -0.901883
C 3.253745 0.039083 0.156179
C 2.453467 1.241607 0.675444
C 1.121026 0.785269 1.301019
C 4.500287 0.390718 -0.718738
C 4.716732 -0.888692 -1.593039
C 3.366559 -1.673142 -1.570557
O -1.035774 -4.102185 -0.178113
O -4.436524 -0.824278 0.040021
C -5.709216 -0.417485 -0.188983
C -6.666287 -1.159102 0.714609
O -6.027178 0.418216 -1.006760
O -3.739713 1.872870 0.485309
C -4.043309 2.848984 -0.415250
C -5.230204 3.652214 0.050915

O	-3.442668	3.015267	-1.452996	C	0.313163	-0.155352	0.384982
C	-0.652545	-1.313559	2.504339	C	1.192734	-1.228140	-0.258706
H	-2.465562	-2.297818	0.870836	C	0.777525	-2.494256	-0.463322
C	3.630691	-0.906223	1.318367	C	-0.591247	-2.947430	-0.163348
C	5.726254	0.926741	-0.007325	C	2.509152	-0.712898	-0.814022
C	6.698041	0.067308	0.761585	C	3.321557	0.106890	0.227101
N	5.880107	2.198604	-0.123572	C	2.461956	1.299298	0.676616
O	7.021911	2.646775	0.574211	C	1.129519	0.820265	1.283798
H	4.192436	1.216061	-1.370298	C	4.595104	0.447358	-0.624090
O	1.880264	0.225192	-1.897775	C	4.863998	-0.866851	-1.426125
H	-0.086812	0.498556	-0.434581	C	3.542386	-1.689483	-1.392784
H	-2.857487	0.002922	2.016283	O	-0.932633	-4.113343	-0.314176
H	-1.627527	1.252010	1.902648	O	-4.369712	-0.891203	0.010603
H	-3.798979	0.193087	-1.647986	C	-5.647321	-0.495582	-0.214784
H	-2.823795	-2.130998	-1.541211	C	-6.597549	-1.264638	0.672537
H	-1.583238	-0.890359	-1.705548	O	-5.972254	0.350324	-1.018934
H	-2.018273	1.432092	-0.559945	O	-3.700525	1.808614	0.501043
H	1.286037	-3.238768	-0.942230	C	-4.013426	2.790570	-0.390257
H	3.034911	1.797511	1.421619	C	-5.203746	3.582387	0.085983
H	2.258806	1.926713	-0.155170	O	-3.416799	2.968563	-1.428464
H	1.332766	0.276714	2.245556	C	-0.579420	-1.377228	2.471446
H	0.530398	1.670925	1.560610	H	-2.373390	-2.361275	0.813435
H	5.524662	-1.511919	-1.199339	C	3.693760	-0.773769	1.441105
H	5.017811	-0.612298	-2.609190	C	5.781150	1.011330	0.136980
H	3.467660	-2.594226	-0.989904	C	6.907010	0.140063	0.642213
H	3.017025	-1.957415	-2.567690	N	5.952863	2.263197	0.375367
H	-7.691127	-0.885806	0.461378	H	4.287425	1.219977	-1.330937
H	-6.527621	-2.239765	0.611534	O	2.143500	0.227406	-1.859077
H	-6.463357	-0.901118	1.759672	H	-0.032495	0.454084	-0.461365
H	-5.270088	4.596320	-0.494193	O	4.909028	3.066219	-0.138526
H	-6.135052	3.072893	-0.165476	H	-2.807356	-0.092050	1.998838
H	-5.190073	3.830153	1.128862	H	-1.597062	1.178271	1.921834
H	0.175204	-2.027973	2.435476	H	-3.742452	0.163872	-1.657585
H	-0.375337	-0.543904	3.231344	H	-2.741749	-2.154081	-1.587672
H	-1.516524	-1.849544	2.912822	H	-1.520075	-0.893868	-1.737093
H	2.750090	-1.369398	1.771374	H	-1.971532	1.399001	-0.543238
H	4.285721	-1.722156	1.000182	H	1.422817	-3.239039	-0.922127
H	4.153093	-0.350142	2.104475	H	3.002604	1.897741	1.418227
H	7.712670	0.221944	0.377610	H	2.276535	1.951897	-0.179909
H	6.720516	0.366731	1.815754	H	1.329361	0.349306	2.250499
H	6.456060	-0.994221	0.704718	H	0.507722	1.696536	1.498569
H	7.017075	3.596075	0.375994	H	5.678750	-1.453785	-0.994481
H	2.611209	0.463913	-2.487820	H	5.160719	-0.626236	-2.451035
Number of Imaginary Frequencies= 0				H	3.646150	-2.572947	-0.755440
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79334988				H	3.245022	-2.048005	-2.384764
Comp_10Z_c01				H	-6.398135	-1.026136	1.722856
B3LYP/6-31G* Geometry				H	-7.624787	-0.996544	0.423597
C	-2.023028	0.337511	1.364069	H	-6.448042	-2.341553	0.547499
C	-1.590759	-1.865460	0.229129	H	-5.248399	4.532703	-0.447838
C	-3.309425	-0.251982	-0.745843	H	-6.106069	3.001656	-0.137167
C	-2.265228	-1.323980	-1.055775	H	-5.164007	3.747592	1.165922
C	-2.684550	0.867997	0.093790	H	0.256562	-2.080434	2.391441
C	-0.947464	-0.752302	1.106188	H	-0.310242	-0.615392	3.209571
				H	-1.437368	-1.928531	2.872312
				H	4.180671	-0.160504	2.207428

H 2.817545 -1.241920 1.898865
H 4.382043 -1.582235 1.177602
H 7.465601 -0.306676 -0.189745
H 7.598954 0.746981 1.230825
H 6.540754 -0.683210 1.265068
H 1.735168 -0.292867 -2.570063
H 5.218757 3.956741 0.087479
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79464479**

Comp_10Z_c02

B3LYP/6-31G* Geometry

C -2.007595 0.602862 1.423882
C -1.703179 -1.674957 0.389933
C -3.354159 -0.024915 -0.634183
C -2.362743 -1.158106 -0.912314
C -2.658187 1.098463 0.133084
C -0.996433 -0.557753 1.211931
C 0.290328 -0.058953 0.460652
C 1.092294 -1.192870 -0.177754
C 0.615102 -2.444835 -0.321175
C -0.762150 -2.821841 0.040388
C 2.410888 -0.753503 -0.790281
C 3.303470 0.033816 0.209371
C 2.522823 1.273616 0.677375
C 1.187884 0.869208 1.331716
C 4.560065 0.298863 -0.692515
C 4.727804 -1.033392 -1.492981
C 3.369364 -1.788314 -1.396497
O -1.155593 -3.978701 -0.029920
O -4.437407 -0.509100 0.198870
C -5.527171 -1.012270 -0.436214
C -6.553437 -1.483465 0.567083
O -5.639836 -1.075189 -1.639777
O -3.599701 2.133602 0.500365
C -3.855379 3.087686 -0.430670
C -4.851436 4.092452 0.097589
O -3.346283 3.113788 -1.529791
C -0.653801 -1.139335 2.602655
H -2.501841 -2.104048 1.004620
C 3.675674 -0.853639 1.418439
C 5.802613 0.802999 0.018718
C 6.899967 -0.124794 0.484684
N 6.049631 2.044954 0.241978
H 4.267686 1.081894 -1.394283
O 2.056415 0.193193 -1.833469
H -0.027054 0.559907 -0.389606
O 5.030006 2.900135 -0.235786
H -2.804446 0.255020 2.091278
H -1.524632 1.447990 1.926187
H -3.780114 0.351193 -1.566037
H -2.885414 -1.980314 -1.411085
H -1.605383 -0.791200 -1.617098
H -1.923552 1.543694 -0.543595

H 1.211169 -3.234593 -0.771050
H 3.119097 1.847596 1.395180
H 2.343096 1.929681 -0.177845
H 1.394647 0.384811 2.290067
H 0.622866 1.777790 1.568715
H 5.529857 -1.658355 -1.092165
H 4.991504 -0.814954 -2.531780
H 3.455215 -2.669440 -0.753168
H 3.014102 -2.142237 -2.370978
H -6.764558 -0.696826 1.297793
H -7.466579 -1.769817 0.044297
H -6.162373 -2.346321 1.117464
H -5.007461 4.874416 -0.646162
H -5.802092 3.594665 0.316232
H -4.489439 4.529884 1.033471
H 0.143119 -1.889268 2.550569
H -0.339223 -0.361082 3.304771
H -1.536954 -1.626096 3.031413
H 4.216506 -0.258456 2.162530
H 4.316168 -1.695183 1.139129
H 2.794632 -1.277582 1.908842
H 7.399230 -0.605226 -0.365955
H 7.646666 0.447055 1.040540
H 6.515751 -0.924078 1.127693
H 1.599144 -0.313029 -2.524545
H 5.396790 3.773871 -0.030716

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79451465**

Comp_10Z_c03

B3LYP/6-31G* Geometry

C -2.071232 0.357193 1.356361
C -1.552050 -1.823856 0.216514
C -3.360402 -0.296309 -0.733495
C -2.270273 -1.316685 -1.058493
C -2.778546 0.853558 0.097043
C -0.948643 -0.679517 1.081536
C 0.269629 -0.027173 0.336029
C 1.194888 -1.064017 -0.303558
C 0.834708 -2.347988 -0.500294
C -0.510252 -2.860167 -0.189705
C 2.485696 -0.497566 -0.865884
C 3.264791 0.359005 0.171377
C 2.356391 1.523980 0.599938
C 1.040834 1.004532 1.212515
C 4.523082 0.749965 -0.684664
C 4.805630 -0.507250 -1.579765
C 3.559369 -1.425056 -1.445060
O -0.803433 -4.039090 -0.340644
O -4.377421 -0.985779 0.037762
C -5.675667 -0.651497 -0.168798
C -6.575480 -1.468890 0.727799
O -6.051801 0.180159 -0.965445
O -3.833411 1.742427 0.521274

C -4.201291 2.715256 -0.358774
 C -5.421767 3.446936 0.136920
 O -3.624669 2.928952 -1.401618
 C -0.527770 -1.283452 2.440998
 H -2.302160 -2.354101 0.813263
 C 3.661951 -0.489799 1.398219
 C 5.689711 1.367142 0.071975
 C 5.734420 2.878952 0.107031
 N 6.676346 0.815949 0.682419
 H 4.175638 1.539170 -1.358105
 O 2.075163 0.425211 -1.912817
 H -0.118651 0.550514 -0.514327
 O 6.662129 -0.598403 0.667783
 H -2.823035 -0.109232 2.004346
 H -1.677770 1.218198 1.907184
 H -3.826068 0.098015 -1.638759
 H -2.714151 -2.169253 -1.583014
 H -1.556891 -0.851981 -1.751123
 H -2.103428 1.419450 -0.551506
 H 1.511929 -3.064413 -0.958167
 H 2.864172 2.149191 1.345827
 H 2.142445 2.157546 -0.266271
 H 1.260624 0.565780 2.189575
 H 0.381668 1.858211 1.405188
 H 5.712441 -1.028776 -1.281116
 H 4.936353 -0.183334 -2.616312
 H 3.755401 -2.261273 -0.766924
 H 3.250010 -1.857628 -2.403951
 H -6.361802 -1.239090 1.777157
 H -7.617606 -1.237936 0.504958
 H -6.387387 -2.537260 0.582277
 H -5.519337 4.396399 -0.391308
 H -6.298107 2.824281 -0.076353
 H -5.375040 3.609191 1.217069
 H 0.337655 -1.947659 2.346066
 H -0.279920 -0.508921 3.173522
 H -1.352536 -1.872080 2.858200
 H 4.101833 0.156039 2.166231
 H 2.800887 -0.998830 1.841554
 H 4.411180 -1.242739 1.153051
 H 4.806579 3.288845 0.525171
 H 6.577834 3.224625 0.708783
 H 5.832190 3.284808 -0.908362
 H 1.706210 -0.115896 -2.629705
 H 7.475599 -0.803104 1.153976

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79097250**

Comp_10Z_c04

B3LYP/6-31G* Geometry

C -2.029648 0.341177 1.377297
 C -1.582251 -1.857955 0.239716
 C -3.292104 -0.249147 -0.749770
 C -2.236551 -1.311252 -1.053448

C -2.686888 0.870931 0.103807
 C -0.950030 -0.746371 1.126234
 C 0.314806 -0.140484 0.418954
 C 1.173640 -1.190797 -0.282404
 C 0.779612 -2.462243 -0.478106
 C -0.573632 -2.935578 -0.138931
 C 2.463250 -0.639335 -0.865250
 C 3.319789 0.092363 0.219183
 C 2.491739 1.267768 0.760859
 C 1.160528 0.772562 1.358972
 C 4.586870 0.462312 -0.628483
 C 4.819322 -0.805350 -1.514481
 C 3.466966 -1.583025 -1.546331
 O -0.897456 -4.109922 -0.257798
 O -4.357654 -0.900679 -0.009859
 C -5.635095 -0.516272 -0.249899
 C -6.589863 -1.303184 0.617151
 O -5.958586 0.332695 -1.051721
 O -3.718334 1.795983 0.510128
 C -4.029506 2.788532 -0.369350
 C -5.240081 3.554202 0.099267
 O -3.417857 2.994453 -1.393521
 C -0.595464 -1.378122 2.491804
 H -2.371733 -2.355357 0.813130
 C 3.701530 -0.873100 1.363672
 C 5.797020 0.961869 0.139946
 C 6.905345 0.039698 0.588852
 N 6.000289 2.197526 0.431203
 H 4.296654 1.298861 -1.273191
 O 1.962262 0.304926 -1.843949
 H -0.025793 0.513506 -0.395255
 O 4.970225 3.046045 -0.034838
 H -2.816369 -0.088994 2.008729
 H -1.607409 1.183554 1.936315
 H -3.717391 0.169329 -1.663947
 H -2.701455 -2.139141 -1.599132
 H -1.481513 -0.873274 -1.718032
 H -1.975788 1.415189 -0.523877
 H 1.415399 -3.188932 -0.976162
 H 3.053763 1.812482 1.527954
 H 2.298227 1.974387 -0.050194
 H 1.369929 0.242948 2.292565
 H 0.554682 1.642873 1.635544
 H 5.605813 -1.443805 -1.105352
 H 5.153189 -0.517918 -2.517296
 H 3.556288 -2.524406 -0.996983
 H 3.135783 -1.830158 -2.559173
 H -6.399697 -1.082622 1.673025
 H -7.616100 -1.034995 0.364147
 H -6.435374 -2.377283 0.474493
 H -5.287976 4.514601 -0.415970
 H -6.129264 2.965469 -0.153700
 H -5.224111 3.697566 1.182932
 H 0.245130 -2.076737 2.416770
 H -0.339821 -0.620468 3.238985

H -1.455078 -1.937401 2.877611
H 4.222715 -0.325397 2.156893
H 2.823941 -1.347938 1.809936
H 4.360041 -1.679992 1.028908
H 7.438730 -0.385634 -0.270285
H 7.622092 0.602851 1.190979
H 6.525841 -0.798362 1.182943
H 2.709693 0.631143 -2.368166
H 5.298298 3.918177 0.233333
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79155018**

Comp_10Z_c05
B3LYP/6-31G* Geometry
C -2.095138 0.569793 1.143547
C -1.716688 -1.800013 0.388421
C -3.393054 -0.317942 -0.846232
C -2.382596 -1.461139 -0.968401
C -2.736907 0.902878 -0.203610
C -1.046139 -0.570774 1.065370
C 0.217265 -0.135278 0.240634
C 1.104471 -1.327175 -0.122651
C 0.653801 -2.598361 -0.115208
C -0.742403 -2.956072 0.186042
C 2.464162 -0.964798 -0.691060
C 3.225860 0.069697 0.182396
C 2.374790 1.345571 0.269645
C 0.991675 1.053872 0.884118
C 4.563511 0.182679 -0.629986
C 4.853364 -1.287372 -1.071540
C 3.507276 -2.061084 -0.954802
O -1.122626 -4.120052 0.190464
O -4.477628 -0.759618 0.005599
C -5.743089 -0.695609 -0.488939
C -6.734112 -1.138727 0.560975
O -6.021813 -0.340029 -1.610922
O -3.764034 1.908170 -0.038582
C -3.359872 3.202373 -0.058305
C -4.541071 4.130253 0.096175
O -2.204705 3.548237 -0.183802
C -0.675896 -0.960693 2.514572
H -2.509347 -2.173913 1.046122
C 3.485804 -0.498948 1.595257
C 5.708895 0.902864 0.057806
C 6.766343 0.168326 0.847670
N 5.902292 2.172519 -0.005501
H 4.324586 0.764187 -1.522357
O 2.183790 -0.293754 -1.948894
H -0.125554 0.243771 -0.732459
O 4.924278 2.837003 -0.779965
H -2.894498 0.262630 1.828332
H -1.645733 1.476239 1.559279
H -3.816052 -0.056229 -1.818301
H -2.890331 -2.352460 -1.351336

H -1.628238 -1.180065 -1.715018
H -1.991513 1.303755 -0.896380
H 1.294730 -3.431300 -0.393006
H 2.886258 2.101206 0.875992
H 2.262977 1.770581 -0.730457
H 1.110383 0.877611 1.957513
H 0.373177 1.952685 0.788394
H 5.611865 -1.763849 -0.445137
H 5.239098 -1.303441 -2.095062
H 3.536241 -2.778664 -0.129047
H 3.270548 -2.631147 -1.860381
H -6.690906 -0.462573 1.421388
H -7.738868 -1.134527 0.137388
H -6.482214 -2.141705 0.919940
H -4.199569 5.164671 0.048071
H -5.275439 3.939157 -0.692836
H -5.037814 3.947533 1.054961
H 0.127482 -1.703522 2.549374
H -0.360551 -0.092393 3.101231
H -1.548055 -1.392642 3.018480
H 3.946890 0.270475 2.224374
H 2.563391 -0.818222 2.088687
H 4.155897 -1.363673 1.584567
H 6.328293 -0.469189 1.623247
H 7.368238 -0.478882 0.197583
H 7.433664 0.892208 1.321298
H 1.805917 -0.964885 -2.540245
H 5.239385 3.753359 -0.748258
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79426870**

Comp_10Z_c08
B3LYP/6-31G* Geometry
C -2.064307 0.609141 1.415729
C -1.661610 -1.648231 0.375362
C -3.407982 -0.084254 -0.623132
C -2.364370 -1.165444 -0.917304
C -2.760105 1.072593 0.136754
C -0.997829 -0.496522 1.184447
C 0.247424 0.062390 0.406606
C 1.104828 -1.039611 -0.216931
C 0.685037 -2.313129 -0.351276
C -0.672727 -2.750730 0.014890
C 2.402523 -0.549638 -0.833353
C 3.252713 0.297641 0.154964
C 2.411371 1.512231 0.584253
C 1.092782 1.065411 1.245956
C 4.496089 0.609753 -0.752165
C 4.698429 -0.686781 -1.611566
C 3.414753 -1.541277 -1.417859
O -1.016221 -3.923295 -0.057354
O -4.451859 -0.626156 0.224206
C -5.532124 -1.168237 -0.395177
C -6.512788 -1.700980 0.622744

O	-5.668950	-1.218050	-1.596800	C	-3.343686	-0.039927	-0.640948
O	-3.750542	2.054358	0.521462	C	-2.340163	-1.163198	-0.915476
C	-4.057435	3.008337	-0.394129	C	-2.664542	1.089047	0.133066
C	-5.104655	3.950171	0.150918	C	-0.994797	-0.556890	1.217469
O	-3.552627	3.078619	-1.493284	C	0.290746	-0.048890	0.469556
C	-0.599214	-1.057879	2.568672	C	1.082905	-1.168126	-0.201066
H	-2.430395	-2.112798	1.002279	C	0.626662	-2.426694	-0.331380
C	3.653901	-0.537988	1.389877	C	-0.739611	-2.819565	0.056008
C	5.712572	1.205083	-0.059311	C	2.383563	-0.702531	-0.832068
C	5.825719	2.713345	-0.094922	C	3.298638	0.029654	0.203527
N	6.695242	0.636501	0.541440	C	2.537456	1.261205	0.718970
H	4.156246	1.388893	-1.440689	C	1.199328	0.849533	1.362807
O	2.002290	0.361806	-1.894391	C	4.559315	0.309762	-0.687356
H	-0.116260	0.640798	-0.453630	C	4.709655	-0.996799	-1.535137
O	6.620235	-0.775095	0.587527	C	3.326329	-1.717667	-1.496661
H	-2.831438	0.217879	2.094018	O	-1.117502	-3.982604	0.008292
H	-1.619401	1.476977	1.914425	O	-4.426678	-0.538355	0.185241
H	-3.866511	0.270979	-1.547754	C	-5.525921	-1.013878	-0.453553
H	-2.851983	-2.013166	-1.408899	C	-6.544414	-1.509837	0.546145
H	-1.636313	-0.761217	-1.632576	O	-5.653283	-1.039046	-1.657051
H	-2.061097	1.558351	-0.549765	O	-3.623059	2.108628	0.502317
H	1.318191	-3.077418	-0.794448	C	-3.872068	3.079709	-0.412386
H	2.969598	2.128700	1.300702	C	-4.893761	4.058004	0.117526
H	2.199560	2.137153	-0.288976	O	-3.341481	3.138751	-1.499854
H	1.321967	0.627924	2.221290	C	-0.655459	-1.137923	2.609275
H	0.482118	1.952547	1.447888	H	-2.492689	-2.109463	1.002737
H	5.587168	-1.240428	-1.315975	C	3.665958	-0.908853	1.374907
H	4.819730	-0.403307	-2.661053	C	5.811179	0.776011	0.033533
H	3.592061	-2.368212	-0.723403	C	6.889400	-0.182357	0.479862
H	3.057116	-1.983258	-2.355401	N	6.078126	2.009015	0.281187
H	-6.735731	-0.939259	1.375901	H	4.291532	1.137226	-1.353100
H	-7.426962	-2.013099	0.116764	O	1.907595	0.227185	-1.837167
H	-6.073496	-2.559061	1.143517	H	-0.025907	0.591049	-0.365170
H	-5.290905	4.744066	-0.572942	O	5.074565	2.889871	-0.183082
H	-6.032708	3.401679	0.344326	H	-2.808985	0.247065	2.091888
H	-4.773739	4.377401	1.102772	H	-1.535111	1.446859	1.927491
H	0.234045	-1.765618	2.501889	H	-3.768967	0.334286	-1.573875
H	-0.312372	-0.263917	3.265218	H	-2.852833	-1.987880	-1.420972
H	-1.448350	-1.588619	3.013668	H	-1.577656	-0.789952	-1.610743
H	4.142754	0.107130	2.128282	H	-1.934396	1.547468	-0.539384
H	2.787728	-1.002058	1.871209	H	1.217718	-3.204096	-0.807487
H	4.364482	-1.326472	1.141467	H	3.141709	1.806460	1.452658
H	4.931777	3.184456	0.332119	H	2.357403	1.945901	-0.113750
H	6.703549	3.046519	0.463066	H	1.405035	0.337880	2.306993
H	5.907714	3.067823	-1.130798	H	0.642127	1.755706	1.626273
H	1.587753	-0.181353	-2.584343	H	5.483224	-1.653792	-1.130946
H	7.440821	-0.995395	1.054553	H	5.020266	-0.757353	-2.557881
Number of Imaginary Frequencies= 0				H	3.392296	-2.637700	-0.909193
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79089759				H	2.956969	-1.993918	-2.488605
Comp_10Z_c09				H	-7.467123	-1.768661	0.025746
B3LYP/6-31G* Geometry				H	-6.155159	-2.395579	1.060318
C	-2.012751	0.598166	1.425391	H	-6.737862	-0.747603	1.306966
C	-1.691354	-1.678237	0.393173	H	-5.035339	4.862174	-0.605164
				H	-5.845644	3.544325	0.289438
				H	-4.565865	4.467619	1.078170

H 0.147682 -1.881567 2.560386
H -0.352054 -0.358991 3.315622
H -1.537116 -1.633352 3.031031
H 4.226501 -0.355366 2.136724
H 2.780264 -1.331595 1.856463
H 4.283669 -1.753859 1.056991
H 6.489664 -0.986546 1.106653
H 7.379857 -0.654192 -0.380611
H 7.646422 0.364014 1.047109
H 2.655794 0.483005 -2.398026
H 5.450794 3.753555 0.046290

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79148086**

Comp_10Z_c10

B3LYP/6-31G* Geometry

C -2.150962 0.589803 1.135787
C -1.671886 -1.771006 0.412262
C -3.432436 -0.388699 -0.822053
C -2.371360 -1.485505 -0.939865
C -2.824747 0.871074 -0.207552
C -1.050308 -0.501366 1.061409
C 0.180602 -0.020168 0.212756
C 1.108584 -1.174437 -0.168769
C 0.720452 -2.465351 -0.134375
C -0.648000 -2.883931 0.212051
C 2.431060 -0.751701 -0.780470
C 3.178384 0.307191 0.077284
C 2.274271 1.546521 0.193154
C 0.923300 1.193595 0.846167
C 4.479385 0.490580 -0.784486
C 4.777920 -0.932541 -1.372092
C 3.513161 -1.791210 -1.094948
O -0.971829 -4.064113 0.250694
O -4.484719 -0.865946 0.050653
C -5.759560 -0.855998 -0.423852
C -6.715459 -1.328537 0.645525
O -6.069625 -0.521900 -1.544194
O -3.894010 1.831764 -0.043906
C -3.549086 3.142218 -0.091223
C -4.768078 4.018820 0.068651
O -2.412671 3.537331 -0.241281
C -0.643232 -0.852618 2.510541
H -2.436898 -2.170170 1.087429
C 3.502066 -0.250440 1.479583
C 5.627090 1.244818 -0.130480
C 5.713558 2.723248 -0.438923
N 6.571020 0.829485 0.635271
H 4.173540 1.117760 -1.626865
O 2.076436 -0.080609 -2.022317
H -0.193523 0.348049 -0.752638
O 6.517875 -0.551250 0.939188
H -2.926204 0.255917 1.835572
H -1.741083 1.523419 1.531706

H -3.879313 -0.162053 -1.792253
H -2.841869 -2.405560 -1.301820
H -1.640835 -1.181592 -1.700965
H -2.107754 1.293938 -0.916746
H 1.393537 -3.269242 -0.421537
H 2.761701 2.319700 0.800990
H 2.108609 1.971899 -0.801378
H 1.087888 1.009102 1.911543
H 0.266075 2.067275 0.781496
H 5.663502 -1.382655 -0.928474
H 4.956145 -0.843353 -2.447722
H 3.667770 -2.457997 -0.241077
H 3.238003 -2.423017 -1.947931
H -6.678870 -0.649044 1.503555
H -7.727449 -1.359590 0.240690
H -6.423396 -2.321582 1.001783
H -4.475369 5.066316 -0.009135
H -5.509538 3.776650 -0.699331
H -5.235246 3.835750 1.042174
H 0.199455 -1.550710 2.544565
H -0.368304 0.038278 3.083592
H -1.485034 -1.324578 3.029832
H 2.607501 -0.620475 1.989260
H 4.232847 -1.058483 1.444938
H 3.935321 0.542200 2.099498
H 4.780754 3.234931 -0.171682
H 6.539999 3.182632 0.107799
H 5.866711 2.882649 -1.514313
H 1.731899 -0.767168 -2.616240
H 7.302313 -0.653982 1.499592

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79062894**

Comp_10Z_c11

B3LYP/6-31G* Geometry

C -2.111491 0.544501 1.167980
C -1.700934 -1.815903 0.404913
C -3.355592 -0.338462 -0.860841
C -2.331292 -1.470466 -0.967021
C -2.729857 0.883124 -0.189137
C -1.051858 -0.587292 1.102734
C 0.222109 -0.130572 0.305586
C 1.093148 -1.305439 -0.134619
C 0.668514 -2.582435 -0.124541
C -0.712152 -2.961917 0.222440
C 2.419965 -0.899952 -0.752016
C 3.225917 0.059525 0.183698
C 2.389873 1.329716 0.398101
C 1.025696 0.991321 1.030653
C 4.543649 0.223013 -0.651615
C 4.807427 -1.213243 -1.210351
C 3.447388 -1.974272 -1.145256
O -1.069727 -4.131945 0.263839
O -4.458867 -0.801802 -0.044072

C	-5.718241	-0.669418	-0.539414	C	-2.151327	0.588691	1.136244
C	-6.728666	-1.143840	0.478255	C	-1.671393	-1.771768	0.412143
O	-5.980287	-0.240095	-1.639428	C	-3.431769	-0.389552	-0.822475
O	-3.774380	1.872193	-0.031761	C	-2.370309	-1.485957	-0.940208
C	-3.392544	3.172764	-0.044090	C	-2.824781	0.870204	-0.207202
C	-4.592506	4.079397	0.092508	C	-1.050403	-0.502209	1.061989
O	-2.241835	3.539342	-0.150740	C	0.180780	-0.020367	0.214076
C	-0.706197	-0.988898	2.554837	C	1.108829	-1.174238	-0.168451
H	-2.506717	-2.196311	1.042295	C	0.721126	-2.465279	-0.134491
C	3.526684	-0.622082	1.537496	C	-0.647153	-2.884364	0.211957
C	5.715866	0.886195	0.048618	C	2.430884	-0.750701	-0.780549
C	6.777920	0.092059	0.770571	C	3.178571	0.307502	0.077738
N	5.923987	2.154889	0.050448	C	2.274163	1.546446	0.195547
H	4.305461	0.891722	-1.486363	C	0.923740	1.192374	0.849049
O	1.979458	-0.206369	-1.946297	C	4.479040	0.491901	-0.784577
H	-0.106244	0.319496	-0.641404	C	4.777387	-0.930550	-1.373831
O	4.937940	2.871504	-0.665292	C	3.512935	-1.789708	-1.096803
H	-2.921361	0.226909	1.835598	O	-0.970582	-4.064662	0.250383
H	-1.677988	1.452750	1.597226	O	-4.484328	-0.867515	0.049546
H	-3.754516	-0.069661	-1.841127	C	-5.759269	-0.855065	-0.424574
H	-2.822016	-2.361582	-1.372242	C	-6.715755	-1.326382	0.644827
H	-1.557755	-1.176545	-1.687857	O	-6.069189	-0.519113	-1.544402
H	-1.976957	1.303279	-0.861758	O	-3.894469	1.830370	-0.043314
H	1.303974	-3.398755	-0.456607	C	-3.550246	3.140978	-0.091216
H	2.924052	2.035960	1.043635	C	-4.769697	4.017008	0.068318
H	2.242892	1.831299	-0.561968	O	-2.414060	3.536598	-0.241582
H	1.182266	0.714178	2.077168	C	-0.643779	-0.853816	2.511151
H	0.412935	1.899179	1.041167	H	-2.436626	-2.171304	1.086836
H	5.559825	-1.742052	-0.620380	C	3.503242	-0.251472	1.479325
H	5.201567	-1.162813	-2.230919	C	5.627027	1.245531	-0.130390
H	3.491360	-2.770422	-0.396477	C	5.713114	2.724325	-0.437203
H	3.169973	-2.437859	-2.096066	N	6.571403	0.829433	0.634393
H	-6.669287	-0.522439	1.378103	H	4.172727	1.119912	-1.626168
H	-7.730465	-1.082496	0.052001	O	2.075323	-0.078476	-2.021499
H	-6.510298	-2.174056	0.777015	H	-0.192994	0.349073	-0.750973
H	-4.269820	5.119797	0.042423	O	6.518670	-0.551695	0.936558
H	-5.314577	3.869698	-0.703007	H	-2.926754	0.254471	1.835681
H	-5.095892	3.892981	1.047155	H	-1.741829	1.522337	1.532510
H	0.116692	-1.710362	2.597559	H	-3.878246	-0.162652	-1.792803
H	-0.429153	-0.122100	3.162782	H	-2.840339	-2.406013	-1.302787
H	-1.577456	-1.453501	3.030400	H	-1.639453	-1.181486	-1.700777
H	4.019647	0.086372	2.212709	H	-2.107796	1.293741	-0.916015
H	2.614648	-0.968201	2.030828	H	1.394359	-3.268870	-0.422175
H	4.180792	-1.492758	1.432827	H	2.761728	2.319111	0.803931
H	6.347141	-0.577565	1.522383	H	2.107654	1.972897	-0.798398
H	7.351737	-0.528979	0.071659	H	1.089210	1.006053	1.913961
H	7.469277	0.778708	1.264562	H	0.266487	2.066185	0.786364
H	2.761430	0.092561	-2.435972	H	5.663317	-1.380981	-0.931230
H	5.261568	3.782170	-0.587410	H	4.954864	-0.840253	-2.449495

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79125960

Comp_10Z_c12
B3LYP/6-31G* Geometry

H -5.509848 3.775791 -0.701245
H -5.238405 3.832280 1.040768
H 0.199270 -1.551478 2.545217
H -0.369529 0.037010 3.084629
H -1.485534 -1.326423 3.029926
H 3.936457 0.540757 2.099783
H 2.609104 -0.622462 1.989053
H 4.234403 -1.059107 1.443428
H 4.780209 3.235510 -0.169411
H 6.539496 3.183303 0.109956
H 5.866210 2.884947 -1.512430
H 1.730989 -0.764566 -2.616085
H 7.303424 -0.654968 1.496417

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79063373

Comp_10Z_c13

B3LYP/6-31G* Geometry

C -2.111909 0.543968 1.168055
C -1.700797 -1.816416 0.405154
C -3.354910 -0.339101 -0.861429
C -2.330447 -1.471013 -0.967102
C -2.729658 0.882567 -0.189381
C -1.052146 -0.587740 1.103335
C 0.222196 -0.130841 0.306910
C 1.093107 -1.305499 -0.134129
C 0.668736 -2.582569 -0.124131
C -0.711775 -2.962329 0.223244
C 2.419547 -0.899435 -0.751975
C 3.226032 0.059341 0.184039
C 2.389890 1.329199 0.400273
C 1.026201 0.989851 1.033344
C 4.543058 0.223789 -0.652185
C 4.806743 -1.212010 -1.212064
C 3.446864 -1.973302 -1.146735
O -1.068992 -4.132423 0.265232
O -4.458602 -0.802532 -0.045264
C -5.717757 -0.668988 -0.540834
C -6.728998 -1.140610 0.477331
O -5.979192 -0.239716 -1.641024
O -3.774427 1.871459 -0.032591
C -3.392653 3.172048 -0.043780
C -4.592740 4.078569 0.092618
O -2.241872 3.538726 -0.149289
C -0.707203 -0.989357 2.555595
H -2.506880 -2.196859 1.042148
C 3.527939 -0.623513 1.536954
C 5.715711 0.886704 0.047597
C 6.778477 0.092239 0.768112
N 5.923594 2.155474 0.050211
H 4.303950 0.893021 -1.486232
O 1.978296 -0.204879 -1.945415
H -0.105707 0.320373 -0.639680
O 4.937046 2.872549 -0.664247

H -2.922096 0.226268 1.835237
H -1.678695 1.452251 1.597490
H -3.753288 -0.070351 -1.841959
H -2.820929 -2.362126 -1.372626
H -1.556568 -1.176995 -1.687522
H -1.976485 1.302796 -0.861685
H 1.304267 -3.398713 -0.456516
H 2.924336 2.034885 1.046204
H 2.242158 1.831714 -0.559200
H 1.183568 0.710869 2.079246
H 0.413457 1.897704 1.045865
H 5.559500 -1.741090 -0.622792
H 5.200388 -1.160859 -2.232789
H 3.491487 -2.770042 -0.398623
H 3.168910 -2.436160 -2.097742
H -6.678556 -0.508145 1.370092
H -7.729374 -1.091275 0.046212
H -6.503979 -2.165414 0.789192
H -4.270312 5.118982 0.041386
H -5.315365 3.867865 -0.702119
H -5.095392 3.892954 1.047828
H 0.115843 -1.710625 2.598711
H -0.430663 -0.122532 3.163732
H -1.578607 -1.454196 3.030665
H 4.020955 0.084476 2.212618
H 2.616365 -0.970634 2.030421
H 4.182447 -1.493723 1.430961
H 6.348464 -0.578263 1.519564
H 7.352035 -0.527975 0.068218
H 7.470000 0.778629 1.262227
H 2.759983 0.092841 -2.436269
H 5.260516 3.783232 -0.585840

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1554.79126269

Comp_10Z_c14

B3LYP/6-31G* Geometry

C -2.118046 0.514423 1.184835
C -1.710207 -1.837224 0.390470
C -3.349325 -0.331669 -0.866682
C -2.330467 -1.467994 -0.979742
C -2.717230 0.875083 -0.175419
C -1.065115 -0.623874 1.118122
C 0.224692 -0.159998 0.349877
C 1.095142 -1.326637 -0.118889
C 0.661512 -2.601326 -0.135343
C -0.722079 -2.982414 0.194465
C 2.424612 -0.910247 -0.729197
C 3.236646 0.041003 0.202120
C 2.392798 1.294809 0.491946
C 1.036969 0.921037 1.123864
C 4.523238 0.235826 -0.671150
C 4.793571 -1.194210 -1.238029
C 3.447547 -1.972810 -1.144330

O -1.084422 -4.151397 0.217500
 O -4.461674 -0.797772 -0.065281
 C -5.718210 -0.619749 -0.556236
 C -6.740117 -1.103027 0.445292
 O -5.968100 -0.148228 -1.641455
 O -3.745619 1.879517 -0.018067
 C -3.343531 3.174176 -0.048180
 C -4.527004 4.101571 0.086899
 O -2.187395 3.519671 -0.168741
 C -0.741241 -1.050105 2.568067
 H -2.521228 -2.227049 1.015201
 C 3.579859 -0.665399 1.533791
 C 5.695494 0.923146 0.002308
 C 6.812868 0.150940 0.661630
 N 5.859537 2.198142 0.031376
 H 4.232088 0.876648 -1.506162
 O 2.094864 -0.252069 -1.979900
 H -0.106906 0.328225 -0.579353
 O 4.817622 2.897785 -0.624394
 H -2.938169 0.193418 1.837873
 H -1.685342 1.414531 1.632286
 H -3.738018 -0.046683 -1.846595
 H -2.822186 -2.351224 -1.400469
 H -1.550649 -1.169359 -1.692159
 H -1.951818 1.291316 -0.836302
 H 1.298625 -3.413888 -0.473396
 H 2.934494 1.968602 1.164291
 H 2.245632 1.884004 -0.423360
 H 1.215643 0.579080 2.146589
 H 0.425371 1.826272 1.202632
 H 5.569872 -1.717425 -0.673067
 H 5.147249 -1.128578 -2.270708
 H 3.505944 -2.773100 -0.401077
 H 3.155739 -2.424124 -2.095805
 H -6.671516 -0.507682 1.362004
 H -7.739316 -1.010316 0.018679
 H -6.542408 -2.144990 0.716211
 H -4.187563 5.135993 0.025748
 H -5.256337 3.896503 -0.703218
 H -5.028637 3.931669 1.045487
 H 0.080630 -1.772636 2.610355
 H -0.473263 -0.193712 3.194757
 H -1.619967 -1.521913 3.021991
 H 4.065933 0.039619 2.217513
 H 2.688897 -1.053415 2.035847
 H 4.258015 -1.511215 1.392330
 H 6.436385 -0.548157 1.416349
 H 7.372825 -0.438358 -0.074893
 H 7.504036 0.848487 1.140504
 H 1.780436 0.645335 -1.791494
 H 5.122288 3.815070 -0.548448
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1554.79227189**

Comp_10Z_c15
B3LYP/6-31G* Geometry
 C -2.030663 0.323572 1.380983
 C -1.591244 -1.872318 0.235161
 C -3.290628 -0.247928 -0.752682
 C -2.243921 -1.319326 -1.055849
 C -2.679011 0.863804 0.107530
 C -0.955228 -0.767382 1.126994
 C 0.313529 -0.167128 0.421353
 C 1.181885 -1.223870 -0.265579
 C 0.773915 -2.491065 -0.465834
 C -0.587040 -2.953754 -0.146779
 C 2.484146 -0.685514 -0.839342
 C 3.323918 0.084845 0.224583
 C 2.483935 1.255539 0.764837
 C 1.150009 0.757917 1.357033
 C 4.579676 0.453526 -0.637236
 C 4.834646 -0.841214 -1.472928
 C 3.497451 -1.640503 -1.478408
 O -0.921017 -4.124177 -0.275114
 O -4.365765 -0.890186 -0.020259
 C -5.637953 -0.489315 -0.266394
 C -6.607214 -1.268145 0.591238
 O -5.944961 0.367097 -1.066540
 O -3.702587 1.797478 0.510716
 C -3.984280 2.807520 -0.359565
 C -5.195554 3.579515 0.095089
 O -3.347345 3.021735 -1.366668
 C -0.600560 -1.403017 2.490466
 H -2.382650 -2.368043 0.807413
 C 3.715499 -0.850808 1.391360
 C 5.772238 1.011186 0.116328
 C 6.914610 0.139054 0.579659
 N 5.932672 2.258590 0.384126
 H 4.260017 1.238351 -1.326018
 O 2.109312 0.187337 -1.934629
 H -0.044196 0.475992 -0.397288
 O 4.866035 3.061115 -0.089308
 H -2.821765 -0.108589 2.005331
 H -1.609232 1.160552 1.948737
 H -3.707273 0.177674 -1.667677
 H -2.716145 -2.143775 -1.600190
 H -1.486757 -0.889959 -1.723910
 H -1.960828 1.404129 -0.515612
 H 1.413667 -3.224571 -0.948550
 H 3.042107 1.801138 1.533246
 H 2.306000 1.999044 -0.023749
 H 1.363108 0.231050 2.290656
 H 0.539408 1.625146 1.632624
 H 5.634823 -1.451416 -1.045474
 H 5.147675 -0.577474 -2.486872
 H 3.587883 -2.562356 -0.897043
 H 3.173473 -1.913222 -2.485764
 H -6.421148 -1.054144 1.649199
 H -7.628516 -0.986656 0.332902

H -6.464623 -2.343400 0.445063
H -5.224987 4.545999 -0.409956
H -6.085437 3.001853 -0.180008
H -5.197889 3.710454 1.180454
H 0.238019 -2.103387 2.412936
H -0.343235 -0.647446 3.239353
H -1.461507 -1.960588 2.875380
H 4.212717 -0.276087 2.180885
H 2.846186 -1.343898 1.835247
H 4.400131 -1.642793 1.076056
H 7.452345 -0.292682 -0.273387
H 7.618400 0.739897 1.160389
H 6.566569 -0.695042 1.198647
H 1.768018 1.019702 -1.574059
H 5.174585 3.950053 0.144451

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1554.79225366

Comp_10Z_c16

B3LYP/6-31G* Geometry

C -2.118005 0.514691 1.184928
C -1.710321 -1.837004 0.390566
C -3.349403 -0.331386 -0.866535
C -2.330553 -1.467727 -0.979648
C -2.717233 0.875337 -0.175315
C -1.065167 -0.623691 1.118240
C 0.224695 -0.159882 0.350034
C 1.095038 -1.326545 -0.118880
C 0.661345 -2.601209 -0.135313
C -0.722248 -2.982234 0.194583
C 2.424511 -0.910200 -0.729224
C 3.236697 0.040868 0.202136
C 2.392940 1.294694 0.492168
C 1.037136 0.920926 1.124160
C 4.523219 0.235704 -0.671234
C 4.793404 -1.194272 -1.238295
C 3.447331 -1.972809 -1.144541
O -1.084610 -4.151210 0.217737
O -4.461731 -0.797418 -0.065061
C -5.718221 -0.620252 -0.556385
C -6.740171 -1.103394 0.445175
O -5.968082 -0.149450 -1.641930
O -3.745541 1.879839 -0.017915
C -3.343400 3.174473 -0.048336
C -4.526789 4.101960 0.086890
O -2.187276 3.519882 -0.169248
C -0.741357 -1.049959 2.568187
H -2.521374 -2.226783 1.015283
C 3.579999 -0.665725 1.533688
C 5.695598 0.922880 0.002191
C 6.813025 0.150531 0.661254
N 5.859700 2.197865 0.031419
H 4.232031 0.876655 -1.506135
O 2.094808 -0.251835 -1.979834

H -0.106879 0.328532 -0.579106
O 4.817767 2.897643 -0.624125
H -2.938127 0.193808 1.838028
H -1.685200 1.414796 1.632295
H -3.738141 -0.046408 -1.846433
H -2.822284 -2.350930 -1.400416
H -1.550727 -1.169079 -1.692051
H -1.951827 1.291498 -0.836252
H 1.298388 -3.413814 -0.473399
H 2.934716 1.968388 1.164543
H 2.245719 1.883959 -0.423080
H 1.215879 0.578750 2.146795
H 0.425638 1.826207 1.203171
H 5.569729 -1.717612 -0.673481
H 5.146957 -1.128562 -2.271011
H 3.505755 -2.773153 -0.401351
H 3.155413 -2.424008 -2.096033
H -7.739282 -1.011603 0.018156
H -6.541926 -2.145023 0.716978
H -6.672248 -0.507287 1.361445
H -4.187327 5.136350 0.025299
H -5.256441 3.896683 -0.702876
H -5.028055 3.932377 1.045728
H 0.080464 -1.772548 2.610488
H -0.473331 -0.193591 3.194889
H -1.620127 -1.521713 3.022082
H 4.066151 0.039196 2.217455
H 2.689081 -1.053801 2.035772
H 4.258130 -1.511533 1.392054
H 7.372916 -0.438618 -0.075439
H 7.504244 0.847971 1.140210
H 6.436612 -0.548725 1.415861
H 1.780026 0.645414 -1.791284
H 5.122465 3.814910 -0.548082

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1554.79227345

Comp_11E_c01

B3LYP/6-31G* Geometry

N 0.007377 3.677784 0.042019
C 0.070262 2.466987 -0.370550
C -1.190342 0.393126 0.238237
C 1.303573 0.375706 0.226333
N 0.053812 -0.388492 0.007621
C 1.312719 1.666358 -0.623310
C -1.217166 1.711731 -0.599158
C 2.536041 -0.449733 -0.120221
C 4.870409 -1.861954 -0.802008
C 2.629718 -1.126227 -1.345297
C 3.624765 -0.494946 0.756981
C 4.786582 -1.192767 0.419025
C 3.785572 -1.829314 -1.682318
C -2.410337 -0.459347 -0.091277
C -4.693654 -1.975383 -0.726096

C -3.433480 -0.637226 0.846505
C -2.542647 -1.059973 -1.352080
C -3.673601 -1.812023 -1.667250
C -4.569560 -1.386964 0.532485
C 0.052266 -1.632589 0.807544
O 1.286232 4.252671 0.224919
H -0.823281 -2.221557 0.520963
H 0.933102 -2.216157 0.524986
C 0.048888 -1.439263 2.270582
C 0.045242 -1.258970 3.465889
H -1.256789 0.690975 1.299844
H 1.382727 0.678094 1.285259
H 2.210110 2.242868 -0.396890
H -1.218863 1.407403 -1.657150
H 5.771971 -2.408516 -1.065755
H 1.780775 -1.110971 -2.023486
H 3.560704 0.018227 1.713695
H 5.622386 -1.216936 1.113435
H 3.840838 -2.352275 -2.633750
H -5.575505 -2.561065 -0.971926
H -3.336224 -0.189390 1.832408
H -1.742023 -0.949533 -2.078306
H -3.759340 -2.272530 -2.648218
H -5.353559 -1.514240 1.274447
H 1.056627 5.144689 0.527053
H 0.044257 -1.113895 4.522417
H 1.348486 1.386741 -1.684562
C -2.474972 2.542362 -0.323822
H -2.450811 3.468968 -0.903359
H -2.540563 2.821914 0.732968
H -3.374856 1.983229 -0.592079

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -997.917142152**

Comp_11E_c02
B3LYP/6-31G* Geometry
N 0.037417 3.824709 -0.122202
C 0.094222 2.576247 -0.402997
C -1.174519 0.580421 0.417074
C 1.308646 0.548168 0.411853
N 0.060099 -0.227315 0.252995
C 1.333402 1.747468 -0.562606
C -1.197657 1.808081 -0.550535
C 2.552161 -0.298402 0.173983
C 4.919465 -1.726817 -0.331788
C 2.642471 -1.159973 -0.927838
C 3.661074 -0.165169 1.017898
C 4.839050 -0.871876 0.767725
C 3.816307 -1.870135 -1.176663
C -2.414999 -0.276369 0.196231
C -4.757463 -1.764742 -0.259714
C -3.451886 -0.284848 1.136499
C -2.563335 -1.033474 -0.974107
C -3.725357 -1.769356 -1.201194

C -4.616621 -1.022344 0.912768
C 0.050730 -1.412497 1.154241
O 1.319067 4.408871 0.001773
H 0.957019 -1.409578 1.771652
H -0.790735 -1.346593 1.855547
C -0.024260 -2.697883 0.449590
C -0.078032 -3.778740 -0.085803
H -1.224248 0.990508 1.445577
H 1.372847 0.961767 1.437569
H 2.232632 2.338839 -0.387980
H -1.202642 1.390865 -1.569035
H 5.833319 -2.281734 -0.527086
H 1.779188 -1.284251 -1.573956
H 3.602508 0.500211 1.876893
H 5.689883 -0.756707 1.434192
H 3.868895 -2.540164 -2.030919
H -5.661831 -2.340795 -0.437025
H -3.348777 0.295566 2.050871
H -1.751845 -1.058925 -1.694860
H -3.823084 -2.353774 -2.112415
H -5.410380 -1.016388 1.655217
H 1.093915 5.330183 0.202335
H -0.130438 -4.725112 -0.573833
H 1.376808 1.357070 -1.587803
C -2.449223 2.672715 -0.365577
H -2.414897 3.533731 -1.038137
H -2.514567 3.062422 0.655884
H -3.353759 2.097273 -0.576654

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -997.909794266**

Comp_11E_c03
B3LYP/6-31G* Geometry
N -1.125705 3.239875 0.230812
C -0.542484 2.154723 0.584103
C -1.206171 -0.281518 0.784189
C 1.215729 0.322399 0.541326
N 0.081521 -0.505295 0.077687
C 0.886184 1.805909 0.268588
C -1.359941 1.164135 1.369254
C 2.518402 -0.036554 -0.164097
C 4.958182 -0.602900 -1.445705
C 3.664205 -0.335134 0.579889
C 2.610105 -0.030333 -1.564389
C 3.817366 -0.315204 -2.200184
C 4.878235 -0.611555 -0.053663
C -2.373215 -0.615843 -0.140919
C -4.595759 -1.147735 -1.781582
C -3.479273 -1.316351 0.356146
C -2.391831 -0.191694 -1.476257
C -3.494538 -0.454243 -2.289139
C -4.584582 -1.580215 -0.455027
C 0.369110 -1.948015 0.017696
O -0.234716 4.097708 -0.458730

H -0.510465 -2.438659 -0.414735
H 1.196850 -2.115521 -0.676833
C 0.689805 -2.575916 1.315080
C 0.954668 -3.059562 2.390890
H -1.266953 -0.963912 1.647818
H 1.387977 0.177572 1.620876
H 1.571873 2.449936 0.835419
H -2.409063 1.454617 1.265811
H 5.900389 -0.821027 -1.941409
H 3.604919 -0.355290 1.665382
H 1.723130 0.186026 -2.154109
H 3.869420 -0.310593 -3.285914
H 5.758149 -0.838635 0.542549
H -5.452825 -1.354323 -2.417227
H -3.473354 -1.662475 1.387941
H -1.529144 0.332702 -1.874488
H -3.493595 -0.117737 -3.322910
H -5.431527 -2.129776 -0.052146
H -0.815470 4.837513 -0.694235
H 1.190501 -3.503244 3.331562
H 1.067253 2.041475 -0.785387
C -1.015336 1.231686 2.873933
H -1.195428 2.243107 3.253027
H 0.027967 0.972193 3.080179
H -1.646756 0.535850 3.438397

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -997.910856154**

Comp_11Z_c01

B3LYP/6-31G* Geometry

N -1.144377 2.402438 -2.281562
C -0.776833 1.665871 -1.300154
C -1.159364 0.245184 0.786868
C 1.177149 0.588494 -0.140599
N 0.254723 -0.191553 0.699703
C 0.487549 0.865896 -1.489386
C -1.481641 1.573669 0.034890
C 2.494755 -0.145971 -0.366190
C 4.947972 -1.431877 -0.866207
C 3.708485 0.505239 -0.119099
C 2.527790 -1.456785 -0.863250
C 3.742650 -2.095093 -1.110241
C 4.927450 -0.129028 -0.368942
C -2.127987 -0.877467 0.387456
C -3.989641 -2.872709 -0.319278
C -3.471080 -0.785370 0.784557
C -1.733019 -1.994108 -0.353596
C -2.655510 -2.982111 -0.708511
C -4.394731 -1.768163 0.434642
C 0.795813 -0.597822 1.999228
O -2.344079 3.100942 -1.995515
H 0.094512 -1.314038 2.444791
H 1.730625 -1.143537 1.833637
C 1.042972 0.503595 2.951914

C 1.243606 1.422902 3.710803
H -1.373368 0.471781 1.840947
H 1.429887 1.556968 0.324889
H 1.166626 1.389997 -2.167755
H -2.557251 1.584517 -0.165333
H 5.894578 -1.929752 -1.058817
H 3.698174 1.518472 0.276222
H 1.594944 -1.981541 -1.047817
H 3.749020 -3.112209 -1.493730
H 5.858837 0.394305 -0.169122
H -4.706772 -3.642222 -0.592530
H -3.796980 0.065838 1.380101
H -0.690553 -2.091002 -0.635246
H -2.326049 -3.841226 -1.287759
H -5.429264 -1.675744 0.755443
H -2.496424 3.576199 -2.826575
H 1.422093 2.225920 4.389603
H 0.246843 -0.099453 -1.954591
C -1.174032 2.824564 0.891820
H -1.428489 3.728701 0.332743
H -0.122271 2.875887 1.187575
H -1.772617 2.804952 1.810104

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -997.907434878**

Comp_11Z_c02

B3LYP/6-31G* Geometry

N 1.691176 -2.916622 -1.319086
C 1.195319 -1.972774 -0.609745
C 1.200378 0.008946 0.910280
C -0.991734 -0.987205 0.147011
N -0.283971 -0.001739 0.983799
C -0.121966 -1.390066 -1.061419
C 1.806052 -1.389412 0.649013
C -2.347597 -0.463561 -0.317128
C -4.830282 0.440427 -1.275580
C -3.466285 -1.304888 -0.308180
C -2.488123 0.841280 -0.807726
C -3.720358 1.288917 -1.284003
C -4.700548 -0.859388 -0.785236
C 1.682528 1.095874 -0.070987
C 2.542452 3.200881 -1.748238
C 1.116786 2.378088 0.025610
C 2.690826 0.893618 -1.022824
C 3.112718 1.934854 -1.856341
C 1.541332 3.418486 -0.798029
C -0.873772 0.058296 2.326543
O 2.944224 -3.345725 -0.809740
H -1.959578 0.146785 2.193433
H -0.713293 -0.871319 2.905975
C -0.411084 1.193563 3.128788
C -0.036123 2.113016 3.816078
H 1.545357 0.326441 1.901177
H -1.183959 -1.912067 0.724375

H -0.658181 -2.109301 -1.685913
H 2.885174 -1.288876 0.496452
H -5.790236 0.792130 -1.644426
H -3.370096 -2.318695 0.076292
H -1.626706 1.502577 -0.802157
H -3.815323 2.304141 -1.660917
H -5.559441 -1.525370 -0.767669
H 2.871952 4.009584 -2.395280
H 0.336501 2.552772 0.759388
H 3.155927 -0.079412 -1.141682
H 3.890528 1.746878 -2.592126
H 1.089325 4.402294 -0.697838
H 3.190732 -4.032219 -1.448430
H 0.291468 2.932015 4.415517
H 0.058170 -0.497932 -1.674842
C 1.628972 -2.350312 1.845929
H 2.131257 -3.297763 1.635310
H 0.576622 -2.564269 2.055840
H 2.072627 -1.915924 2.749570

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -997.905950546**

Comp_11Z_c03
B3LYP/6-31G* Geometry
N -1.082573 3.109314 0.025210
C -0.424251 2.159276 -0.526634
C 1.259769 0.290651 -0.754099
C -1.190084 -0.120874 -1.180000
N 0.090446 -0.606614 -0.597102
C -1.100549 1.371228 -1.602569
C 0.969067 1.702494 -0.162098
C -2.373748 -0.333605 -0.238774
C -4.620988 -0.602413 1.431309
C -3.650050 -0.531499 -0.780716
C -2.238050 -0.274887 1.151107
C -3.352872 -0.408210 1.980389
C -4.766583 -0.664880 0.043854
C 2.497016 -0.290128 -0.076482
C 4.807028 -1.277052 1.192602
C 2.462595 -0.679406 1.271299
C 3.703318 -0.408799 -0.775968
C 4.852741 -0.894726 -0.147649
C 3.605890 -1.170704 1.899206
C 0.392685 -1.965942 -1.080179
O -0.337454 3.728144 1.059152
H 0.550963 -1.968941 -2.178039
H 1.337543 -2.287360 -0.633594
C -0.631337 -2.962083 -0.756013
C -1.437597 -3.829225 -0.522858
H 1.510223 0.418335 -1.825819
H -1.399800 -0.685845 -2.102424
H -0.517337 1.445334 -2.531402
H 1.019116 1.636326 0.931166
H -5.488026 -0.709507 2.078044

H -3.769784 -0.589931 -1.861334
H -1.249369 -0.144806 1.577914
H -3.228518 -0.363273 3.059573
H -5.747875 -0.824187 -0.396155
H 5.698131 -1.658914 1.683560
H 1.526884 -0.612987 1.819105
H 3.743730 -0.118385 -1.823515
H 5.779962 -0.977457 -0.708606
H 3.559869 -1.472370 2.942393
H -0.971138 4.381340 1.393303
H -2.170239 -4.569815 -0.295723
H -2.100420 1.763254 -1.800659
C 2.021412 2.729912 -0.627079
H 1.820766 3.701165 -0.170522
H 1.999184 2.849592 -1.717358
H 3.028189 2.409604 -0.341768

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -997.906946032**

Comp_11Z_c04
B3LYP/6-31G* Geometry
N -1.152168 3.222476 -1.063751
C -0.819730 2.147060 -0.453208
C -1.176925 0.020669 0.858981
C 1.161600 0.799367 0.283091
N 0.287805 -0.216557 0.890292
C 0.442728 1.462073 -0.909897
C -1.566074 1.520384 0.704982
C 2.507574 0.225677 -0.162293
C 4.995211 -0.715864 -1.084586
C 2.679657 -1.121586 -0.500904
C 3.604451 1.090649 -0.280509
C 4.836270 0.628917 -0.742406
C 3.914393 -1.588626 -0.957343
C -1.913747 -0.863594 -0.159561
C -3.368240 -2.471666 -1.965707
C -3.315037 -0.929679 -0.104445
C -1.257242 -1.632947 -1.123939
C -1.976498 -2.425105 -2.023072
C -4.036803 -1.721601 -0.995306
C 0.788433 -0.647994 2.202505
O -2.359261 3.762546 -0.553588
H 1.874169 -0.771771 2.118338
H 0.625336 0.119321 2.983431
C 0.206540 -1.916069 2.652402
C -0.272347 -2.951522 3.046944
H -1.558313 -0.286330 1.840088
H 1.389745 1.605012 1.007934
H 1.104062 2.180735 -1.400345
H -2.634535 1.575260 0.473585
H 5.955458 -1.080309 -1.439706
H 1.846564 -1.806365 -0.381359
H 3.490347 2.138320 -0.007773
H 5.673551 1.316792 -0.827564

H 4.030045 -2.639394 -1.210578
H -3.927481 -3.089883 -2.662957
H -3.851662 -0.362317 0.653616
H -0.174815 -1.620304 -1.161367
H -1.441836 -3.011432 -2.766299
H -5.121285 -1.756418 -0.928776
H -2.485427 4.535363 -1.125108
H -0.693394 -3.873881 3.377268
H 0.202322 0.686392 -1.648231
C -1.346979 2.326498 2.005642
H -1.669794 3.360593 1.861425
H -0.297242 2.337200 2.316272
H -1.934604 1.891364 2.822788

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -997.905432669

Comp_11Z_c05

B3LYP/6-31G* Geometry

N 1.691469 -2.916457 -1.318997
C 1.195400 -1.972752 -0.609627
C 1.200200 0.008868 0.910480
C -0.991783 -0.987274 0.146826
N -0.284161 -0.001735 0.983717
C -0.121824 -1.390068 -1.061494
C 1.805838 -1.389527 0.649352
C -2.347611 -0.463671 -0.317398
C -4.830221 0.440478 -1.275900
C -2.487906 0.841016 -0.808580
C -3.466471 -1.304714 -0.307939
C -4.700728 -0.859124 -0.785005
C -3.720076 1.288722 -1.284875
C 1.682620 1.095712 -0.070780
C 2.543110 3.200645 -1.747842
C 2.691310 0.893434 -1.022200
C 1.116791 2.377916 0.025505
C 1.541607 3.418270 -0.798045
C 3.113477 1.934637 -1.855620
C -0.874092 0.058393 2.326399
O 2.944483 -3.345398 -0.809471
H -1.959912 0.146545 2.193188
H -0.713383 -0.871050 2.906036
C -0.411802 1.193978 3.128436
C -0.037220 2.113712 3.815558
H 1.545016 0.326416 1.901424
H -1.183987 -1.912162 0.724146
H -0.657947 -2.109300 -1.686076
H 2.885001 -1.289041 0.497108
H -5.790135 0.792271 -1.644765
H -1.626345 1.502130 -0.803396
H -3.370463 -2.318394 0.076914
H -5.559760 -1.524913 -0.766999
H -3.814899 2.303788 -1.662247
H 2.872841 4.009320 -2.394800
H 3.156504 -0.079572 -1.140851

H 0.336207 2.552591 0.758963
H 1.089505 4.402062 -0.698109
H 3.891591 1.746636 -2.591078
H 3.191176 -4.031799 -1.448188
H 0.290264 2.932931 4.414754
H 0.058385 -0.497919 -1.674875
C 1.628460 -2.350535 1.846136
H 2.130742 -3.297980 1.635475
H 0.576072 -2.564459 2.055880
H 2.072014 -1.916281 2.749894

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -997.905950408

Comp_11Z_c06

B3LYP/6-31G* Geometry

N -1.863113 -2.041924 -1.816122
C -1.903219 -1.027159 -1.033531
C -1.104024 -0.102112 1.177306
C -0.664687 1.178742 -0.939605
N -0.904676 1.209859 0.520458
C -1.740480 0.330093 -1.664462
C -2.122512 -1.048790 0.463321
C 0.788068 0.841494 -1.291742
C 3.489980 0.444483 -1.982992
C 1.799444 1.636654 -0.731070
C 1.152944 -0.153313 -2.205359
C 2.494976 -0.351226 -2.545736
C 3.135255 1.442416 -1.070744
C 0.246620 -0.763141 1.497516
C 2.716766 -1.877947 2.272519
C 1.103621 -0.083052 2.376414
C 0.649703 -2.012103 1.013304
C 1.877840 -2.561609 1.396026
C 2.323089 -0.630033 2.763814
C -1.830691 2.271434 0.934100
O -2.046484 -3.263511 -1.117763
H -2.801408 2.250706 0.404076
H -2.064839 2.119676 1.994291
C -1.251755 3.611557 0.766756
C -0.797709 4.720457 0.616293
H -1.546520 0.133549 2.153162
H -0.807727 2.213966 -1.271103
H -2.694085 0.869867 -1.578747
H -1.959339 -2.063852 0.827302
H 4.532512 0.290284 -2.249309
H 1.524243 2.408791 -0.018245
H 0.400992 -0.796952 -2.648709
H 2.756942 -1.134199 -3.253066
H 3.902314 2.070615 -0.624620
H 3.668483 -2.309670 2.571186
H 0.808170 0.894726 2.748777
H 0.020186 -2.572889 0.330179
H 2.174090 -3.530523 1.002157
H 2.966997 -0.084686 3.449323

H -1.944316 -3.912683 -1.830731
H -0.387710 5.697165 0.492148
H -1.532157 0.232007 -2.732680
C -3.591402 -0.697676 0.789992
H -4.262256 -1.438593 0.343026
H -3.887009 0.287759 0.416147
H -3.752130 -0.707549 1.874460

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -997.899419349

Comp_11Z_c07

B3LYP/6-31G* Geometry

N -1.019109 3.063941 0.750553
C -0.422992 2.266333 -0.055281
C 1.179563 0.457710 -0.754132
C -1.246365 0.191384 -1.216551
N -0.035551 -0.373713 -0.585856
C -1.195295 1.748388 -1.228467
C 1.001284 1.775605 0.059477
C -2.515475 -0.308452 -0.536107
C -4.922090 -1.103794 0.678882
C -3.632123 -0.642582 -1.311595
C -2.616249 -0.384856 0.858575
C -3.811262 -0.778037 1.460404
C -4.829172 -1.037166 -0.711701
C 2.450239 -0.249021 -0.304110
C 4.849399 -1.453885 0.540546
C 3.554385 -0.327961 -1.161827
C 2.564318 -0.788551 0.986100
C 3.751868 -1.387695 1.402704
C 4.747914 -0.921898 -0.744441
C 0.112181 -1.807758 -0.919677
O -0.164970 3.466177 1.808197
H -0.623968 -2.081883 -1.688244
H 1.096334 -1.992148 -1.366249
C -0.059608 -2.709770 0.227475
C -0.193467 -3.485211 1.143281
H 1.322487 0.724927 -1.819248
H -1.299184 -0.124202 -2.276120
H -0.691085 2.077382 -2.148294
H 1.184613 1.549398 1.115432
H -5.850915 -1.414006 1.150554
H -3.564023 -0.595012 -2.397080
H -1.747036 -0.151227 1.463734
H -3.874085 -0.834491 2.544195
H -5.684216 -1.297590 -1.330366
H 5.774800 -1.919954 0.868350
H 3.479757 0.082099 -2.166639
H 1.710597 -0.755201 1.655750
H 3.820032 -1.806261 2.403347
H 5.593769 -0.969859 -1.425256
H -0.756377 4.024380 2.335897
H -0.322662 -4.156723 1.961201
H -2.206152 2.160777 -1.240389

C 1.998697 2.864793 -0.379320
H 1.880526 3.753576 0.244928
H 1.836132 3.154062 -1.425095
H 3.028535 2.505495 -0.284264

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -997.905304103

Comp_11Z_c08

B3LYP/6-31G* Geometry

N -0.798682 -3.164677 0.535612
C -1.222229 -2.042792 0.081896
C -1.281160 0.466997 0.452679
C -0.418438 -0.463504 -1.713111
N -1.085377 0.650800 -1.007748
C -1.102987 -1.818703 -1.401538
C -1.854157 -0.924441 0.880267
C 1.104539 -0.442079 -1.530716
C 3.916916 -0.314147 -1.410058
C 1.859343 -1.578782 -1.220168
C 1.783252 0.760061 -1.780678
C 3.172272 0.826844 -1.721434
C 3.254904 -1.513306 -1.158123
C -0.020667 0.883869 1.224790
C 2.223558 1.830285 2.641726
C 0.761578 0.010994 1.988541
C 0.338937 2.239908 1.185852
C 1.445865 2.711877 1.885874
C 1.877487 0.481787 2.687694
C -2.244730 1.176462 -1.744877
O -0.972472 -3.272520 1.939201
H -1.921166 1.335377 -2.781765
H -3.100985 0.478810 -1.801259
C -2.733620 2.455097 -1.218723
C -3.164811 3.504427 -0.804754
H -2.041124 1.206106 0.726472
H -0.586385 -0.272656 -2.781362
H -2.112426 -1.781308 -1.834486
H -1.618709 -1.073703 1.934901
H 5.001668 -0.264843 -1.361902
H 1.371542 -2.522207 -1.001220
H 1.205333 1.651899 -2.004455
H 3.675663 1.770469 -1.916167
H 3.820783 -2.407283 -0.908127
H 3.089014 2.193775 3.189840
H 0.517428 -1.044795 2.048146
H -0.261035 2.924763 0.591791
H 1.701432 3.767951 1.845244
H 2.475558 -0.214895 3.269696
H -0.571459 -4.136667 2.119703
H -3.537231 4.434844 -0.439810
H -0.589785 -2.658692 -1.875857
C -3.394207 -1.005021 0.764030
H -3.751405 -1.948078 1.190729
H -3.746852 -0.953969 -0.271121

H -3.861530 -0.182600 1.317315
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -997.898851312

Comp_11Z_c09
B3LYP/6-31G* Geometry
N -1.218554 -3.146755 0.035905
C -1.410790 -1.962489 -0.418696
C -1.418940 0.490577 0.188339
C -0.073465 -0.321946 -1.835739
N -0.913398 0.705821 -1.186631
C -0.834740 -1.665846 -1.779173
C -2.195023 -0.855095 0.249437
C 1.407012 -0.404670 -1.424902
C 4.157211 -0.491948 -0.784001
C 1.916891 -1.388527 -0.566191
C 2.312889 0.515735 -1.975532
C 3.670047 0.483011 -1.654852
C 3.275572 -1.431164 -0.248933
C -0.422316 0.700189 1.341183
C 1.358197 1.217705 3.472939
C -0.116519 2.014940 1.731175
C 0.159686 -0.349272 2.066319
C 1.040186 -0.093461 3.119107
C 0.770130 2.274028 2.776709
C -0.531061 2.077834 -1.515901
O -1.830588 -3.342524 1.300457
H 0.362796 2.425284 -0.968850
H -0.260172 2.093302 -2.580030
C -1.615959 3.046896 -1.309558
C -2.480711 3.873880 -1.145278
H -2.173684 1.275754 0.313457
H -0.059524 -0.026612 -2.893889
H -1.669188 -1.588389 -2.488316
H -2.344643 -1.118614 1.297783
H 5.214521 -0.526727 -0.534984
H 1.255607 -2.139279 -0.148349
H 1.957195 1.259950 -2.684365
H 4.346734 1.210074 -2.096607
H 3.644928 -2.206365 0.417671
H 2.044129 1.414387 4.292788
H -0.600422 2.847830 1.226936
H -0.088772 -1.379363 1.834725
H 1.473953 -0.925744 3.667842
H 0.988007 3.301869 3.055972
H -1.569832 -4.254131 1.503173
H -3.253608 4.596456 -1.011379
H -0.200732 -2.494158 -2.105515
C -3.584260 -0.715807 -0.410228
H -4.100936 -1.680792 -0.439749
H -3.499725 -0.327601 -1.429695
H -4.202485 -0.017830 0.165446
Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-
31+G**) = -997.900299812

Comp_11Z_c10
B3LYP/6-31G* Geometry
N 2.557833 -0.175395 -2.169147
C 1.958697 -0.794361 -1.218531
C 1.080890 -0.561738 1.137557
C -0.445748 -1.466967 -0.708315
N 0.009568 -1.480665 0.699595
C 0.792101 -1.662761 -1.611794
C 2.337265 -0.775927 0.246574
C -1.387236 -0.331021 -1.136769
C -3.227064 1.664827 -1.914554
C -2.752071 -0.439057 -0.822789
C -0.969874 0.786303 -1.873557
C -1.879191 1.773106 -2.257778
C -3.662030 0.550323 -1.196716
C 0.703659 0.917011 1.349596
C -0.004599 3.603791 1.871665
C -0.017167 1.271412 2.501567
C 1.089093 1.947756 0.480713
C 0.737748 3.274361 0.738101
C -0.377450 2.593893 2.758985
C -1.034669 -1.714669 1.694589
O 3.664006 0.582560 -1.704062
H -0.547166 -1.761603 2.677175
H -1.771199 -0.894519 1.756425
C -1.755479 -2.978262 1.483500
C -2.374797 -4.004428 1.334586
H 1.357393 -0.932543 2.134496
H -1.038364 -2.383819 -0.802718
H 1.101281 -2.710870 -1.505493
H 3.029433 0.049985 0.418360
H -3.933377 2.434590 -2.214489
H -3.111030 -1.322348 -0.299560
H 0.069624 0.886471 -2.165751
H -1.530652 2.627881 -2.832041
H -4.712741 0.441262 -0.939779
H -0.276978 4.637125 2.069460
H -0.284370 0.505319 3.225016
H 1.688351 1.730625 -0.396610
H 1.052580 4.053495 0.048441
H -0.936463 2.835021 3.659560
H 3.975007 0.994913 -2.524652
H -2.907573 -4.919402 1.206477
H 0.543362 -1.498833 -2.663353
C 3.058406 -2.087837 0.624829
H 3.897920 -2.279178 -0.051455
H 2.372649 -2.939560 0.587053
H 3.455551 -2.016600 1.644046
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -997.900447380

Comp_11Z_c11**B3LYP/6-31G* Geometry**

N -1.223119 0.668677 2.808256
 C -1.481916 0.397308 1.581764
 C -0.892522 0.910088 -0.832348
 C -0.789232 -1.463637 0.030336
 N -0.981845 -0.540981 -1.100579
 C -1.674245 -1.053368 1.233223
 C -1.638748 1.394045 0.454351
 C 0.694889 -1.689916 0.357902
 C 3.406823 -2.287752 0.847232
 C 1.207505 -1.677017 1.660164
 C 1.567041 -2.005926 -0.694700
 C 2.906239 -2.302010 -0.457587
 C 2.553313 -1.971449 1.901441
 C 0.567036 1.389919 -0.908623
 C 3.235805 2.247493 -1.212464
 C 1.178129 1.423004 -2.171030
 C 1.316285 1.802300 0.198935
 C 2.641125 2.222473 0.047254
 C 2.495352 1.846682 -2.327480
 C -1.876642 -1.003839 -2.155526
 O -1.075058 2.063376 3.028613
 H -1.878945 -0.251024 -2.952558
 H -1.443402 -1.910491 -2.603066
 C -3.277416 -1.319910 -1.795624
 C -4.414096 -1.624677 -1.517600
 H -1.404155 1.389477 -1.674826
 H -1.172157 -2.432651 -0.315033
 H -2.716009 -1.210029 0.927478
 H -1.193260 2.339787 0.765954
 H 4.452331 -2.517135 1.036221
 H 0.572471 -1.415144 2.499167
 H 1.187528 -1.999827 -1.712564
 H 3.561787 -2.541994 -1.290956
 H 2.930460 -1.948279 2.920857
 H 4.264405 2.579167 -1.327788
 H 0.610274 1.107936 -3.044243
 H 0.879501 1.802385 1.192242
 H 3.206415 2.531452 0.922769
 H 2.943062 1.869183 -3.317998
 H -0.850913 2.087843 3.971564
 H -5.420407 -1.877932 -1.270260
 H -1.496267 -1.681360 2.109571
 C -3.135699 1.669677 0.193377
 H -3.620460 2.020395 1.110541
 H -3.666759 0.782479 -0.162260
 H -3.244451 2.453973 -0.565440

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -997.898256635

Comp_12E_c01**B3LYP/6-31G* Geometry**

C 2.955626 -0.026073 1.090203

C 2.846768 -1.340212 1.337082
 C 2.367043 0.518527 -0.127699
 C 1.470198 -0.416572 -0.924624
 O 1.989601 -1.715011 -0.924070
 C 2.185595 -2.279019 0.372429
 O 0.165373 -0.463817 -0.369654
 H 1.427756 -0.097791 -1.973806
 N 2.475443 1.715470 -0.588743
 O 3.289365 2.523745 0.225828
 C -0.667848 0.643371 -0.702523
 C -2.081824 0.356116 -0.255671
 C -4.741955 -0.141217 0.492047
 C -2.868042 1.373757 0.294171
 C -2.639759 -0.917618 -0.422884
 C -3.959707 -1.165208 -0.048138
 C -4.192895 1.130134 0.661480
 H 3.456959 0.650765 1.772372
 H 3.227470 -1.771503 2.260662
 H 1.224029 -2.624113 0.784152
 H 2.808581 -3.165971 0.210369
 H 3.274692 3.368904 -0.249140
 H -0.297219 1.566806 -0.237050
 H -0.635322 0.801729 -1.794495
 H -5.771144 -0.335026 0.782655
 H -2.440634 2.363689 0.439116
 H -2.026199 -1.712879 -0.835056
 H -4.379866 -2.159237 -0.178785
 H -4.791129 1.931074 1.088136

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -745.303572304

Comp_12E_c02**B3LYP/6-31G* Geometry**

C 3.338713 0.290653 0.239443
 C 3.602400 -1.024754 0.238891
 C 2.021859 0.755543 -0.177767
 C 0.959965 -0.306612 -0.386709
 O 1.521162 -1.466308 -0.969163
 C 2.598474 -2.037062 -0.227963
 O 0.382483 -0.576826 0.875696
 H 0.203555 0.035738 -1.098913
 N 1.638712 1.968010 -0.370374
 O 2.674196 2.890086 -0.143704
 C -0.816633 -1.352875 0.812993
 C -2.036071 -0.560319 0.377952
 C -4.352232 0.857090 -0.336650
 C -3.105105 -1.212154 -0.248035
 C -2.134762 0.812299 0.635444
 C -3.284770 1.516381 0.276109
 C -4.259800 -0.511212 -0.597987
 H 4.072078 1.026328 0.548648
 H 4.558597 -1.405433 0.592053
 H 2.212473 -2.602132 0.636593
 H 3.066063 -2.760876 -0.905046

H 2.233587 3.735436 -0.320526
H -0.672643 -2.221881 0.157872
H -0.953339 -1.728230 1.834032
H -5.247432 1.406885 -0.615118
H -3.033136 -2.276296 -0.464768
H -1.297804 1.324736 1.099800
H -3.346499 2.583265 0.474990
H -5.081428 -1.031102 -1.083955
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.306015150**

Comp_12E_c03

B3LYP/6-31G* Geometry

C 1.673935 0.931290 1.212809
C 2.472611 -0.032240 1.696582
C 1.354483 0.936341 -0.209902
C 1.744773 -0.305251 -0.994359
O 2.996357 -0.769107 -0.579663
C 3.092966 -1.072715 0.811346
O 0.814371 -1.369523 -0.827861
H 1.843058 -0.058099 -2.057982
N 0.755228 1.854168 -0.883038
O 0.414640 2.957597 -0.084109
C -0.443523 -1.204465 -1.479035
C -1.560493 -0.739035 -0.562613
C -3.708174 0.009791 1.085508
C -2.654038 -0.043200 -1.090271
C -1.551944 -1.053767 0.800344
C -2.617263 -0.678362 1.619875
C -3.723952 0.326252 -0.274179
H 1.247225 1.702015 1.844256
H 2.693398 -0.097899 2.760118
H 2.643803 -2.057815 1.014570
H 4.166823 -1.157931 1.014022
H -0.055289 3.526806 -0.712795
H -0.347390 -0.518539 -2.331581
H -0.692146 -2.194694 -1.883641
H -4.537982 0.300811 1.724201
H -2.667542 0.215344 -2.147397
H -0.699020 -1.582219 1.214001
H -2.595656 -0.925139 2.678445
H -4.565106 0.868617 -0.698534

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.301261263**

Comp_12E_c04

B3LYP/6-31G* Geometry

C -2.938345 0.246465 1.098779
C -2.500844 1.500753 1.286461
C -2.542744 -0.473256 -0.105638
C -1.459245 0.168372 -0.949286
O -1.640663 1.570408 -1.005159
C -1.655914 2.211084 0.270446

O -0.217630 -0.185436 -0.384576
H -1.526145 -0.171496 -1.988908
N -2.988343 -1.600034 -0.535624
O -3.980218 -2.128587 0.306126
C 0.900764 0.144459 -1.204255
C 2.188593 -0.077701 -0.442737
C 4.618962 -0.418137 0.922890
C 3.404715 -0.064417 -1.138057
C 2.201115 -0.267386 0.942326
C 3.410805 -0.438187 1.619654
C 4.612164 -0.230259 -0.461494
H -3.575683 -0.257058 1.816405
H -2.738915 2.047894 2.196361
H -0.628772 2.323523 0.654845
H -2.043130 3.219214 0.084104
H -4.192022 -2.966871 -0.132725
H 0.885331 -0.475632 -2.115369
H 0.826637 1.193148 -1.526147
H 5.559020 -0.551648 1.451630
H 3.406756 0.075209 -2.217625
H 1.259911 -0.290264 1.480317
H 3.406017 -0.589248 2.696211
H 5.547322 -0.218348 -1.015414

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.305792937**

Comp_12E_c05

B3LYP/6-31G* Geometry

C 3.356652 0.092768 0.166890
C 3.512909 -1.236373 0.260306
C 2.071997 0.627799 -0.269580
C 0.924669 -0.363007 -0.375623
O 1.374430 -1.589764 -0.875604
C 2.423870 -2.194593 -0.121556
O 0.351808 -0.588360 0.909671
H 0.166975 -0.001966 -1.077703
N 1.777452 1.853668 -0.531633
O 2.882689 2.709194 -0.365356
C -0.638257 0.360599 1.299055
C -1.966460 0.182201 0.584505
C -4.474144 -0.146400 -0.635710
C -2.401113 -1.088057 0.186528
C -2.797497 1.285108 0.357500
C -4.047047 1.123220 -0.243004
C -3.645468 -1.250288 -0.423083
H 4.150824 0.786880 0.416398
H 4.440474 -1.667826 0.631129
H 2.013985 -2.675453 0.780740
H 2.819532 -2.990141 -0.763237
H 2.509596 3.570250 -0.609133
H -0.763235 0.199378 2.376317
H -0.266929 1.385402 1.161432
H -5.443660 -0.274082 -1.109996
H -1.748607 -1.941578 0.344694

H -2.463236 2.278472 0.650292
H -4.681168 1.989406 -0.413714
H -3.968795 -2.240837 -0.732836
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.303588215**

Comp_12E_c06
B3LYP/6-31G* Geometry
C -2.647950 1.300170 0.397450
C -1.605305 2.112935 0.168668
C -2.591540 -0.079423 -0.068833
C -1.245795 -0.570769 -0.567544
O -0.588724 0.440362 -1.302158
C -0.397088 1.667809 -0.599462
O -0.517328 -1.006434 0.558758
H -1.377232 -1.394813 -1.278373
N -3.543066 -0.943920 -0.095281
O -4.750549 -0.410840 0.389473
C 0.674182 -1.749210 0.264341
C 1.923596 -0.896645 0.197386
C 4.252308 0.672267 0.112730
C 2.363419 -0.210636 1.338478
C 2.662620 -0.783263 -0.984325
C 3.822807 -0.007241 -1.027803
C 3.517375 0.571344 1.297239
H -3.535383 1.632506 0.923534
H -1.598225 3.134019 0.544937
H 0.469938 1.587415 0.075197
H -0.139587 2.404808 -1.369068
H -5.347058 -1.172266 0.323518
H 0.760171 -2.474526 1.081307
H 0.544361 -2.310397 -0.671362
H 5.154751 1.277075 0.080618
H 1.792291 -0.290917 2.260496
H 2.323285 -1.300398 -1.878648
H 4.387388 0.069499 -1.953377
H 3.847793 1.096706 2.189648

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.304677073**

Comp_12E_c07
B3LYP/6-31G* Geometry
C -3.389494 0.698769 -0.348156
C -4.070204 -0.457108 -0.315562
C -1.997243 0.738083 0.095206
C -1.475401 -0.535546 0.773167
O -2.000179 -1.671344 0.089121
C -3.415213 -1.746860 0.088770
O -0.100920 -0.650320 0.852674
H -1.826427 -0.542418 1.818494
N -1.211522 1.755790 0.066521
O -1.821338 2.877585 -0.522246
C 0.596795 -0.833344 -0.391967

C 2.040050 -0.436952 -0.200010
C 4.722773 0.336595 0.087250
C 3.071371 -1.272341 -0.639160
C 2.364283 0.791590 0.391719
C 3.696918 1.173363 0.536326
C 4.407131 -0.887323 -0.502483
H -3.851895 1.627474 -0.662200
H -5.125842 -0.494001 -0.576733
H -3.674731 -2.549627 -0.611065
H -3.786323 -2.058153 1.084005
H -1.121585 3.545381 -0.454596
H 0.518699 -1.880948 -0.703331
H 0.130345 -0.215887 -1.169655
H 5.761391 0.636534 0.200666
H 2.828796 -2.233016 -1.088546
H 1.560565 1.434215 0.738242
H 3.938205 2.126606 1.000288
H 5.198362 -1.547614 -0.848219

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.299720382**

Comp_12E_c08
B3LYP/6-31G* Geometry
C 3.196006 0.205793 -0.802166
C 3.345869 -1.083435 -1.143313
C 2.045222 0.626783 -0.004442
C 0.992503 -0.445110 0.239909
O 1.630048 -1.704128 0.457419
C 2.401821 -2.142871 -0.647583
O 0.241805 -0.145111 1.363506
H 0.349856 -0.529139 -0.657435
N 1.792485 1.814705 0.417470
O 2.816225 2.718159 0.080355
C -0.987498 -0.867758 1.461981
C -2.074971 -0.326592 0.552433
C -4.152524 0.682154 -1.043429
C -3.081887 -1.174208 0.076273
C -2.112912 1.032428 0.214725
C -3.144377 1.531278 -0.581603
C -4.119186 -0.673486 -0.711975
H 3.888709 0.970166 -1.134259
H 4.157662 -1.399974 -1.794955
H 2.954182 -3.022872 -0.298960
H 1.747877 -2.480603 -1.474853
H 2.485098 3.545175 0.462813
H -0.817562 -1.935784 1.277119
H -1.280586 -0.759072 2.512198
H -4.955953 1.073113 -1.662220
H -3.054663 -2.233776 0.323775
H -1.319161 1.685430 0.565876
H -3.161256 2.586609 -0.841908
H -4.894610 -1.343430 -1.074575

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -745.301260228

Comp_12E_c09

B3LYP/6-31G* Geometry

C -3.245796 0.567780 -0.703593
C -2.941384 1.873116 -0.766444
C -2.298036 -0.367390 -0.102194
C -0.919503 0.204354 0.232104
O -1.063438 1.517321 0.746084
C -1.681001 2.419194 -0.157101
O -0.259531 -0.514440 1.225882
H -0.313622 0.239334 -0.692615
N -2.465667 -1.627160 0.088857
O -3.747384 -2.053571 -0.304438
C 0.760674 -1.398601 0.768407
C 2.008411 -0.693676 0.267093
C 4.380178 0.540328 -0.590803
C 2.385838 0.552331 0.783234
C 2.825530 -1.308897 -0.688647
C 4.008082 -0.700348 -1.111669
C 3.563215 1.165733 0.353622
H -4.166641 0.171606 -1.116065
H -3.599587 2.580254 -1.267094
H -1.893797 3.323419 0.424473
H -0.974586 2.711678 -0.957612
H -3.717862 -2.998867 -0.091164
H 0.997468 -2.007415 1.648388
H 0.365644 -2.080614 0.003549
H 5.297626 1.019021 -0.923053
H 1.739346 1.040743 1.505781
H 2.534808 -2.271638 -1.105050
H 4.632720 -1.190305 -1.854212
H 3.843736 2.134885 0.758405

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -745.297856604

Comp_12E_c10

B3LYP/6-31G* Geometry

C 2.057506 1.417525 0.624279
C 2.934633 0.638628 1.275337
C 1.246344 0.865429 -0.459428
C 1.583277 -0.569173 -0.883045
O 1.935367 -1.333923 0.263992
C 3.051346 -0.829285 0.979162
O 0.596580 -1.235176 -1.601883
H 2.449531 -0.524880 -1.565865
N 0.380590 1.498663 -1.166664
O 0.220596 2.828071 -0.738688
C -0.438853 -1.923638 -0.871350
C -1.457315 -1.045542 -0.177575
C -3.380746 0.545756 1.109252
C -1.450723 -0.906375 1.214238
C -2.440134 -0.376242 -0.918606

C -3.395027 0.414409 -0.282562
C -2.406532 -0.116064 1.856681
H 1.953366 2.472597 0.849613
H 3.594315 1.048968 2.037061
H 3.100187 -1.411496 1.906491
H 3.986866 -1.030893 0.423802
H -0.476015 3.144273 -1.334109
H -0.927140 -2.515811 -1.650851
H 0.019243 -2.611239 -0.155732
H -4.127898 1.158734 1.606885
H -0.686269 -1.416311 1.795287
H -2.448046 -0.474281 -2.001497
H -4.155418 0.923928 -0.869310
H -2.389844 -0.018577 2.939203

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -745.294145814

Comp_12E_c11

B3LYP/6-31G* Geometry

C 3.730827 0.243815 0.063515
C 4.002205 -1.040961 0.339693
C 2.357636 0.664210 -0.213615
C 1.353698 -0.469833 -0.365119
O 1.629357 -1.475828 0.610984
C 2.910124 -2.065783 0.466218
O 0.064415 -0.014060 -0.180530
H 1.469318 -0.924350 -1.371223
N 1.944169 1.862654 -0.424183
O 2.980839 2.802528 -0.289629
C -0.945002 -0.963516 -0.528609
C -2.305570 -0.393292 -0.205925
C -4.865002 0.563981 0.437288
C -3.420944 -0.786636 -0.953850
C -2.482197 0.489984 0.865310
C -3.754477 0.967465 1.181390
C -4.694773 -0.316290 -0.632438
H 4.511002 0.993560 0.002448
H 5.026300 -1.380584 0.480027
H 3.059436 -2.685059 1.358004
H 2.931110 -2.748140 -0.405608
H 2.520842 3.633321 -0.485360
H -0.874369 -1.204202 -1.601445
H -0.775566 -1.893675 0.030440
H -5.855118 0.937070 0.685717
H -3.293136 -1.463463 -1.796472
H -1.615718 0.809028 1.434845
H -3.878092 1.657801 2.011959
H -5.551218 -0.629851 -1.223798

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -745.300446877

Comp_13Z_c01

B3LYP/6-31G* Geometry

C 3.018606 -0.195236 1.303704
 C 2.951048 -1.532190 1.235722
 C 2.435287 0.619688 0.244331
 C 1.604069 -0.124981 -0.799406
 O 2.174375 -1.371177 -1.074778
 C 2.333248 -2.226829 0.058286
 O 0.285941 -0.338405 -0.321142
 H 1.587998 0.418857 -1.749486
 N 2.634226 1.891059 0.290461
 C -0.585588 0.788795 -0.386534
 C -2.000624 0.334586 -0.115282
 C -4.660837 -0.453093 0.317970
 C -2.863790 1.131194 0.643995
 C -2.481768 -0.866286 -0.651990
 C -3.801827 -1.258739 -0.433833
 C -4.188499 0.744323 0.856138
 O 2.011746 2.565564 -0.780177
 H 3.493502 0.322440 2.132118
 H 3.336600 -2.157229 2.037802
 H 1.363191 -2.665803 0.338080
 H 2.975367 -3.044033 -0.288757
 H -0.285164 1.558403 0.337313
 H -0.511195 1.245575 -1.386838
 H -5.689783 -0.759790 0.486672
 H -2.496766 2.059981 1.075734
 H -1.809036 -1.494486 -1.227787
 H -4.161787 -2.195439 -0.851875
 H -4.846671 1.373827 1.449423
 H 2.271723 3.485031 -0.615462

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.301329339**

Comp_13Z_c02

B3LYP/6-31G* Geometry

C 3.506345 0.586431 0.139725
 C 3.849101 -0.709270 0.119009
 C 2.132891 0.987989 -0.131863
 C 1.115135 -0.124253 -0.333236
 O 1.714588 -1.256523 -0.928775
 C 2.854580 -1.773417 -0.241945
 O 0.571535 -0.407903 0.940018
 H 0.334111 0.179233 -1.035723
 N 1.872486 2.248553 -0.157011
 C -0.546384 -1.302546 0.914591
 C -1.836295 -0.671784 0.425617
 C -4.287628 0.435434 -0.379487
 C -2.768657 -1.442111 -0.278751
 C -2.139842 0.664352 0.715803
 C -3.356490 1.214043 0.311698
 C -3.990632 -0.895873 -0.674684
 O 0.512080 2.500307 -0.392172
 H 4.218662 1.373089 0.370456
 H 4.856763 -1.029543 0.372975
 H 2.542436 -2.324271 0.660435

H 3.298100 -2.502146 -0.929462
 H -0.305778 -2.189065 0.314503
 H -0.653400 -1.625338 1.956725
 H -5.235798 0.865496 -0.691498
 H -2.536648 -2.477514 -0.520507
 H -1.406592 1.272768 1.235049
 H -3.579278 2.253816 0.537820
 H -4.704438 -1.506693 -1.221380
 H 0.486076 3.469282 -0.421732

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.304670886**

Comp_13Z_c03

B3LYP/6-31G* Geometry

C 3.334764 0.262481 1.074712
 C 3.478365 -1.069377 1.131682
 C 2.380901 0.855582 0.148605
 C 1.551579 -0.091298 -0.705205
 O 2.238483 -1.298918 -0.955075
 C 2.717399 -1.975160 0.207049
 O 0.332686 -0.277104 -0.032020
 H 1.381679 0.337418 -1.699156
 N 2.269126 2.138152 0.133529
 C -0.700429 -0.876347 -0.819847
 C -2.047555 -0.451416 -0.285210
 C -4.574979 0.363983 0.619169
 C -3.092449 -1.373264 -0.173107
 C -2.276272 0.885581 0.066339
 C -3.531793 1.288763 0.517940
 C -4.352994 -0.968626 0.271841
 O 1.276542 2.565329 -0.765963
 H 3.889299 0.936914 1.720490
 H 4.139783 -1.533650 1.859217
 H 1.882086 -2.453209 0.744458
 H 3.362159 -2.776243 -0.170441
 H -0.585335 -0.551802 -1.866541
 H -0.604500 -1.970067 -0.809198
 H -5.553290 0.680782 0.971159
 H -2.919951 -2.415601 -0.433334
 H -1.458839 1.597027 -0.007616
 H -3.698435 2.327384 0.792323
 H -5.156292 -1.696121 0.354867
 H 1.336840 3.530239 -0.690289

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.304824743**

Comp_13Z_c04

B3LYP/6-31G* Geometry

C -1.991753 0.856717 1.445702
 C -2.916171 1.468477 0.691860
 C -1.350573 -0.362475 0.967411
 C -1.655228 -0.770030 -0.471548
 O -2.987657 -0.477765 -0.782011

C -3.363921 0.889820 -0.618506
O -0.822411 -0.078585 -1.393192
H -1.547839 -1.850720 -0.600425
N -0.564532 -0.983057 1.775757
C 0.452912 -0.651025 -1.674636
C 1.589745 -0.074175 -0.851459
C 3.767359 1.014095 0.549040
C 2.703494 -0.862872 -0.542982
C 1.575616 1.265432 -0.447725
C 2.655361 1.804881 0.251958
C 3.789225 -0.322883 0.148187
O -0.002932 -2.132623 1.188096
H -1.681883 1.240024 2.413556
H -3.370130 2.405747 1.005136
H -2.977718 1.489360 -1.457485
H -4.457416 0.896035 -0.689211
H 0.417367 -1.741868 -1.556709
H 0.628549 -0.439594 -2.737571
H 4.608998 1.435669 1.092324
H 2.720729 -1.908267 -0.844760
H 0.706359 1.875879 -0.672811
H 2.628948 2.845532 0.565267
H 4.647781 -0.948116 0.380349
H 0.595581 -2.442263 1.885082

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.298841700**

Comp_13Z_c05

B3LYP/6-31G* Geometry

C -2.726951 1.624312 0.350568
C -1.674427 2.407218 0.072615
C -2.679060 0.200302 0.052317
C -1.365820 -0.351504 -0.481028
O -0.679794 0.611843 -1.247749
C -0.451102 1.866577 -0.606879
O -0.643150 -0.811601 0.638414
H -1.549711 -1.175320 -1.178643
N -3.732849 -0.503021 0.281773
C 0.484882 -1.642077 0.335684
C 1.786762 -0.878203 0.215345
C 4.229926 0.499167 0.046876
C 2.217755 -0.059171 1.268826
C 2.592953 -0.995136 -0.920796
C 3.809830 -0.314714 -1.005365
C 3.428439 0.627585 1.184757
O -3.531586 -1.861004 -0.014699
H -3.631025 2.007346 0.814798
H -1.672790 3.461561 0.339368
H 0.383274 1.782224 0.107000
H -0.124490 2.541118 -1.406442
H 0.542409 -2.350493 1.170306
H 0.293588 -2.218934 -0.579601
H 5.175443 1.031176 -0.017478
H 1.594449 0.039267 2.154269

H 2.264296 -1.619303 -1.748730
H 4.424849 -0.416458 -1.895731
H 3.750684 1.258834 2.009032
H -4.403911 -2.239903 0.174183

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.303718966**

Comp_13Z_c06

B3LYP/6-31G* Geometry

C 3.568606 -0.286125 0.018110
C 3.364760 -1.608847 0.093519
C 2.447424 0.612976 -0.220980
C 1.055776 -0.009565 -0.270869
O 1.115092 -1.308914 -0.801412
C 2.004474 -2.201222 -0.132405
O 0.525338 -0.027837 1.045728
H 0.404974 0.549149 -0.946042
N 2.701776 1.869990 -0.330866
C -0.628989 0.787200 1.263988
C -1.886361 0.303026 0.566230
C -4.280693 -0.561782 -0.620166
C -2.833560 1.229420 0.114877
C -2.147031 -1.063662 0.407763
C -3.334874 -1.492580 -0.183748
C -4.027225 0.802189 -0.469329
O 1.525839 2.628384 -0.511829
H 4.549080 0.161193 0.153184
H 4.176947 -2.292063 0.330400
H 1.566653 -2.529221 0.824116
H 2.068884 -3.082470 -0.780252
H -0.767471 0.763103 2.351355
H -0.414586 1.825648 0.982172
H -5.205834 -0.897876 -1.081008
H -2.634818 2.294123 0.220816
H -1.403908 -1.784452 0.733436
H -3.522738 -2.556271 -0.305855
H -4.752452 1.534196 -0.815371
H 1.878831 3.525772 -0.612723

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.301152769**

Comp_13Z_c08

B3LYP/6-31G* Geometry

C -3.470104 0.392268 -0.847607
C -4.061290 -0.751020 -0.475554
C -2.211770 0.827605 -0.242304
C -1.564860 -0.114151 0.793540
O -1.995552 -1.453961 0.575264
C -3.397048 -1.661186 0.516337
O -0.180716 -0.129190 0.819710
H -1.868901 0.220619 1.799182
N -1.845434 2.024683 -0.550920
C 0.466191 -0.493696 -0.407538

C 1.957404 -0.354536 -0.223300
 C 4.736442 -0.065962 0.048217
 C 2.496259 0.792292 0.375137
 C 2.823619 -1.353230 -0.678377
 C 4.206950 -1.209370 -0.549871
 C 3.876190 0.932582 0.513515
 O -0.693591 2.456286 0.116901
 H -3.925246 1.074410 -1.560089
 H -5.033695 -1.037721 -0.868231
 H -3.528294 -2.712311 0.237007
 H -3.851343 -1.536233 1.517451
 H 0.202510 -1.521477 -0.679701
 H 0.116767 0.171117 -1.210916
 H 5.812253 0.046033 0.155809
 H 1.821548 1.561499 0.737533
 H 2.413736 -2.252479 -1.133175
 H 4.867642 -1.994778 -0.907841
 H 4.283502 1.823627 0.984867
 H -0.581467 3.350254 -0.243626

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -745.295949149**

Comp_14E_c01
B3LYP/6-31G* Geometry

C -0.660310 1.665516 -0.070606
 O -1.149396 -0.287766 1.261574
 C 0.935312 -0.132665 0.116030
 C -0.271678 -1.003739 0.418322
 C 0.620256 1.268545 -0.168679
 C -1.714718 0.661529 0.340055
 N 2.081739 -0.712226 0.115328
 C -2.071316 -0.288552 -0.826782
 O -1.002820 -1.240293 -0.792349
 O 3.120447 0.173045 -0.216611
 H -0.964331 2.682719 -0.304310
 H 0.002829 -1.952269 0.881964
 H 1.423324 1.942607 -0.443038
 H -2.581314 1.123200 0.817009
 H -2.092397 0.201921 -1.804606
 H -3.029597 -0.791188 -0.643407
 H 3.898194 -0.405116 -0.181852

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -513.086428098**

Comp_15Z_c01
B3LYP/6-31G* Geometry

C -1.266364 1.529574 -0.078868
 O -0.874845 -0.421365 1.283878
 C 0.910480 0.478370 -0.020167
 C 0.154154 -0.783462 0.390219
 C 0.059304 1.641647 -0.265095
 C -1.820725 0.206078 0.397477
 N 2.178184 0.595144 -0.201889

O 2.860088 -0.602313 0.070961
 C -1.850136 -0.844475 -0.737581
 O -0.499396 -1.320992 -0.766768
 H -1.948414 2.350818 -0.280588
 H 0.789304 -1.539852 0.847061
 H 0.534843 2.562897 -0.588345
 H -2.768127 0.305761 0.930501
 H 3.780645 -0.357261 -0.109655
 H -2.111971 -0.427887 -1.714682
 H -2.530621 -1.669520 -0.491540

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -513.084537875**

Comp_16E_c01
B3LYP/6-31G* Geometry

C -3.978356 -0.190746 0.681639
 C -3.487749 -1.504158 0.023041
 C -2.242921 -1.310358 -0.837889
 C -2.801854 0.542800 1.363937
 C -1.619356 0.781102 0.407390
 C -1.085505 -0.556435 -0.182861
 C -0.367920 -1.480978 0.834501
 C -0.532256 1.668682 1.070892
 H -0.380457 -0.320891 -0.987090
 C 0.331262 -2.696297 0.197093
 C 1.546627 -2.348266 -0.681354
 N 2.466547 -1.400847 -0.047521
 C 3.067415 -1.935729 1.170274
 C 3.485838 -0.890609 -0.964626
 C 4.097394 0.446104 -0.515774
 C 3.109733 1.621826 -0.549730
 C 2.026380 1.555186 0.522093
 C 0.625615 2.001671 0.163165
 O 2.269562 1.238633 1.675840
 N 0.567294 2.737941 -0.891594
 O -0.711723 3.251444 -1.117424
 C -4.719168 0.694112 -0.334545
 H -4.700107 -0.462150 1.463862
 O -2.165301 -1.755227 -1.970037
 H -1.996801 1.357413 -0.443848
 H -3.231697 -2.224998 0.813261
 H -4.264855 -1.963012 -0.596280
 H -2.465245 -0.035603 2.235268
 H -3.156426 1.506122 1.754161
 H -1.082412 -1.841859 1.584785
 H 0.379091 -0.892523 1.374345
 H -1.014519 2.608944 1.368023
 H -0.130791 1.208019 1.976897
 H 0.636672 -3.379374 0.999140
 H -0.371707 -3.263284 -0.425985
 H 2.054874 -3.291878 -0.966652
 H 1.195858 -1.892435 -1.614279
 H 2.292520 -2.243217 1.876260
 H 3.659208 -1.164118 1.666505

H 3.718257 -2.809791 0.970600
H 3.013483 -0.744897 -1.944531
H 4.299190 -1.628691 -1.115938
H 4.527116 0.361900 0.487521
H 4.931024 0.677421 -1.191127
H 2.654808 1.719691 -1.538342
H 3.659485 2.556978 -0.369650
H -0.586821 3.776579 -1.924325
H -5.601677 0.175594 -0.726480
H -5.056411 1.628173 0.130148
H -4.089938 0.955990 -1.192958

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.634304916

Comp_16E_c02

B3LYP/6-31G* Geometry

C 3.984020 -0.006963 -0.540458
C 3.422749 -1.434221 -0.332638
C 2.126376 -1.444628 0.469154
C 2.878136 0.918910 -1.090419
C 1.614176 0.935471 -0.210681
C 1.027495 -0.493533 -0.004350
C 0.313534 -1.083709 -1.247911
C 0.597341 1.975395 -0.759355
H 0.289189 -0.446298 0.801191
C -0.419719 -2.419182 -1.012502
C -1.288962 -2.522351 0.253278
N -2.204081 -1.402369 0.521851
C -2.826726 -1.598811 1.828681
C -3.197449 -1.192808 -0.531911
C -4.026711 0.097154 -0.361617
C -3.229484 1.325651 0.122147
C -1.975905 1.568216 -0.698281
C -0.713192 2.035162 -0.015321
O -1.967573 1.395964 -1.909757
N -0.887822 2.509648 1.168356
O 0.295967 2.999599 1.721018
C 4.627444 0.531990 0.747564
H 4.775144 -0.068956 -1.300052
O 1.966026 -2.194241 1.418215
H 1.903762 1.289164 0.785329
H 3.206800 -1.877809 -1.315983
H 4.143105 -2.087283 0.169868
H 2.612598 0.600298 -2.108184
H 3.271904 1.940071 -1.181905
H 1.028401 -1.226293 -2.069298
H -0.406531 -0.349001 -1.610433
H 1.072884 2.961908 -0.696786
H 0.373446 1.782875 -1.811622
H -1.018016 -2.633844 -1.907298
H 0.306290 -3.240096 -0.940233
H -1.844456 -3.481185 0.204559
H -0.620759 -2.594128 1.117790
H -2.049655 -1.695093 2.593868

H -3.459018 -2.507624 1.867434
H -3.453860 -0.742917 2.092837
H -3.894261 -2.051906 -0.613997
H -2.663510 -1.128943 -1.482881
H -4.487746 0.318091 -1.330221
H -4.850836 -0.062982 0.343914
H -2.964932 1.243909 1.176385
H -3.863472 2.219040 0.027351
H 0.005567 3.320188 2.590195
H 5.017217 1.545734 0.597116
H 3.917687 0.567203 1.582087
H 5.462288 -0.106110 1.059422

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.632780665

Comp_16E_c03

B3LYP/6-31G* Geometry

C 3.951568 -0.319270 -0.449909
C 3.321102 -1.646982 0.038642
C 1.980441 -1.452356 0.740165
C 2.906945 0.526450 -1.214387
C 1.624337 0.754945 -0.395027
C 0.953358 -0.593637 0.002314
C 0.346608 -1.403952 -1.175165
C 0.666233 1.760398 -1.089418
H 0.147523 -0.395781 0.716132
C -0.454030 -2.651853 -0.730207
C -1.973367 -2.433455 -0.714010
N -2.426951 -1.378002 0.199644
C -2.453776 -1.839387 1.584440
C -3.703889 -0.803061 -0.232607
C -4.045758 0.551874 0.418576
C -2.847404 1.482049 0.659301
C -1.880292 1.612828 -0.504270
C -0.493722 2.138589 -0.205174
O -2.168385 1.332875 -1.657363
N -0.438945 2.923548 0.812192
O 0.841290 3.454601 1.006688
C 4.596224 0.448756 0.716183
H 4.754495 -0.573353 -1.155017
O 1.732009 -1.977960 1.812373
H 1.920769 1.236144 0.544588
H 3.142441 -2.297893 -0.829807
H 3.988276 -2.187532 0.717276
H 2.661023 0.033790 -2.165172
H 3.351253 1.495692 -1.476716
H 1.145245 -1.706896 -1.862500
H -0.314923 -0.745157 -1.747617
H 1.239337 2.665809 -1.320222
H 0.272584 1.365220 -2.029319
H -0.264288 -3.477879 -1.428205
H -0.105151 -3.004313 0.247167
H -2.279550 -2.144931 -1.726012
H -2.478850 -3.395224 -0.496215

H -2.762338 -1.026005 2.248470
H -3.152175 -2.685713 1.736165
H -1.454106 -2.156904 1.897102
H -4.548587 -1.501073 -0.066055
H -3.627100 -0.641703 -1.309406
H -4.781354 1.044194 -0.228310
H -4.543353 0.404959 1.385357
H -3.202293 2.491304 0.911732
H -2.273046 1.158090 1.531836
H 0.713195 4.026973 1.780085
H 5.398402 -0.143805 1.170782
H 5.030604 1.394440 0.371234
H 3.876468 0.680976 1.509537

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.630414340

Comp_16E_c04

B3LYP/6-31G* Geometry

C 3.670959 -0.135102 0.097225
C 3.561920 -1.649487 -0.205191
C 2.149549 -2.063531 -0.596766
C 2.550183 0.313782 1.052192
C 1.137425 -0.093984 0.583451
C 1.063342 -1.643758 0.394564
C -0.321535 -2.203268 0.035188
C 0.693373 0.686717 -0.689634
H 1.366773 -2.065381 1.367866
C -1.368945 -2.064111 1.153251
C -2.809144 -2.186605 0.633019
N -3.228886 -1.028426 -0.173290
C -4.270514 -1.393922 -1.128898
C -3.642929 0.097972 0.673311
C -3.698702 1.452438 -0.051722
C -2.385301 1.839591 -0.740015
C -1.245796 2.144994 0.222195
C 0.165304 2.057626 -0.343249
O -1.427575 2.440838 1.388315
N 0.775476 3.179683 -0.429351
O 2.086941 3.035746 -0.929755
C 5.057339 0.221305 0.646012
H 3.546244 0.403507 -0.851835
O 1.907027 -2.666614 -1.626517
H 0.438662 0.166352 1.387164
H 4.248415 -1.949920 -1.003130
H 3.837511 -2.209840 0.702243
H 2.596111 1.401479 1.178918
H 2.728496 -0.127658 2.044249
H -0.206538 -3.260995 -0.229684
H -0.700012 -1.720533 -0.871155
H 1.514080 0.781206 -1.403949
H -0.106295 0.136411 -1.192247
H -1.205204 -2.838297 1.915602
H -1.257552 -1.106885 1.676606
H -2.875175 -3.077864 -0.002776

H -3.503944 -2.355259 1.477531
H -3.912523 -2.202393 -1.774314
H -4.514150 -0.541945 -1.770911
H -5.207776 -1.728882 -0.642492
H -2.927824 0.187250 1.495415
H -4.630357 -0.099204 1.136937
H -4.501235 1.457043 -0.798627
H -3.956579 2.215374 0.690788
H -2.077806 1.061669 -1.445875
H -2.520462 2.754702 -1.337710
H 2.389330 3.957052 -0.961892
H 5.849773 -0.081638 -0.048421
H 5.148035 1.301518 0.809114
H 5.243560 -0.279365 1.605116

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.629402637

Comp_16E_c05

B3LYP/6-31G* Geometry

C 3.978605 -0.025930 -0.437772
C 3.415899 -1.447889 -0.200244
C 2.055629 -1.452667 0.491740
C 2.900838 0.871198 -1.084863
C 1.594139 0.901566 -0.272813
C 0.991675 -0.521827 -0.089084
C 0.398097 -1.169867 -1.373229
C 0.600765 1.939991 -0.858303
H 0.185944 -0.458797 0.646100
C -0.499111 -2.396309 -1.104530
C -1.957650 -2.091848 -0.716185
N -2.162290 -1.379493 0.554934
C -1.721182 -2.185276 1.698222
C -3.571449 -1.001582 0.730239
C -4.052637 0.180437 -0.122012
C -3.247618 1.470521 0.107161
C -1.959633 1.495299 -0.700785
C -0.695459 2.047060 -0.094865
O -1.943260 1.120281 -1.865967
N -0.847585 2.622935 1.046893
O 0.343819 3.165749 1.527874
C 4.548617 0.570994 0.859385
H 4.811006 -0.113618 -1.149121
O 1.825265 -2.197154 1.431408
H 1.838302 1.258589 0.734888
H 3.286626 -1.945496 -1.172573
H 4.100830 -2.064724 0.389966
H 2.693855 0.516874 -2.104539
H 3.293585 1.891650 -1.187577
H 1.211161 -1.470357 -2.046622
H -0.187452 -0.423847 -1.917066
H 1.093396 2.919229 -0.834323
H 0.361845 1.710652 -1.899440
H -0.559880 -2.982497 -2.031348
H -0.030603 -3.059099 -0.367522

H -2.394062 -1.481440 -1.512963
H -2.516253 -3.050857 -0.704664
H -1.911440 -1.632564 2.624119
H -0.647964 -2.381819 1.649549
H -2.254678 -3.153701 1.762140
H -3.699782 -0.726157 1.784289
H -4.240168 -1.868126 0.552692
H -4.041643 -0.058497 -1.190315
H -5.101831 0.360657 0.143917
H -3.837333 2.330925 -0.240876
H -3.041995 1.634660 1.167023
H 0.069024 3.562349 2.370359
H 5.373778 -0.043820 1.236774
H 4.933825 1.583481 0.690034
H 3.797295 0.628024 1.655418

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.634448452

Comp_16E_c06

B3LYP/6-31G* Geometry

C 3.304763 0.167212 0.529536
C 3.511687 -1.309786 0.119792
C 2.308574 -1.887474 -0.612819
C 1.943503 0.344059 1.223786
C 0.752504 -0.208952 0.411842
C 0.968595 -1.730962 0.120731
C -0.174516 -2.486397 -0.583860
C 0.480250 0.610565 -0.880162
H 1.125265 -2.191686 1.110957
C -1.292356 -3.026346 0.326450
C -2.189092 -1.998438 1.035057
N -2.771408 -0.979248 0.154610
C -3.705192 -1.557746 -0.806862
C -3.392360 0.098306 0.934467
C -3.711550 1.363398 0.121523
C -2.536314 1.855859 -0.734755
C -1.308114 2.242452 0.080195
C 0.051970 2.023666 -0.563967
O -1.395623 2.718705 1.196577
N 0.722944 3.102502 -0.732700
O 1.988693 2.865823 -1.301771
C 4.457644 0.662086 1.410591
H 3.301433 0.774628 -0.384202
O 2.409289 -2.424969 -1.700597
H -0.140052 -0.120951 1.039571
H 4.395940 -1.432867 -0.513502
H 3.666853 -1.909004 1.031341
H 1.776515 1.405633 1.442981
H 1.968716 -0.171963 2.195574
H 0.276028 -3.338356 -1.104153
H -0.612109 -1.868713 -1.374151
H 1.353873 0.633087 -1.535278
H -0.329942 0.125750 -1.431735
H -1.916368 -3.703276 -0.271369

H -0.850853 -3.658758 1.110126
H -2.978238 -2.549109 1.587086
H -1.601275 -1.471503 1.795205
H -4.084848 -0.781860 -1.477875
H -4.573900 -2.042580 -0.319184
H -3.201045 -2.305521 -1.424807
H -2.689591 0.375697 1.726996
H -4.317346 -0.246387 1.438528
H -4.578366 1.203620 -0.530349
H -3.994421 2.148018 0.831296
H -2.270458 1.116711 -1.494930
H -2.829537 2.767143 -1.278520
H 2.343112 3.765386 -1.381864
H 5.422853 0.549437 0.902791
H 4.331567 1.721586 1.662209
H 4.506586 0.097576 2.350943

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.628444462

Comp_16E_c07

B3LYP/6-31G* Geometry

C 3.795266 -0.326352 -0.602877
C 3.563736 -0.652684 0.885184
C 2.129209 -1.080489 1.183717
C 2.797696 0.753238 -1.110199
C 1.544216 0.913498 -0.219780
C 1.034736 -0.443145 0.325874
C 0.550597 -1.438417 -0.763157
C 0.470009 1.767739 -0.941461
H 0.191190 -0.253749 0.999944
C -0.151414 -2.701226 -0.234111
C -1.443315 -2.440315 0.557787
N -2.350536 -1.488616 -0.091390
C -2.832797 -1.972100 -1.382073
C -3.460402 -1.091538 0.775677
C -4.137414 0.221813 0.352533
C -3.231343 1.455619 0.481442
C -2.101218 1.504634 -0.540649
C -0.753818 2.037030 -0.103282
O -2.267889 1.212331 -1.714019
N -0.799516 2.772564 0.951973
O 0.434455 3.358467 1.249677
C 5.250208 0.077383 -0.870322
H 3.607119 -1.252969 -1.162534
O 1.871959 -1.890156 2.058366
H 1.845486 1.492761 0.660232
H 4.236140 -1.440124 1.241563
H 3.775513 0.239361 1.496644
H 2.500972 0.514218 -2.139625
H 3.304586 1.726454 -1.161325
H -0.139653 -0.901339 -1.421358
H 1.398448 -1.749248 -1.387191
H 0.930408 2.729108 -1.203889
H 0.144816 1.296752 -1.872592

H -0.360620 -3.355718 -1.089749
 H 0.522067 -3.263895 0.421273
 H -1.938573 -3.413416 0.752054
 H -1.176924 -2.027886 1.537309
 H -1.991911 -2.220782 -2.033459
 H -3.469680 -2.873055 -1.282325
 H -3.403967 -1.189940 -1.886179
 H -3.062688 -0.965188 1.790933
 H -4.229134 -1.888369 0.837969
 H -5.012596 0.368785 0.998088
 H -4.517563 0.154209 -0.671792
 H -3.832249 2.361855 0.317961
 H -2.826059 1.535671 1.493227
 H 0.230775 3.881542 2.041713
 H 5.411017 0.287200 -1.934515
 H 5.514279 0.982847 -0.308789
 H 5.947253 -0.715979 -0.575675
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632018324**

Comp_16E_c08

B3LYP/6-31G* Geometry

C -3.989907 -0.199774 0.732960
 C -3.496743 -1.510606 0.072289
 C -2.286908 -1.298282 -0.832854
 C -2.803781 0.550155 1.377402
 C -1.653520 0.807390 0.386524
 C -1.118868 -0.517784 -0.227026
 C -0.331412 -1.428652 0.752662
 C -0.564761 1.697553 1.039896
 H -0.461356 -0.264902 -1.066045
 C 0.409199 -2.585964 0.056670
 C 1.671058 -2.163510 -0.713634
 N 2.637869 -1.408483 0.087597
 C 3.189480 -2.186209 1.191710
 C 3.687628 -0.805708 -0.741238
 C 3.324640 0.585818 -1.273365
 C 3.232075 1.670587 -0.175725
 C 2.026306 1.568845 0.745705
 C 0.664658 1.952827 0.202870
 O 2.126597 1.263691 1.923164
 N 0.702041 2.577367 -0.922481
 O -0.556845 3.019085 -1.332813
 C -4.768911 0.668685 -0.268467
 H -4.686517 -0.475186 1.536353
 O -2.243823 -1.746401 -1.965615
 H -2.058738 1.383657 -0.451288
 H -3.200397 -2.216804 0.861618
 H -4.284158 -1.991281 -0.516646
 H -2.430136 -0.025806 2.235362
 H -3.158100 1.507720 1.782200
 H 0.401941 -0.826414 1.297547
 H -1.012631 -1.843452 1.505859
 H -1.028072 2.669020 1.259516

H -0.230335 1.279187 1.992516
 H 0.675302 -3.338114 0.809089
 H -0.254712 -3.094151 -0.653573
 H 2.136673 -3.071820 -1.148751
 H 1.380217 -1.534324 -1.562675
 H 2.390230 -2.518204 1.859657
 H 3.749859 -3.082027 0.858679
 H 3.860393 -1.553558 1.779908
 H 3.959182 -1.464760 -1.587417
 H 4.592445 -0.709849 -0.129384
 H 2.390112 0.554035 -1.844568
 H 4.105665 0.891127 -1.982385
 H 4.119139 1.631046 0.465616
 H 3.202598 2.650531 -0.663442
 H -0.359757 3.467617 -2.170994
 H -5.105944 1.601093 0.199778
 H -4.166367 0.933717 -1.144872
 H -5.654727 0.136488 -0.633619
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632919333**

Comp_16E_c09

B3LYP/6-31G* Geometry

C -3.429232 0.461035 -0.476709
 C -3.718632 -0.994941 -0.038513
 C -2.547993 -1.637786 0.696056
 C -2.052226 0.566263 -1.156404
 C -0.906605 -0.045458 -0.320806
 C -1.211924 -1.552706 -0.048415
 C -0.087140 -2.365175 0.614778
 C -0.614636 0.771038 0.978442
 H -1.410816 -1.985629 -1.043477
 C 0.903725 -3.033781 -0.356308
 C 1.813417 -2.118736 -1.196314
 N 2.525302 -1.083480 -0.436373
 C 3.348618 -1.648205 0.632148
 C 3.327030 -0.238705 -1.328743
 C 3.823044 1.077842 -0.706726
 C 2.710099 2.085238 -0.376955
 C 1.818718 1.645334 0.776952
 C 0.326046 1.906026 0.673078
 O 2.256614 1.126357 1.787719
 N 0.038036 3.109913 0.339801
 O -1.348938 3.357563 0.353190
 C -4.547954 0.998671 -1.376787
 H -3.409866 1.082157 0.428800
 O -2.675124 -2.167901 1.784271
 H 0.005943 -0.020844 -0.924880
 H -4.606295 -1.053722 0.599240
 H -3.914657 -1.599366 -0.938693
 H -1.837435 1.618132 -1.371968
 H -2.092229 0.043351 -2.124393
 H -0.555409 -3.150564 1.217908
 H 0.465235 -1.740260 1.323384

H -1.536592 1.155744 1.420663
H -0.125518 0.143053 1.726647
H 1.526602 -3.728993 0.220234
H 0.348999 -3.665213 -1.065101
H 2.522488 -2.766746 -1.752107
H 1.211705 -1.604415 -1.956989
H 2.737696 -2.256722 1.301336
H 3.774436 -0.845543 1.235877
H 4.169858 -2.280307 0.240898
H 2.706657 0.004013 -2.202102
H 4.203851 -0.796758 -1.716045
H 4.415558 0.887084 0.193362
H 4.504165 1.543186 -1.430329
H 3.161156 3.043413 -0.081844
H 2.097769 2.293979 -1.260044
H -1.387659 4.301360 0.130967
H -5.522367 0.942245 -0.877425
H -4.367247 2.046544 -1.643557
H -4.615948 0.421913 -2.308433

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.627966277**

Comp_16E_c10

B3LYP/6-31G* Geometry

C 3.769316 -0.437983 -0.418347
C 3.325763 -0.882936 0.989018
C 1.843862 -1.243477 1.073676
C 2.888004 0.726968 -0.954277
C 1.539306 0.872893 -0.215889
C 0.905286 -0.500218 0.122039
C 0.573518 -1.388502 -1.111320
C 0.595796 1.852949 -0.960550
H -0.032845 -0.349395 0.665693
C -0.259563 -2.650323 -0.799122
C -1.778279 -2.443185 -0.885333
N -2.335155 -1.468096 0.061219
C -2.396757 -2.007089 1.417580
C -3.629746 -0.960990 -0.403905
C -4.088266 0.342314 0.281582
C -2.964251 1.340145 0.598208
C -1.963601 1.571546 -0.520018
C -0.628717 2.178640 -0.146075
O -2.180498 1.305560 -1.691301
N -0.671539 2.964536 0.870473
O 0.569829 3.557721 1.135521
C 5.260200 -0.079433 -0.447667
H 3.630710 -1.302186 -1.082005
O 1.438769 -2.075279 1.869296
H 1.753693 1.350455 0.748466
H 3.906352 -1.739038 1.348702
H 3.502320 -0.066048 1.707291
H 2.717235 0.585606 -2.029541
H 3.432513 1.675778 -0.857429
H 1.506513 -1.688142 -1.604093

H 0.028100 -0.774680 -1.838716
H 1.149896 2.778934 -1.153588
H 0.274057 1.448184 -1.923797
H -0.015448 -3.424648 -1.538869
H 0.029549 -3.062588 0.172638
H -2.008148 -2.082288 -1.894608
H -2.281015 -3.426050 -0.781892
H -1.392490 -2.260006 1.770811
H -3.031652 -2.912331 1.484550
H -2.809063 -1.258151 2.101282
H -4.430756 -1.719796 -0.299961
H -3.521614 -0.750988 -1.469355
H -4.832572 0.807793 -0.375209
H -4.607969 0.126668 1.223461
H -3.392286 2.315742 0.869077
H -2.402936 1.022557 1.481866
H 0.367946 4.129170 1.893664
H 5.882550 -0.926888 -0.136746
H 5.574335 0.215444 -1.455994
H 5.473856 0.759878 0.226724

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.628188663**

Comp_16E_c11

B3LYP/6-31G* Geometry

C 3.808077 -0.731844 -0.668378
C 3.184162 -1.948684 0.058502
C 1.962208 -1.587618 0.898623
C 2.714720 0.092556 -1.387249
C 1.572446 0.503346 -0.439899
C 0.892564 -0.746228 0.197886
C 0.109534 -1.646876 -0.796711
C 0.577591 1.489923 -1.116283
H 0.207043 -0.409083 0.983242
C -0.728919 -2.756052 -0.134499
C -1.944376 -2.235336 0.653619
N -2.806453 -1.356235 -0.140963
C -3.628736 -2.091743 -1.092366
C -3.590321 -0.401946 0.648115
C -3.883876 0.904825 -0.110858
C -2.626330 1.551987 -0.704466
C -1.614938 1.996381 0.344768
C -0.198190 2.312445 -0.109560
O -1.929130 2.147488 1.511678
N 0.279241 3.352985 0.480041
O 1.588158 3.635265 0.072565
C 4.647270 0.119870 0.298842
H 4.490770 -1.119018 -1.436815
O 1.829526 -1.975668 2.045385
H 2.027050 1.064435 0.385433
H 2.859943 -2.685151 -0.691204
H 3.909387 -2.447605 0.708802
H 2.313969 -0.484804 -2.231932
H 3.170418 0.993792 -1.817145

H -0.573861 -1.026455 -1.383487
H 0.803375 -2.106158 -1.510607
H 1.158328 2.185221 -1.732134
H -0.100897 0.957586 -1.786744
H -1.063630 -3.447811 -0.918406
H -0.115055 -3.351914 0.552674
H -2.501695 -3.099877 1.063831
H -1.586594 -1.664082 1.515719
H -3.002227 -2.696876 -1.755039
H -4.193455 -1.396695 -1.721824
H -4.353039 -2.767316 -0.595808
H -3.016800 -0.148466 1.543046
H -4.544434 -0.841422 0.996539
H -4.364344 1.599612 0.586469
H -4.598440 0.727795 -0.924431
H -2.158143 0.869925 -1.418549
H -2.894767 2.454834 -1.275675
H 1.783461 4.446463 0.568601
H 5.082639 0.984394 -0.215895
H 4.056679 0.496309 1.141953
H 5.469045 -0.471587 0.718307

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.625537154**

Comp_16E_c12

B3LYP/6-31G* Geometry

C -3.899068 -0.519166 1.080244
C -3.466865 -1.658644 0.125484
C -2.512417 -1.183629 -0.967155
C -2.656222 0.244803 1.585733
C -1.778450 0.780997 0.441097
C -1.308007 -0.362430 -0.502549
C -0.223147 -1.292880 0.101074
C -0.626942 1.657275 1.015352
H -0.893075 0.095837 -1.406890
C 0.659371 -1.984007 -0.950332
C 1.944803 -2.543166 -0.319887
N 2.767706 -1.474244 0.262273
C 3.397880 -1.839805 1.523825
C 3.717950 -0.889584 -0.683132
C 4.124335 0.558849 -0.361530
C 3.015092 1.596418 -0.590813
C 1.925599 1.593253 0.475519
C 0.512249 1.958507 0.071618
O 2.166291 1.365278 1.649780
N 0.432252 2.579736 -1.052197
O -0.867999 2.998369 -1.336836
C -4.938255 0.400690 0.418387
H -4.381940 -0.982215 1.951574
O -2.688136 -1.461368 -2.140281
H -2.394719 1.442311 -0.176162
H -2.947603 -2.432136 0.709949
H -4.326225 -2.135727 -0.355845
H -2.056605 -0.420535 2.223395

H -2.975771 1.077984 2.226358
H 0.439412 -0.706432 0.743377
H -0.677230 -2.051497 0.753177
H -1.069098 2.609291 1.338119
H -0.189848 1.195600 1.904930
H 0.114641 -2.789902 -1.459059
H 0.928112 -1.259531 -1.731119
H 1.671392 -3.238177 0.483210
H 2.508110 -3.137546 -1.061484
H 4.201171 -2.594355 1.408332
H 2.644611 -2.242700 2.207802
H 3.824635 -0.952949 2.000220
H 3.259189 -0.904751 -1.679563
H 4.634980 -1.509690 -0.754046
H 4.970279 0.815578 -1.012055
H 4.488710 0.639643 0.667602
H 3.454208 2.604756 -0.573492
H 2.569184 1.483364 -1.582665
H -0.767989 3.427383 -2.202131
H -5.230749 1.212937 1.094434
H -4.563922 0.854252 -0.506730
H -5.842251 -0.162354 0.159326

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.630750813**

Comp_16E_c13

B3LYP/6-31G* Geometry

C 3.312856 0.382997 0.517770
C 3.661654 -1.045475 0.035248
C 2.503746 -1.707460 -0.698437
C 1.956099 0.394040 1.245186
C 0.808955 -0.246882 0.435727
C 1.181563 -1.718362 0.073168
C 0.097251 -2.554012 -0.626419
C 0.428747 0.579861 -0.822979
H 1.409631 -2.203109 1.037318
C -1.084620 -2.997579 0.274860
C -2.460105 -2.405624 -0.074804
N -2.656690 -0.994566 0.298499
C -2.849921 -0.864657 1.745351
C -3.795728 -0.423256 -0.432602
C -3.911409 1.105509 -0.361814
C -2.678706 1.839742 -0.906662
C -1.542141 1.986618 0.095689
C -0.131605 1.934061 -0.467731
O -1.732280 2.179507 1.281643
N 0.430404 3.079041 -0.573353
O 1.739757 2.988987 -1.093703
C 4.429658 0.956430 1.397707
H 3.226606 1.025751 -0.366942
O 2.622465 -2.179812 -1.814916
H -0.080210 -0.283373 1.073941
H 4.537732 -1.046501 -0.621077
H 3.900724 -1.665474 0.914034

H 1.690043 1.424889 1.507861
H 2.054488 -0.151828 2.196018
H -0.278100 -2.023120 -1.508167
H 0.594984 -3.441426 -1.030527
H 1.281474 0.701995 -1.495145
H -0.348702 0.035414 -1.367903
H -1.195108 -4.086618 0.196509
H -0.852700 -2.810699 1.331170
H -2.597650 -2.486780 -1.159913
H -3.247316 -3.035423 0.385137
H -3.780250 -1.360068 2.084416
H -2.882204 0.187764 2.032209
H -2.012217 -1.321078 2.279145
H -4.752011 -0.867120 -0.089431
H -3.682571 -0.706063 -1.486879
H -4.102922 1.446900 0.660545
H -4.790714 1.389080 -0.953132
H -2.314065 1.372943 -1.829366
H -2.947037 2.872648 -1.176776
H 2.005662 3.921259 -1.125464
H 4.203528 1.987417 1.694049
H 4.555406 0.364401 2.313736
H 5.390203 0.961729 0.868878

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.626600657

Comp_16E_c14

B3LYP/6-31G* Geometry

C 3.812458 -0.178898 -0.562239
C 3.499987 -0.885051 0.769082
C 2.048047 -1.342326 0.844251
C 2.887436 1.049537 -0.771105
C 1.571746 1.001555 0.044759
C 1.001948 -0.433754 0.190196
C 0.466015 -1.044911 -1.132701
C 0.577630 2.049178 -0.527952
H 0.152856 -0.398100 0.882412
C -0.288564 -2.384822 -1.017829
C -1.292093 -2.540983 0.136677
N -2.248973 -1.443918 0.352224
C -3.000076 -1.704799 1.578006
C -3.134486 -1.209523 -0.789138
C -4.008836 0.054077 -0.651941
C -3.291974 1.275313 -0.041942
C -1.968065 1.569307 -0.721540
C -0.792820 2.044826 0.098521
O -1.831562 1.432186 -1.929813
N -1.089350 2.459197 1.280109
O 0.026690 2.947514 1.961890
C 5.293789 0.200899 -0.670694
H 3.600567 -0.903076 -1.361542
O 1.741893 -2.388243 1.392727
H 1.806215 1.328674 1.064882
H 4.141399 -1.756749 0.934997

H 3.681391 -0.192796 1.606992
H 2.661835 1.147564 -1.840740
H 3.426764 1.965453 -0.492937
H 1.290104 -1.179710 -1.846483
H -0.198686 -0.306141 -1.585981
H 1.023192 3.041441 -0.384409
H 0.443305 1.900287 -1.602092
H -0.780860 -2.567057 -1.982168
H 0.428764 -3.204256 -0.889154
H -1.826968 -3.501550 -0.010831
H -0.715837 -2.643335 1.060979
H -3.666711 -0.870121 1.811411
H -2.305043 -1.824567 2.415398
H -3.616286 -2.623068 1.512400
H -3.797513 -2.078833 -0.976792
H -2.507574 -1.094458 -1.676451
H -4.375961 0.306819 -1.652365
H -4.895115 -0.152887 -0.040096
H -3.930775 2.161812 -0.165655
H -3.132134 1.155921 1.029746
H -0.351775 3.226674 2.811239
H 5.940022 -0.681463 -0.594210
H 5.505577 0.690398 -1.628842
H 5.578486 0.896774 0.129063

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.629221176

Comp_16E_c15

B3LYP/6-31G* Geometry

C 3.977286 -0.271694 -0.474929
C 3.824531 0.987477 0.410761
C 2.398773 1.218222 0.903452
C 2.850862 -0.347828 -1.524057
C 1.430986 -0.215388 -0.924806
C 1.335111 1.162977 -0.193165
C -0.055593 1.616701 0.278577
C 1.122620 -1.478745 -0.068398
H 1.676250 1.893567 -0.947565
C -0.976779 2.037387 -0.877397
C -2.422530 2.311992 -0.436525
N -3.136948 1.106002 0.002315
C -4.236178 1.424606 0.904996
C -3.580493 0.278021 -1.122822
C -3.897225 -1.178559 -0.739235
C -2.842353 -1.823218 0.174076
C -1.437562 -1.763182 -0.405113
C -0.259721 -1.619227 0.518787
O -1.233333 -1.834514 -1.610506
N -0.541473 -1.689082 1.774528
O 0.576055 -1.578009 2.590888
C 5.363766 -0.321753 -1.128159
H 3.893828 -1.147208 0.183634
O 2.145967 1.452888 2.070393
H 0.716490 -0.208596 -1.753233

H 4.492366 0.952406 1.277403
H 4.105468 1.870411 -0.185896
H 2.933387 -1.292205 -2.078250
H 2.996239 0.455458 -2.261728
H -0.542026 0.840276 0.871449
H 0.079283 2.465461 0.960544
H 1.265638 -2.338424 -0.735711
H 1.840725 -1.575495 0.747282
H -0.584378 2.952218 -1.344607
H -0.973915 1.275910 -1.666580
H -2.400693 3.008901 0.410512
H -2.968943 2.828753 -1.249947
H -4.694174 0.504652 1.282371
H -5.034067 2.025425 0.424716
H -3.858117 1.985333 1.766095
H -2.778762 0.260175 -1.864307
H -4.464344 0.721575 -1.624286
H -3.987434 -1.752868 -1.667833
H -4.869015 -1.246008 -0.234719
H -2.844285 -1.367178 1.164090
H -3.086223 -2.886419 0.317667
H 0.190762 -1.573734 3.481833
H 5.492445 -1.240311 -1.712947
H 5.510382 0.529405 -1.805642
H 6.159538 -0.289578 -0.374703

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.634209160

Comp_16E_c16

B3LYP/6-31G* Geometry

C 3.645914 -0.785643 -0.650660
C 3.896055 0.640623 -0.111358
C 2.688640 1.222512 0.615229
C 2.315175 -0.828584 -1.419431
C 1.112903 -0.324361 -0.592067
C 1.365474 1.158291 -0.164438
C 0.218144 1.895364 0.557230
C 0.830753 -1.297087 0.593409
H 1.575982 1.692379 -1.107468
C -0.702345 2.726280 -0.355260
C -1.641834 1.949395 -1.291435
N -2.568021 1.040243 -0.606977
C -3.556315 1.762706 0.187083
C -3.199214 0.103842 -1.540405
C -3.893528 -1.085919 -0.851098
C -3.116005 -1.653353 0.355781
C -1.638736 -1.828776 0.050280
C -0.606756 -1.369684 1.045142
O -1.260506 -2.332908 -0.999594
N -1.053508 -1.156915 2.233296
O -0.054950 -0.789368 3.132317
C 4.821097 -1.268452 -1.508399
H 3.565292 -1.458262 0.215511
O 2.787104 1.707540 1.727210

H 0.241025 -0.341734 -1.249626
H 4.755519 0.673865 0.565650
H 4.118950 1.301429 -0.964485
H 2.112787 -1.851166 -1.762659
H 2.408446 -0.210204 -2.325186
H -0.380382 1.195330 1.144759
H 0.678161 2.572291 1.284599
H 1.091084 -2.307630 0.254501
H 1.461042 -1.065904 1.454364
H -1.293659 3.403824 0.274079
H -0.089216 3.384237 -0.988214
H -2.193076 2.678435 -1.920054
H -1.042764 1.345091 -1.982664
H -4.191423 2.429109 -0.429592
H -3.063694 2.371818 0.949383
H -4.211897 1.057836 0.705593
H -2.406872 -0.292641 -2.182068
H -3.925977 0.610296 -2.206512
H -4.026935 -1.867359 -1.606985
H -4.898653 -0.811554 -0.508808
H -3.233926 -1.022964 1.237210
H -3.524047 -2.641456 0.610045
H -0.553616 -0.638476 3.951297
H 4.662894 -2.297827 -1.850980
H 4.943935 -0.635407 -2.396720
H 5.762010 -1.241689 -0.946296

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.631994455

Comp_16E_c17

B3LYP/6-31G* Geometry

C 3.811664 -0.204285 -0.484114
C 3.413953 -0.889436 0.836248
C 1.952759 -1.327988 0.856275
C 2.893478 1.012167 -0.783609
C 1.544462 0.983337 -0.028001
C 0.959144 -0.445416 0.098607
C 0.569619 -1.120233 -1.250770
C 0.573484 2.026344 -0.638989
H 0.048630 -0.397959 0.704400
C -0.347575 -2.353103 -1.128896
C -1.842586 -2.071820 -0.887196
N -2.192797 -1.438258 0.395079
C -1.849432 -2.301298 1.530378
C -3.622319 -1.103132 0.450653
C -4.060800 0.100220 -0.394406
C -3.321549 1.401634 -0.042972
C -1.964080 1.490613 -0.721489
C -0.783225 2.067624 0.015501
O -1.821235 1.145976 -1.887370
N -1.054007 2.592079 1.159569
O 0.073836 3.148727 1.763954
C 5.294330 0.186296 -0.493525
H 3.664601 -0.945302 -1.281979

O 1.609913 -2.341599 1.444406
H 1.736652 1.316828 0.999648
H 4.035227 -1.765765 1.048782
H 3.561474 -0.189663 1.674669
H 2.714756 1.067675 -1.865269
H 3.415169 1.941311 -0.516181
H 0.072281 -0.375944 -1.880563
H 1.481247 -1.417368 -1.786448
H 1.037577 3.015059 -0.540924
H 0.421738 1.831293 -1.703140
H -0.303719 -2.894745 -2.083692
H 0.048855 -3.042962 -0.377068
H -2.195740 -1.415336 -1.688404
H -2.390069 -3.031518 -0.993433
H -2.127471 -1.798752 2.462979
H -0.775193 -2.493529 1.562515
H -2.380153 -3.272828 1.495249
H -3.856109 -0.877220 1.498506
H -4.244937 -1.978920 0.176269
H -5.134720 0.240088 -0.217954
H -3.946467 -0.093493 -1.465669
H -3.900807 2.258784 -0.416038
H -3.223361 1.532336 1.036917
H -0.286810 3.507292 2.590980
H 5.570865 0.658152 -1.443949
H 5.516162 0.900463 0.310014
H 5.939877 -0.688711 -0.352852

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.632255821

Comp_16E_c18

B3LYP/6-31G* Geometry

C -3.978617 -0.230607 0.351554
C -3.484132 -1.695003 0.338517
C -1.964986 -1.776797 0.367494
C -3.289866 0.552072 -0.777674
C -1.750232 0.516343 -0.707654
C -1.231208 -0.959497 -0.702140
C 0.287971 -1.032185 -0.537156
C -1.207499 1.371047 0.489346
H -1.534377 -1.388133 -1.672360
C 1.007883 -2.317768 -0.965822
C 2.385951 -2.397200 -0.277513
N 3.160490 -1.149427 -0.394969
C 4.177728 -1.206273 -1.430872
C 3.642104 -0.600550 0.873347
C 3.867742 0.925313 0.861826
C 2.721538 1.749104 0.257271
C 1.376624 1.573573 0.946817
C 0.129868 2.015446 0.206062
O 1.259361 1.090121 2.060825
N 0.326358 2.990811 -0.608952
O -0.863777 3.425119 -1.208187
C -5.506278 -0.158032 0.252206

H -3.680870 0.213027 1.313349
O -1.375767 -2.435574 1.206146
H -1.375844 0.980028 -1.626207
H -3.877100 -2.265473 1.185957
H -3.840578 -2.175812 -0.586310
H -3.627684 1.596458 -0.774289
H -3.608639 0.126313 -1.741549
H 0.504210 -0.866274 0.521496
H 0.741674 -0.203282 -1.087814
H -1.925464 2.176268 0.684473
H -1.115627 0.780154 1.405037
H 0.432904 -3.206066 -0.677885
H 1.116418 -2.344560 -2.059581
H 2.211191 -2.600868 0.785000
H 2.958952 -3.255477 -0.665396
H 4.602870 -0.212078 -1.607935
H 3.732324 -1.544282 -2.372984
H 5.013582 -1.891839 -1.184373
H 4.581160 -1.086842 1.206886
H 2.887135 -0.815591 1.632294
H 4.043559 1.234771 1.898813
H 4.781686 1.174060 0.307265
H 2.968290 2.819837 0.290638
H 2.595255 1.510961 -0.802596
H -0.559918 4.162773 -1.761148
H -5.984789 -0.713150 1.067356
H -5.856153 0.879911 0.300947
H -5.858168 -0.585773 -0.695560

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.628603500

Comp_16E_c19

B3LYP/6-31G* Geometry

C 3.786758 -0.331905 -0.610076
C 3.573029 -0.642715 0.883439
C 2.138803 -1.054517 1.203730
C 2.795422 0.755914 -1.109992
C 1.551437 0.934552 -0.208287
C 1.037454 -0.410459 0.358388
C 0.518127 -1.408780 -0.712637
C 0.478960 1.780242 -0.939710
H 0.212398 -0.202235 1.049883
C -0.211458 -2.640860 -0.150952
C -1.538314 -2.337481 0.560824
N -2.466492 -1.515696 -0.219812
C -2.899698 -2.155489 -1.457192
C -3.596947 -1.040282 0.586946
C -3.363215 0.345517 1.200658
C -3.333310 1.490137 0.161475
C -2.109835 1.508986 -0.740802
C -0.797064 2.003485 -0.166775
O -2.159118 1.210791 -1.923283
N -0.916850 2.677376 0.923581
O 0.297820 3.216613 1.355527

C 5.242302 0.050698 -0.903704
H 3.577631 -1.260334 -1.159242
O 1.886395 -1.856167 2.087053
H 1.862479 1.522565 0.661972
H 4.242383 -1.433440 1.238207
H 3.800902 0.253000 1.483667
H 2.485465 0.515477 -2.135128
H 3.312449 1.723289 -1.171310
H -0.165410 -0.869087 -1.376296
H 1.354998 -1.750387 -1.335349
H 0.922391 2.761124 -1.157836
H 0.207112 1.328988 -1.897214
H -0.387814 -3.340677 -0.977570
H 0.429428 -3.167881 0.563861
H -2.005902 -3.299853 0.854770
H -1.326991 -1.805037 1.495067
H -3.477134 -3.086102 -1.291082
H -2.035390 -2.403305 -2.079209
H -3.516639 -1.455086 -2.027215
H -3.844706 -1.760560 1.387387
H -4.484246 -0.985393 -0.055228
H -2.439501 0.352683 1.791276
H -4.180005 0.552638 1.905078
H -4.208139 1.421910 -0.494206
H -3.375384 2.443577 0.697561
H 0.038306 3.702497 2.154922
H 5.388594 0.250762 -1.971879
H 5.527028 0.956618 -0.353122
H 5.933610 -0.749655 -0.614518

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.629909079

Comp_16Z_c01

B3LYP/6-31G* Geometry

C 3.871730 0.201318 0.051225
C 3.867425 -1.318261 -0.243971
C 2.489865 -1.814395 -0.663529
C 2.711784 0.577444 0.992150
C 1.332305 0.069222 0.519974
C 1.369939 -1.481966 0.321785
C 0.030031 -2.137398 -0.046404
C 0.846557 0.834119 -0.747228
H 1.698002 -1.887502 1.293841
C -0.988413 -2.184476 1.103728
C -2.408190 -2.514625 0.615606
N -3.024767 -1.410757 -0.137112
C -4.020886 -1.892809 -1.088213
C -3.580650 -0.387443 0.756377
C -3.785276 0.987478 0.096382
C -2.546020 1.530231 -0.623595
C -1.348578 1.775255 0.271946
C -0.023406 2.027063 -0.435850
O -1.387332 1.735244 1.488591
N 0.375625 3.187449 -0.798621

C 5.225368 0.654991 0.609862
H 3.721480 0.717164 -0.907894
O 2.299707 -2.406314 -1.710754
H 0.619317 0.270997 1.325457
O -0.580876 4.180045 -0.479498
H 4.587262 -1.575321 -1.027421
H 4.159114 -1.856254 0.671554
H 2.675474 1.668100 1.111677
H 2.916010 0.162634 1.990314
H 0.231937 -3.156083 -0.398382
H -0.426886 -1.624079 -0.898974
H 1.689214 1.191447 -1.347131
H 0.270936 0.162489 -1.395116
H -0.684749 -2.944003 1.837682
H -1.006105 -1.232162 1.647402
H -2.353797 -3.384298 -0.050768
H -3.042563 -2.817402 1.470228
H -4.409628 -1.060330 -1.683470
H -4.883497 -2.388834 -0.600858
H -3.560259 -2.607199 -1.778167
H -2.892180 -0.257059 1.593077
H -4.545058 -0.722064 1.188308
H -4.611128 0.949930 -0.624634
H -4.090603 1.688771 0.881559
H -2.234424 0.844977 -1.422111
H -2.762493 2.490598 -1.114714
H 5.241686 1.739317 0.770637
H 5.435875 0.170776 1.572197
H 6.042608 0.404354 -0.076422
H -0.155074 4.987907 -0.805918

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.628809374

Comp_16Z_c02

B3LYP/6-31G* Geometry

C 3.353829 0.639089 0.473516
C 3.784608 -0.787955 0.058024
C 2.688055 -1.541029 -0.684645
C 1.977870 0.604005 1.160765
C 0.892966 -0.122836 0.339047
C 1.337646 -1.592129 0.041875
C 0.315868 -2.498203 -0.671325
C 0.512747 0.653472 -0.946087
H 1.557776 -2.031066 1.029817
C -0.695780 -3.223872 0.233300
C -1.709195 -2.362751 1.006553
N -2.465180 -1.403025 0.190226
C -3.315845 -2.073165 -0.789672
C -3.241027 -0.495711 1.045726
C -3.784359 0.753986 0.329023
C -2.754222 1.472867 -0.554107
C -1.480230 1.863634 0.172267
C -0.216312 1.945831 -0.671570
O -1.425721 2.061530 1.371882

N 0.239811 3.031573 -1.171041
C 4.415276 1.302160 1.358912
H 3.267602 1.238919 -0.443122
O 2.877754 -2.051906 -1.773365
H -0.005441 -0.179258 0.958218
O -0.608004 4.125471 -0.879204
H 4.681474 -0.772140 -0.569212
H 4.023773 -1.359040 0.969260
H 1.644060 1.624913 1.382300
H 2.078127 0.095740 2.131768
H 0.882659 -3.257876 -1.220240
H -0.226176 -1.936368 -1.438385
H 1.387618 0.880389 -1.563891
H -0.150358 0.027255 -1.554163
H -1.235102 -3.954665 -0.382936
H -0.154078 -3.821338 0.980692
H -2.393259 -3.045273 1.551402
H -1.180741 -1.786293 1.774729
H -3.852952 -1.333344 -1.390293
H -4.066326 -2.737488 -0.317652
H -2.712166 -2.674212 -1.475070
H -2.579071 -0.160104 1.848773
H -4.087553 -1.021996 1.530282
H -4.653901 0.504489 -0.290786
H -4.144360 1.439748 1.103963
H -2.490907 0.865189 -1.426380
H -3.177694 2.407587 -0.952228
H 4.128939 2.329493 1.612289
H 4.545302 0.749473 2.298440
H 5.388143 1.338516 0.854736
H -0.141408 4.863785 -1.300717

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.627478097**

Comp_16Z_c03

B3LYP/6-31G* Geometry

C -4.040731 0.080172 0.461272
C -3.594652 -1.246991 -0.201364
C -2.255772 -1.132656 -0.923683
C -2.885489 0.684532 1.291891
C -1.594785 0.855844 0.470178
C -1.116598 -0.501228 -0.124607
C -0.591424 -1.511986 0.927389
C -0.501546 1.621717 1.254943
H -0.310526 -0.303391 -0.839162
C -0.008908 -2.808614 0.337418
C 1.214667 -2.597308 -0.571899
N 2.196783 -1.668011 -0.008476
C 2.811150 -2.175976 1.214246
C 3.209833 -1.251550 -0.977989
C 3.868403 0.094753 -0.640322
C 2.902190 1.285047 -0.700103
C 2.004371 1.442842 0.518117
C 0.637931 2.101383 0.369613

O 2.343601 1.091197 1.635634
N 0.343348 3.095073 -0.389911
C -4.593767 1.062574 -0.584500
H -4.860726 -0.154495 1.153327
O -2.094939 -1.549270 -2.057918
H -1.835922 1.500971 -0.385764
O 1.403159 3.555442 -1.184962
H -3.481063 -2.014577 0.578357
H -4.339083 -1.615400 -0.914158
H -2.691973 0.048678 2.166596
H -3.198401 1.660259 1.686707
H -1.391747 -1.774983 1.629971
H 0.189728 -1.019540 1.512282
H -0.971372 2.501307 1.708900
H -0.084420 1.025208 2.069770
H 0.249425 -3.476490 1.168749
H -0.766105 -3.342595 -0.250639
H 1.661635 -3.585752 -0.801569
H 0.873830 -2.180821 -1.526059
H 3.454158 -1.411095 1.654795
H 3.414198 -3.088016 1.035793
H 2.045747 -2.415982 1.956677
H 2.719900 -1.158178 -1.955490
H 3.998479 -2.021515 -1.096889
H 4.348454 0.064038 0.342954
H 4.669320 0.262509 -1.371634
H 3.467917 2.223986 -0.773507
H 2.289363 1.252571 -1.607716
H -4.897765 2.005667 -0.115229
H -3.858887 1.297943 -1.362887
H -5.471088 0.638158 -1.085889
H 0.992199 4.297813 -1.655209

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.626378931**

Comp_16Z_c04

B3LYP/6-31G* Geometry

C 4.015871 0.146542 -0.283646
C 3.535557 -1.233509 0.231147
C 2.125031 -1.210031 0.813171
C 2.926615 0.813072 -1.155970
C 1.568118 0.892645 -0.435940
C 1.057428 -0.522194 -0.036605
C 0.678304 -1.440510 -1.230669
C 0.535950 1.746506 -1.215091
H 0.169668 -0.422762 0.593923
C 0.003343 -2.767700 -0.818533
C -1.529313 -2.692460 -0.777292
N -2.067857 -1.703243 0.162842
C -2.020974 -2.189097 1.539459
C -3.403467 -1.254001 -0.235889
C -3.875940 0.028263 0.472711
C -2.803887 1.108244 0.681596
C -1.976201 1.457148 -0.538838

C -0.640989 2.172217 -0.353776
O -2.314078 1.183917 -1.679000
N -0.404802 3.163285 0.427887
C 4.469908 1.044169 0.879347
H 4.893433 -0.025862 -0.921258
O 1.860346 -1.744794 1.877199
H 1.732276 1.438943 0.503290
O -1.498517 3.551959 1.218658
H 3.524786 -1.943465 -0.609008
H 4.211889 -1.641606 0.988712
H 2.820788 0.260561 -2.099498
H 3.255563 1.824441 -1.429012
H 1.572643 -1.657676 -1.826775
H -0.002559 -0.894116 -1.893423
H 1.044986 2.652656 -1.560807
H 0.155662 1.230433 -2.100419
H 0.258109 -3.545059 -1.551100
H 0.400233 -3.120597 0.140419
H -1.875985 -2.414660 -1.779568
H -1.938765 -3.702092 -0.573922
H -0.987189 -2.391923 1.835223
H -2.616793 -3.111815 1.682623
H -2.411654 -1.428308 2.222110
H -4.167736 -2.043155 -0.086910
H -3.360995 -1.044802 -1.306841
H -4.702368 0.438255 -0.119723
H -4.297455 -0.204812 1.458530
H -3.277768 2.035977 1.024866
H -2.111120 0.833567 1.485432
H 4.806971 2.020849 0.512468
H 3.669688 1.219382 1.607655
H 5.303916 0.582238 1.419966
H -1.135737 4.310638 1.701992

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623014526

Comp_16Z_c05

B3LYP/6-31G* Geometry

C 3.354154 0.905480 0.501868
C 3.878144 -0.497139 0.113562
C 2.852054 -1.311573 -0.664524
C 1.950634 0.811684 1.128370
C 0.940416 0.012874 0.277449
C 1.485598 -1.429238 0.019223
C 0.529514 -2.397147 -0.698936
C 0.557624 0.775104 -1.024590
H 1.703338 -1.835390 1.021726
C -0.393189 -3.224370 0.215206
C -1.392300 -2.465765 1.104785
N -2.216473 -1.461223 0.419574
C -2.983876 -2.030152 -0.687929
C -3.097720 -0.787978 1.380567
C -3.714549 0.528199 0.885324
C -2.689331 1.634669 0.601625

C -1.924909 1.448024 -0.700102
C -0.456098 1.856774 -0.749366
O -2.436656 1.004394 -1.711173
N -0.039485 3.059136 -0.602831
C 4.340403 1.628501 1.426668
H 3.278934 1.494464 -0.422527
O 3.107398 -1.819156 -1.740875
H 0.020006 -0.105889 0.857176
O -1.101310 3.955487 -0.332019
H 4.795871 -0.432832 -0.479427
H 4.114002 -1.051568 1.035829
H 1.565896 1.824216 1.301479
H 2.033383 0.333703 2.116453
H 1.139084 -3.093768 -1.284503
H -0.075613 -1.856483 -1.433175
H 1.439010 1.225780 -1.490107
H 0.114704 0.094939 -1.757110
H -0.935634 -3.942632 -0.412322
H 0.221638 -3.837037 0.890106
H -2.026959 -3.218471 1.616345
H -0.842681 -1.942171 1.897776
H -2.315480 -2.507544 -1.407277
H -3.509673 -1.235730 -1.220495
H -3.720613 -2.783858 -0.347652
H -2.502717 -0.570826 2.277712
H -3.914552 -1.463262 1.706822
H -4.325013 0.367616 -0.008903
H -4.399665 0.878943 1.667387
H -3.197637 2.603814 0.509399
H -1.983119 1.745284 1.433557
H 3.991745 2.641651 1.658679
H 4.458631 1.088911 2.375365
H 5.330847 1.711686 0.964140
H -0.640891 4.807588 -0.286309

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.627308051

Comp_16Z_c06

B3LYP/6-31G* Geometry

C 4.051221 0.280818 -0.341898
C 3.573157 -1.179928 -0.171405
C 2.237131 -1.267544 0.555108
C 2.927340 1.126981 -0.975306
C 1.600640 1.065613 -0.193303
C 1.103828 -0.400511 0.002969
C 0.509590 -1.043477 -1.276390
C 0.564429 2.022148 -0.836787
H 0.314420 -0.402745 0.760701
C -0.068143 -2.463299 -1.109129
C -0.950503 -2.723122 0.125576
N -1.962962 -1.706518 0.441065
C -2.611474 -2.053277 1.702535
C -2.933186 -1.474976 -0.629255
C -3.834105 -0.246225 -0.385103

C -3.106102 0.977372 0.196006
C -1.976875 1.478536 -0.683536
C -0.748316 2.147984 -0.081714
O -2.004222 1.330752 -1.896885
N -0.702192 2.877464 0.975795
C 4.558491 0.861146 0.988254
H 4.898502 0.274961 -1.040999
O 2.076711 -2.008124 1.511065
H 1.785322 1.463023 0.814330
O -1.929440 3.025095 1.633949
H 3.442383 -1.629653 -1.166954
H 4.301890 -1.788825 0.372579
H 2.759664 0.787860 -2.007328
H 3.256728 2.172138 -1.047702
H 1.262289 -1.072633 -2.075484
H -0.281882 -0.387587 -1.642713
H 1.024068 3.015493 -0.882392
H 0.336812 1.727424 -1.864294
H -0.615612 -2.707661 -2.028628
H 0.747207 -3.196835 -1.050476
H -1.416169 -3.722399 0.001976
H -0.297291 -2.788230 1.001615
H -1.853788 -2.165370 2.484758
H -3.183905 -2.999897 1.642045
H -3.301470 -1.264156 2.014561
H -3.579832 -2.360691 -0.796142
H -2.377965 -1.313427 -1.556138
H -4.300446 0.020154 -1.339459
H -4.652176 -0.501701 0.299124
H -3.814941 1.809227 0.313926
H -2.720996 0.777903 1.197347
H 4.885619 1.900141 0.863527
H 3.789210 0.844125 1.768965
H 5.411114 0.282546 1.361733
H -1.689817 3.598948 2.378746

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624034595

Comp_16Z_c07

B3LYP/6-31G* Geometry

C 3.992699 0.311665 -0.316420
C 3.619178 -1.142500 0.051364
C 2.251632 -1.243784 0.714452
C 2.842401 0.968565 -1.108577
C 1.488774 0.922319 -0.369877
C 1.091590 -0.541526 0.004584
C 0.615219 -1.422760 -1.182772
C 0.418502 1.707657 -1.176923
H 0.283276 -0.496402 0.735435
C 0.110216 -2.821591 -0.781901
C -1.043106 -2.801249 0.236846
N -2.151227 -1.926781 -0.164507
C -3.008188 -2.551177 -1.163848
C -2.911306 -1.391029 0.966966

C -3.702555 -0.113369 0.626631
C -2.914234 0.927275 -0.178425
C -1.643454 1.428483 0.475584
C -0.734700 2.294415 -0.391419
O -1.321272 1.188680 1.624164
N -0.907410 3.560000 -0.496723
C 4.389209 1.117234 0.931670
H 4.870567 0.274726 -0.975666
O 2.077314 -1.889315 1.733745
H 1.612621 1.456426 0.581310
O -2.036762 3.992099 0.236822
H 3.584080 -1.746474 -0.867909
H 4.358678 -1.600575 0.715499
H 2.746200 0.474231 -2.086138
H 3.103099 2.014091 -1.318690
H 1.415287 -1.530943 -1.926679
H -0.211113 -0.910186 -1.683477
H 0.901021 2.561568 -1.665394
H 0.019515 1.080213 -1.984362
H -0.197042 -3.346277 -1.696258
H 0.920841 -3.420377 -0.347948
H -1.384904 -3.838764 0.415879
H -0.649782 -2.438466 1.190649
H -2.414361 -2.877250 -2.023614
H -3.752348 -1.837138 -1.531702
H -3.549396 -3.433884 -0.769429
H -2.197296 -1.143109 1.754725
H -3.611417 -2.140084 1.387309
H -4.611029 -0.357834 0.061801
H -4.038305 0.329154 1.571705
H -2.646381 0.533241 -1.166990
H -3.529170 1.819550 -0.367313
H 4.638604 2.152061 0.668910
H 3.587969 1.145418 1.678996
H 5.266406 0.672493 1.415303
H -2.030647 4.948562 0.077194

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.622890716

Comp_16Z_c08

B3LYP/6-31G* Geometry

C 3.240361 0.867397 0.502530
C 3.849101 -0.482241 0.050976
C 2.849895 -1.356150 -0.696964
C 1.890278 0.634824 1.202120
C 0.898446 -0.203547 0.370346
C 1.523984 -1.590485 0.032948
C 0.625753 -2.599481 -0.703457
C 0.423517 0.529231 -0.907812
H 1.796804 -2.032601 1.006217
C -0.537790 -3.207871 0.120502
C -1.961730 -2.711264 -0.190839
N -2.324439 -1.377484 0.318777
C -2.455676 -1.395114 1.778019

C -3.576964 -0.925052 -0.304418
C -3.928731 0.552325 -0.075617
C -2.912395 1.535416 -0.673571
C -1.639922 1.685394 0.146604
C -0.339843 1.797742 -0.631960
O -1.633201 1.723874 1.363068
N 0.113108 2.903169 -1.090321
C 4.217610 1.643523 1.392871
H 3.062032 1.471589 -0.397786
O 3.089716 -1.818785 -1.798055
H 0.011017 -0.384038 0.981932
O -0.762439 3.976385 -0.791089
H 4.727996 -0.337013 -0.585166
H 4.172363 -1.035542 0.947114
H 1.430051 1.596371 1.458486
H 2.069695 0.115557 2.155788
H 1.282144 -3.411159 -1.034348
H 0.242209 -2.162167 -1.632341
H 1.257417 0.774480 -1.574153
H -0.243853 -0.141434 -1.461290
H -0.561781 -4.287194 -0.077366
H -0.328110 -3.122635 1.194362
H -2.081834 -2.692178 -1.281234
H -2.680777 -3.466435 0.186175
H -2.613938 -0.383563 2.155519
H -1.537092 -1.770156 2.235473
H -3.291083 -2.041094 2.111033
H -4.430671 -1.546028 0.034995
H -3.484202 -1.089627 -1.385657
H -4.904896 0.726313 -0.545090
H -4.055691 0.772360 0.989081
H -2.661677 1.262051 -1.705969
H -3.345583 2.544803 -0.720567
H 5.171800 1.816168 0.881152
H 3.803970 2.619612 1.671799
H 4.429120 1.092472 2.318515
H -0.304092 4.731622 -1.190902

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.626408345

Comp_16Z_c09

B3LYP/6-31G* Geometry

C 3.890859 -0.017386 -0.422270
C 3.564441 -0.329019 1.051869
C 2.160867 -0.897763 1.239604
C 2.836607 0.939468 -1.048634
C 1.502684 0.996158 -0.270011
C 1.087762 -0.392484 0.274604
C 0.804849 -1.449425 -0.826916
C 0.409008 1.720247 -1.088949
H 0.168722 -0.283435 0.861386
C 0.214495 -2.781963 -0.334197
C -1.093823 -2.653035 0.462956
N -2.066804 -1.736256 -0.140910

C -2.536383 -2.197659 -1.444496
C -3.190048 -1.455300 0.755126
C -3.937388 -0.154168 0.428589
C -3.082105 1.106463 0.612297
C -2.123408 1.390779 -0.533578
C -0.805187 2.104334 -0.259476
O -2.378015 1.097663 -1.689845
N -0.614934 3.070384 0.565643
C 5.314774 0.530313 -0.578452
H 3.848370 -0.972426 -0.963697
O 1.911546 -1.715203 2.109434
H 1.668856 1.631438 0.611277
O -1.753037 3.435939 1.301298
H 4.280096 -1.032637 1.489901
H 3.630072 0.595390 1.647908
H 2.653911 0.642955 -2.089752
H 3.245344 1.957976 -1.094190
H 0.105367 -1.001277 -1.539054
H 1.723983 -1.663210 -1.387465
H 0.848192 2.636831 -1.499680
H 0.072087 1.120732 -1.938382
H 0.064808 -3.426733 -1.209789
H 0.933013 -3.303111 0.307974
H -1.520055 -3.665867 0.610620
H -0.850790 -2.268111 1.459102
H -1.690434 -2.376954 -2.112435
H -3.156951 -1.429481 -1.911344
H -3.121922 -3.135330 -1.373021
H -2.790746 -1.374235 1.774210
H -3.913552 -2.295154 0.768674
H -4.798701 -0.091039 1.105690
H -4.343671 -0.174805 -0.587562
H -3.728181 1.992112 0.685428
H -2.530828 1.075995 1.558246
H 5.545473 0.731852 -1.631314
H 5.434808 1.470673 -0.025175
H 6.060792 -0.178996 -0.201165
H -1.417874 4.173402 1.834996

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.624163376

Comp_16Z_c10

B3LYP/6-31G* Geometry

C 3.242094 0.879382 0.672926
C 3.838545 -0.468920 0.202996
C 2.890066 -1.250901 -0.697974
C 1.803544 0.692857 1.191516
C 0.881602 -0.062596 0.210553
C 1.492798 -1.461438 -0.109843
C 0.629848 -2.429585 -0.938379
C 0.582489 0.781420 -1.061689
H 1.663828 -1.928238 0.874859
C -0.461283 -3.211389 -0.164830
C -1.904187 -2.677821 -0.222004

N -2.204081 -1.480468 0.578132
C -2.215991 -1.783195 2.007004
C -3.479254 -0.887759 0.148581
C -3.750693 0.524370 0.697380
C -2.550253 1.480316 0.625301
C -1.870297 1.521667 -0.729281
C -0.393182 1.895649 -0.775872
O -2.429525 1.233779 -1.771152
N 0.052004 3.084455 -0.613526
C 4.140802 1.545586 1.721402
H 3.206876 1.545508 -0.199763
O 3.224509 -1.665041 -1.792879
H -0.078314 -0.259517 0.698756
O -0.995750 3.995263 -0.328777
H 4.786185 -0.326391 -0.325904
H 4.040776 -1.090247 1.089919
H 1.376133 1.676969 1.419345
H 1.835466 0.137636 2.141404
H 1.320246 -3.153214 -1.384399
H 0.178909 -1.912548 -1.793808
H 1.498621 1.212316 -1.476462
H 0.140071 0.152177 -1.840517
H -0.514726 -4.219091 -0.597401
H -0.147669 -3.366852 0.876378
H -2.132197 -2.436817 -1.266998
H -2.587609 -3.503549 0.061717
H -1.249134 -2.186723 2.320569
H -2.395328 -0.872499 2.586244
H -2.998013 -2.519948 2.276503
H -4.334221 -1.541025 0.413815
H -3.452240 -0.821914 -0.941276
H -4.585330 0.936423 0.119076
H -4.090851 0.483966 1.739389
H -2.863712 2.509252 0.850507
H -1.798453 1.228781 1.381832
H 3.744324 2.524766 2.014539
H 4.213936 0.928540 2.626451
H 5.156385 1.696044 1.336876
H -0.523174 4.840412 -0.278141

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624378832

Comp_16Z_c11

B3LYP/6-31G* Geometry

C 3.886874 -0.000322 -0.304217
C 3.436445 -0.461764 1.096267
C 2.015497 -1.021070 1.125381
C 2.876965 1.004643 -0.931866
C 1.493157 1.002706 -0.245824
C 1.032799 -0.430404 0.115063
C 0.892007 -1.386985 -1.104977
C 0.460012 1.828747 -1.048714
H 0.054985 -0.393411 0.604834
C 0.181218 -2.722882 -0.809478

C -1.347582 -2.661392 -0.929840
N -2.009946 -1.748647 0.010020
C -2.048318 -2.306486 1.360159
C -3.335423 -1.358221 -0.477034
C -3.946613 -0.147978 0.250600
C -2.966926 0.985397 0.590719
C -2.074525 1.434302 -0.549088
C -0.776912 2.172684 -0.236627
O -2.332114 1.222188 -1.722541
N -0.621766 3.118153 0.617902
C 5.309016 0.573145 -0.271749
H 3.914305 -0.896682 -0.938648
O 1.690907 -1.889385 1.918964
H 1.605736 1.538986 0.707182
O -1.777932 3.423539 1.355375
H 4.110040 -1.218412 1.512216
H 3.462726 0.391553 1.793086
H 2.767188 0.786263 -2.002034
H 3.284544 2.022750 -0.872391
H 1.885672 -1.596654 -1.519380
H 0.340369 -0.861217 -1.894675
H 0.940345 2.764924 -1.355013
H 0.146783 1.313440 -1.960974
H 0.518144 -3.468232 -1.542637
H 0.487793 -3.104237 0.169808
H -1.588970 -2.317371 -1.942890
H -1.758669 -3.687331 -0.841595
H -2.538192 -1.606131 2.043574
H -2.600076 -3.265953 1.403894
H -1.032083 -2.470335 1.730385
H -4.055481 -2.200012 -0.431320
H -3.221185 -1.091301 -1.530010
H -4.751264 0.237924 -0.386111
H -4.424453 -0.457661 1.188353
H -3.524551 1.867329 0.929815
H -2.323625 0.716972 1.436175
H 5.634869 0.873835 -1.274593
H 5.359292 1.459130 0.374343
H 6.028768 -0.161182 0.108860
H -1.474056 4.161018 1.907252

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.621727799

Comp_16Z_c12

B3LYP/6-31G* Geometry

C 3.847316 0.720452 -0.418647
C 3.614541 -0.736494 -0.893221
C 2.593024 -1.499482 -0.052621
C 2.499739 1.438882 -0.171453
C 1.593244 0.646819 0.786165
C 1.278052 -0.770773 0.228931
C 0.392731 -0.809628 -1.044382
C 0.366285 1.431115 1.328651
H 0.773981 -1.337069 1.018505

C -0.235291 -2.181078 -1.342068
 C -1.175296 -2.692314 -0.235328
 N -2.121355 -1.680991 0.255077
 C -2.619534 -2.010524 1.588284
 C -3.216189 -1.429270 -0.685123
 C -3.929474 -0.085093 -0.475844
 C -3.012006 1.134538 -0.653442
 C -2.115507 1.401215 0.547019
 C -0.693978 1.928724 0.358973
 O -2.507293 1.243088 1.691069
 N -0.347747 2.865933 -0.447673
 C 4.777741 0.762270 0.805255
 H 4.360717 1.252091 -1.231259
 O 2.797716 -2.635207 0.338820
 H 2.180716 0.467677 1.698888
 O -1.401936 3.330094 -1.257933
 H 3.234401 -0.717075 -1.925048
 H 4.544559 -1.313419 -0.904501
 H 1.985273 1.602982 -1.125398
 H 2.691215 2.437336 0.241671
 H 0.967764 -0.483291 -1.919351
 H -0.415394 -0.088301 -0.927490
 H -0.145196 0.816065 2.074493
 H 0.759731 2.303755 1.864270
 H -0.773707 -2.109571 -2.296296
 H 0.542379 -2.941262 -1.490876
 H -1.696057 -3.601961 -0.592123
 H -0.567475 -3.008911 0.618155
 H -3.196174 -1.175086 1.992280
 H -3.255161 -2.917013 1.595700
 H -1.774165 -2.181696 2.262120
 H -3.964827 -2.245968 -0.647737
 H -2.800452 -1.438514 -1.699458
 H -4.740310 -0.024206 -1.212690
 H -4.402829 -0.038388 0.509971
 H -2.413285 1.054169 -1.565922
 H -3.618166 2.041934 -0.779931
 H 4.931385 1.792944 1.146116
 H 4.383386 0.185736 1.650154
 H 5.758846 0.340508 0.558702
 H -0.967742 4.031990 -1.767334
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.620983851**

Comp_16Z_c13

B3LYP/6-31G* Geometry

C -3.768865 0.457642 -0.160229
 C -3.938944 -1.052773 0.135082
 C -2.646295 -1.699658 0.617720
 C -2.519176 0.719343 -1.023836
 C -1.236580 0.066109 -0.466523
 C -1.450973 -1.472118 -0.305668
 C -0.194689 -2.256514 0.093786
 C -0.763255 0.773435 0.842063

H -1.778366 -1.822264 -1.299389
 C 0.804844 -2.462186 -1.059896
 C 2.239760 -2.649092 -0.545581
 N 2.795917 -1.384520 -0.035284
 C 3.615041 -1.561468 1.161183
 C 3.509104 -0.651831 -1.083864
 C 3.714606 0.846961 -0.815389
 C 2.417952 1.664335 -0.769581
 C 1.678925 1.617590 0.556270
 C 0.180779 1.916592 0.554725
 O 2.214444 1.378431 1.621091
 N -0.318012 3.080479 0.365379
 C -5.032120 1.041307 -0.803911
 H -3.630247 0.961586 0.806477
 O -2.576720 -2.331626 1.655723
 H -0.445279 0.191107 -1.216474
 O 0.681336 4.041089 0.075753
 H -4.720143 -1.227810 0.881465
 H -4.242780 -1.561797 -0.793282
 H -2.364428 1.801294 -1.120657
 H -2.699974 0.333423 -2.038217
 H -0.498808 -3.228295 0.498715
 H 0.317702 -1.742421 0.913175
 H -1.622469 1.163837 1.395100
 H -0.248564 0.075808 1.507670
 H 0.511585 -3.334504 -1.660421
 H 0.791206 -1.604130 -1.745736
 H 2.228878 -3.379541 0.271740
 H 2.882084 -3.080072 -1.334049
 H 3.854362 -0.587907 1.594969
 H 4.559166 -2.105852 0.963513
 H 3.047539 -2.120414 1.911309
 H 2.932765 -0.752904 -2.012542
 H 4.498145 -1.114054 -1.281660
 H 4.273159 1.006919 0.112310
 H 4.343811 1.235341 -1.626227
 H 2.625301 2.730011 -0.941284
 H 1.732527 1.369242 -1.575410
 H -4.929659 2.120919 -0.964441
 H -5.228847 0.574585 -1.777781
 H -5.912157 0.877634 -0.171108
 H 0.164997 4.859362 0.012934
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624915141**

Comp_16Z_c14

B3LYP/6-31G* Geometry

C -4.039911 0.256568 0.231365
 C -3.554812 -1.195985 0.017513
 C -2.154127 -1.280543 -0.581286
 C -2.954418 1.074277 0.962747
 C -1.589156 1.028916 0.251286
 C -1.070456 -0.431415 0.086789
 C -0.623875 -1.124206 1.405947

C -0.592348 2.003238 0.926153
H -0.209110 -0.427202 -0.587429
C 0.158866 -2.438738 1.208148
C 1.648177 -2.287241 0.849263
N 1.945753 -1.707095 -0.468751
C 1.493147 -2.580197 -1.555642
C 3.378705 -1.421839 -0.610936
C 3.872356 -0.169658 0.128990
C 3.097772 1.099674 -0.258471
C 1.918873 1.386159 0.656248
C 0.716560 2.186844 0.179201
O 1.906582 0.998949 1.816268
N 0.680487 3.072158 -0.753685
C -4.476131 0.899394 -1.095775
H -4.924821 0.219671 0.881163
O -1.914449 -2.022802 -1.519946
H -1.732227 1.418433 -0.766766
O 1.893474 3.279050 -1.419257
H -3.525366 -1.708734 0.990062
H -4.234063 -1.762685 -0.626956
H -2.846420 0.699443 1.990373
H -3.285955 2.117509 1.050839
H -1.502328 -1.329639 2.031196
H 0.002258 -0.434509 1.979022
H -1.080861 2.981441 0.983366
H -0.363374 1.691871 1.948310
H 0.138190 -2.987900 2.159073
H -0.351013 -3.084304 0.483433
H 2.112037 -1.646829 1.606224
H 2.125499 -3.285551 0.938222
H 0.405711 -2.675812 -1.549107
H 1.943585 -3.590775 -1.502596
H 1.773162 -2.135391 -2.516115
H 3.570128 -1.271782 -1.680504
H 3.994865 -2.291414 -0.305263
H 3.835038 -0.298496 1.214781
H 4.930718 -0.042458 -0.130329
H 3.746064 1.985306 -0.193701
H 2.761606 1.065646 -1.298135
H -5.309752 0.342312 -1.538468
H -4.806898 1.933242 -0.941186
H -3.668009 0.914243 -1.836267
H 1.657463 3.975867 -2.051950

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624368217

Comp_16Z_c15

B3LYP/6-31G* Geometry

C -4.048747 -0.098509 -0.785449
C -3.695477 1.264544 -0.144441
C -2.490733 1.187907 0.787888
C -2.784865 -0.741343 -1.396941
C -1.633647 -0.878219 -0.383029
C -1.241192 0.500876 0.231408

C -0.511363 1.475575 -0.735573
C -0.445261 -1.646951 -0.994819
H -0.593085 0.317628 1.093660
C 0.129372 2.688322 -0.032602
C 1.467046 2.374778 0.658090
N 2.528569 1.951683 -0.267177
C 3.086251 3.082858 -1.002134
C 3.577901 1.170050 0.400379
C 3.168700 -0.290562 0.642616
C 2.936277 -1.047529 -0.679872
C 2.042946 -2.269507 -0.588327
C 0.642341 -2.052413 -0.017896
O 2.346810 -3.360988 -1.027203
N 0.328315 -2.261326 1.203315
C -4.755926 -1.020210 0.221680
H -4.754563 0.092281 -1.605106
O -2.509997 1.677991 1.903561
H -1.992120 -1.490891 0.452665
O 1.444174 -2.678216 1.961782
H -3.451135 1.981109 -0.942561
H -4.536651 1.680467 0.418755
H -2.452489 -0.142329 -2.256805
H -3.040801 -1.732331 -1.794856
H -1.208455 1.829285 -1.505139
H 0.283881 0.944607 -1.268182
H -0.819832 -2.568759 -1.463591
H 0.007558 -1.074113 -1.813159
H 0.276765 3.488524 -0.768262
H -0.552229 3.094356 0.724685
H 1.788379 3.257823 1.243948
H 1.308344 1.571180 1.384103
H 3.816108 2.724726 -1.735556
H 3.588637 3.820618 -0.346678
H 2.296900 3.606186 -1.549498
H 3.882945 1.632320 1.358178
H 4.464561 1.184940 -0.245273
H 3.949948 -0.790687 1.226430
H 2.267374 -0.325875 1.262045
H 2.447911 -0.344965 -1.372626
H 3.880427 -1.363987 -1.135780
H -5.694284 -0.569265 0.564062
H -4.994810 -1.989139 -0.232426
H -4.144567 -1.209266 1.111490
H 1.067452 -2.765250 2.851523

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624173692

Comp_16Z_c16

B3LYP/6-31G* Geometry

C 3.534175 0.595092 0.100924
C 3.865586 -0.899409 -0.121402
C 2.643174 -1.703058 -0.543104
C 2.306275 0.733895 1.016591
C 1.074241 -0.064427 0.540201

C 1.429312 -1.574479 0.384253
C 0.292645 -2.516175 -0.047630
C 0.451619 0.522593 -0.752620
H 1.780945 -1.893845 1.379999
C -0.876055 -2.730363 0.941073
C -2.040126 -1.716752 1.005278
N -2.636609 -1.338640 -0.288347
C -2.958174 -2.506383 -1.112633
C -3.870024 -0.555274 -0.110607
C -3.751828 0.830846 0.538396
C -2.817736 1.814978 -0.193600
C -1.419948 1.844587 0.403232
C -0.234804 1.847522 -0.542051
O -1.229106 1.811127 1.606751
N 0.175691 2.880665 -1.174054
C 4.745160 1.356036 0.652754
H 3.288463 1.029767 -0.878171
O 2.632602 -2.383523 -1.553302
H 0.324453 0.009716 1.331560
O -0.637264 4.005728 -0.884708
H 4.646939 -1.033001 -0.876261
H 4.238158 -1.319413 0.826379
H 2.035106 1.791715 1.117621
H 2.576775 0.387448 2.025525
H 0.756322 -3.494393 -0.218887
H -0.082750 -2.215236 -1.029714
H 1.197868 0.644736 -1.544758
H -0.314016 -0.168555 -1.125010
H -1.303881 -3.717243 0.725643
H -0.477961 -2.810323 1.962696
H -2.811095 -2.166925 1.664733
H -1.715549 -0.798370 1.501677
H -3.394441 -2.170603 -2.058911
H -3.683559 -3.188293 -0.627367
H -2.059248 -3.078617 -1.347833
H -4.614106 -1.137472 0.471229
H -4.300583 -0.418891 -1.110880
H -4.768353 1.242256 0.552235
H -3.440072 0.765836 1.585848
H -2.769223 1.607564 -1.268041
H -3.193857 2.841887 -0.089952
H 4.519078 2.422373 0.769201
H 5.039597 0.967032 1.636162
H 5.609985 1.266256 -0.015092
H -0.229376 4.698397 -1.427086

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.622778454

Comp_16Z_c17

B3LYP/6-31G* Geometry

C -4.052782 -0.592903 -0.806657
C -3.925391 0.867860 -0.315980
C -2.758345 1.075219 0.644522
C -2.688567 -1.097604 -1.322988

C -1.564149 -0.964281 -0.278342
C -1.405556 0.505791 0.213373
C -0.751885 1.483877 -0.804601
C -0.261483 -1.597017 -0.810134
H -0.789665 0.485895 1.114736
C -0.131611 2.729346 -0.146484
C 1.154378 2.427788 0.643897
N 2.193240 1.771442 -0.160596
C 2.893206 2.718557 -1.020556
C 3.115658 0.964367 0.642726
C 3.910883 -0.067982 -0.174571
C 3.072132 -0.963471 -1.119715
C 2.258633 -2.049716 -0.433571
C 0.897286 -1.693128 0.160489
O 2.621067 -3.210042 -0.402617
N 0.669473 -1.588199 1.413970
C -4.648726 -1.499075 0.283227
H -4.751387 -0.599383 -1.654331
O -2.885663 1.702995 1.681573
H -1.850807 -1.549106 0.604396
O 1.847027 -1.751018 2.178578
H -3.755880 1.521090 -1.184760
H -4.838846 1.215394 0.176597
H -2.415769 -0.537289 -2.229229
H -2.783673 -2.148238 -1.628601
H -1.486361 1.797934 -1.556705
H 0.046492 0.970773 -1.347460
H -0.481920 -2.623252 -1.141642
H 0.078989 -1.075533 -1.713611
H 0.076579 3.474082 -0.925499
H -0.848211 3.196679 0.540648
H 1.526777 3.364662 1.100893
H 0.909058 1.759756 1.475573
H 2.176555 3.274456 -1.631922
H 3.566711 2.192752 -1.704403
H 3.493524 3.451305 -0.445751
H 2.530368 0.434123 1.397489
H 3.841458 1.597893 1.191700
H 4.659434 0.439980 -0.794338
H 4.473428 -0.696764 0.525822
H 2.405407 -0.317309 -1.702449
H 3.747569 -1.486158 -1.804881
H -4.727787 -2.535020 -0.067204
H -4.045243 -1.501106 1.198388
H -5.653730 -1.160356 0.559524
H 1.516395 -1.651213 3.085321

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.621593986

Comp_16Z_c18

B3LYP/6-31G* Geometry

C 4.011887 -0.120102 -0.636062
C 3.615384 -1.340918 0.230001
C 2.336801 -1.120551 1.033691

C 2.792471 0.401129 -1.430430
C 1.587423 0.714083 -0.523492
C 1.141557 -0.555985 0.261839
C 0.522846 -1.678168 -0.614585
C 0.454819 1.436207 -1.302401
H 0.411709 -0.263990 1.023170
C -0.252719 -2.755068 0.169851
C -1.652515 -2.319911 0.655244
N -2.414229 -1.598787 -0.365345
C -2.695752 -2.425996 -1.534937
C -3.660255 -0.995081 0.113058
C -3.520985 0.073927 1.213603
C -2.310602 1.014578 1.118728
C -1.962608 1.560137 -0.249495
C -0.555676 2.137431 -0.410749
O -2.712309 1.572342 -1.206385
N -0.173023 3.236199 0.124464
C 4.672886 0.974720 0.217951
H 4.760746 -0.460052 -1.364050
O 2.259180 -1.410601 2.214526
H 1.922485 1.442471 0.226857
O -1.173747 3.817517 0.935717
H 3.444180 -2.205183 -0.427925
H 4.411239 -1.619912 0.927418
H 2.505018 -0.339004 -2.190044
H 3.082908 1.306983 -1.978456
H 1.312466 -2.168776 -1.195827
H -0.158801 -1.225863 -1.339034
H 0.926638 2.202200 -1.928187
H -0.074528 0.757621 -1.977905
H -0.351735 -3.640676 -0.469596
H 0.322242 -3.080006 1.045796
H -2.193677 -3.218898 1.014581
H -1.545031 -1.662355 1.523475
H -3.209858 -1.822804 -2.289939
H -3.334322 -3.300232 -1.299776
H -1.769582 -2.798319 -1.980875
H -4.372322 -1.765869 0.472122
H -4.117675 -0.520335 -0.758784
H -4.446004 0.662104 1.195420
H -3.485633 -0.396467 2.204104
H -2.461379 1.889347 1.765403
H -1.410831 0.531002 1.514494
H 4.940643 1.843317 -0.395112
H 4.020245 1.325178 1.026010
H 5.590006 0.597421 0.684526
H -0.743141 4.632550 1.236538

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.619042320

Comp_16Z_c19

B3LYP/6-31G* Geometry

C 3.859996 0.106529 -0.381309
C 3.521399 -0.367568 1.044229

C 2.149953 -1.028614 1.116572
C 2.780671 1.086082 -0.916761
C 1.418734 1.002838 -0.182221
C 1.058610 -0.456229 0.206136
C 0.802229 -1.402508 -1.000906
C 0.349198 1.762653 -1.009809
H 0.150409 -0.439198 0.813034
C 0.278175 -2.806610 -0.649694
C -0.998933 -2.813322 0.205367
N -2.066361 -1.957627 -0.326841
C -2.741024 -2.567822 -1.465398
C -3.008685 -1.511900 0.702559
C -3.815195 -0.262001 0.300725
C -2.981556 0.843108 -0.359210
C -1.821413 1.362119 0.464453
C -0.854678 2.292026 -0.261842
O -1.631103 1.088897 1.634607
N -1.033168 3.560755 -0.292748
C 5.264787 0.716438 -0.456989
H 3.857839 -0.787195 -1.021041
O 1.934124 -1.975309 1.853790
H 1.523565 1.550890 0.764169
O -2.215258 3.933534 0.386775
H 4.262649 -1.074771 1.430434
H 3.518740 0.493756 1.731201
H 2.635506 0.909111 -1.990737
H 3.146369 2.118096 -0.829692
H 1.717363 -1.507739 -1.598469
H 0.062379 -0.922064 -1.649076
H 0.820599 2.640509 -1.466467
H 0.005440 1.130562 -1.839835
H 0.112283 -3.347406 -1.591339
H 1.038132 -3.372890 -0.100425
H -1.340937 -3.858673 0.334005
H -0.737685 -2.450412 1.203271
H -3.294748 -3.487363 -1.190204
H -2.014735 -2.831581 -2.240493
H -3.455007 -1.866045 -1.909078
H -2.426706 -1.263026 1.592069
H -3.716529 -2.314502 0.990004
H -4.628370 -0.527287 -0.386446
H -4.293832 0.128142 1.206497
H -2.577497 0.503094 -1.321072
H -3.607228 1.718899 -0.587865
H 5.500729 1.037085 -1.478765
H 5.345104 1.595517 0.195273
H 6.030455 -0.003856 -0.145920
H -2.213295 4.898171 0.287297

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.621106604

Comp_16Z_c20

B3LYP/6-31G* Geometry

C 4.040793 -0.337311 -0.812740

C 3.541146 -1.592130 -0.061523
C 2.424752 -1.268514 0.924774
C 2.843884 0.407723 -1.438164
C 1.758203 0.795202 -0.412775
C 1.251377 -0.443387 0.388495
C 0.284636 -1.364767 -0.399154
C 0.653950 1.617455 -1.130666
H 0.714054 -0.084755 1.270392
C -0.460959 -2.380982 0.483306
C -1.776276 -2.861153 -0.153503
N -2.698719 -1.773315 -0.507142
C -3.730420 -2.231996 -1.428809
C -3.272624 -1.095085 0.660118
C -3.770378 0.333315 0.369881
C -2.748812 1.238081 -0.330993
C -1.480662 1.505859 0.456868
C -0.393132 2.294168 -0.271708
O -1.307251 1.141945 1.604435
N -0.350087 3.574410 -0.223407
C 4.892005 0.560855 0.099561
H 4.686657 -0.674641 -1.634888
O 2.445181 -1.674170 2.073053
H 2.214353 1.474175 0.320218
O -1.405429 4.100012 0.554050
H 3.143234 -2.310474 -0.793799
H 4.347185 -2.092365 0.484254
H 2.397006 -0.224654 -2.219385
H 3.205361 1.312333 -1.945351
H 0.809635 -1.885581 -1.211909
H -0.475415 -0.747406 -0.884929
H 1.148159 2.422326 -1.685904
H 0.150462 0.987855 -1.876169
H 0.161026 -3.261704 0.685554
H -0.655875 -1.933883 1.464746
H -1.542793 -3.393052 -1.085144
H -2.255775 -3.602081 0.516147
H -4.392422 -3.004110 -0.989200
H -3.267298 -2.653353 -2.327718
H -4.360197 -1.392799 -1.741070
H -2.504651 -1.024720 1.430275
H -4.106402 -1.682208 1.093095
H -4.678371 0.308563 -0.245267
H -4.058287 0.782600 1.327458
H -2.464017 0.817133 -1.304095
H -3.186243 2.224356 -0.546052
H 5.227727 1.457559 -0.434735
H 4.343082 0.888018 0.990133
H 5.781693 0.023984 0.447748
H -1.245164 5.054927 0.499343

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623799800

Comp_16Z_c21
B3LYP/6-31G* Geometry

C 3.508435 0.793028 0.615326
C 3.885094 -0.566731 -0.020975
C 2.781988 -1.108811 -0.922708
C 2.107621 0.727050 1.252311
C 1.021088 0.196202 0.294989
C 1.414627 -1.217009 -0.243467
C 0.335666 -1.891890 -1.110814
C 0.712419 1.227116 -0.842048
H 1.593488 -1.830083 0.654992
C -0.505913 -2.974005 -0.407789
C -1.179518 -2.631364 0.931803
N -2.011598 -1.419538 0.989673
C -2.531569 -1.271451 2.347002
C -3.080423 -1.397764 -0.012795
C -3.865466 -0.072035 -0.066539
C -3.014889 1.206782 0.034074
C -1.870728 1.257080 -0.958260
C -0.576005 1.971749 -0.588639
O -1.928152 0.703604 -2.044026
N -0.485106 3.158942 -0.111818
C 4.571790 1.249185 1.621052
H 3.483355 1.533209 -0.197237
O 2.983866 -1.408923 -2.085036
H 0.099652 0.046736 0.867769
O -1.742610 3.764831 0.092136
H 4.808882 -0.492596 -0.603267
H 4.053598 -1.298055 0.785144
H 1.820915 1.723959 1.612628
H 2.151236 0.075642 2.138389
H 0.830090 -2.355761 -1.971371
H -0.331167 -1.135596 -1.532677
H 1.516778 1.963154 -0.922135
H 0.628144 0.734562 -1.815261
H -1.259502 -3.333129 -1.120048
H 0.131348 -3.845232 -0.198341
H -1.768390 -3.520031 1.239357
H -0.403890 -2.506842 1.699125
H -1.699100 -1.248024 3.058596
H -3.205193 -2.100898 2.638497
H -3.085999 -0.335339 2.451748
H -3.801787 -2.225242 0.144887
H -2.621678 -1.557925 -0.990060
H -4.421537 -0.065644 -1.010248
H -4.616022 -0.035215 0.732184
H -3.645973 2.084703 -0.157209
H -2.613502 1.350137 1.041590
H 4.326794 2.235089 2.033487
H 4.648113 0.545003 2.459714
H 5.560062 1.317632 1.151558
H -1.491920 4.641075 0.423469

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623575883

Comp_16Z_c22

B3LYP/6-31G* Geometry

C 4.044749 -0.034544 -0.660822
 C 3.672004 -1.354410 0.050284
 C 2.418668 -1.236034 0.912350
 C 2.808241 0.546352 -1.378376
 C 1.605424 0.757085 -0.435653
 C 1.196071 -0.573291 0.270324
 C 0.494436 -1.623368 -0.639141
 C 0.465336 1.490179 -1.197385
 H 0.525778 -0.330601 1.096249
 C -0.304689 -2.680690 0.148887
 C -1.707760 -2.219867 0.586330
 N -2.536395 -1.695910 -0.510934
 C -2.774659 -2.702565 -1.543137
 C -3.814990 -1.152814 -0.038699
 C -3.725471 0.166713 0.743621
 C -2.944667 1.269688 0.010303
 C -1.533006 1.467602 0.534003
 C -0.557359 2.222614 -0.356963
 O -1.162231 1.072572 1.623910
 N -0.554306 3.501652 -0.438252
 C 4.689475 0.963532 0.315089
 H 4.793893 -0.268736 -1.429404
 O 2.375680 -1.695720 2.040108
 H 1.926977 1.442360 0.359848
 O -1.561806 4.078426 0.369131
 H 3.475617 -2.125200 -0.709541
 H 4.485695 -1.724053 0.681993
 H 2.517844 -0.122357 -2.201813
 H 3.079493 1.504071 -1.841850
 H 1.235828 -2.126567 -1.272334
 H -0.198494 -1.121161 -1.320572
 H 0.921081 2.255682 -1.835076
 H -0.053919 0.793920 -1.867949
 H -0.390179 -3.590570 -0.457207
 H 0.244558 -2.971651 1.052296
 H -2.212554 -3.071128 1.086607
 H -1.608052 -1.429947 1.335883
 H -1.832471 -3.020475 -1.997429
 H -3.395546 -2.273460 -2.336465
 H -3.288612 -3.605204 -1.157889
 H -4.367282 -1.893319 0.574196
 H -4.429150 -0.973590 -0.930457
 H -4.755091 0.497520 0.924514
 H -3.276305 0.016423 1.730055
 H -2.896558 1.084222 -1.069905
 H -3.425459 2.251243 0.127817
 H 4.936028 1.904867 -0.190249
 H 4.034887 1.199874 1.161945
 H 5.616813 0.551922 0.729607
 H -1.433885 5.026404 0.210155

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.620935081

Comp_16Z_c23**B3LYP/6-31G* Geometry**

C 4.045958 -0.389471 -0.841711
 C 3.578386 -1.520598 0.106545
 C 2.483906 -1.062902 1.064662
 C 2.827130 0.268781 -1.524945
 C 1.778998 0.781584 -0.521061
 C 1.289684 -0.351506 0.427969
 C 0.344565 -1.382141 -0.238235
 C 0.631676 1.529790 -1.244548
 H 0.741773 0.109458 1.258116
 C -0.449473 -2.245531 0.756689
 C -1.749108 -2.763508 0.117832
 N -2.615716 -1.659171 -0.312145
 C -3.376101 -1.952522 -1.520036
 C -3.463921 -1.139050 0.759643
 C -3.878575 0.331490 0.587620
 C -2.740425 1.348379 0.759237
 C -1.863564 1.552672 -0.467080
 C -0.435441 2.068986 -0.302762
 O -2.255771 1.333471 -1.600068
 N -0.038025 2.977687 0.512792
 C 4.934413 0.625215 -0.103533
 H 4.659533 -0.848748 -1.628607
 O 2.545581 -1.270174 2.263553
 H 2.261395 1.529628 0.121891
 O -1.043359 3.480179 1.353060
 H 3.172075 -2.345001 -0.497584
 H 4.405946 -1.924593 0.697799
 H 2.357585 -0.456579 -2.204474
 H 3.168958 1.100952 -2.154999
 H 0.895211 -2.028974 -0.934258
 H -0.391575 -0.842566 -0.839844
 H 1.073517 2.371322 -1.791135
 H 0.145242 0.896731 -1.990474
 H 0.144045 -3.094768 1.118355
 H -0.691215 -1.651138 1.647750
 H -1.493357 -3.354410 -0.770127
 H -2.267818 -3.452785 0.809155
 H -3.864925 -1.044353 -1.883032
 H -4.151673 -2.729423 -1.369293
 H -2.697916 -2.293172 -2.308671
 H -2.914796 -1.231270 1.704495
 H -4.378287 -1.756349 0.871840
 H -4.360107 0.488780 -0.382739
 H -4.640005 0.543794 1.349110
 H -3.157199 2.337694 0.990530
 H -2.109349 1.103485 1.622205
 H 5.254212 1.429644 -0.776480
 H 4.419991 1.086230 0.747551
 H 5.834321 0.137532 0.288328
 H -0.559657 4.143445 1.869985

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623550212

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623839067

Comp_16Z_c24

B3LYP/6-31G* Geometry

C 3.192156 0.892980 0.795026
C 3.809528 -0.468761 0.402290
C 2.967696 -1.194707 -0.637895
C 1.710562 0.718215 1.172105
C 0.864374 0.007831 0.093327
C 1.493615 -1.373823 -0.263376
C 0.750318 -2.233141 -1.302249
C 0.596958 0.932394 -1.129136
H 1.505760 -1.917198 0.696054
C -0.786893 -2.332569 -1.207916
C -1.388523 -2.751389 0.155655
N -1.989875 -1.629524 0.901653
C -2.146294 -1.953906 2.315630
C -3.261879 -1.196452 0.306863
C -3.702179 0.225788 0.702357
C -2.605223 1.297494 0.600099
C -1.922153 1.370599 -0.753134
C -0.499317 1.921980 -0.816813
O -2.432468 0.964764 -1.781824
N -0.191657 3.151006 -0.636382
C 3.990624 1.561879 1.919813
H 3.250332 1.546736 -0.086932
O 3.436953 -1.584369 -1.691885
H -0.106989 -0.233916 0.537166
O -1.331968 3.934387 -0.332818
H 4.824960 -0.353890 0.010088
H 3.865758 -1.102366 1.301680
H 1.273789 1.701039 1.390288
H 1.651582 0.137003 2.105090
H 1.179464 -3.242326 -1.250287
H 1.008224 -1.874225 -2.304944
H 1.495121 1.482417 -1.427166
H 0.275464 0.342289 -1.994259
H -1.234292 -1.383558 -1.516094
H -1.098624 -3.058458 -1.969335
H -2.133375 -3.556232 0.007228
H -0.605654 -3.182644 0.791289
H -1.172883 -2.204592 2.750816
H -2.831317 -2.806415 2.490023
H -2.542742 -1.090381 2.859174
H -4.075973 -1.904760 0.558052
H -3.153004 -1.221202 -0.778377
H -4.541542 0.496531 0.051728
H -4.091151 0.241520 1.728004
H -3.026913 2.294399 0.789292
H -1.837329 1.151013 1.367757
H 3.577636 2.547876 2.163111
H 3.967408 0.953885 2.833586
H 5.040678 1.698009 1.635827
H -0.954026 4.824330 -0.259406

Number of Imaginary Frequencies= 0

Comp_16Z_c26

B3LYP/6-31G* Geometry

C -3.995842 0.444732 0.178656
C -3.960789 -1.057644 0.543922
C -2.532810 -1.545188 0.737298
C -3.055742 0.714389 -1.007890
C -1.605236 0.238757 -0.777437
C -1.588317 -1.289958 -0.441706
C -0.203560 -1.902411 -0.189620
C -0.874043 1.088387 0.300554
H -2.047712 -1.787968 -1.312176
C 0.764412 -1.854397 -1.378270
C 2.169089 -2.355742 -1.005503
N 2.831471 -1.546535 0.027666
C 3.865281 -2.309508 0.718685
C 3.346640 -0.279963 -0.499993
C 3.622373 0.784684 0.574947
C 2.437483 1.107963 1.519850
C 1.400046 2.091926 1.006410
C 0.460995 1.674714 -0.121481
O 1.216988 3.178367 1.522741
N 0.675030 1.913957 -1.358049
C -5.426247 0.918011 -0.102397
H -3.622081 1.002989 1.050167
O -2.163392 -2.066098 1.774748
H -1.071256 0.377012 -1.720919
O 1.929926 2.537616 -1.558548
H -4.527532 -1.265166 1.456897
H -4.418209 -1.630045 -0.278087
H -3.050067 1.786956 -1.242741
H -3.457116 0.205571 -1.897421
H -0.345881 -2.946032 0.118290
H 0.265189 -1.418073 0.672305
H -1.494216 1.945470 0.600110
H -0.725166 0.514038 1.222945
H 0.389002 -2.484649 -2.197279
H 0.826736 -0.838887 -1.784560
H 2.076913 -3.374877 -0.610212
H 2.792766 -2.431362 -1.917973
H 3.428851 -3.215212 1.151867
H 4.699519 -2.611101 0.054452
H 4.288014 -1.722321 1.539452
H 2.618701 0.118015 -1.207886
H 4.281765 -0.441139 -1.074328
H 4.455521 0.459382 1.208976
H 3.961309 1.696051 0.070725
H 1.935314 0.162164 1.765784
H 2.815473 1.547275 2.448483
H -5.450963 1.992602 -0.318322
H -5.850476 0.392729 -0.967840
H -6.082129 0.732142 0.755952
H 1.951661 2.650889 -2.521647

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623225387

Comp_16Z_c27

B3LYP/6-31G* Geometry

C -4.098155 -0.211449 -0.682991
C -3.780904 1.135868 0.008715
C -2.533024 1.078504 0.884601
C -2.833807 -0.760765 -1.379389
C -1.636323 -0.893884 -0.421619
C -1.284124 0.465315 0.250320
C -0.620236 1.507535 -0.690598
C -0.432235 -1.560723 -1.117707
H -0.596378 0.267482 1.078143
C 0.096359 2.642501 0.061115
C 1.432548 2.235794 0.704218
N 2.376235 1.574103 -0.206798
C 2.755142 2.423735 -1.333139
C 3.557381 1.086699 0.517951
C 3.378386 -0.306106 1.134484
C 3.373696 -1.448923 0.096501
C 2.138469 -1.547498 -0.780351
C 0.754656 -1.832042 -0.201745
O 2.219085 -1.448895 -1.994755
N 0.448015 -2.369886 0.925083
C -4.716519 -1.213928 0.305340
H -4.848958 -0.016138 -1.460713
O -2.522197 1.530427 2.016886
H -1.930830 -1.567811 0.392197
O 1.523523 -2.684833 1.763629
H -3.605754 1.898832 -0.763922
H -4.614799 1.485039 0.625599
H -2.566207 -0.102880 -2.218714
H -3.059906 -1.740908 -1.820416
H -1.370753 1.939150 -1.364370
H 0.113147 1.004021 -1.326353
H -0.765207 -2.519619 -1.537650
H -0.079225 -0.975109 -1.968365
H 0.262590 3.477618 -0.630041
H -0.545877 3.035088 0.859199
H 1.890722 3.140601 1.153624
H 1.240116 1.547579 1.535079
H 3.255597 3.361903 -1.022902
H 1.874545 2.691249 -1.923294
H 3.432841 1.870583 -1.990178
H 3.857948 1.801573 1.307376
H 4.395318 1.043465 -0.187702
H 4.217500 -0.482431 1.820047
H 2.473630 -0.349265 1.749472
H 4.219303 -1.335860 -0.590942
H 3.486955 -2.400670 0.624963
H -4.931351 -2.169441 -0.187690
H -4.057774 -1.418079 1.157235
H -5.658175 -0.825793 0.710327

H 1.070091 -3.067080 2.531684
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623887606

Comp_16Z_c28

B3LYP/6-31G* Geometry

C -4.011641 0.217077 0.121568
C -3.578699 -1.231342 -0.213650
C -2.135747 -1.326189 -0.700935
C -2.956724 0.897484 1.023640
C -1.545067 0.844361 0.412249
C -1.093023 -0.623689 0.167190
C -0.864946 -1.476454 1.462224
C -0.516864 1.693614 1.205093
H -0.164059 -0.619724 -0.409230
C 0.585994 -1.929979 1.715813
C 1.245379 -2.658453 0.526893
N 1.938417 -1.743042 -0.394050
C 2.014814 -2.290982 -1.745408
C 3.247400 -1.345393 0.128361
C 3.817808 -0.066823 -0.510192
C 2.799601 1.063162 -0.722524
C 1.996291 1.434223 0.508548
C 0.656448 2.140592 0.347581
O 2.362218 1.172063 1.643395
N 0.417674 3.142594 -0.418728
C -4.308478 1.019395 -1.156310
H -4.948166 0.157934 0.692496
O -1.831131 -1.956869 -1.699310
H -1.609235 1.321260 -0.575054
O 1.515632 3.540678 -1.199540
H -3.653273 -1.840955 0.699039
H -4.229977 -1.688047 -0.965352
H -2.958968 0.417553 2.012211
H -3.244555 1.943842 1.190322
H -1.484986 -2.382267 1.414544
H -1.221099 -0.930927 2.345440
H -1.024353 2.593634 1.568583
H -0.134149 1.160858 2.080405
H 1.200795 -1.073577 2.010066
H 0.571666 -2.605491 2.581622
H 1.938606 -3.437025 0.897966
H 0.472966 -3.184891 -0.045648
H 2.505484 -1.574811 -2.412750
H 1.001957 -2.464038 -2.122836
H 2.582510 -3.240446 -1.795549
H 3.987309 -2.163890 0.022249
H 3.135238 -1.162282 1.198597
H 4.633689 0.285460 0.131540
H 4.269219 -0.288570 -1.485203
H 3.316017 1.971763 -1.056521
H 2.095722 0.819079 -1.525770
H -4.601213 2.048080 -0.915243
H -3.444726 1.066893 -1.829430

H -5.129750 0.558799 -1.717192
H 1.155665 4.304324 -1.677068
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.619052407**

Comp_16Z_c29
B3LYP/6-31G* Geometry

C 3.566053 0.274296 -0.085124
C 3.733192 -1.249834 -0.287778
C 2.404299 -1.938553 -0.567844
C 2.457510 0.553794 0.943744
C 1.111634 -0.127329 0.620071
C 1.303211 -1.671835 0.462139
C 0.026381 -2.472596 0.152254
C 0.407014 0.497593 -0.612532
H 1.709801 -2.011316 1.429896
C -1.082448 -2.366856 1.218540
C -2.494658 -2.532207 0.633684
N -2.868145 -1.447908 -0.287062
C -3.927837 -1.856468 -1.202977
C -3.213495 -0.205116 0.410407
C -3.167971 1.030379 -0.517993
C -2.621796 2.301739 0.176183
C -1.193261 2.118048 0.657711
C -0.109378 1.900604 -0.392014
O -0.896822 2.063063 1.838270
N 0.383251 2.846232 -1.101293
C 4.892559 0.929392 0.316303
H 3.262398 0.706392 -1.049067
O 2.231003 -2.635945 -1.551242
H 0.461073 0.035794 1.484138
O -0.224558 4.088702 -0.799866
H 4.422389 -1.475738 -1.107619
H 4.153717 -1.680954 0.634521
H 2.302562 1.635352 1.038639
H 2.796007 0.203592 1.930585
H -0.372068 -2.157496 -0.816347
H 0.308718 -3.523018 0.016953
H 1.070808 0.521777 -1.483639
H -0.449913 -0.129336 -0.884940
H -0.939805 -3.135631 1.989679
H -1.025398 -1.411149 1.751399
H -2.529730 -3.468547 0.063391
H -3.230953 -2.638149 1.453833
H -4.878306 -2.097025 -0.686994
H -3.610930 -2.740145 -1.766135
H -4.131082 -1.057746 -1.923486
H -2.495170 -0.068339 1.223069
H -4.207730 -0.276308 0.894799
H -2.539998 0.792739 -1.384435
H -4.164200 1.260591 -0.912135
H -2.643320 3.140390 -0.529439
H -3.227953 2.563421 1.050404
H 4.780212 2.015270 0.416547

H 5.248856 0.539610 1.278762
H 5.672386 0.739234 -0.430472
H 0.228849 4.691582 -1.409359
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.625627352**

Comp_16Z_c30
B3LYP/6-31G* Geometry

C 3.850020 -0.172985 -0.553466
C 3.651905 -0.228216 0.974909
C 2.271003 -0.736707 1.379032
C 2.737281 0.666148 -1.245890
C 1.483945 0.887706 -0.368883
C 1.118142 -0.383481 0.436337
C 0.775535 -1.623781 -0.436593
C 0.324463 1.494276 -1.198393
H 0.257643 -0.167591 1.078492
C -0.018175 -2.731985 0.278737
C -1.485890 -2.386274 0.601976
N -2.187669 -1.721897 -0.499249
C -2.259572 -2.560076 -1.693995
C -3.539274 -1.265652 -0.160353
C -3.650745 -0.229924 0.972799
C -2.570088 0.862434 1.022845
C -2.148144 1.461911 -0.302566
C -0.769695 2.119005 -0.349254
O -2.825610 1.451998 -1.312268
N -0.478121 3.211341 0.251383
C 5.250364 0.334517 -0.918587
H 3.773450 -1.205962 -0.919061
O 2.098062 -1.398792 2.387351
H 1.738999 1.658289 0.371172
O -1.558469 3.708470 1.015514
H 4.403982 -0.857668 1.461767
H 3.767979 0.782146 1.399046
H 2.456022 0.182239 -2.190301
H 3.136268 1.651846 -1.520296
H 1.702628 -2.063157 -0.826232
H 0.206122 -1.285680 -1.306726
H 0.744889 2.280130 -1.837296
H -0.125675 0.751631 -1.864299
H 0.014005 -3.631096 -0.349304
H 0.480155 -2.997674 1.217735
H -2.002534 -3.317313 0.912877
H -1.515133 -1.718953 1.469129
H -2.748315 -2.001892 -2.498964
H -2.831929 -3.493728 -1.527582
H -1.259908 -2.836665 -2.038570
H -4.199286 -2.119951 0.094128
H -3.941972 -0.811867 -1.069661
H -4.638086 0.235130 0.869853
H -3.654894 -0.726876 1.950603
H -2.912095 1.702114 1.642762
H -1.667765 0.496217 1.524939

H 6.032074 -0.300804 -0.485871
H 5.392793 0.348471 -2.005706
H 5.404731 1.356528 -0.549100
H -1.191916 4.531122 1.374815
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.617696380**

Comp_16Z_c31

B3LYP/6-31G* Geometry

C 3.927066 0.567971 -0.203029
C 3.657167 -0.915306 0.140790
C 2.251658 -1.166618 0.677132
C 2.771791 1.141464 -1.052945
C 1.393651 0.958107 -0.387036
C 1.094817 -0.547221 -0.109752
C 0.831223 -1.424482 -1.367636
C 0.287046 1.701819 -1.185774
H 0.215593 -0.610013 0.529233
C 0.243813 -2.817328 -1.051401
C -1.291889 -2.852822 -0.974165
N -1.873734 -1.928282 0.002551
C -1.639494 -2.368813 1.379215
C -3.295757 -1.673892 -0.239725
C -3.794388 -0.338191 0.332817
C -3.085142 0.882403 -0.266749
C -1.786969 1.277599 0.414498
C -0.879370 2.217566 -0.372870
O -1.471657 0.940428 1.538814
N -1.062119 3.486147 -0.383686
C 4.192992 1.393683 1.066698
H 4.839296 0.607302 -0.813777
O 2.059380 -1.874446 1.651837
H 1.437428 1.443707 0.596592
O -2.194722 3.857223 0.378722
H 3.765211 -1.518985 -0.772676
H 4.375804 -1.303391 0.869376
H 2.771169 0.662311 -2.042557
H 2.953324 2.209810 -1.228803
H 1.759864 -1.544131 -1.939619
H 0.135993 -0.903071 -2.036296
H 0.724236 2.584180 -1.666164
H -0.094038 1.066727 -1.995653
H 0.529645 -3.516452 -1.848532
H 0.687141 -3.216624 -0.132467
H -1.683254 -2.574757 -1.961363
H -1.615714 -3.897850 -0.791980
H -2.016791 -1.618076 2.076779
H -0.569427 -2.474723 1.573852
H -2.133888 -3.336188 1.593582
H -3.929161 -2.494968 0.150828
H -3.452403 -1.653407 -1.325938
H -4.868480 -0.269418 0.119340
H -3.691459 -0.312175 1.422420
H -2.894314 0.744647 -1.340230

H -3.717374 1.779839 -0.193745
H 4.369624 2.447335 0.820202
H 3.357037 1.351610 1.774469
H 5.079028 1.018132 1.591104
H -2.196421 4.822289 0.284578
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.620962327**

Comp_16Z_c32

B3LYP/6-31G* Geometry

C 3.866348 -0.076802 -0.610225
C 3.731165 -0.213765 0.919082
C 2.393444 -0.825253 1.321649
C 2.701351 0.760750 -1.208313
C 1.472256 0.896535 -0.276645
C 1.177127 -0.421863 0.482090
C 0.777060 -1.620986 -0.427128
C 0.283462 1.487635 -1.082072
H 0.369774 -0.239825 1.194937
C -0.080216 -2.689135 0.274886
C -1.549746 -2.299608 0.518817
N -2.254371 -1.788025 -0.669591
C -2.231973 -2.749970 -1.771069
C -3.645590 -1.424978 -0.372092
C -3.847364 -0.169829 0.489797
C -3.155844 1.083563 -0.068591
C -1.788851 1.343672 0.538910
C -0.805533 2.165110 -0.281150
O -1.468616 0.944929 1.643859
N -0.861742 3.443525 -0.341749
C 5.233719 0.492357 -1.007249
H 3.803040 -1.092331 -1.025370
O 2.301593 -1.617334 2.243086
H 1.722843 1.644596 0.488028
O -1.931999 3.953793 0.429619
H 4.530733 -0.826113 1.348186
H 3.805348 0.780561 1.387598
H 2.394281 0.317816 -2.165134
H 3.059024 1.771730 -1.446128
H 1.681870 -2.103278 -0.819313
H 0.230463 -1.246997 -1.298571
H 0.678103 2.252666 -1.760524
H -0.171388 0.709037 -1.707701
H -0.039008 -3.614189 -0.313639
H 0.366848 -2.927957 1.246290
H -2.073380 -3.187399 0.928667
H -1.596788 -1.526155 1.290121
H -2.712129 -3.714060 -1.512471
H -2.760104 -2.330332 -2.633701
H -1.205294 -2.959447 -2.081086
H -4.185706 -2.269551 0.101744
H -4.139042 -1.247871 -1.336545
H -4.929157 0.001788 0.544775
H -3.510440 -0.328367 1.518752

H -3.067479 1.047018 -1.161261
H -3.736040 1.989582 0.158424
H 5.327047 0.569409 -2.097200
H 5.375585 1.497192 -0.588780
H 6.051456 -0.141147 -0.644179
H -1.850382 4.909420 0.286769

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.619762806

Comp_16Z_c33

B3LYP/6-31G* Geometry

C 3.860410 -0.431330 -0.704356
C 3.854317 -0.367695 0.834923
C 2.475730 -0.670600 1.409946
C 2.834535 0.562441 -1.313595
C 1.706956 0.988872 -0.342631
C 1.274981 -0.149037 0.613485
C 0.523763 -1.319249 -0.070090
C 0.541868 1.634839 -1.131046
H 0.591082 0.276289 1.359416
C -0.322042 -2.185194 0.879810
C -1.499603 -2.825875 0.128410
N -2.414665 -1.805003 -0.402848
C -3.009912 -2.167257 -1.682715
C -3.420622 -1.378182 0.569526
C -3.960267 0.044653 0.349383
C -2.941554 1.164439 0.609143
C -1.989950 1.448242 -0.541842
C -0.626755 2.080523 -0.266102
O -2.271791 1.206620 -1.702767
N -0.368601 3.011908 0.579202
C 5.266985 -0.213761 -1.274506
H 3.549849 -1.449376 -0.979124
O 2.331582 -1.310931 2.436148
H 2.107260 1.781598 0.304266
O -1.474432 3.421172 1.341509
H 4.571606 -1.065396 1.279274
H 4.146007 0.642635 1.163983
H 2.400066 0.114884 -2.216973
H 3.356410 1.468800 -1.649887
H 1.224018 -1.955745 -0.628746
H -0.163804 -0.893028 -0.806855
H 0.938358 2.506347 -1.666143
H 0.156377 0.955160 -1.895070
H 0.285101 -2.960400 1.360472
H -0.710270 -1.564456 1.697786
H -1.107965 -3.401403 -0.719161
H -2.023695 -3.550165 0.778180
H -3.718791 -3.015647 -1.609731
H -2.221750 -2.440126 -2.391516
H -3.541561 -1.309118 -2.102810
H -2.967900 -1.420119 1.567591
H -4.275494 -2.084375 0.588192
H -4.369291 0.155163 -0.660046

H -4.801070 0.182280 1.041243
H -3.467295 2.110510 0.795967
H -2.365661 0.979747 1.523793
H 5.261702 -0.272497 -2.369504
H 5.652697 0.775312 -0.995528
H 5.971134 -0.966487 -0.901076
H -1.090174 4.121426 1.891960

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.620230733

Comp_17E_c01

B3LYP/6-31G* Geometry

C 3.748396 -0.030982 -0.416900
C 3.007691 0.682436 0.721209
C 1.475693 0.723770 0.548838
C 3.243683 -1.483338 -0.489322
C 1.733888 -1.580755 -0.640209
C 0.843386 -0.661002 0.202324
O 1.238300 -2.398095 -1.399279
H 3.501339 0.466080 -1.367414
C 5.269314 0.023122 -0.237087
C 1.020570 1.806278 -0.479654
C -0.406363 2.208059 -0.203815
C -1.536868 1.590627 -0.993290
C -2.921442 1.556444 -0.365699
O -1.302289 1.127342 -2.098922
N -0.782344 3.043896 0.699419
O 0.299541 3.605896 1.385060
C -3.830903 0.445073 -0.911782
C -3.218767 -0.968351 -0.877910
N -2.496290 -1.291899 0.357160
C -3.390338 -1.418714 1.501396
C 0.318904 -1.387493 1.472301
H -0.036012 -0.491582 -0.420989
H 1.069566 1.040876 1.516396
C -1.654394 -2.484314 0.183678
C -0.535320 -2.644237 1.228053
H 3.381041 1.708191 0.837899
H 3.246548 0.162827 1.661825
H 3.699365 -2.046907 -1.309906
H 3.519355 -1.993976 0.448516
H 5.628559 1.058799 -0.216746
H 5.785539 -0.496426 -1.052793
H 5.569214 -0.453614 0.705299
H 1.084315 1.433548 -1.506084
H 1.658537 2.690951 -0.387913
H -3.389374 2.536565 -0.538014
H -2.805889 1.470281 0.716965
H -0.138872 4.217369 1.998470
H -4.094512 0.656590 -1.954304
H -4.770030 0.476837 -0.345209
H -2.500562 -1.042176 -1.697734
H -4.021211 -1.704365 -1.085763
H -2.814165 -1.604840 2.413157

H -3.953362 -0.492023 1.651416
 H -4.119506 -2.245104 1.384005
 H 1.153843 -1.642776 2.140552
 H -0.291440 -0.650872 2.007744
 H -1.180611 -2.415543 -0.798728
 H -2.265617 -3.408729 0.176684
 H -0.948076 -2.961753 2.195179
 H 0.095268 -3.473083 0.883762
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.631481089**

Comp_17E_c03

B3LYP/6-31G* Geometry

C 4.304289 0.054799 -0.306074
 C 3.223793 1.094167 -0.646306
 C 1.816129 0.789176 -0.085288
 C 3.840242 -1.326474 -0.814936
 C 2.495316 -1.689402 -0.209905
 C 1.354432 -0.671999 -0.400461
 O 2.337160 -2.732218 0.400223
 H 5.214909 0.327948 -0.856632
 C 4.657914 0.021726 1.188999
 C 0.865404 1.875477 -0.675579
 C -0.498429 2.028136 -0.057238
 C -1.710166 1.536218 -0.813533
 C -3.067966 1.555451 -0.130976
 O -1.564330 1.137580 -1.960252
 N -0.751956 2.606697 1.064557
 O 0.407755 3.069997 1.688613
 C -4.067858 0.553057 -0.726201
 C -3.569062 -0.904484 -0.730870
 N -2.947314 -1.320692 0.528514
 C -3.938465 -1.534510 1.574893
 C 0.106086 -1.122361 0.383135
 H 1.131482 -0.695019 -1.481495
 H 1.838208 0.909555 1.004955
 C -2.064578 -2.485875 0.374618
 C -0.740798 -2.177851 -0.341135
 H 3.151229 1.174240 -1.741616
 H 3.537711 2.083149 -0.287065
 H 3.733886 -1.288170 -1.909103
 H 4.553830 -2.119163 -0.570162
 H 4.984800 1.009684 1.534140
 H 5.470187 -0.688487 1.381419
 H 3.806893 -0.283280 1.808853
 H 0.724384 1.682981 -1.743258
 H 1.373892 2.841338 -0.570576
 H -3.465038 2.577141 -0.225348
 H -2.928758 1.384391 0.938034
 H 0.060868 3.480565 2.497148
 H -4.300568 0.826157 -1.761644
 H -5.005788 0.640502 -0.163773
 H -2.824027 -0.996743 -1.522227
 H -4.410127 -1.572256 -1.006508

H -4.529822 -0.625638 1.727213
 H -3.437326 -1.768508 2.520153
 H -4.641757 -2.359471 1.344510
 H 0.429881 -1.525030 1.350489
 H -0.531081 -0.266286 0.606477
 H -2.580627 -3.317068 -0.145909
 H -1.834180 -2.850844 1.383477
 H -0.174240 -3.112767 -0.421382
 H -0.936324 -1.845342 -1.369195
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.635316701**

Comp_17E_c04

B3LYP/6-31G* Geometry

C -3.620304 0.227016 0.848763
 C -2.525468 1.219968 0.413031
 C -1.633011 0.708435 -0.737444
 C -2.961088 -1.118002 1.235671
 C -2.084424 -1.618529 0.098909
 C -0.977973 -0.661870 -0.359296
 O -2.282675 -2.697518 -0.433524
 H -4.098954 0.636425 1.748865
 C -4.718179 0.032265 -0.208976
 C -0.627053 1.805134 -1.215056
 C 0.555065 2.095955 -0.320459
 C 1.909231 1.522172 -0.676692
 C 2.970968 1.393127 0.400474
 O 2.128565 1.201554 -1.835435
 N 0.607223 2.915689 0.670056
 O -0.601509 3.574999 0.899630
 C 3.946079 0.231200 0.140063
 C 3.266593 -1.125328 -0.135253
 N 2.115111 -1.393877 0.729620
 C 2.511505 -1.544054 2.126692
 C -0.113109 -1.276340 -1.471171
 H -0.339976 -0.470528 0.517126
 H -2.275388 0.530523 -1.612332
 C 1.335220 -2.569263 0.312784
 C 0.702916 -2.532164 -1.087804
 H -1.892390 1.449469 1.278820
 H -2.986832 2.170159 0.116937
 H -2.330556 -0.964257 2.123299
 H -3.704119 -1.886252 1.470980
 H -4.337348 -0.441498 -1.120909
 H -5.163243 0.993936 -0.490585
 H -5.518863 -0.609074 0.176794
 H -1.193665 2.733101 -1.352182
 H -0.215901 1.523744 -2.187461
 H 2.483872 1.297753 1.372668
 H 3.530129 2.339194 0.431926
 H -0.378848 4.166541 1.636654
 H 4.621965 0.160810 1.000853
 H 4.573629 0.463907 -0.726976
 H 4.028226 -1.927566 -0.058204

H 2.911986 -1.121860 -1.167373
H 3.188373 -2.405663 2.289617
H 3.021852 -0.644706 2.482990
H 1.622299 -1.692799 2.749020
H 0.573455 -0.513799 -1.839522
H -0.762320 -1.544165 -2.314517
H 1.946286 -3.491995 0.385380
H 0.532916 -2.684510 1.052851
H 1.476709 -2.678717 -1.852127
H 0.053514 -3.411475 -1.141098

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.630053759

Comp_17E_c05

B3LYP/6-31G* Geometry

C -3.770150 0.061408 0.247649
C -2.967503 0.586849 -0.951215
C -1.448281 0.658888 -0.698182
C -3.279141 -1.355886 0.592642
C -1.774713 -1.441916 0.806792
C -0.854219 -0.668683 -0.140278
O -1.305739 -2.154597 1.678639
H -3.574450 0.710668 1.114078
C -5.279280 0.078414 -0.020052
C -1.068820 1.861654 0.216784
C 0.413966 2.132899 0.169709
C 1.298614 1.561580 1.246241
C 2.811190 1.564453 1.088302
O 0.776413 1.091704 2.247177
N 1.021708 2.812424 -0.739704
O 0.141812 3.320473 -1.696403
C 3.438814 0.185164 1.403055
C 3.754925 -0.670153 0.167981
N 2.609410 -1.099892 -0.647094
C 3.077936 -1.473637 -1.981146
C -0.331767 -1.608968 -1.258272
H 0.013947 -0.426669 0.469457
H -0.972803 0.855518 -1.666458
C 1.875271 -2.202420 -0.005071
C 0.636042 -2.701836 -0.773412
H -3.331998 1.579927 -1.245993
H -3.157002 -0.075309 -1.809902
H -3.769823 -1.764732 1.481967
H -3.528933 -2.024406 -0.248386
H -5.633060 1.095185 -0.227964
H -5.840270 -0.303417 0.841008
H -5.531469 -0.547059 -0.886428
H -1.343600 1.663823 1.256606
H -1.601361 2.755045 -0.124481
H 3.180291 2.297735 1.818244
H 3.097850 1.920725 0.096992
H 0.736279 3.810022 -2.287592
H 2.797301 -0.344985 2.114860
H 4.394619 0.340538 1.918512

H 4.353159 -1.545948 0.492094
H 4.409912 -0.078364 -0.483746
H 3.773858 -2.335892 -1.969538
H 2.235709 -1.731353 -2.628041
H 3.598671 -0.625296 -2.437355
H -1.168724 -2.079310 -1.793879
H 0.184112 -0.974150 -1.987712
H 1.557031 -1.866920 0.986706
H 2.545288 -3.071433 0.159405
H 0.946942 -3.293688 -1.643988
H 0.113507 -3.395475 -0.105323

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.630531369

Comp_17E_c06

B3LYP/6-31G* Geometry

C 3.503801 0.180995 -0.925513
C 2.476451 1.196143 -0.394010
C 1.624404 0.684916 0.787436
C 2.762855 -1.114304 -1.327234
C 1.953349 -1.638886 -0.152501
C 0.921843 -0.670864 0.443706
O 2.143326 -2.756738 0.297079
H 3.952389 0.607114 -1.833450
C 4.645815 -0.103188 0.063183
C 0.649948 1.798829 1.282794
C -0.493698 2.138285 0.357518
C -1.844364 1.505835 0.595904
C -2.902125 1.547121 -0.497910
O -2.086027 1.038486 1.699086
N -0.509191 3.031860 -0.569048
O 0.696788 3.723530 -0.683149
C -3.867354 0.354183 -0.433765
C -3.351414 -0.901778 -1.151286
N -2.047703 -1.405841 -0.700797
C -1.517867 -2.338064 -1.696417
C 0.181771 -1.319370 1.630209
H 0.197248 -0.460367 -0.357173
H 2.294765 0.498543 1.639269
C -2.137168 -2.034573 0.630133
C -0.801930 -2.452396 1.270705
H 1.807225 1.477630 -1.216789
H 2.988447 2.118446 -0.093228
H 2.076288 -0.890154 -2.156331
H 3.452464 -1.898868 -1.653539
H 4.290811 -0.585286 0.981371
H 5.155178 0.825231 0.347616
H 5.390042 -0.771806 -0.384603
H 1.238800 2.705867 1.455084
H 0.206813 1.503713 2.236415
H -2.428317 1.633074 -1.479520
H -3.459674 2.482497 -0.345152
H 0.502992 4.364889 -1.385875
H -4.811445 0.629728 -0.919918

H -4.108190 0.148618 0.613728
 H -3.248583 -0.659204 -2.216895
 H -4.126358 -1.692370 -1.086662
 H -0.520495 -2.681800 -1.412378
 H -2.157441 -3.232863 -1.825775
 H -1.438303 -1.835274 -2.666311
 H 0.936552 -1.731932 2.310760
 H -0.368888 -0.555059 2.183725
 H -2.791205 -2.929523 0.577797
 H -2.625955 -1.321002 1.298557
 H -1.073257 -2.960272 2.206311
 H -0.292233 -3.211234 0.670038
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632703054**

Comp_17E_c07

B3LYP/6-31G* Geometry

C 3.722429 -0.196895 -0.444621
 C 2.612925 -0.067008 -1.503285
 C 1.185395 -0.232635 -0.936769
 C 3.474465 0.801864 0.706057
 C 2.060244 0.726920 1.267803
 C 0.918257 0.737104 0.249292
 O 1.847329 0.708726 2.466936
 H 3.683516 -1.209704 -0.018962
 C 5.115449 -0.005263 -1.055580
 C 0.919506 -1.726155 -0.581338
 C -0.413061 -1.939240 0.082435
 C -1.656257 -1.757686 -0.740866
 C -3.006166 -1.684654 -0.049451
 O -1.549867 -1.646637 -1.955550
 N -0.605761 -2.217704 1.325051
 O 0.580968 -2.361089 2.033450
 C -3.936359 -0.630641 -0.676837
 C -3.318233 0.768593 -0.847507
 N -2.541546 1.251220 0.301178
 C -3.377515 1.391827 1.492430
 C 0.684421 2.201247 -0.218773
 H 0.022068 0.427867 0.793526
 H 0.478048 0.013519 -1.735855
 C -1.896775 2.539979 -0.005447
 C -0.659278 2.482909 -0.921598
 H 2.773010 -0.805951 -2.299884
 H 2.702722 0.917895 -1.983748
 H 4.180677 0.659887 1.530401
 H 3.624454 1.823153 0.319323
 H 5.214581 0.992252 -1.503190
 H 5.307570 -0.744655 -1.842138
 H 5.900112 -0.109844 -0.297094
 H 1.702303 -2.121752 0.067856
 H 0.931951 -2.294755 -1.517586
 H -2.857530 -1.506175 1.015790
 H -3.477317 -2.674141 -0.139342
 H 0.274716 -2.457938 2.949491

H -4.846825 -0.579009 -0.067788
 H -4.248464 -0.964784 -1.672243
 H -4.130664 1.480639 -1.101136
 H -2.648495 0.738354 -1.710604
 H -4.193953 2.129003 1.359650
 H -3.831124 0.433316 1.757692
 H -2.760325 1.713246 2.337351
 H 1.495661 2.505038 -0.892795
 H 0.756004 2.861246 0.657044
 H -2.638550 3.233464 -0.450218
 H -1.595056 2.990681 0.947986
 H -0.820326 1.776237 -1.743715
 H -0.571744 3.468703 -1.397775
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632809713**

Comp_17E_c09

B3LYP/6-31G* Geometry

C -3.959768 0.121796 0.951080
 C -2.712984 0.959615 1.278970
 C -1.554822 0.856127 0.258104
 C -3.534834 -1.354797 0.787988
 C -2.465208 -1.463619 -0.283690
 C -1.188436 -0.634392 -0.062608
 O -2.634426 -2.145344 -1.280039
 H -4.638492 0.183461 1.812769
 C -4.724894 0.633356 -0.279559
 C -0.385273 1.695346 0.856281
 C 0.833284 1.947892 0.007017
 C 2.184559 1.477968 0.498487
 C 3.305585 1.255046 -0.509265
 O 2.363266 1.358905 1.700481
 N 0.884630 2.659425 -1.063161
 O -0.364104 3.195034 -1.399195
 C 4.131581 -0.006961 -0.212669
 C 3.384238 -1.321939 -0.481768
 N 2.203980 -1.527240 0.362137
 C 2.574543 -1.800625 1.748767
 C -0.231237 -0.792107 -1.259586
 H -0.719539 -1.036923 0.849377
 H -1.866356 1.330126 -0.679560
 C 1.307632 -2.567719 -0.161525
 C 0.486828 -2.147032 -1.389482
 H -2.334702 0.647514 2.264205
 H -2.997774 2.015063 1.381370
 H -3.125342 -1.716646 1.742142
 H -4.375374 -1.996943 0.507994
 H -5.012544 1.683315 -0.149970
 H -5.639280 0.050429 -0.438801
 H -4.130427 0.560201 -1.197407
 H -0.042946 1.236989 1.789183
 H -0.804500 2.676713 1.115761
 H 3.961117 2.135153 -0.448911
 H 2.905669 1.233973 -1.526487

H -0.163988 3.703551 -2.201411
H 4.490059 0.034399 0.820787
H 5.024170 0.002806 -0.850953
H 4.096642 -2.165568 -0.376237
H 3.056402 -1.322500 -1.527721
H 1.668792 -1.951120 2.345109
H 3.207521 -2.703383 1.852176
H 3.104979 -0.946702 2.174819
H -0.803985 -0.618373 -2.178060
H 0.527036 -0.012608 -1.209416
H 0.617794 -2.826266 0.649998
H 1.860251 -3.499422 -0.394465
H 1.133450 -2.099929 -2.275945
H -0.241558 -2.939096 -1.592405

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.631870089

Comp_17E_c12

B3LYP/6-31G* Geometry

C 3.723483 0.214931 -0.746503
C 2.618544 1.134110 -0.193852
C 1.641432 0.452556 0.789879
C 3.068624 -1.025234 -1.401662
C 2.156202 -1.695710 -0.391254
C 1.005274 -0.829424 0.148087
O 2.378011 -2.821829 0.018978
H 4.249964 0.770041 -1.535011
C 4.766500 -0.185285 0.308639
C 0.617794 1.480090 1.368914
C -0.380243 2.070616 0.400579
C -1.822852 1.596103 0.413860
C -2.623792 1.705811 -0.878193
O -2.307613 1.244161 1.474796
N -0.223285 3.100612 -0.354093
O 1.033999 3.698510 -0.220004
C -3.801870 0.730253 -0.987234
C -3.371403 -0.717572 -1.274019
N -2.584376 -1.306986 -0.193353
C -3.428248 -1.697106 0.930775
C 0.102029 -1.635320 1.096031
H 0.424423 -0.487497 -0.723272
H 2.214655 0.114795 1.665697
C -1.695774 -2.383934 -0.628985
C -0.671658 -2.797182 0.441232
H 2.044001 1.534167 -1.038423
H 3.073953 2.002148 0.296655
H 2.475684 -0.700945 -2.268348
H 3.814695 -1.750328 -1.740477
H 5.213323 0.703467 0.769698
H 5.574038 -0.770489 -0.146130
H 4.336086 -0.798284 1.108322
H 1.196901 2.300888 1.807392
H 0.042193 1.019109 2.174772
H -1.947006 1.599226 -1.733115

H -2.989656 2.741522 -0.922961
H 0.961534 4.464511 -0.811894
H -4.451901 1.057145 -1.808994
H -4.404236 0.784487 -0.074630
H -2.753337 -0.719208 -2.181514
H -4.268800 -1.324945 -1.508392
H -4.119911 -2.522637 0.670429
H -2.815665 -2.017802 1.776524
H -4.014674 -0.841838 1.271341
H 0.731003 -2.051300 1.892403
H -0.618655 -0.961666 1.566600
H -1.166473 -2.026439 -1.521592
H -2.258150 -3.286710 -0.945692
H -1.179471 -3.355946 1.237146
H 0.029688 -3.503791 -0.012329

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.629260098

Comp_17E_c13

B3LYP/6-31G* Geometry

C 3.519963 -0.195673 -0.895921
C 2.270018 0.419992 -1.550303
C 0.959995 0.098510 -0.800668
C 3.616431 0.228122 0.584571
C 2.318954 0.068256 1.372924
C 1.033400 0.539178 0.684967
O 2.319564 -0.336079 2.521578
H 3.421790 -1.289709 -0.922669
C 4.798638 0.169085 -1.659644
C 0.593280 -1.407736 -0.982714
C -0.632337 -1.820341 -0.215397
C -1.988993 -1.550819 -0.804072
C -3.222716 -1.697369 0.075760
O -2.079913 -1.253264 -1.987557
N -0.635875 -2.408207 0.931732
O 0.648892 -2.677453 1.390765
C -4.105770 -0.437341 0.078192
C -3.458199 0.791576 0.729448
N -2.293098 1.332008 0.013732
C -2.689005 1.839911 -1.301986
C 0.953303 2.076537 0.908798
H 0.205432 0.090484 1.239246
H 0.146322 0.658982 -1.270540
C -1.652304 2.386457 0.819013
C -0.259180 2.830049 0.331118
H 2.190593 0.073953 -2.589454
H 2.400154 1.511024 -1.602357
H 4.404689 -0.315614 1.115371
H 3.885815 1.296270 0.624659
H 5.682559 -0.283799 -1.195255
H 4.950387 1.256276 -1.676463
H 4.750673 -0.177276 -2.698874
H 1.423848 -2.050708 -0.684443
H 0.393179 -1.572008 -2.046136

H -2.934988 -1.968669 1.093467
H -3.804565 -2.532726 -0.336150
H 0.500097 -2.988073 2.298327
H -5.019055 -0.662004 0.643430
H -4.426204 -0.214659 -0.944438
H -3.128105 0.518389 1.739948
H -4.236248 1.573174 0.851225
H -2.988086 1.015564 -1.951433
H -3.519216 2.569736 -1.233788
H -1.846311 2.337099 -1.786824
H 0.981404 2.239713 1.994711
H 1.855617 2.559735 0.510893
H -1.564811 2.013287 1.847114
H -2.313220 3.274836 0.869579
H -0.219322 2.820520 -0.763043
H -0.130814 3.883597 0.612848

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.633079103

Comp_17E_c14

B3LYP/6-31G* Geometry

C 3.960478 0.226111 0.927076
C 2.917079 1.333158 0.717164
C 1.519524 0.839493 0.278570
C 4.116711 -0.552253 -0.393030
C 2.790218 -1.119577 -0.871791
C 1.579127 -0.165975 -0.916850
O 2.706760 -2.273523 -1.254953
H 4.921063 0.711277 1.148554
C 3.629292 -0.705205 2.103664
C 0.684883 2.120047 -0.017150
C -0.789500 1.970922 -0.287219
C -1.685216 1.524217 0.838160
C -3.159026 1.265146 0.571574
O -1.195932 1.380203 1.950764
N -1.395520 2.248417 -1.389071
O -0.529730 2.662245 -2.400627
C -3.718060 0.100437 1.405139
C -2.939133 -1.215294 1.229936
N -2.629929 -1.541802 -0.164644
C -3.819572 -1.963815 -0.894047
C 0.279786 -0.965389 -1.172492
H 1.770456 0.443779 -1.818722
H 1.055932 0.337933 1.133183
C -1.543175 -2.525576 -0.279902
C -0.143988 -1.932925 -0.053394
H 3.301749 2.029629 -0.043662
H 2.806075 1.918109 1.639688
H 4.489433 0.133273 -1.169532
H 4.829026 -1.379132 -0.311358
H 3.511587 -0.135493 3.032873
H 4.430107 -1.437871 2.256813
H 2.702325 -1.267429 1.939897
H 1.139931 2.659854 -0.851728

H 0.767099 2.756254 0.872907
H -3.310971 1.096678 -0.494654
H -3.700057 2.188218 0.827715
H -1.137863 2.820523 -3.140585
H -4.773858 -0.032087 1.138941
H -3.694734 0.359988 2.469230
H -3.499551 -2.036003 1.721641
H -1.994277 -1.117719 1.769178
H -4.270080 -2.892895 -0.491499
H -4.583696 -1.180615 -0.857128
H -3.568619 -2.134905 -1.946081
H -0.540311 -0.273947 -1.374745
H 0.429232 -1.549687 -2.087745
H -1.582049 -2.941229 -1.294469
H -1.702319 -3.377308 0.409731
H 0.570775 -2.760924 -0.000953
H -0.113616 -1.437108 0.924589

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.633164373

Comp_17E_c15

B3LYP/6-31G* Geometry

C 3.681975 0.146673 -0.546398
C 2.990262 0.838960 0.635014
C 1.451299 0.782873 0.570412
C 3.255625 -1.331637 -0.565715
C 1.745959 -1.529462 -0.573111
C 0.883556 -0.648144 0.334610
O 1.245961 -2.413509 -1.251465
H 3.336508 0.615136 -1.480314
C 5.206886 0.286904 -0.484999
C 0.875262 1.772832 -0.487625
C -0.564945 2.101431 -0.186989
C -1.675182 1.479768 -1.000132
C -3.113288 1.623176 -0.518792
O -1.399780 0.924485 -2.052713
N -0.957409 2.913714 0.732597
O 0.113082 3.498172 1.414733
C -3.948441 0.342047 -0.676285
C -3.616296 -0.760443 0.341037
N -2.272880 -1.334555 0.209742
C -2.164645 -2.149908 -1.003729
C 0.582640 -1.410203 1.659579
H -0.077816 -0.556457 -0.171774
H 1.085876 1.131181 1.542869
C -1.915690 -2.104629 1.411226
C -0.445036 -2.549212 1.526189
H 3.307783 1.887841 0.702300
H 3.329515 0.356750 1.564621
H 3.668651 -1.877303 -1.420295
H 3.645457 -1.816484 0.345033
H 5.508114 1.340980 -0.505864
H 5.687994 -0.217329 -1.331306
H 5.604517 -0.156117 0.437502

H 0.927301 1.352967 -1.495978
H 1.454003 2.702783 -0.466361
H -3.561298 2.416339 -1.134690
H -3.133727 1.980371 0.513277
H -0.336797 4.083676 2.045049
H -3.856491 -0.026076 -1.702821
H -5.005080 0.603431 -0.536172
H -4.392415 -1.550051 0.272157
H -3.699682 -0.331825 1.348487
H -2.380139 -1.537228 -1.881262
H -1.145741 -2.522326 -1.122807
H -2.864532 -3.008302 -0.987613
H 1.512892 -1.809014 2.088553
H 0.205123 -0.677800 2.386396
H -2.555124 -3.007351 1.498274
H -2.149070 -1.475766 2.280870
H -0.388594 -3.170089 2.430815
H -0.168947 -3.205400 0.694485

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632998565**

Comp_17E_c16

B3LYP/6-31G* Geometry

C 3.704606 0.245955 -0.523615
C 2.940568 0.822039 0.676508
C 1.410032 0.687438 0.553487
C 3.386536 -1.254291 -0.636106
C 1.900447 -1.582609 -0.627448
C 0.954622 -0.770996 0.265847
O 1.471809 -2.528320 -1.268139
H 3.347979 0.742623 -1.438262
C 5.214174 0.488864 -0.415861
C 0.831219 1.672770 -0.505649
C -0.631530 1.946805 -0.270746
C -1.672328 1.307596 -1.156983
C -3.146633 1.489677 -0.825458
O -1.311054 0.706810 -2.158270
N -1.094169 2.726554 0.645023
O -0.076590 3.316022 1.400144
C -3.951120 0.181299 -0.893748
C -3.665412 -0.786398 0.263104
N -2.301199 -1.324267 0.280465
C -2.080755 -2.274411 -0.813633
C 0.679580 -1.576071 1.569118
H 0.013857 -0.740879 -0.285074
H 0.990078 0.990075 1.519096
C -1.918683 -1.883578 1.594269
C -0.670005 -1.251338 2.238677
H 3.196798 1.880002 0.820240
H 3.278221 0.299918 1.585308
H 3.829675 -1.715223 -1.525176
H 3.823492 -1.767215 0.237805
H 5.748470 0.065745 -1.274722
H 5.622131 0.025562 0.492095

H 5.440242 1.560903 -0.374007
H 0.944063 1.274872 -1.517659
H 1.370638 2.624529 -0.443254
H -3.541811 2.187468 -1.577206
H -3.263353 1.969483 0.148543
H -0.573719 3.876585 2.017505
H -3.778227 -0.300243 -1.861587
H -5.019503 0.429932 -0.857841
H -4.416668 -1.601844 0.234766
H -3.824184 -0.245634 1.204335
H -2.200940 -1.773419 -1.777405
H -1.058052 -2.657655 -0.784914
H -2.780931 -3.130641 -0.770077
H 0.708158 -2.649762 1.343054
H 1.492076 -1.389115 2.285250
H -1.767656 -2.970767 1.509823
H -2.753944 -1.753641 2.295138
H -0.815267 -0.164809 2.299955
H -0.629261 -1.615478 3.275402

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.630658016**

Comp_17E_c18

B3LYP/6-31G* Geometry

C -3.614908 0.060024 0.890654
C -2.596816 1.062990 0.317566
C -1.674972 0.488298 -0.780833
C -2.856389 -1.184525 1.411416
C -1.998776 -1.752635 0.295073
C -0.937357 -0.802899 -0.284747
O -2.191883 -2.869305 -0.153600
H -4.103132 0.538845 1.750477
C -4.715891 -0.325554 -0.109834
C -0.739534 1.597576 -1.354467
C 0.288691 2.153067 -0.399040
C 1.711568 1.630014 -0.454230
C 2.488380 1.569055 0.846586
O 2.167494 1.309801 -1.539413
N 0.156755 3.150816 0.401348
O -1.108259 3.746179 0.332553
C 3.822518 0.812853 0.789109
C 3.753701 -0.561350 0.092693
N 2.517035 -1.300453 0.361942
C 2.492730 -1.847924 1.712772
C -0.103021 -1.521961 -1.357851
H -0.279995 -0.507023 0.548261
H -2.301994 0.185822 -1.632384
C 2.254544 -2.332965 -0.651203
C 0.772002 -2.685484 -0.825791
H -1.974092 1.437092 1.140230
H -3.124751 1.937332 -0.080368
H -2.208449 -0.884598 2.247197
H -3.539804 -1.963333 1.763068
H -5.235052 0.566473 -0.479758

H -5.460371 -0.976289 0.363057
H -4.318815 -0.866837 -0.975897
H -1.375133 2.420852 -1.697928
H -0.195545 1.216388 -2.222236
H 1.823427 1.121894 1.594145
H 2.644068 2.601456 1.188231
H -1.018445 4.490742 0.948805
H 4.188184 0.712233 1.818902
H 4.572494 1.412003 0.258943
H 4.652691 -1.148378 0.366629
H 3.794573 -0.388874 -0.982922
H 1.539323 -2.350680 1.902102
H 3.304559 -2.580743 1.890444
H 2.597170 -1.045959 2.451454
H -0.797621 -1.912117 -2.110436
H 0.544501 -0.798524 -1.862749
H 2.829058 -3.255703 -0.436095
H 2.626065 -1.953765 -1.609685
H 0.725821 -3.522012 -1.534218
H 0.357088 -3.083710 0.106140

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.627768284**

Comp_17E_c21

B3LYP/6-31G* Geometry

C -3.526905 -0.273028 -0.977775
C -3.166132 -0.927915 0.366740
C -1.665915 -0.764191 0.717069
C -3.364063 1.256448 -0.824016
C -2.312539 1.640897 0.212552
C -1.132569 0.676231 0.366061
O -2.434588 2.652325 0.881002
H -2.814889 -0.628857 -1.735307
C -4.936224 -0.641670 -1.453280
C -0.869341 -1.902169 0.017745
C 0.616444 -1.940531 0.259350
C 1.549104 -1.511992 -0.846748
C 3.046946 -1.518345 -0.601133
O 1.071790 -1.203289 -1.930825
N 1.190058 -2.375095 1.327037
O 0.266664 -2.788759 2.287791
C 3.807052 -0.474184 -1.437307
C 3.157736 0.924187 -1.417417
N 2.587724 1.277258 -0.116242
C 3.621223 1.575409 0.867650
C -0.105075 1.185637 1.394568
H -0.671785 0.609256 -0.631504
H -1.553816 -0.897477 1.798726
C 1.584088 2.342578 -0.213778
C 0.667975 2.461333 1.012839
H -3.427050 -1.993942 0.360248
H -3.780917 -0.465866 1.153579
H -3.086868 1.719789 -1.782132
H -4.303760 1.726492 -0.510787

H -5.029243 -1.721499 -1.618981
H -5.183906 -0.135298 -2.393891
H -5.689029 -0.349851 -0.709882
H -1.016733 -1.840198 -1.063932
H -1.285159 -2.854842 0.366447
H 3.414552 -2.525322 -0.849109
H 3.231460 -1.384935 0.465579
H 0.837933 -3.090753 3.012390
H 3.865734 -0.796407 -2.482889
H 4.839471 -0.435588 -1.068639
H 2.337230 0.921957 -2.138325
H 3.893552 1.674917 -1.767056
H 4.323266 0.739181 0.941002
H 3.179352 1.721021 1.857302
H 4.200917 2.484739 0.612917
H 0.610260 0.384626 1.603454
H -0.644917 1.383422 2.328798
H 2.058388 3.327494 -0.398850
H 0.973320 2.127616 -1.098227
H 1.256605 2.775912 1.884496
H -0.040208 3.274879 0.826544

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632880842**

Comp_17E_c29

B3LYP/6-31G* Geometry

C 3.397708 -0.161508 1.146482
C 2.004322 -0.721142 1.475289
C 0.870583 -0.120081 0.618837
C 3.698369 -0.378364 -0.350555
C 2.591730 0.132161 -1.263636
C 1.152803 -0.257377 -0.902922
O 2.839625 0.776715 -2.266810
H 3.393302 0.921760 1.335309
C 4.486454 -0.783093 2.028581
C 0.581653 1.354627 1.029909
C -0.648129 1.873073 0.336924
C -1.995832 1.471402 0.875520
C -3.209994 1.532956 -0.041063
O -2.092839 1.126859 2.044590
N -0.682558 2.638504 -0.697687
O 0.589341 3.026707 -1.114197
C -4.057930 0.250834 0.015650
C -3.398379 -0.988551 -0.606054
N -2.199850 -1.481401 0.087154
C -2.528833 -1.996698 1.417772
C 0.865083 -1.671341 -1.487069
H 0.525795 0.443612 -1.460678
H -0.047590 -0.673797 0.832117
C -1.518622 -2.512379 -0.715281
C -0.606023 -1.994445 -1.844181
H 1.777675 -0.559749 2.537565
H 2.026868 -1.812080 1.332120
H 4.639200 0.090962 -0.655827

H 3.800256 -1.461569 -0.530501
H 5.475064 -0.374400 1.788599
H 4.531741 -1.871067 1.888322
H 4.291952 -0.591264 3.090493
H 1.428769 2.008183 0.808642
H 0.391909 1.378723 2.107766
H -2.903247 1.756707 -1.065292
H -3.824454 2.376693 0.302019
H 0.408768 3.531965 -1.923114
H -4.989032 0.430977 -0.536340
H -4.348767 0.058070 1.053140
H -3.114180 -0.748858 -1.637847
H -4.159530 -1.793226 -0.670591
H -1.622009 -2.388812 1.888853
H -2.903062 -1.192108 2.053294
H -3.279989 -2.809375 1.386248
H 1.438194 -1.757859 -2.419276
H 1.256262 -2.451479 -0.819121
H -2.265367 -3.205260 -1.149284
H -0.911095 -3.118892 -0.033494
H -0.577086 -2.784271 -2.606723
H -1.062297 -1.126011 -2.336549

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.631200685**

Comp_17E_c30

B3LYP/6-31G* Geometry

C -3.790777 0.367558 0.254651
C -2.851309 0.698341 -0.913846
C -1.358258 0.516229 -0.573102
C -3.566631 -1.095402 0.680166
C -2.106981 -1.441950 0.939759
C -1.048279 -0.907375 -0.033717
O -1.785932 -2.179347 1.854308
H -3.530156 1.013849 1.106065
C -5.259788 0.626402 -0.098084
C -0.862079 1.612742 0.421312
C 0.607110 1.897294 0.252412
C 1.606140 1.270985 1.192696
C 3.089263 1.402328 0.895670
O 1.197918 0.679969 2.182379
N 1.108582 2.655204 -0.659938
O 0.124765 3.208981 -1.484381
C 3.893277 0.133545 1.243863
C 3.243686 -1.183706 0.776034
N 2.584920 -1.083655 -0.528635
C 3.532265 -0.872494 -1.617240
C -0.832054 -1.952803 -1.163299
H -0.131773 -0.873573 0.560972
H -0.800214 0.658522 -1.505863
C 1.708886 -2.230039 -0.811051
C 0.568257 -1.888579 -1.803539
H -3.015926 1.728724 -1.254939
H -3.111809 0.049464 -1.763923

H -4.143555 -1.365847 1.570610
H -3.911305 -1.750715 -0.137695
H -5.920200 0.383540 0.742692
H -5.571185 0.014313 -0.954705
H -5.424157 1.677906 -0.361849
H -1.032804 1.305821 1.456886
H -1.412074 2.541630 0.238540
H 3.470562 2.242808 1.493563
H 3.222178 1.684460 -0.149008
H 0.647439 3.756908 -2.091857
H 4.025417 0.061117 2.328831
H 4.897907 0.248063 0.818444
H 2.472246 -1.455471 1.501527
H 4.006722 -1.986860 0.797763
H 4.114777 0.038265 -1.451171
H 4.240418 -1.716877 -1.731985
H 2.995074 -0.753499 -2.563693
H -0.973318 -2.958823 -0.746817
H -1.598295 -1.828021 -1.940496
H 1.274076 -2.556412 0.139645
H 2.296193 -3.088879 -1.187452
H 0.742429 -0.886518 -2.213284
H 0.586436 -2.580017 -2.655352

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.631359428**

Comp_17E_c31

B3LYP/6-31G* Geometry

C 4.126251 -0.074957 -0.405363
C 3.017272 0.864420 -0.936504
C 1.705280 0.813379 -0.126445
C 3.513657 -1.396105 0.141592
C 2.152559 -1.679564 -0.469988
C 1.086192 -0.617143 -0.201258
O 1.907951 -2.695324 -1.097933
H 4.766225 -0.337183 -1.257317
C 5.010703 0.600120 0.651618
C 0.765048 1.921189 -0.677286
C -0.609159 2.013237 -0.068254
C -1.791073 1.502519 -0.857717
C -3.168315 1.485609 -0.218367
O -1.611364 1.134201 -2.010198
N -0.895700 2.548101 1.067054
O 0.239845 3.029025 1.721846
C -4.083459 0.383754 -0.780442
C -3.426088 -1.009983 -0.825870
N -2.600075 -1.298021 0.347746
C -3.406609 -1.534765 1.538534
C 0.334529 -1.000307 1.107688
H 0.386126 -0.662339 -1.043142
H 1.925788 1.049846 0.922819
C -1.624563 -2.368973 0.115864
C -0.431719 -2.333451 1.083931
H 2.779761 0.591137 -1.975006

H 3.396556 1.893834 -0.971294
H 4.172875 -2.252518 -0.023460
H 3.365951 -1.293461 1.227177
H 5.529597 1.470851 0.233689
H 5.770459 -0.092425 1.033285
H 4.415434 0.943889 1.507365
H 0.630235 1.765489 -1.751668
H 1.263785 2.886386 -0.530526
H -3.625720 2.469484 -0.400973
H -3.059058 1.400156 0.863723
H -0.132195 3.410998 2.533190
H -4.391381 0.635652 -1.801283
H -4.999571 0.368097 -0.177068
H -2.771018 -1.044242 -1.699155
H -4.211324 -1.776096 -0.980568
H -4.066288 -0.681848 1.726107
H -4.038407 -2.440730 1.450484
H -2.766616 -1.653688 2.417739
H 1.063884 -1.024828 1.929912
H -0.368989 -0.197514 1.345021
H -1.246785 -2.263325 -0.905986
H -2.098795 -3.368622 0.169171
H -0.771619 -2.547910 2.105675
H 0.237019 -3.156742 0.808366

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632069754**

Comp_17E_c32

B3LYP/6-31G* Geometry

C -4.166587 0.460920 0.107395
C -2.988411 1.218145 0.749697
C -1.603753 0.629008 0.413508
C -4.107166 -1.029696 0.510274
C -2.742377 -1.638398 0.219314
C -1.540284 -0.879526 0.797203
O -2.625365 -2.676441 -0.407741
H -5.095572 0.881223 0.516419
C -4.220577 0.626380 -1.420019
C -0.489168 1.473852 1.114335
C 0.716569 1.782932 0.262543
C 2.103135 1.372099 0.712138
C 3.279191 1.626796 -0.224899
O 2.258043 0.952472 1.848760
N 0.692621 2.501381 -0.806911
O -0.591184 2.970874 -1.099689
C 4.303289 0.483146 -0.279906
C 3.776921 -0.770121 -0.997348
N 2.685400 -1.418044 -0.278646
C 3.153277 -2.163812 0.882844
C -0.202898 -1.581724 0.505083
H -1.693865 -0.915863 1.890960
H -1.463873 0.711321 -0.668069
C 1.703974 -2.146891 -1.098280
C 0.286131 -1.566767 -0.951359

H -3.117732 1.218856 1.842955
H -3.009613 2.267669 0.430619
H -4.286299 -1.115029 1.592612
H -4.869159 -1.624849 -0.002533
H -4.251771 1.686506 -1.697783
H -5.114790 0.143346 -1.830468
H -3.353054 0.176809 -1.916861
H -0.142510 0.990227 2.031073
H -0.925512 2.438409 1.404420
H 3.774092 2.531184 0.157642
H 2.918039 1.870543 -1.226351
H -0.444763 3.488954 -1.907560
H 4.632361 0.238771 0.735660
H 5.191432 0.837952 -0.818681
H 4.622428 -1.466407 -1.171676
H 3.406264 -0.471588 -1.985601
H 3.610845 -1.488002 1.611393
H 3.891359 -2.946136 0.617422
H 2.309598 -2.648560 1.379406
H 0.562901 -1.120100 1.135521
H -0.296958 -2.625567 0.831318
H 1.698924 -3.213228 -0.825556
H 1.998727 -2.107345 -2.155112
H 0.308464 -0.539204 -1.336011
H -0.405653 -2.136554 -1.582030

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.630332509**

Comp_17E_c33

B3LYP/6-31G* Geometry

C -3.994100 -0.151515 0.564881
C -2.814440 0.625267 1.203826
C -1.583683 0.747728 0.282019
C -3.472283 -1.246809 -0.406612
C -2.096804 -1.737808 0.002581
C -1.000498 -0.670731 0.011414
O -1.867488 -2.902932 0.281478
H -4.532037 -0.660536 1.374544
C -4.986440 0.777689 -0.146586
C -0.565430 1.719916 0.941701
C 0.663533 2.039041 0.131206
C 2.020866 1.565322 0.603303
C 3.163186 1.484478 -0.402181
O 2.183415 1.332917 1.790601
N 0.701176 2.785016 -0.916761
O -0.559846 3.294252 -1.247274
C 4.067095 0.256299 -0.207328
C 3.415409 -1.077479 -0.606656
N 2.258433 -1.453548 0.207122
C 2.649061 -1.813301 1.569167
C -0.211431 -0.752947 -1.324944
H -0.315647 -0.928714 0.826435
H -1.898585 1.193417 -0.670207
C 1.451694 -2.516086 -0.409825

C 0.571700 -2.052108 -1.581303
H -2.496519 0.115981 2.125278
H -3.157763 1.621716 1.509178
H -4.160116 -2.093929 -0.474634
H -3.377313 -0.809341 -1.411985
H -4.487165 1.364052 -0.928680
H -5.443413 1.481519 0.558923
H -5.792933 0.207062 -0.622358
H -0.233872 1.315995 1.903250
H -1.089090 2.663593 1.139191
H 3.762396 2.395563 -0.262338
H 2.773874 1.526469 -1.422740
H -0.364804 3.844731 -2.022649
H 4.414836 0.225453 0.830151
H 4.961694 0.385038 -0.829619
H 4.189605 -1.871690 -0.581181
H 3.085465 -1.000641 -1.649851
H 1.761470 -2.116219 2.132930
H 3.081169 -0.950314 2.079921
H 3.376027 -2.648024 1.598088
H 0.489300 0.083395 -1.344874
H -0.905005 -0.583718 -2.161626
H 0.786387 -2.911678 0.362529
H 2.082280 -3.363893 -0.742332
H 1.174072 -1.904322 -2.487903
H -0.114830 -2.876882 -1.806392

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.630484119

Comp_17E_c34

B3LYP/6-31G* Geometry

C -3.838436 0.026029 0.721529
C -3.291867 0.756381 -0.517081
C -1.747981 0.660770 -0.630195
C -3.599582 -1.484605 0.522793
C -2.309386 -1.795277 -0.232151
C -1.212011 -0.733253 -0.145524
O -2.179022 -2.834884 -0.853431
H -3.267928 0.361691 1.599726
C -5.317277 0.332309 0.980863
C -1.098508 1.842812 0.150170
C 0.379319 2.031036 -0.070374
C 1.361476 1.498388 0.943472
C 2.850658 1.628405 0.668518
O 0.930175 0.981929 1.965405
N 0.907959 2.646444 -1.071001
O -0.050239 3.121404 -1.965697
C 3.711191 0.597139 1.412594
C 3.329064 -0.867352 1.125843
N 3.101284 -1.154828 -0.292572
C 4.347233 -1.172313 -1.047828
C 0.077444 -1.181400 -0.851600
H -1.004232 -0.626486 0.931380
H -1.478104 0.774937 -1.686505

C 2.324434 -2.382635 -0.514116
C 0.850101 -2.276414 -0.097215
H -3.596947 1.810334 -0.512194
H -3.753206 0.308653 -1.409973
H -3.561659 -2.010407 1.487960
H -4.420661 -1.941326 -0.043745
H -5.693897 -0.227961 1.845004
H -5.931934 0.059008 0.113588
H -5.472655 1.399445 1.178662
H -1.264627 1.709754 1.223308
H -1.596055 2.766262 -0.164662
H 3.146134 2.644143 0.971754
H 3.016429 1.576433 -0.408726
H 0.492625 3.558544 -2.641646
H 3.629907 0.752819 2.494244
H 4.759868 0.783954 1.150627
H 2.404638 -1.076834 1.665491
H 4.106119 -1.532599 1.553709
H 5.039534 -1.975141 -0.724439
H 4.134128 -1.316107 -2.112506
H 4.870914 -0.217009 -0.938769
H -0.178614 -1.539393 -1.856794
H 0.737922 -0.320402 -0.983247
H 2.787868 -3.250391 -0.003365
H 2.368710 -2.598922 -1.589258
H 0.374726 -3.248533 -0.266251
H 0.783743 -2.093493 0.983233

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.634417684

Comp_17E_c35

B3LYP/6-31G* Geometry

C 3.713079 -0.114329 -0.397392
C 2.651627 -0.098619 -1.510387
C 1.212433 -0.317623 -1.001825
C 3.374639 0.956994 0.658981
C 1.945989 0.863348 1.179533
C 0.838932 0.655239 0.149807
O 1.687706 1.007015 2.362892
H 3.685941 -1.095203 0.099160
C 5.126705 0.085130 -0.955915
C 0.968723 -1.805857 -0.625406
C -0.396062 -2.047075 -0.030945
C -1.620498 -1.817188 -0.882864
C -2.997465 -1.910855 -0.242971
O -1.475416 -1.610411 -2.078110
N -0.640473 -2.440641 1.170981
O 0.512515 -2.642421 1.924962
C -3.390568 -0.791257 0.750246
C -3.713297 0.573139 0.123439
N -2.555752 1.379115 -0.288612
C -2.966443 2.362703 -1.288672
C 0.363983 2.035530 -0.386475
H 0.004480 0.227123 0.708372

H 0.528087 -0.111053 -1.830133
C -1.910288 2.017229 0.866603
C -0.606988 2.774951 0.547286
H 2.891716 -0.859730 -2.264973
H 2.703796 0.870904 -2.028088
H 4.052923 0.920185 1.517628
H 3.493435 1.950416 0.196308
H 5.212218 1.050415 -1.471790
H 5.381776 -0.701548 -1.675869
H 5.877359 0.066081 -0.157056
H 1.722570 -2.170444 0.074922
H 1.047836 -2.397662 -1.545125
H -3.047962 -2.864604 0.294866
H -3.716506 -1.946752 -1.068470
H 0.156264 -2.892117 2.792725
H -2.627277 -0.701449 1.528978
H -4.301091 -1.128773 1.262512
H -4.348432 1.144442 0.830277
H -4.329206 0.400967 -0.767420
H -3.719703 3.079538 -0.905567
H -3.393324 1.846044 -2.154038
H -2.105268 2.937972 -1.638228
H -0.130538 1.860988 -1.347645
H 1.223145 2.687728 -0.594612
H -1.690193 1.234524 1.599130
H -2.606715 2.720057 1.368829
H -0.840896 3.748779 0.098266
H -0.116299 2.991631 1.504242

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632292869**

Comp_17E_c36

B3LYP/6-31G* Geometry

C 4.230465 -0.207550 -0.037126
C 3.244054 0.766830 -0.732885
C 1.805292 0.687245 -0.183441
C 3.495911 -1.488932 0.443889
C 2.301223 -1.808596 -0.435572
C 1.220360 -0.723742 -0.479884
O 2.185680 -2.860653 -1.038557
H 4.972898 -0.515738 -0.783942
C 4.982087 0.456398 1.124341
C 0.963429 1.834012 -0.813219
C -0.403650 2.048937 -0.218929
C -1.619242 1.505294 -0.931564
C -2.979826 1.617701 -0.262658
O -1.474484 0.989190 -2.030564
N -0.651601 2.694548 0.867522
O 0.510530 3.179692 1.469022
C -4.000076 0.581901 -0.756951
C -3.548839 -0.881645 -0.591240
N -2.961231 -1.178715 0.718360
C -3.970549 -1.216254 1.768683
C 0.076447 -1.140377 0.483564

H 0.819121 -0.726748 -1.501524
H 1.832756 0.849920 0.902783
C -2.142146 -2.399082 0.717811
C -0.821554 -2.263203 -0.056056
H 3.205860 0.543121 -1.808992
H 3.624278 1.792508 -0.647373
H 4.164995 -2.352780 0.481570
H 3.115126 -1.314624 1.461710
H 4.283961 0.843579 1.877824
H 5.591942 1.296083 0.770701
H 5.648782 -0.256362 1.624332
H 0.839449 1.641539 -1.883062
H 1.524514 2.767497 -0.694319
H -3.355694 2.632078 -0.463505
H -2.848002 1.555430 0.818942
H 0.163980 3.647264 2.246163
H -4.209126 0.742410 -1.820553
H -4.943083 0.760376 -0.225486
H -2.794984 -1.082628 -1.353450
H -4.406951 -1.548936 -0.808664
H -3.489534 -1.369690 2.740759
H -4.718439 -2.021447 1.624807
H -4.510330 -0.264685 1.810979
H -0.550987 -0.270898 0.691762
H 0.500216 -1.434283 1.456077
H -1.913894 -2.630828 1.766301
H -2.707797 -3.266702 0.324077
H -0.298583 -3.225540 -0.023222
H -1.024764 -2.080203 -1.117646

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.632949169**

Comp_17E_c37

B3LYP/6-31G* Geometry

C 3.692753 -0.182510 -0.357652
C 2.684285 -0.146121 -1.521192
C 1.220443 -0.327848 -1.071111
C 3.319482 0.869346 0.709253
C 1.853531 0.820341 1.131067
C 0.826140 0.719710 0.006456
O 1.521283 0.912311 2.300196
H 3.638376 -1.170977 0.119500
C 5.131738 0.015394 -0.848443
C 0.958817 -1.804847 -0.640879
C -0.333493 -1.984089 0.108358
C -1.632104 -1.806703 -0.631522
C -2.923988 -1.728253 0.163054
O -1.610849 -1.720357 -1.852037
N -0.446738 -2.223285 1.368643
O 0.781547 -2.359575 2.006867
C -3.972639 -0.774738 -0.438278
C -3.454769 0.611644 -0.862169
N -2.505035 1.237897 0.065961
C -3.091867 1.488104 1.379772

C 0.601198 2.137992 -0.606497
H -0.117477 0.424415 0.467606
H 0.568474 -0.148597 -1.933388
C -1.966619 2.484960 -0.503395
C -0.578836 2.910432 0.012751
H 2.943113 -0.919286 -2.257255
H 2.782813 0.817629 -2.042461
H 3.936810 0.775698 1.608516
H 3.510999 1.870261 0.290375
H 5.414521 -0.761861 -1.568335
H 5.844869 -0.021882 -0.016465
H 5.247396 0.988055 -1.344223
H 1.771427 -2.185990 -0.021182
H 0.917149 -2.409480 -1.553498
H -2.689097 -1.463602 1.194521
H -3.346954 -2.742906 0.201144
H 0.528886 -2.420477 2.942162
H -4.785847 -0.676188 0.291336
H -4.417093 -1.228700 -1.331129
H -4.332727 1.264057 -1.046018
H -2.934922 0.499874 -1.817910
H -3.960628 2.174045 1.330551
H -3.421597 0.552892 1.839531
H -2.344724 1.933139 2.043186
H 1.509430 2.746572 -0.509798
H 0.428868 2.037110 -1.687203
H -2.682138 3.315201 -0.342619
H -1.896430 2.352669 -1.589833
H -0.461655 3.974344 -0.234044
H -0.529703 2.845796 1.107061

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.630111946**

Comp_17Z_c01

B3LYP/6-31G* Geometry

C 3.675439 0.890029 0.526172
C 2.528018 1.483189 -0.309875
C 1.318263 0.542251 -0.466533
C 4.133586 -0.434432 -0.122398
C 2.980704 -1.408663 -0.316311
C 1.726336 -0.859829 -1.014875
O 3.069344 -2.573516 0.029849
H 4.518748 1.592617 0.480840
C 3.310933 0.700546 2.006935
C 0.247945 1.215355 -1.369848
C -0.671723 2.157896 -0.635002
C -1.589871 1.545281 0.414221
C -2.934422 1.052599 -0.084984
O -1.208313 1.429471 1.564334
N -0.662940 3.400196 -0.939918
C -3.644183 0.079859 0.863163
C -2.876337 -1.229754 1.114754
N -2.442625 -1.930343 -0.101055
C -3.573047 -2.533204 -0.800588

C 0.585151 -1.900547 -1.037284
H 2.049411 -0.699000 -2.060111
H 0.877261 0.397233 0.524907
C -1.398593 -2.925996 0.201117
C 0.004261 -2.312374 0.328841
O -1.628313 4.115641 -0.192656
H 2.189106 2.428974 0.131453
H 2.914187 1.730668 -1.310554
H 4.555250 -0.216999 -1.115711
H 4.908804 -0.937089 0.464268
H 2.510760 -0.035318 2.147501
H 2.973580 1.643997 2.451050
H 4.178597 0.349060 2.577075
H -0.382138 0.448983 -1.836139
H 0.731571 1.771133 -2.181687
H -2.788016 0.594070 -1.070292
H -3.543870 1.952957 -0.255164
H -4.642334 -0.128219 0.459616
H -3.796650 0.562807 1.834998
H -1.987244 -0.989571 1.701368
H -3.503217 -1.890343 1.747173
H -4.299943 -1.764091 -1.081084
H -3.225930 -3.013576 -1.721227
H -4.104532 -3.293136 -0.194267
H -0.232412 -1.517907 -1.658002
H 0.959682 -2.799663 -1.540138
H -1.387877 -3.657243 -0.616637
H -1.648848 -3.492549 1.117852
H 0.672696 -3.038628 0.801175
H -0.043346 -1.455300 1.010649
H -1.510833 5.021164 -0.519371

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.627164833**

Comp_17Z_c02

B3LYP/6-31G* Geometry

C -3.753972 0.338169 0.084362
C -2.828333 0.730353 -1.077104
C -1.332351 0.726950 -0.697184
C -3.365570 -1.065446 0.592318
C -1.884185 -1.190730 0.918875
C -0.884877 -0.637515 -0.099999
O -1.505704 -1.745797 1.936796
H -3.599689 1.050795 0.908423
C -5.232428 0.396190 -0.315593
C -0.983978 1.912086 0.254346
C 0.429877 2.429346 0.093653
C 1.584457 1.613611 0.673948
C 2.663927 1.122755 -0.270806
O 1.561827 1.366158 1.866375
N 0.551277 3.576340 -0.466606
C 3.664255 0.135301 0.341831
C 3.054979 -1.215864 0.758651
N 2.247602 -1.845081 -0.290987

C 3.062879 -2.413227 -1.355943
 C -0.579335 -1.691545 -1.197022
 H 0.043118 -0.488689 0.454759
 H -0.766530 0.887241 -1.625139
 C 1.269420 -2.806197 0.229649
 C 0.050841 -3.002029 -0.691655
 O 1.894081 4.003676 -0.554580
 H -2.992816 0.029304 -1.908639
 H -3.101808 1.723642 -1.456476
 H -3.935144 -1.357833 1.480236
 H -3.596347 -1.797273 -0.199072
 H -5.441925 -0.292223 -1.144630
 H -5.514720 1.404876 -0.639510
 H -5.882514 0.117587 0.521951
 H -1.122471 1.621341 1.303409
 H -1.652127 2.755351 0.051108
 H 3.175144 2.013918 -0.654576
 H 2.161981 0.670169 -1.136330
 H 4.124210 0.580270 1.231872
 H 4.475294 -0.015965 -0.381501
 H 3.870716 -1.881601 1.103737
 H 2.404568 -1.041705 1.619252
 H 2.424555 -2.806399 -2.153599
 H 3.705296 -1.645401 -1.798773
 H 3.712425 -3.238462 -1.001999
 H -1.487245 -1.926375 -1.768777
 H 0.117149 -1.218073 -1.898590
 H 0.906025 -2.431083 1.190133
 H 1.730470 -3.792556 0.431651
 H -0.685235 -3.593249 -0.132175
 H 0.319277 -3.607473 -1.567576
 H 1.800934 4.875517 -0.968703

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.626803270

Comp_17Z_c03

B3LYP/6-31G* Geometry

C -4.068426 0.448687 0.862206
 C -2.720245 1.000806 1.358924
 C -1.547081 0.821925 0.371688
 C -3.906790 -1.047989 0.512582
 C -2.775701 -1.250539 -0.482581
 C -1.410869 -0.670182 -0.076920
 O -2.949968 -1.832807 -1.538530
 H -4.786226 0.524492 1.690287
 C -4.639841 1.244027 -0.322335
 C -0.253847 1.353378 1.045479
 C 0.844181 1.841796 0.114858
 C 2.267602 1.412958 0.434792
 C 3.213979 1.000104 -0.684094
 O 2.614142 1.420771 1.604767
 N 0.500352 2.668667 -0.803077
 C 4.030294 -0.257187 -0.344948
 C 3.220123 -1.558406 -0.445758

N 2.072051 -1.622742 0.462837
 C 2.496067 -1.811181 1.848754
 C -0.362687 -0.909309 -1.179165
 H -1.126259 -1.220882 0.834985
 H -1.737388 1.435775 -0.517603
 C 1.096846 -2.650338 0.065763
 C 0.274036 -2.308251 -1.188109
 O 1.589145 3.137849 -1.562824
 H -2.826397 2.068124 1.593655
 H -2.461853 0.502081 2.305800
 H -3.665212 -1.606045 1.429239
 H -4.822236 -1.472129 0.088833
 H -4.740887 2.305689 -0.068165
 H -5.631024 0.868167 -0.600727
 H -4.004308 1.172396 -1.212498
 H 0.170677 0.588215 1.701906
 H -0.524165 2.194690 1.696813
 H 3.890383 1.850998 -0.841533
 H 2.664120 0.874290 -1.621444
 H 4.472593 -0.140794 0.649703
 H 4.867497 -0.334846 -1.049849
 H 2.843905 -1.643938 -1.471105
 H 3.898435 -2.420845 -0.287108
 H 3.072670 -2.744830 1.995273
 H 3.106292 -0.966767 2.176547
 H 1.615375 -1.850632 2.498118
 H -0.842343 -0.738161 -2.148667
 H 0.436214 -0.174735 -1.084091
 H 0.415071 -2.780126 0.914313
 H 1.584714 -3.634421 -0.079985
 H -0.503217 -3.074043 -1.299526
 H 0.902150 -2.394146 -2.084253
 H 1.152211 3.722656 -2.201365

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.626735079

Comp_17Z_c04

B3LYP/6-31G* Geometry

C -3.541303 0.650078 0.815323
 C -2.335036 1.376061 0.190623
 C -1.567485 0.538852 -0.854096
 C -3.070054 -0.698954 1.412793
 C -2.328985 -1.509228 0.362454
 C -1.096166 -0.827744 -0.246874
 O -2.723182 -2.603771 -0.002064
 H -3.908641 1.270301 1.643963
 C -4.706979 0.456858 -0.167533
 C -0.454086 1.396307 -1.520220
 C 0.465157 2.189757 -0.616429
 C 1.397261 1.508015 0.379705
 C 2.790405 1.202767 -0.127497
 O 1.000718 1.252907 1.502695
 N 0.446082 3.463832 -0.756347
 C 3.655294 0.328339 0.788559

C 3.018786 -1.025829 1.157945
N 2.368789 -1.693163 0.027883
C 3.334857 -2.261926 -0.903617
C -0.374015 -1.749020 -1.245497
H -0.428498 -0.584952 0.589211
H -2.252907 0.291300 -1.677842
C 1.359809 -2.673754 0.445766
C 0.311732 -2.985632 -0.634495
O 1.386801 4.092461 0.091872
H -2.667666 2.314826 -0.271806
H -1.636063 1.654038 0.990262
H -2.385593 -0.498088 2.248935
H -3.909193 -1.293286 1.787159
H -5.025886 1.418743 -0.586375
H -5.569885 0.007343 0.337069
H -4.443388 -0.201874 -1.003152
H -0.938978 2.135514 -2.167571
H 0.158086 0.764465 -2.174803
H 3.270197 2.177131 -0.302038
H 2.683083 0.740232 -1.116764
H 3.864192 0.863143 1.722521
H 4.624417 0.182562 0.295448
H 3.789293 -1.666593 1.630431
H 2.251920 -0.837505 1.911555
H 4.019834 -1.486741 -1.262698
H 3.943124 -3.067587 -0.446771
H 2.823283 -2.678266 -1.776529
H -1.099242 -2.090820 -1.993963
H 0.391966 -1.175146 -1.774745
H 0.851493 -2.260627 1.323799
H 1.826462 -3.621501 0.780002
H -0.440796 -3.647687 -0.194181
H 0.774275 -3.555973 -1.451110
H 1.261165 5.029909 -0.122247

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.625480919

Comp_17Z_c05

B3LYP/6-31G* Geometry

C -3.746465 -0.050892 0.107489
C -2.948492 0.359357 -1.140410
C -1.455204 0.629921 -0.856737
C -3.110050 -1.308868 0.732885
C -1.614477 -1.164900 0.973818
C -0.771076 -0.582375 -0.162792
O -1.099074 -1.538534 2.013870
H -3.682351 0.761974 0.845600
C -5.228922 -0.277885 -0.209543
C -1.264585 1.954247 -0.061501
C 0.151934 2.484808 -0.115943
C 1.160696 1.924862 0.879507
C 2.432657 1.286439 0.349841
O 0.868546 1.947804 2.061377
N 0.393087 3.400801 -0.979126

C 2.959708 0.146480 1.243659
C 3.558810 -1.004372 0.420062
N 2.593009 -1.639613 -0.487593
C 3.267748 -2.338799 -1.575999
C -0.372798 -1.690352 -1.174836
H 0.156282 -0.252799 0.308625
H -0.960355 0.781806 -1.825734
C 1.656919 -2.520196 0.222830
C 0.394454 -2.884016 -0.578455
O 1.739133 3.823864 -0.952765
H -3.035081 -0.440685 -1.890113
H -3.397381 1.252451 -1.594779
H -3.583097 -1.584266 1.680798
H -3.254325 -2.153297 0.038866
H -5.354263 -1.075766 -0.953110
H -5.690564 0.630863 -0.613287
H -5.787078 -0.567957 0.688251
H -1.537779 1.826917 0.992841
H -1.921350 2.718802 -0.489557
H 3.172843 2.088656 0.237139
H 2.236625 0.913476 -0.662016
H 2.153959 -0.219836 1.887963
H 3.729683 0.519414 1.928634
H 4.373320 -0.606814 -0.198491
H 4.019391 -1.744094 1.103114
H 3.884509 -3.191151 -1.228405
H 2.534761 -2.726914 -2.289860
H 3.920489 -1.643896 -2.114771
H -1.263727 -2.066561 -1.695196
H 0.254430 -1.210347 -1.935221
H 1.339566 -2.020427 1.140832
H 2.158643 -3.458124 0.535326
H -0.255906 -3.454734 0.096393
H 0.645614 -3.568192 -1.399399
H 1.746493 4.517355 -1.630521

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.626204744

Comp_17Z_c06

B3LYP/6-31G* Geometry

C -2.563071 -2.000893 0.981405
C -1.327535 -2.111239 0.072789
C -0.801863 -0.757625 -0.441426
C -3.688940 -1.280087 0.213104
C -3.247741 0.066656 -0.343048
C -1.920224 0.095781 -1.118159
O -3.954046 1.053788 -0.230975
H -2.906992 -3.020826 1.200925
C -2.264736 -1.317253 2.325252
C 0.373360 -0.990134 -1.422343
C 1.592037 -1.616969 -0.792429
C 2.232567 -0.872819 0.368317
C 3.229610 0.210398 0.000296
O 1.905305 -1.127261 1.512827

N 2.046079 -2.710929 -1.275503
 C 3.291429 1.373171 1.001722
 C 1.921176 1.992159 1.329929
 N 1.058653 2.228749 0.164173
 C 1.585386 3.297262 -0.680354
 C -1.527996 1.530894 -1.554002
 H -2.168841 -0.446760 -2.049999
 H -0.413578 -0.196858 0.412343
 C -0.315674 2.507324 0.606942
 C -1.372853 2.647195 -0.497269
 O 3.232273 -3.107781 -0.612560
 H -0.518508 -2.620327 0.609655
 H -1.578005 -2.746864 -0.790316
 H -3.993197 -1.902956 -0.642349
 H -4.577414 -1.114866 0.830803
 H -1.435207 -1.813144 2.841576
 H -3.143024 -1.349442 2.980435
 H -1.993024 -0.261710 2.202605
 H 0.686032 -0.028208 -1.843697
 H 0.054326 -1.630564 -2.253864
 H 2.996492 0.572966 -1.006614
 H 4.209482 -0.284716 -0.073832
 H 3.981412 2.128584 0.606589
 H 3.723848 1.024113 1.945928
 H 1.389860 1.300351 1.989034
 H 2.080807 2.924192 1.907968
 H 2.606030 3.059729 -0.994743
 H 1.608458 4.276815 -0.163423
 H 0.979625 3.404198 -1.584241
 H -2.314506 1.873988 -2.236494
 H -0.616611 1.474310 -2.158967
 H -0.347578 3.436490 1.212522
 H -0.604085 1.698117 1.287336
 H -1.191428 3.578777 -1.049728
 H -2.334940 2.785855 0.003646
 H 3.449590 -3.938864 -1.062479

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.623661162**

Comp_17Z_c07

B3LYP/6-31G* Geometry

C -3.571931 0.653476 0.928484
 C -2.412554 1.513317 0.388299
 C -1.627560 0.862013 -0.768817
 C -3.033103 -0.740534 1.331636
 C -2.277875 -1.367082 0.170038
 C -1.095770 -0.551831 -0.360879
 O -2.626275 -2.425499 -0.325764
 H -3.952199 1.140371 1.836893
 C -4.745702 0.538368 -0.057315
 C -0.543637 1.835216 -1.318699
 C 0.638621 2.129855 -0.412018
 C 1.953477 1.417481 -0.712735
 C 2.914222 1.052012 0.402343

O 2.191557 1.138295 -1.877751
 N 0.457902 3.045386 0.472985
 C 3.779648 -0.177438 0.085130
 C 2.986282 -1.461836 -0.222996
 N 1.854339 -1.680836 0.680181
 C 2.291214 -1.922241 2.051626
 C -0.341447 -1.273919 -1.488510
 H -0.406445 -0.403962 0.484608
 H -2.319049 0.713808 -1.611481
 C 0.959473 -2.764994 0.252345
 C 0.310506 -2.628947 -1.133823
 O 1.592664 3.328305 1.248449
 H -2.802688 2.484307 0.055790
 H -1.716871 1.732792 1.208448
 H -2.341869 -0.625345 2.178941
 H -3.838414 -1.416771 1.634674
 H -4.469622 0.001697 -0.972133
 H -5.109463 1.531199 -0.347358
 H -5.581478 -0.006786 0.396051
 H -1.045950 2.783837 -1.537013
 H -0.142107 1.462067 -2.263247
 H 2.352570 0.923266 1.330753
 H 3.558145 1.926324 0.568639
 H 4.456783 -0.336692 0.933021
 H 4.414896 0.034494 -0.781505
 H 2.593678 -1.383633 -1.238574
 H 3.686459 -2.321879 -0.215137
 H 2.874004 -1.076486 2.427694
 H 1.416776 -2.040543 2.700835
 H 2.912458 -2.834209 2.149599
 H -1.033506 -1.443160 -2.323595
 H 0.433420 -0.603265 -1.864904
 H 0.162308 -2.821644 1.004728
 H 1.479069 -3.744307 0.289024
 H -0.448995 -3.414911 -1.183060
 H 1.044047 -2.864140 -1.915479
 H 1.271608 4.045424 1.817504

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624229682**

Comp_17Z_c08

B3LYP/6-31G* Geometry

C 4.003730 0.168267 -0.385940
 C 2.858354 1.083413 0.092551
 C 1.744520 0.335050 0.850977
 C 3.428085 -0.991914 -1.235008
 C 2.306404 -1.706389 -0.496499
 C 1.154485 -0.807971 -0.036265
 O 2.336730 -2.904148 -0.273936
 H 4.656271 0.766292 -1.036262
 C 4.866471 -0.362619 0.770412
 C 0.697057 1.329461 1.425529
 C -0.093188 2.179291 0.453670
 C -1.192589 1.577874 -0.421007

C -2.571750 1.517395 0.204286
O -0.937059 1.187447 -1.545109
N 0.157196 3.436546 0.446637
C -3.633531 0.784246 -0.624371
C -3.340311 -0.708935 -0.862983
N -3.008803 -1.452690 0.356410
C -4.192737 -1.722732 1.162701
C 0.020819 -1.612068 0.615906
H 0.768908 -0.324279 -0.945252
H 2.186038 -0.136881 1.741242
C -2.249407 -2.684845 0.093078
C -0.808956 -2.439481 -0.383516
O -0.693842 4.128961 -0.443465
H 3.267632 1.876140 0.732825
H 2.413876 1.588653 -0.775890
H 3.013261 -0.581597 -2.167065
H 4.198517 -1.723316 -1.498029
H 4.306916 -1.037328 1.428688
H 5.251671 0.461603 1.382446
H 5.724411 -0.926059 0.386221
H 1.227685 2.028707 2.081518
H -0.011315 0.782867 2.059878
H -2.869171 2.560869 0.385874
H -2.472273 1.054824 1.194907
H -3.728481 1.264435 -1.605294
H -4.600691 0.911988 -0.122809
H -4.205430 -1.162808 -1.385991
H -2.491922 -0.772668 -1.544272
H -4.703323 -0.787390 1.414239
H -4.924966 -2.378770 0.651319
H -3.901631 -2.205792 2.101615
H 0.440193 -2.271262 1.385979
H -0.668021 -0.929179 1.119930
H -2.773016 -3.334371 -0.635929
H -2.215076 -3.245138 1.036281
H -0.824395 -1.932096 -1.356621
H -0.331070 -3.408631 -0.561035
H -0.404718 5.047843 -0.330895

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.626450577**

Comp_17Z_c09

B3LYP/6-31G* Geometry

C 3.107808 1.078807 0.677238
C 1.640515 0.817813 1.058239
C 0.796679 0.194846 -0.077248
C 3.762170 -0.231748 0.188747
C 2.963569 -0.875869 -0.933627
C 1.470610 -1.074255 -0.672379
O 3.480206 -1.223837 -1.980261
H 3.131814 1.794608 -0.157426
C 3.895898 1.693779 1.839298
C 0.416465 1.255150 -1.149425
C -0.724046 2.115487 -0.662977

C -2.101829 1.459184 -0.644719
C -2.694888 1.071024 0.699190
O -2.643309 1.220306 -1.708421
N -0.491259 3.320794 -0.302800
C -3.700955 -0.088378 0.631697
C -3.176121 -1.358697 -0.059361
N -1.903914 -1.876976 0.467914
C -2.098619 -2.581151 1.731207
C 1.242050 -2.301812 0.267013
H 1.033757 -1.299214 -1.651928
H -0.139426 -0.166279 0.361661
C -1.244042 -2.710522 -0.547261
C 0.139171 -3.278117 -0.191025
O -1.669603 3.959991 0.155089
H 1.623238 0.151772 1.933367
H 1.172489 1.756739 1.379306
H 4.787062 -0.073866 -0.161581
H 3.802991 -0.937330 1.033942
H 3.451761 2.644111 2.157866
H 4.936923 1.887249 1.555278
H 3.905832 1.020759 2.706571
H 0.087782 0.755050 -2.069011
H 1.264307 1.897537 -1.408643
H -3.176433 1.975173 1.097499
H -1.876785 0.841871 1.390604
H -4.590129 0.231286 0.076326
H -4.037410 -0.307330 1.652745
H -3.964905 -2.134977 -0.022238
H -3.023327 -1.121390 -1.114628
H -2.601770 -1.925445 2.448256
H -1.136245 -2.866118 2.165905
H -2.712361 -3.496676 1.619644
H 1.020610 -1.941825 1.278703
H 2.164748 -2.890581 0.353725
H -1.151395 -2.093859 -1.448860
H -1.885228 -3.570852 -0.828979
H 0.487978 -3.798566 -1.093315
H 0.037841 -4.057746 0.575322
H -1.352469 4.854255 0.355181

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624351879**

Comp_17Z_c10

B3LYP/6-31G* Geometry

C -3.384087 0.967224 -0.254000
C -2.030923 0.905153 -0.985739
C -0.913962 0.231131 -0.161141
C -3.808252 -0.442193 0.215430
C -2.710697 -1.161087 0.989389
C -1.323371 -1.175528 0.344380
O -2.927101 -1.714785 2.052290
H -3.265300 1.590590 0.643848
C -4.469371 1.613946 -1.122469
C -0.430663 1.152766 1.001755

C 0.701745 2.035532 0.545747
C 2.095662 1.419659 0.568190
C 2.827427 1.202422 -0.746342
O 2.575232 1.125527 1.647759
N 0.444219 3.235407 0.181572
C 3.733647 -0.036943 -0.753861
C 3.009617 -1.368538 -1.004746
N 2.006153 -1.754607 -0.003942
C 2.632333 -2.078318 1.280468
C -1.297148 -2.263987 -0.762298
H -0.627710 -1.486845 1.130023
H -0.052128 0.082019 -0.818224
C 1.212394 -2.899134 -0.494167
C 0.062508 -2.516398 -1.445223
O 1.609390 3.909630 -0.259191
H -2.166806 0.361667 -1.932234
H -1.712481 1.920231 -1.256250
H -4.705027 -0.410215 0.842332
H -4.050693 -1.048461 -0.671860
H -4.633772 1.036641 -2.041658
H -4.186023 2.632276 -1.413439
H -5.425106 1.670377 -0.588410
H -0.065757 0.550096 1.840040
H -1.244503 1.780569 1.376596
H 3.428223 2.109634 -0.898142
H 2.108262 1.181814 -1.574176
H 4.300634 -0.066705 0.181866
H 4.472676 0.075150 -1.557101
H 2.503196 -1.302456 -1.975732
H 3.774908 -2.165055 -1.109572
H 3.359532 -2.909457 1.202184
H 3.141501 -1.201538 1.683981
H 1.858541 -2.368677 1.998127
H -1.632524 -3.204686 -0.304149
H -2.032614 -2.028252 -1.542465
H 0.790151 -3.412066 0.377650
H 1.873418 -3.637121 -0.987050
H -0.088071 -3.337112 -2.159106
H 0.354603 -1.650753 -2.051690
H 1.268944 4.795513 -0.457899

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624805269**

Comp_17Z_c11

B3LYP/6-31G* Geometry

C 3.712979 0.728393 -0.442819
C 2.423432 1.357162 0.114781
C 1.529795 0.371281 0.892585
C 3.338663 -0.471813 -1.342211
C 2.464630 -1.465751 -0.593988
C 1.187458 -0.894404 0.041207
O 2.766614 -2.643773 -0.509862
H 4.200665 1.480895 -1.077344
C 4.717071 0.327913 0.649568

C 0.292453 1.111680 1.484839
C -0.485562 2.031502 0.568758
C -1.327941 1.469114 -0.565831
C -2.839057 1.503913 -0.420571
O -0.778911 1.032912 -1.563667
N -0.410951 3.287555 0.813535
C -3.548348 0.338563 -1.128160
C -3.775345 -0.884493 -0.228885
N -2.574386 -1.465803 0.385121
C -2.972998 -2.339807 1.489395
C 0.430431 -1.987706 0.817282
H 0.585425 -0.540993 -0.805013
H 2.085173 0.016808 1.773369
C -1.750831 -2.177104 -0.608635
C -0.494589 -2.864420 -0.044256
O -1.201542 4.044980 -0.082264
H 2.671458 2.210001 0.760540
H 1.842027 1.762188 -0.723650
H 2.771147 -0.103086 -2.208831
H 4.223150 -0.999274 -1.712718
H 4.963194 1.185153 1.287628
H 5.649409 -0.038349 0.204592
H 4.333612 -0.470460 1.295635
H 0.641163 1.741817 2.310530
H -0.409379 0.384935 1.909137
H -3.139509 2.463827 -0.862451
H -3.109399 1.559849 0.640440
H -2.987142 0.079957 -2.031831
H -4.538202 0.668824 -1.466081
H -4.435397 -0.574660 0.591378
H -4.334945 -1.648611 -0.805319
H -3.562699 -3.215630 1.155345
H -2.096262 -2.709368 2.026091
H -3.583612 -1.772864 2.199843
H 1.170483 -2.639905 1.293170
H -0.160393 -1.538490 1.620262
H -1.457599 -1.449352 -1.371035
H -2.355385 -2.949368 -1.127363
H 0.073679 -3.262048 -0.893686
H -0.791739 -3.741821 0.543412
H -1.054296 4.950666 0.231345

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624637357**

Comp_17Z_c12

B3LYP/6-31G* Geometry

C -3.473085 0.695763 -0.124954
C -2.175629 0.802989 -0.944170
C -0.937411 0.219866 -0.229355
C -3.719157 -0.772472 0.285951
C -2.511386 -1.397402 0.970289
C -1.163453 -1.233819 0.266255
O -2.611529 -2.016445 2.015009
H -3.353792 1.281927 0.798067

C -4.674285 1.270183 -0.884598
C -0.449410 1.141876 0.924368
C 0.518862 2.202362 0.459586
C 1.778458 1.717846 -0.247385
C 2.850891 1.106844 0.636583
O 1.871535 1.784861 -1.458508
N 0.248016 3.431806 0.688628
C 3.786893 0.133762 -0.090918
C 3.095472 -1.089726 -0.719050
N 2.168939 -1.811384 0.165838
C 2.866840 -2.374753 1.321176
C -1.047487 -2.288220 -0.865915
H -0.400210 -1.477874 1.011048
H -0.131170 0.182372 -0.966986
C 1.474792 -2.887273 -0.568281
C 0.345324 -2.431905 -1.512018
O 1.286121 4.281953 0.251566
H -2.321307 0.281674 -1.901419
H -1.980499 1.853175 -1.197257
H -4.581353 -0.871978 0.953099
H -3.936884 -1.357963 -0.621933
H -4.513012 2.324603 -1.137650
H -5.591307 1.203503 -0.287524
H -4.844878 0.723739 -1.821307
H 0.060774 0.527125 1.677537
H -1.280267 1.639801 1.434410
H 2.373490 0.626258 1.497191
H 3.425459 1.953102 1.044440
H 4.566559 -0.183659 0.611558
H 4.298703 0.664044 -0.901513
H 2.530723 -0.748883 -1.590063
H 3.883771 -1.772103 -1.098205
H 3.651717 -3.102787 1.036834
H 3.340998 -1.582267 1.906917
H 2.148983 -2.884213 1.971876
H -1.336202 -3.263020 -0.448843
H -1.773686 -2.068965 -1.660040
H 1.048137 -3.570466 0.176544
H 2.209324 -3.483628 -1.144564
H 0.251765 -3.187058 -2.303708
H 0.628965 -1.507314 -2.026962
H 0.940114 5.159433 0.477274

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624721003

Comp_17Z_c13

B3LYP/6-31G* Geometry

C 3.724827 0.755793 -0.653841
C 2.513062 1.466625 -0.023881
C 1.630320 0.568012 0.868350
C 3.225514 -0.477420 -1.444916
C 2.418915 -1.375048 -0.523733
C 1.180775 -0.735123 0.123870
O 2.779886 -2.511022 -0.267774

H 4.180350 1.451289 -1.371949
C 4.806569 0.374424 0.368829
C 0.467611 1.391404 1.499322
C -0.544312 2.010129 0.547761
C -1.958556 1.431049 0.512145
C -2.728526 1.398500 -0.798912
O -2.441538 1.068176 1.570531
N -0.169436 3.088437 -0.043828
C -3.775342 0.282587 -0.905916
C -3.169657 -1.091853 -1.222613
N -2.275744 -1.588810 -0.177553
C -3.029138 -2.085720 0.970166
C 0.447859 -1.732900 1.036151
H 0.517902 -0.418436 -0.697233
H 2.234635 0.241214 1.727443
C -1.309957 -2.568672 -0.681527
C -0.214141 -2.931752 0.332542
O -1.152809 3.670737 -0.862576
H 2.855696 2.326390 0.566574
H 1.895876 1.883979 -0.828073
H 2.585116 -0.136450 -2.270727
H 4.053222 -1.057969 -1.863431
H 4.452019 -0.368057 1.092649
H 5.139736 1.256512 0.928416
H 5.681215 -0.056087 -0.132138
H 0.931069 2.206114 2.067124
H -0.088561 0.785607 2.217220
H -2.024040 1.363549 -1.638164
H -3.217109 2.378783 -0.876751
H -4.470959 0.535043 -1.716319
H -4.369410 0.250984 0.013030
H -3.984968 -1.811525 -1.436984
H -2.586066 -1.002212 -2.148311
H -2.349818 -2.389254 1.769793
H -3.661816 -1.292066 1.372683
H -3.667082 -2.953526 0.710989
H 1.170802 -2.121836 1.763732
H -0.320583 -1.196925 1.598859
H -0.846049 -2.131437 -1.574897
H -1.805772 -3.502558 -1.017179
H 0.545795 -3.525214 -0.184162
H -0.631233 -3.588663 1.106393
H -0.702960 4.472026 -1.173149

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624867215

Comp_17Z_c14

B3LYP/6-31G* Geometry

C -2.583066 -1.955090 1.035990
C -1.400431 -2.128576 0.069172
C -0.830712 -0.807165 -0.482650
C -3.712691 -1.206100 0.303835
C -3.253144 0.102865 -0.325016
C -1.940689 0.081208 -1.127064

O -3.945732 1.103183 -0.251257
H -2.955562 -2.957162 1.289054
C -2.196642 -1.265014 2.353052
C 0.298963 -1.123882 -1.504585
C 1.581248 -1.565678 -0.844203
C 2.575841 -0.485845 -0.434956
C 2.907772 -0.318192 1.038860
O 3.088733 0.188217 -1.309437
N 1.797538 -2.820611 -0.704953
C 3.082332 1.146247 1.463842
C 1.759799 1.914351 1.597139
N 0.982166 2.034177 0.357948
C 1.627100 2.952309 -0.580374
C -1.500923 1.500852 -1.565174
H -2.229630 -0.449993 -2.053914
H -0.379130 -0.239516 0.336643
C -0.395836 2.439088 0.674082
C -1.350749 2.622621 -0.513238
O 3.033697 -3.071704 -0.061890
H -0.595604 -2.694754 0.551920
H -1.734292 -2.744810 -0.779484
H -4.087184 -1.841481 -0.513816
H -4.562450 -0.983476 0.957015
H -1.383876 -1.804363 2.853968
H -3.050384 -1.229874 3.039540
H -1.863893 -0.231957 2.196976
H 0.538612 -0.243280 -2.106061
H -0.040943 -1.912762 -2.186114
H 3.843148 -0.870858 1.198753
H 2.149735 -0.821517 1.650985
H 3.761992 1.643228 0.764312
H 3.574391 1.172257 2.444151
H 1.132486 1.387698 2.328547
H 1.968128 2.913698 2.029957
H 1.052632 3.010975 -1.507333
H 2.619162 2.579408 -0.840944
H 1.724179 3.975744 -0.168655
H -2.251578 1.860767 -2.278491
H -0.570519 1.410979 -2.135515
H -0.400764 3.391694 1.242968
H -0.805150 1.682289 1.355461
H -1.067932 3.530125 -1.062217
H -2.335913 2.831082 -0.087576
H 3.069795 -4.040655 -0.062682

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623145457

Comp_17Z_c15

B3LYP/6-31G* Geometry

C -3.395255 0.736607 1.014971
C -2.246068 1.497812 0.329673
C -1.570272 0.734159 -0.828974
C -2.869023 -0.637737 1.493952
C -2.251443 -1.386602 0.324829

C -1.080923 -0.683973 -0.381098
O -2.703054 -2.452753 -0.056795
H -3.690749 1.310964 1.903528
C -4.639554 0.588083 0.125703
C -0.492242 1.635523 -1.501467
C 0.592717 2.200113 -0.606085
C 1.883862 1.405065 -0.417104
C 2.313209 1.043309 0.989605
O 2.497058 1.094721 -1.422750
N 0.409928 3.395159 -0.175657
C 3.484427 0.058509 1.097597
C 3.318341 -1.235705 0.279532
N 1.969707 -1.805036 0.351269
C 1.727206 -2.464456 1.629118
C -0.538565 -1.554428 -1.529197
H -0.288018 -0.548781 0.368847
H -2.320224 0.568224 -1.616504
C 1.673100 -2.687702 -0.785616
C 0.179259 -2.851532 -1.096442
O 1.490359 3.875923 0.595385
H -2.610152 2.464314 -0.041911
H -1.486328 1.735322 1.085900
H -2.100638 -0.478290 2.263914
H -3.665332 -1.253657 1.922732
H -4.989157 1.567773 -0.220859
H -5.458523 0.115045 0.679450
H -4.447098 -0.031813 -0.757186
H -1.018696 2.490862 -1.938350
H -0.002929 1.105433 -2.324142
H 1.426272 0.653139 1.505388
H 2.553991 1.984054 1.499649
H 3.629514 -0.167342 2.161711
H 4.408597 0.544033 0.761772
H 3.514447 -0.994368 -0.765815
H 4.089936 -1.964241 0.597982
H 0.696140 -2.827037 1.682821
H 1.875307 -1.760343 2.454809
H 2.400355 -3.328589 1.794540
H -1.384610 -1.819610 -2.173938
H 0.155446 -0.966710 -2.141024
H 2.126070 -3.688992 -0.641078
H 2.155933 -2.253660 -1.668600
H -0.352408 -3.317318 -0.260926
H 0.111659 -3.575633 -1.919249
H 1.206181 4.780974 0.796535

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623862314

Comp_17Z_c16

B3LYP/6-31G* Geometry

C 4.379634 0.228160 -0.205420
C 3.266201 1.191613 -0.651566
C 1.853029 0.854281 -0.123394
C 4.000987 -1.208209 -0.627908

C 2.641313 -1.583857 -0.065231
C 1.477354 -0.636019 -0.408526
O 2.490401 -2.575033 0.627058
H 5.296007 0.506518 -0.743552
C 4.680797 0.313983 1.299109
C 0.866981 1.873341 -0.765724
C -0.451634 2.117173 -0.050321
C -1.719918 1.621241 -0.738169
C -2.988393 1.354217 0.052926
O -1.662325 1.413585 -1.941179
N -0.356700 2.788550 1.042387
C -3.944800 0.375081 -0.640920
C -3.365351 -1.040430 -0.816089
N -2.798809 -1.598970 0.414545
C -3.835360 -2.004493 1.354549
C 0.180730 -1.112898 0.270487
H 1.361987 -0.709931 -1.504374
H 1.834518 1.012448 0.963524
C -1.843981 -2.687933 0.174355
C -0.528688 -2.244458 -0.483858
O -1.573847 3.062479 1.675106
H 3.522280 2.214077 -0.344395
H 3.232046 1.201781 -1.751806
H 3.950722 -1.257967 -1.725527
H 4.734122 -1.945376 -0.286581
H 4.939910 1.339430 1.587712
H 5.524053 -0.334092 1.563959
H 3.827080 0.000164 1.910821
H 0.641470 1.577587 -1.794349
H 1.384372 2.837721 -0.816355
H -3.478976 2.324451 0.212029
H -2.719128 0.996944 1.049897
H -4.210525 0.753360 -1.634022
H -4.874624 0.341830 -0.059969
H -4.148779 -1.702538 -1.236598
H -2.571303 -0.985175 -1.563325
H -4.483485 -1.156167 1.596422
H -4.478332 -2.820349 0.967397
H -3.375946 -2.348607 2.287363
H 0.420855 -1.451141 1.285247
H -0.517748 -0.283887 0.385044
H -2.296667 -3.501650 -0.427755
H -1.607231 -3.123505 1.153231
H -0.706902 -1.934175 -1.522524
H 0.127571 -3.121215 -0.534538
H -1.286032 3.569397 2.450819

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.626017060

Comp_17Z_c17

B3LYP/6-31G* Geometry

C -3.126684 1.156608 -0.592712
C -1.693505 0.846571 -1.060004
C -0.820519 0.146384 0.004561

C -3.804661 -0.130462 -0.072203
C -2.956811 -0.831984 0.978671
C -1.506081 -1.119130 0.586473
O -3.405181 -1.155491 2.063776
H -3.075129 1.865727 0.245839
C -3.956706 1.811897 -1.702458
C -0.381477 1.132922 1.125056
C 0.778386 1.980573 0.670699
C 2.145552 1.306888 0.665357
C 2.914904 1.199777 -0.641628
O 2.574448 0.869709 1.718268
N 0.561535 3.198483 0.339151
C 3.756310 -0.079851 -0.761494
C 2.975578 -1.324924 -1.209400
N 1.892944 -1.760443 -0.315914
C 2.425548 -2.257058 0.954654
C -1.464590 -2.337081 -0.382688
H -1.001283 -1.414013 1.513586
H 0.097941 -0.206108 -0.474621
C 1.083753 -2.786599 -0.995693
C -0.216047 -3.242364 -0.306064
O 1.744963 3.851354 -0.080291
H -1.750092 0.215457 -1.958925
H -1.201906 1.777167 -1.370674
H -4.791349 0.072062 0.356339
H -3.944237 -0.820372 -0.919834
H -4.045915 1.146331 -2.570964
H -3.493505 2.745701 -2.042293
H -4.970137 2.045853 -1.355871
H -0.050993 0.571131 2.005976
H -1.203334 1.784694 1.437110
H 3.567471 2.082681 -0.671017
H 2.226254 1.310675 -1.487658
H 4.275324 -0.254491 0.186066
H 4.538389 0.084790 -1.513138
H 2.523707 -1.108588 -2.186344
H 3.699890 -2.148128 -1.377164
H 2.980141 -1.467108 1.462613
H 1.608735 -2.552402 1.617300
H 3.089335 -3.132527 0.814700
H -2.323724 -2.981824 -0.153635
H -1.609296 -2.002498 -1.418795
H 1.701135 -3.691590 -1.169317
H 0.825803 -2.398124 -1.989656
H -0.027963 -3.511705 0.740109
H -0.485362 -4.185731 -0.800274
H 1.427199 4.749092 -0.262908

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624677274

Comp_17Z_c18

B3LYP/6-31G* Geometry

C -2.559376 -1.921048 1.064200
C -1.317172 -2.055824 0.166055

C -0.833595 -0.725533 -0.442075
C -3.703285 -1.273495 0.253871
C -3.279163 0.047528 -0.369601
C -1.974605 0.031028 -1.182775
O -3.959170 1.052882 -0.258293
H -2.880162 -2.933761 1.343987
C -2.279239 -1.150255 2.363839
C 0.349667 -0.977279 -1.405523
C 1.571419 -1.570982 -0.753809
C 2.248438 -0.783808 0.355869
C 3.420291 0.096443 -0.052445
O 1.861425 -0.887333 1.505352
N 2.012235 -2.691955 -1.185872
C 3.452311 1.461557 0.648331
C 2.430940 2.466863 0.097169
N 1.022606 2.086449 0.274135
C 0.659620 2.128034 1.693240
C -1.631301 1.442661 -1.707743
H -2.222989 -0.587297 -2.065473
H -0.467416 -0.082566 0.363222
C 0.154701 2.978177 -0.516492
C -1.316773 2.551069 -0.667598
O 3.200434 -3.067654 -0.510426
H -0.495414 -2.499851 0.739639
H -1.544802 -2.758880 -0.650044
H -3.989511 -1.952048 -0.564272
H -4.594492 -1.093437 0.863343
H -2.015669 -0.103106 2.174256
H -1.448160 -1.603862 2.915174
H -3.161833 -1.150060 3.014013
H 0.651363 -0.026090 -1.859131
H 0.043325 -1.649282 -2.216919
H 3.434131 0.216319 -1.142828
H 4.319494 -0.481273 0.204185
H 4.447351 1.903091 0.511801
H 3.325594 1.315153 1.725737
H 2.629834 3.457406 0.554333
H 2.609550 2.580206 -0.980049
H -0.403638 1.912098 1.818303
H 1.211774 1.367257 2.247720
H 0.858662 3.120169 2.142853
H -0.805439 1.369934 -2.425388
H -2.500663 1.767749 -2.288087
H 0.595132 3.062755 -1.518492
H 0.175113 3.998836 -0.084019
H -1.854886 3.454610 -0.978196
H -1.750865 2.297771 0.303475
H 3.411946 -3.917263 -0.927119

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624019964

Comp_17Z_c19

B3LYP/6-31G* Geometry

C 3.464873 1.196700 0.702521

C 2.310178 1.705779 -0.176663
C 1.232803 0.647108 -0.479367
C 4.131440 -0.002581 -0.002387
C 3.134212 -1.101061 -0.342197
C 1.832006 -0.676404 -1.042477
O 3.381873 -2.271115 -0.109722
H 4.210017 2.000953 0.771581
C 3.031437 0.847439 2.135027
C 0.171173 1.255443 -1.446558
C -0.913824 2.016962 -0.723973
C -2.171201 1.246821 -0.324480
C -2.403880 0.983222 1.152126
O -2.937112 0.901885 -1.203296
N -0.748199 3.270253 -0.521209
C -3.294032 -0.226432 1.460304
C -2.569627 -1.579620 1.394833
N -2.083239 -1.970076 0.069299
C -3.178953 -2.343244 -0.821643
C 0.816798 -1.836529 -1.097104
H 2.148343 -0.454177 -2.078362
H 0.728048 0.396108 0.462048
C -1.047022 -3.013875 0.169445
C 0.362808 -2.413641 0.259764
O -1.835132 3.835450 0.188891
H 1.832296 2.579460 0.283237
H 2.730400 2.056564 -1.131474
H 4.577766 0.344037 -0.947132
H 4.932769 -0.446493 0.596681
H 2.545726 1.704253 2.616789
H 3.897229 0.564877 2.744794
H 2.328858 0.005978 2.163247
H -0.316285 0.474987 -2.037002
H 0.672291 1.931930 -2.148132
H -2.860034 1.906221 1.537227
H -1.434380 0.903955 1.661706
H -4.163393 -0.212535 0.794884
H -3.684525 -0.120091 2.480315
H -1.703062 -1.532523 2.066611
H -3.241064 -2.359065 1.810431
H -3.790096 -3.180099 -0.430065
H -2.772773 -2.642253 -1.792760
H -3.829928 -1.482941 -0.993142
H -0.071009 -1.489506 -1.636103
H 1.249118 -2.647962 -1.693202
H -1.103813 -3.645445 -0.725182
H -1.237334 -3.683075 1.027410
H 1.074921 -3.175283 0.591700
H 0.360865 -1.639285 1.038720
H -1.593057 4.773902 0.218525

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623416973

Comp_17Z_c20

B3LYP/6-31G* Geometry

C -4.248772 -0.517670 -0.618955
 C -2.964242 -1.276751 -0.991044
 C -1.707011 -0.880804 -0.183065
 C -3.994087 0.998485 -0.770057
 C -2.804384 1.416902 0.075895
 C -1.482923 0.668920 -0.186891
 O -2.902458 2.282739 0.927219
 H -5.025727 -0.801989 -1.341661
 C -4.768436 -0.869526 0.783872
 C -0.510338 -1.662379 -0.784843
 C 0.701683 -1.903750 0.102229
 C 2.060244 -1.674970 -0.542746
 C 3.250277 -1.189845 0.267620
 O 2.139160 -1.839180 -1.750999
 N 0.471213 -2.378763 1.272215
 C 4.133192 -0.212487 -0.527054
 C 3.367022 1.019509 -1.045987
 N 2.516992 1.639610 -0.028719
 C 3.295159 2.387667 0.950089
 C -0.397091 1.165487 0.785949
 H -1.202965 0.931330 -1.222789
 H -1.836145 -1.204652 0.857453
 C 1.397306 2.417700 -0.569847
 C 0.218967 2.528505 0.413318
 O 1.630767 -2.676367 2.002369
 H -3.130129 -2.356085 -0.876041
 H -2.757373 -1.110908 -2.059452
 H -3.773162 1.220847 -1.824268
 H -4.861208 1.594162 -0.469127
 H -4.065964 -0.575379 1.572271
 H -4.941027 -1.948312 0.876059
 H -5.716354 -0.358401 0.987556
 H -0.169134 -1.172890 -1.701970
 H -0.873539 -2.649468 -1.100298
 H 3.832926 -2.076311 0.554865
 H 2.901676 -0.740543 1.198361
 H 4.570140 -0.722847 -1.392029
 H 4.970098 0.089442 0.114324
 H 4.089944 1.738064 -1.480358
 H 2.719747 0.692860 -1.864903
 H 3.829659 3.248123 0.500797
 H 2.647736 2.769422 1.744299
 H 4.039267 1.736791 1.419695
 H -0.848639 1.230541 1.781053
 H 0.416635 0.441336 0.855101
 H 1.054980 1.911319 -1.481178
 H 1.716314 3.431961 -0.880390
 H -0.541089 3.188789 -0.020723
 H 0.552521 3.034503 1.327099
 H 1.264241 -2.995117 2.842176
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G) = -999.623642229**

Comp_17Z_c21

B3LYP/6-31G* Geometry
 C -3.317000 1.005128 0.878508
 C -2.080684 1.605577 0.188345
 C -1.455315 0.704499 -0.897507
 C -2.929606 -0.367036 1.477346
 C -2.366625 -1.273259 0.396824
 C -1.147548 -0.736250 -0.369014
 O -2.873941 -2.352775 0.141822
 H -3.586311 1.668564 1.711586
 C -4.541938 0.899710 -0.042954
 C -0.236335 1.425290 -1.545909
 C 0.736474 2.116564 -0.615310
 C 1.609839 1.332052 0.357832
 C 3.015512 1.025206 -0.126634
 O 1.190417 1.045562 1.463572
 N 0.815640 3.392164 -0.714959
 C 3.721527 -0.127937 0.595123
 C 3.346509 -1.508600 0.036628
 N 1.925238 -1.839208 0.167879
 C 1.605129 -2.215313 1.544046
 C -0.729180 -1.728715 -1.471933
 H -0.340495 -0.642368 0.367022
 H -2.181267 0.586545 -1.715429
 C 1.505986 -2.868412 -0.792685
 C -0.012944 -3.003081 -0.978603
 O 1.787498 3.925568 0.164103
 H -2.333534 2.577936 -0.255175
 H -1.319746 1.802350 0.954147
 H -2.157625 -0.213300 2.244622
 H -3.784270 -0.869014 1.941332
 H -4.798080 1.879047 -0.464414
 H -5.414299 0.532731 0.509964
 H -4.375980 0.208949 -0.877720
 H -0.613613 2.208632 -2.212486
 H 0.322284 0.720575 -2.173835
 H 3.563379 1.969306 0.010836
 H 2.989869 0.855413 -1.211619
 H 3.513502 -0.063236 1.667965
 H 4.806248 -0.009330 0.480705
 H 3.594309 -1.518705 -1.032449
 H 3.986771 -2.278473 0.511839
 H 1.804416 -1.378111 2.216741
 H 0.543819 -2.459771 1.634407
 H 2.186150 -3.095025 1.882683
 H -0.078133 -1.230725 -2.200563
 H -1.634550 -2.025228 -2.013354
 H 1.923696 -3.860906 -0.526565
 H 1.942275 -2.600029 -1.763583
 H -0.495143 -3.374121 -0.068918
 H -0.159110 -3.796845 -1.723222
 H 1.734694 4.875072 -0.025553
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G) = -999.624577111**

Comp_17Z_c22**B3LYP/6-31G* Geometry**

C 3.857460 0.415539 0.014723
 C 2.537695 1.173123 -0.262174
 C 1.275272 0.272984 -0.369756
 C 3.584833 -0.866440 0.815237
 C 2.670662 -1.814705 0.055054
 C 1.600718 -1.168942 -0.845831
 O 2.786798 -3.023757 0.141164
 H 4.283277 0.106258 -0.951548
 C 4.889103 1.315423 0.703936
 C 0.207309 0.959911 -1.260054
 C -0.511457 2.093433 -0.573634
 C -1.486112 1.681908 0.519497
 C -2.909894 1.418042 0.063309
 O -1.101310 1.518369 1.662729
 N -0.319478 3.296935 -0.959329
 C -3.693547 0.458286 0.966425
 C -3.068221 -0.940718 1.106322
 N -2.699538 -1.590738 -0.159511
 C -3.881771 -1.943995 -0.940874
 C 0.384862 -2.112559 -0.988075
 H 2.075733 -1.094981 -1.840386
 H 0.850806 0.188397 0.637236
 C -1.849557 -2.771304 0.088890
 C -0.373129 -2.414738 0.321805
 O -1.129253 4.199672 -0.227456
 H 2.365516 1.907649 0.534903
 H 2.656599 1.757332 -1.183730
 H 4.501921 -1.406793 1.072258
 H 3.088597 -0.609418 1.765311
 H 4.538772 1.620334 1.698228
 H 5.069145 2.226520 0.120892
 H 5.848916 0.800398 0.828292
 H -0.560721 0.232648 -1.544406
 H 0.664619 1.337335 -2.181994
 H -2.883024 1.048725 -0.968145
 H -3.401597 2.401506 0.021410
 H -4.719593 0.388603 0.585544
 H -3.765708 0.883033 1.973875
 H -2.161936 -0.844199 1.708508
 H -3.765848 -1.579027 1.685482
 H -4.552548 -2.653031 -0.417203
 H -4.463108 -1.047148 -1.176991
 H -3.576010 -2.400045 -1.887992
 H -0.312598 -1.695480 -1.721653
 H 0.746648 -3.056612 -1.408387
 H -1.919481 -3.426971 -0.787815
 H -2.237928 -3.357435 0.943009
 H 0.119874 -3.246663 0.836631
 H -0.321670 -1.563746 1.010423
 H -0.890766 5.053678 -0.620165

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -999.622914586**

Comp_17Z_c23**B3LYP/6-31G* Geometry**

C -3.789373 0.251017 -0.324702
 C -2.709836 -0.013710 -1.390714
 C -1.264808 0.193425 -0.881723
 C -3.506792 -0.578169 0.947925
 C -2.066231 -0.464063 1.436031
 C -0.976904 -0.666642 0.380455
 O -1.799982 -0.261652 2.606838
 H -3.746880 1.312335 -0.042868
 C -5.197994 -0.024578 -0.864017
 C -1.001622 1.706333 -0.659237
 C 0.348319 2.075742 -0.084627
 C 1.577727 1.607805 -0.836748
 C 2.882962 1.362132 -0.104280
 O 1.459796 1.390677 -2.034613
 N 0.306855 2.817282 0.965903
 C 3.760990 0.295720 -0.770884
 C 3.100212 -1.086782 -0.902441
 N 2.406605 -1.552776 0.304588
 C 3.334053 -1.745004 1.417582
 C -0.868946 -2.187825 0.074133
 H -0.034400 -0.355665 0.840732
 H -0.582258 -0.128030 -1.675298
 C 1.670732 -2.798526 0.040186
 C 0.354718 -2.651684 -0.742769
 O 1.559606 3.228084 1.434119
 H -2.823967 -1.042418 -1.760118
 H -2.884206 0.637452 -2.257769
 H -4.171036 -0.297144 1.771468
 H -3.698458 -1.639629 0.723301
 H -5.304648 -1.074474 -1.166496
 H -5.415569 0.598776 -1.739497
 H -5.961924 0.183407 -0.105650
 H -1.750433 2.143173 0.008211
 H -1.101293 2.204261 -1.632582
 H 2.665526 1.110293 0.936299
 H 3.418665 2.320774 -0.065474
 H 4.695729 0.222879 -0.202140
 H 4.036620 0.622763 -1.779266
 H 2.366015 -1.035680 -1.710024
 H 3.872053 -1.817787 -1.220529
 H 2.779735 -2.063540 2.306055
 H 4.112457 -2.504326 1.204737
 H 3.839644 -0.806540 1.661226
 H -0.868670 -2.729564 1.030428
 H -1.772792 -2.515284 -0.454179
 H 1.438541 -3.256527 1.009476
 H 2.322831 -3.520566 -0.491511
 H 0.118855 -3.648181 -1.140237
 H 0.497328 -2.015189 -1.623652
 H 1.319726 3.734864 2.226147

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.626740945

Comp_17Z_c24

B3LYP/6-31G* Geometry

C 3.448250 0.685892 -0.999542
C 2.332806 1.542726 -0.373911
C 1.605397 0.879970 0.814659
C 2.857200 -0.681415 -1.413437
C 2.184229 -1.344326 -0.222463
C 1.062438 -0.540094 0.447734
O 2.545939 -2.436398 0.183276
H 3.787861 1.195190 -1.911847
C 4.669942 0.519063 -0.082209
C 0.531524 1.849714 1.388542
C -0.643501 2.166258 0.481522
C -1.904296 1.325890 0.643085
C -2.870555 1.123153 -0.512670
O -2.118358 0.848354 1.746828
N -0.499244 3.199335 -0.272193
C -3.720074 -0.151158 -0.389675
C -3.108234 -1.373109 -1.089467
N -1.750867 -1.730392 -0.661618
C -1.140914 -2.621776 -1.647973
C 0.463233 -1.304259 1.644959
H 0.282670 -0.406034 -0.317409
H 2.330973 0.746766 1.630881
C -1.743955 -2.332407 0.683524
C -0.357370 -2.564443 1.306283
O -1.617091 3.508134 -1.059928
H 2.748039 2.504933 -0.046132
H 1.596038 1.781814 -1.151663
H 2.104951 -0.523003 -2.199510
H 3.624025 -1.358551 -1.802273
H 5.070131 1.495649 0.215128
H 5.468486 -0.030080 -0.594149
H 4.430558 -0.037421 0.831127
H 1.036006 2.793384 1.620471
H 0.126695 1.458816 2.324443
H -2.327236 1.160552 -1.462147
H -3.514029 2.013587 -0.516154
H -4.696713 0.022761 -0.858080
H -3.919070 -0.349927 0.667489
H -3.800797 -2.232405 -0.981507
H -3.056997 -1.153240 -2.163666
H -1.139009 -2.137475 -2.630421
H -1.677703 -3.585968 -1.742807
H -0.105039 -2.842645 -1.380023
H -0.175529 -0.630820 2.223318
H 1.290134 -1.604393 2.300608
H -2.284242 -3.301592 0.663303
H -2.307456 -1.669230 1.345854
H 0.243987 -3.248658 0.701269
H -0.542577 -3.097620 2.248871
H -1.324015 4.314222 -1.513461

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.625648846

Comp_17Z_c25

B3LYP/6-31G* Geometry

C -3.099344 0.934241 -0.577638
C -1.667478 0.672380 -1.073736
C -0.749472 0.024446 -0.015527
C -3.713592 -0.377124 -0.037535
C -2.819764 -1.048063 0.995209
C -1.361143 -1.269181 0.585600
O -3.238639 -1.401266 2.083110
H -3.056964 1.651354 0.254633
C -3.977563 1.547642 -1.674097
C -0.353480 1.013245 1.109424
C 0.562912 2.116334 0.635903
C 1.786715 1.699945 -0.169287
C 2.902538 1.019635 0.604436
O 1.819085 1.873692 -1.372805
N 0.272280 3.326731 0.933162
C 3.786562 0.093467 -0.241624
C 3.033686 -1.041895 -0.956692
N 2.088789 -1.792715 -0.115017
C 2.782252 -2.497537 0.960776
C -1.266597 -2.497883 -0.363633
H -0.831525 -1.527232 1.510061
H 0.179204 -0.273417 -0.507926
C 1.309378 -2.726117 -0.945773
C 0.039953 -3.319134 -0.302066
O 1.261863 4.226438 0.485438
H -1.719614 0.017650 -1.955805
H -1.211309 1.607245 -1.422142
H -4.698790 -0.214510 0.410991
H -3.842732 -1.073491 -0.881728
H -4.056991 0.872819 -2.536354
H -3.558525 2.496215 -2.029534
H -4.992415 1.743368 -1.308388
H 0.169839 0.444392 1.891110
H -1.223631 1.473375 1.589841
H 2.468987 0.481928 1.454217
H 3.509623 1.829141 1.038738
H 4.577909 -0.308880 0.402046
H 4.288694 0.681774 -1.017420
H 2.458863 -0.602909 -1.777244
H 3.782769 -1.718553 -1.415497
H 2.068015 -3.040035 1.585516
H 3.525893 -3.225683 0.580709
H 3.305110 -1.786742 1.606813
H -2.078292 -3.191414 -0.105692
H -1.453208 -2.189873 -1.401289
H 1.956518 -3.563918 -1.274609
H 1.018416 -2.192464 -1.858865
H 0.234358 -3.606551 0.738692
H -0.159604 -4.261035 -0.830537

H 0.900063 5.082018 0.764247
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624171916

Comp_17Z_c26

B3LYP/6-31G* Geometry

C 3.180951 1.409524 1.027729
C 1.987580 1.941726 0.217581
C 1.098823 0.849184 -0.406647
C 4.049224 0.529925 0.104622
C 3.258049 -0.597775 -0.542194
C 1.904886 -0.239408 -1.176363
O 3.705350 -1.729825 -0.599610
H 3.787783 2.274426 1.329337
C 2.772526 0.669601 2.310854
C 0.042935 1.517401 -1.341098
C -1.227621 1.906529 -0.621424
C -2.381935 0.909628 -0.690052
C -3.109389 0.518071 0.578393
O -2.657459 0.441450 -1.781861
N -1.261120 3.058498 -0.058693
C -3.776599 -0.865931 0.524229
C -2.880689 -2.014620 0.024312
N -1.508161 -1.969726 0.535485
C -1.454288 -2.152121 1.983262
C 1.063448 -1.503333 -1.456251
H 2.184281 0.208064 -2.147913
H 0.556983 0.333241 0.396387
C -0.623534 -2.939164 -0.137472
C 0.825895 -2.437436 -0.241913
O -2.486533 3.322589 0.587928
H 1.362511 2.598169 0.835590
H 2.381324 2.573727 -0.592683
H 4.450390 1.157756 -0.706035
H 4.902227 0.086675 0.628326
H 2.205629 -0.245640 2.102761
H 2.149562 1.308206 2.948217
H 3.656812 0.377091 2.888798
H -0.245013 0.845061 -2.152911
H 0.483888 2.409496 -1.799447
H -3.866308 1.289849 0.768403
H -2.404726 0.594538 1.413395
H -4.649556 -0.827166 -0.137108
H -4.163449 -1.085622 1.526994
H -3.379643 -2.974943 0.265493
H -2.817982 -1.948777 -1.064558
H -1.879612 -3.123384 2.303817
H -0.416003 -2.111776 2.326834
H -2.002545 -1.356801 2.496715
H 0.094829 -1.180751 -1.853853
H 1.547238 -2.077778 -2.252955
H -1.014840 -3.120313 -1.145383
H -0.653825 -3.914043 0.382822
H 1.508527 -3.290050 -0.306658

H 1.084230 -1.930469 0.696053
H -2.350179 4.225291 0.914957
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.620703905

Comp_17Z_c27

B3LYP/6-31G* Geometry

C 4.209671 -0.509250 -0.187444
C 2.926561 -1.346631 -0.379890
C 1.671078 -0.482284 -0.617466
C 4.004276 0.536877 0.935762
C 2.709208 1.321111 0.760643
C 1.453695 0.459981 0.609007
O 2.682852 2.539173 0.753793
H 5.006421 -1.192316 0.136527
C 4.683999 0.159329 -1.488504
C 0.439176 -1.323753 -1.039746
C -0.476260 -1.901361 0.020892
C -1.939132 -1.989537 -0.395277
C -3.012070 -1.293672 0.432928
O -2.198879 -2.543998 -1.448843
N -0.001116 -2.317784 1.133369
C -3.901690 -0.389821 -0.443517
C -3.200139 0.873463 -0.975795
N -2.726757 1.782219 0.072504
C -3.828394 2.515674 0.685349
C 0.151343 1.277434 0.667429
H 1.444921 -0.202762 1.487657
H 1.872350 0.155074 -1.489740
C -1.671975 2.701975 -0.383378
C -0.294468 2.044082 -0.583998
O -1.012561 -2.861351 1.956428
H 3.068484 -2.027621 -1.229804
H 2.757897 -1.977695 0.502525
H 3.942192 0.015331 1.902351
H 4.838590 1.243094 0.988675
H 3.977554 0.915080 -1.851357
H 4.818758 -0.582800 -2.284276
H 5.644263 0.664823 -1.335002
H 0.779486 -2.153915 -1.674359
H -0.192188 -0.719667 -1.697301
H -2.564961 -0.728985 1.253734
H -3.623339 -2.087491 0.882111
H -4.793158 -0.113971 0.131160
H -4.252536 -0.972241 -1.302694
H -2.337341 0.563969 -1.575485
H -3.885925 1.392818 -1.674930
H -4.348963 3.188873 -0.024510
H -4.570232 1.822418 1.092946
H -3.451916 3.121948 1.515613
H -0.661189 0.609294 0.962571
H 0.256042 1.998678 1.487938
H -1.568083 3.470829 0.391906
H -1.968276 3.233099 -1.309601

H 0.427746 2.834396 -0.818240
H -0.320358 1.385529 -1.460925
H -0.521708 -3.099116 2.758412
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.619788143**

Comp_17Z_c28

B3LYP/6-31G* Geometry

C -3.746823 0.201304 0.125789
C -2.965942 0.488735 -1.167485
C -1.448330 0.647503 -0.941738
C -3.166808 -1.046852 0.823972
C -1.649728 -1.023266 0.973757
C -0.837752 -0.597166 -0.249860
O -1.109155 -1.391118 2.003244
H -3.618210 1.055530 0.805615
C -5.248351 0.040074 -0.138045
C -1.136162 1.952054 -0.154713
C 0.331608 2.322741 -0.143199
C 1.219282 1.682643 0.919707
C 2.625418 1.233461 0.556320
O 0.752008 1.533425 2.035664
N 0.691032 3.203227 -1.006037
C 3.122383 0.002513 1.333529
C 2.500885 -1.348394 0.921673
N 2.421895 -1.555798 -0.532253
C 3.746144 -1.534150 -1.150306
C -0.643285 -1.817294 -1.190894
H 0.157863 -0.345296 0.110204
H -0.969414 0.753434 -1.924911
C 1.748567 -2.810634 -0.895378
C 0.247680 -2.921475 -0.580404
O 2.054224 3.538346 -0.934213
H -3.142307 -0.332035 -1.877980
H -3.361170 1.395483 -1.644476
H -3.603675 -1.204700 1.815187
H -3.417773 -1.932289 0.216949
H -5.439239 -0.797692 -0.821418
H -5.669123 0.944654 -0.592797
H -5.796843 -0.155235 0.790845
H -1.461956 1.867690 0.888061
H -1.687305 2.778797 -0.614570
H 3.278697 2.090160 0.771573
H 2.685394 1.078531 -0.523616
H 2.922591 0.147304 2.400446
H 4.212622 -0.041925 1.226004
H 3.089481 -2.155210 1.404665
H 1.490705 -1.414751 1.334965
H 4.412267 -2.332887 -0.767678
H 3.647962 -1.667166 -2.232961
H 4.240631 -0.574705 -0.978131
H -1.618667 -2.240869 -1.462820
H -0.193714 -1.455594 -2.125286
H 2.261668 -3.680362 -0.435157

H 1.869942 -2.923929 -1.980633
H 0.082329 -2.979432 0.500666
H -0.064730 -3.895678 -0.979154
H 2.132157 4.210171 -1.629483
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.623643938**

Comp_17Z_c29

B3LYP/6-31G* Geometry

C 3.881074 -1.078858 0.331939
C 2.497979 -1.668200 -0.002883
C 1.580258 -0.703712 -0.785267
C 3.693541 0.244801 1.109467
C 2.808378 1.210052 0.336515
C 1.426608 0.675853 -0.066890
O 3.184679 2.333640 0.051360
H 4.391016 -1.787653 0.998416
C 4.773603 -0.885827 -0.904288
C 0.229561 -1.372916 -1.143063
C -0.793225 -1.632718 -0.054817
C -2.183339 -2.044880 -0.544552
C -3.123997 -0.976934 -1.079285
O -2.465496 -3.227323 -0.559043
N -0.461353 -1.602892 1.179554
C -3.925292 -0.201049 -0.005167
C -3.112750 0.805312 0.827291
N -2.276356 1.699197 0.022418
C -3.070099 2.675678 -0.715055
C 0.644551 1.724221 -0.880936
H 0.905958 0.464194 0.877338
H 2.054452 -0.504910 -1.758072
C -1.212423 2.338621 0.807600
C -0.023861 2.824579 -0.038311
O -1.557568 -1.902960 2.023617
H 2.625779 -2.589519 -0.587528
H 1.996338 -1.953634 0.927697
H 3.207260 0.026503 2.071411
H 4.648539 0.738547 1.314316
H 4.893312 -1.829233 -1.450256
H 5.771097 -0.537048 -0.613435
H 4.364564 -0.145323 -1.601592
H 0.442459 -2.345836 -1.612259
H -0.270643 -0.789604 -1.924935
H -3.826113 -1.500150 -1.736648
H -2.555635 -0.250618 -1.671068
H -4.401182 -0.909004 0.683982
H -4.743069 0.312556 -0.524833
H -3.819644 1.371528 1.467299
H -2.458324 0.248587 1.502178
H -3.780391 2.170676 -1.376913
H -3.643510 3.348570 -0.046999
H -2.422704 3.294051 -1.342721
H 1.337480 2.194632 -1.586804
H -0.138532 1.235991 -1.466938

H -0.855113 1.598466 1.531851
H -1.604519 3.187026 1.402660
H 0.713017 3.281456 0.632940
H -0.350384 3.629746 -0.709078
H -1.153865 -1.865134 2.904920
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.621524358**

Comp_17Z_c30

B3LYP/6-31G* Geometry

C -4.097656 0.226130 0.463145
C -2.858683 0.819770 1.182459
C -1.587440 0.839962 0.308593
C -3.674931 -0.868254 -0.556612
C -2.387655 -1.547551 -0.131212
C -1.173485 -0.624617 -0.012231
O -2.309536 -2.745902 0.082172
H -4.721514 -0.258860 1.224406
C -4.946696 1.306789 -0.219376
C -0.479415 1.641931 1.038941
C 0.733222 2.022727 0.205288
C 2.081799 1.425811 0.591228
C 3.125231 1.117924 -0.472958
O 2.297344 1.245241 1.778511
N 0.524050 2.916206 -0.693696
C 3.971254 -0.125781 -0.166573
C 3.253440 -1.445796 -0.483512
N 2.034174 -1.667445 0.295796
C 2.337587 -2.013738 1.682541
C -0.317909 -0.754421 -1.301046
H -0.579208 -1.000134 0.828072
H -1.811240 1.371395 -0.627828
C 1.140383 -2.655699 -0.323828
C 0.351524 -2.120500 -1.530213
O 1.674217 3.292358 -1.407968
H -3.092783 1.832866 1.532843
H -2.639704 0.228385 2.083634
H -4.457696 -1.618051 -0.699289
H -3.486186 -0.389329 -1.529381
H -5.341072 2.019557 0.514330
H -5.798414 0.865615 -0.750817
H -4.355231 1.872356 -0.950979
H -0.128349 1.089845 1.915905
H -0.929043 2.570978 1.407973
H 3.768855 2.006934 -0.525957
H 2.652317 1.042771 -1.456734
H 4.297630 -0.093791 0.877599
H 4.881646 -0.090630 -0.778232
H 2.978668 -1.437134 -1.544894
H 3.965441 -2.285668 -0.352794
H 2.874327 -1.194832 2.167323
H 1.404267 -2.167094 2.233497
H 2.943270 -2.936375 1.770498
H -0.940585 -0.508840 -2.173654

H 0.456514 0.014026 -1.261192
H 0.415953 -2.967603 0.434023
H 1.688511 -3.570096 -0.622770
H -0.399201 -2.878405 -1.782250
H 1.001351 -2.031917 -2.411364
H 1.324301 3.971013 -2.006199
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.622911967**

Comp_17Z_c31

B3LYP/6-31G* Geometry

C -3.693957 0.468539 0.264108
C -2.845676 0.868538 -0.954052
C -1.328190 0.784325 -0.693124
C -3.313779 -0.957879 0.715963
C -1.813145 -1.144931 0.902245
C -0.902264 -0.631239 -0.212124
O -1.364542 -1.707476 1.888975
H -3.459234 1.155612 1.090806
C -5.195995 0.578964 -0.020670
C -0.868248 1.863694 0.327059
C 0.536129 2.390667 0.111875
C 1.685383 1.460112 -0.272680
C 2.521308 0.930235 0.871872
O 1.859193 1.195564 -1.447536
N 0.705720 3.652718 0.248309
C 3.676955 -0.012138 0.507289
C 3.300525 -1.236757 -0.350328
N 2.040125 -1.872656 0.039014
C 2.113900 -2.546947 1.330654
C -0.820338 -1.677211 -1.357367
H 0.102248 -0.588414 0.213317
H -0.812269 0.983067 -1.640072
C 1.510139 -2.756217 -1.007509
C -0.018173 -2.942619 -0.995116
O 2.064316 4.012088 0.075469
H -3.104341 0.210084 -1.796116
H -3.105623 1.887177 -1.271065
H -3.811187 -1.239927 1.649439
H -3.646809 -1.667881 -0.058036
H -5.470422 1.602832 -0.300803
H -5.789493 0.300039 0.857885
H -5.488699 -0.083301 -0.845750
H -0.931498 1.456392 1.347426
H -1.530234 2.736565 0.303712
H 1.827322 0.442696 1.571066
H 2.904761 1.810101 1.408283
H 4.149498 -0.328303 1.445659
H 4.443753 0.546978 -0.042682
H 3.182127 -0.897996 -1.380828
H 4.148938 -1.950361 -0.333075
H 2.760620 -3.446162 1.303497
H 1.113143 -2.838599 1.660376
H 2.515931 -1.867229 2.088017

H -0.346706 -1.190582 -2.221106
H -1.828079 -1.966081 -1.685514
H 1.991382 -3.753640 -0.962002
H 1.786070 -2.324476 -1.976884
H -0.352034 -3.338837 -0.028709
H -0.245037 -3.721712 -1.735520
H 2.035775 4.975299 0.183575
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.623484118**

Comp_17Z_c32

B3LYP/6-31G* Geometry

C 3.169016 1.497761 0.368032
C 1.698359 1.740289 -0.045458
C 0.898537 0.465698 -0.435863
C 3.336139 0.086534 0.953229
C 2.975531 -0.974863 -0.073070
C 1.803749 -0.653346 -1.016827
O 3.604102 -2.014311 -0.168726
H 3.793550 1.544370 -0.536547
C 3.670007 2.581761 1.328654
C -0.245741 0.845785 -1.404066
C -1.255136 1.791839 -0.804893
C -2.020628 1.283279 0.405710
C -3.254047 0.448210 0.110702
O -1.610111 1.500791 1.530890
N -1.447030 2.932918 -1.349214
C -3.524348 -0.655404 1.144867
C -2.314283 -1.560694 1.436757
N -1.576826 -2.013993 0.248815
C -2.374537 -2.938062 -0.553082
C 1.111097 -1.954936 -1.505823
H 2.293648 -0.223745 -1.909485
H 0.432869 0.074979 0.474022
C -0.295721 -2.610131 0.658453
C 0.670583 -3.008023 -0.466788
O -2.479247 3.643909 -0.690254
H 1.161330 2.226316 0.778810
H 1.679859 2.456644 -0.877233
H 4.355616 -0.107998 1.301961
H 2.668988 -0.031296 1.822539
H 3.539684 3.580642 0.895586
H 4.733779 2.451087 1.559764
H 3.112502 2.553769 2.273375
H -0.789486 -0.060549 -1.690429
H 0.158744 1.304695 -2.314365
H -3.161800 0.028317 -0.896579
H -4.100685 1.149629 0.071648
H -4.382967 -1.244480 0.800661
H -3.823271 -0.201748 2.096255
H -1.612711 -0.992896 2.053982
H -2.654857 -2.419510 2.049074
H -2.624708 -3.869387 -0.007793
H -1.838818 -3.212428 -1.465812

H -3.312774 -2.462002 -0.852998
H 1.829473 -2.462898 -2.158365
H 0.264408 -1.687026 -2.145671
H -0.470259 -3.513800 1.278022
H 0.197883 -1.886898 1.318118
H 0.249816 -3.853720 -1.026216
H 1.566322 -3.403161 0.023815
H -2.508554 4.473319 -1.191841
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.620778612**

Comp_17Z_c33

B3LYP/6-31G* Geometry

C -3.921852 0.157658 0.878106
C -2.715245 1.105326 1.075990
C -1.517174 0.883009 0.107446
C -4.008928 -0.297712 -0.583824
C -2.748161 -1.030440 -1.020264
C -1.432280 -0.602825 -0.345703
O -2.785361 -1.910254 -1.861408
H -3.750190 -0.743544 1.485222
C -5.227280 0.795340 1.365644
C -0.239222 1.400545 0.812775
C 0.924364 1.808176 -0.075196
C 2.316475 1.416523 0.395309
C 3.335048 0.870131 -0.595253
O 2.578446 1.558981 1.578521
N 0.659684 2.545744 -1.089727
C 4.075154 -0.368630 -0.063975
C 3.225274 -1.647906 -0.095096
N 2.000034 -1.571574 0.706591
C 2.293973 -1.620792 2.137619
C -0.231996 -0.975532 -1.246887
H -1.381275 -1.202895 0.579483
H -1.672361 1.500277 -0.786277
C 1.011984 -2.597987 0.337827
C 0.338220 -2.385679 -1.027789
O 1.813743 2.946015 -1.792791
H -3.047485 2.147183 0.969755
H -2.366512 1.006481 2.112833
H -4.868040 -0.950146 -0.772705
H -4.128671 0.579858 -1.239863
H -5.477814 1.681178 0.767899
H -5.144326 1.112864 2.411981
H -6.066069 0.093153 1.293379
H 0.120280 0.653467 1.526773
H -0.510947 2.281131 1.410174
H 4.052820 1.681514 -0.775827
H 2.859429 0.664370 -1.558686
H 4.442940 -0.160517 0.945969
H 4.961022 -0.545654 -0.686669
H 2.938188 -1.837463 -1.134962
H 3.851077 -2.507049 0.219335
H 1.359766 -1.557720 2.705225

H 2.812735 -2.552551 2.434353
H 2.911063 -0.767506 2.427932
H -0.541678 -0.885027 -2.293467
H 0.575033 -0.260897 -1.094366
H 0.243625 -2.585286 1.120193
H 1.454983 -3.612998 0.367620
H -0.458960 -3.130754 -1.133405
H 1.051561 -2.598679 -1.834444
H 1.437034 3.464864 -2.520455
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.622246984**

Comp_17Z_c34

B3LYP/6-31G* Geometry

C 3.266235 1.518518 0.510884
C 2.014238 1.757690 -0.352596
C 1.094118 0.527993 -0.462483
C 4.052493 0.314824 -0.055322
C 3.175759 -0.919515 -0.210213
C 1.862462 -0.720623 -0.982831
O 3.519022 -2.004924 0.224690
H 3.907219 2.406355 0.423129
C 2.941960 1.328988 2.001410
C -0.125108 0.840481 -1.364118
C -1.099203 1.821472 -0.764046
C -1.760023 1.405712 0.535418
C -3.185123 0.879719 0.486307
O -1.124051 1.452235 1.574373
N -1.350194 2.916638 -1.374967
C -3.371814 -0.397907 1.329576
C -3.256579 -1.714136 0.548448
N -1.995883 -1.984620 -0.161303
C -2.195952 -3.173997 -0.992925
C 1.055702 -2.032808 -1.095087
H 2.191254 -0.467538 -2.007926
H 0.724023 0.300125 0.540863
C -0.868636 -2.142551 0.777006
C 0.452731 -2.670256 0.180660
O -2.335329 3.666179 -0.683103
H 1.439497 2.597484 0.055296
H 2.329759 2.056941 -1.364015
H 4.435479 0.576556 -1.053456
H 4.909953 0.049226 0.570979
H 2.366841 0.414895 2.187962
H 2.354246 2.170458 2.384728
H 3.863054 1.258717 2.591536
H -0.690114 -0.081341 -1.546746
H 0.207300 1.234588 -2.332482
H -3.502199 0.731446 -0.551513
H -3.804268 1.691272 0.891600
H -4.378551 -0.395366 1.764683
H -2.678480 -0.363611 2.176390
H -3.486002 -2.542690 1.249777
H -4.051638 -1.723139 -0.208318

H -1.314819 -3.378490 -1.603610
H -2.418350 -4.081568 -0.398459
H -3.038493 -3.002319 -1.670795
H 0.275424 -1.899580 -1.851482
H 1.748775 -2.774175 -1.508106
H -1.145846 -2.848955 1.586957
H -0.706576 -1.176369 1.262344
H 0.319469 -3.737182 -0.036567
H 1.199823 -2.638464 0.980175
H -2.430957 4.449055 -1.247263
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.620664763**

Comp_17Z_c35

B3LYP/6-31G* Geometry

C -3.717215 0.562524 0.301182
C -2.863120 1.029424 -0.886227
C -1.349175 0.850741 -0.654599
C -3.426809 -0.925345 0.574005
C -1.943640 -1.242337 0.718830
C -0.971215 -0.608467 -0.278463
O -1.559640 -2.027532 1.571191
H -3.418920 1.135843 1.191719
C -5.212396 0.804545 0.066622
C -0.805166 1.864869 0.397242
C 0.640677 2.252979 0.151332
C 1.742999 1.394522 0.765093
C 3.054000 1.192995 0.020995
O 1.533289 0.915801 1.866964
N 0.798178 3.340190 -0.516174
C 3.824627 -0.080833 0.397959
C 3.393238 -1.332229 -0.381791
N 2.009033 -1.745981 -0.141817
C 1.860109 -2.359899 1.180271
C -0.825035 -1.541443 -1.516378
H 0.005578 -0.603901 0.204923
H -0.850843 1.090553 -1.603230
C 1.513047 -2.627306 -1.207420
C -0.013460 -2.823378 -1.251108
O 2.139045 3.699302 -0.731227
H -3.162631 0.459539 -1.778782
H -3.073277 2.083480 -1.110732
H -3.938508 -1.292728 1.469384
H -3.805793 -1.514179 -0.277718
H -5.421226 1.869914 -0.086621
H -5.809464 0.463948 0.920663
H -5.562653 0.263962 -0.822417
H -0.883940 1.461970 1.412600
H -1.397825 2.783933 0.350742
H 3.658996 2.080026 0.251735
H 2.872876 1.248878 -1.058691
H 3.752317 -0.241620 1.477894
H 4.888134 0.080653 0.180771
H 3.497062 -1.115084 -1.452940

H 4.103720 -2.154298 -0.160185
H 2.197419 -1.663585 1.950813
H 0.808938 -2.571504 1.385935
H 2.442894 -3.297644 1.266854
H -1.815151 -1.810727 -1.909933
H -0.331138 -0.966883 -2.312677
H 1.992377 -3.626386 -1.152010
H 1.823009 -2.188481 -2.165014
H -0.370103 -3.309205 -0.336531
H -0.207827 -3.534653 -2.065346
H 2.045148 4.539964 -1.205962

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624740124**

Comp_17Z_c36

B3LYP/6-31G* Geometry

C 4.081883 0.766159 0.454945
C 2.696115 1.392555 0.727357
C 1.552847 0.360437 0.669357
C 4.067788 -0.013130 -0.884525
C 2.874048 -0.955443 -0.993812
C 1.519375 -0.296523 -0.745211
O 2.997491 -2.136042 -1.268701
H 4.804035 1.587386 0.352815
C 4.567376 -0.127963 1.608214
C 0.190232 0.912191 1.157244
C -0.700365 1.659077 0.183178
C -2.194877 1.484398 0.423766
C -3.144385 1.198624 -0.730224
O -2.591164 1.563799 1.575279
N -0.169168 2.425349 -0.695673
C -4.155100 0.084724 -0.399375
C -3.579244 -1.333578 -0.543045
N -2.395691 -1.580476 0.282922
C -2.726355 -1.728835 1.697948
C 0.321674 -1.207783 -1.053262
H 1.465719 0.542764 -1.455999
H 1.794735 -0.430035 1.393626
C -1.532285 -2.680842 -0.189734
C -0.039089 -2.329534 -0.064629
O -1.133347 3.096124 -1.479076
H 2.707675 1.872021 1.715503
H 2.495559 2.186267 -0.003440
H 3.991837 0.705378 -1.714271
H 4.986355 -0.591148 -1.026321
H 4.563517 0.419934 2.557932
H 5.590725 -0.474641 1.424304
H 3.943034 -1.020264 1.733054
H 0.364869 1.564068 2.024470
H -0.409472 0.083829 1.538505
H -2.583646 0.974688 -1.642467
H -3.680376 2.138027 -0.921674
H -5.009726 0.161959 -1.083123
H -4.548926 0.253022 0.608465

H -4.384466 -2.066735 -0.337502
H -3.285401 -1.475432 -1.589761
H -3.167941 -0.808348 2.088527
H -3.427546 -2.565492 1.880688
H -1.814475 -1.924425 2.271291
H -0.555787 -0.560452 -1.145827
H 0.485651 -1.654775 -2.041743
H -1.757735 -2.873665 -1.245524
H -1.756299 -3.616487 0.350019
H 0.572229 -3.217903 -0.257588
H 0.167893 -2.033981 0.971577
H -0.579689 3.612078 -2.085451

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G) = -999.622491631**

Comp_17Z_c37

B3LYP/6-31G* Geometry

C -3.367627 0.907689 -0.599672
C -1.960528 0.636356 -1.164350
C -0.944609 0.191584 -0.091791
C -3.880513 -0.309547 0.203669
C -2.867353 -0.827272 1.219169
C -1.445078 -1.047041 0.698702
O -3.175386 -1.068847 2.371966
H -3.301801 1.754231 0.098409
C -4.356939 1.298866 -1.703642
C -0.563579 1.374981 0.857083
C 0.697322 2.062717 0.393235
C 2.009089 1.418747 0.831196
C 3.083668 1.105739 -0.193194
O 2.126414 1.125308 2.008995
N 0.579016 3.135060 -0.298830
C 3.961107 -0.093974 0.197597
C 3.180834 -1.387339 0.493712
N 2.166569 -1.710882 -0.514706
C 2.774084 -2.139188 -1.770975
C -1.412328 -2.383742 -0.100164
H -0.817171 -1.173440 1.587124
H -0.024316 -0.112812 -0.601103
C 1.186054 -2.693334 -0.029766
C -0.114418 -2.698546 -0.871680
O 1.826072 3.673259 -0.683088
H -2.033199 -0.137655 -1.942888
H -1.584143 1.539947 -1.661494
H -4.809036 -0.080333 0.736129
H -4.103651 -1.126177 -0.500610
H -4.466675 0.490306 -2.438025
H -4.016905 2.193154 -2.239019
H -5.350041 1.511616 -1.290809
H -0.382632 1.011818 1.873864
H -1.367885 2.113530 0.911158
H 3.701553 2.007271 -0.297182
H 2.608416 0.956110 -1.167808
H 4.536515 0.150584 1.097246

H 4.693512 -0.254651 -0.603053
H 3.904005 -2.216068 0.628499
H 2.664627 -1.259819 1.448839
H 2.000753 -2.347459 -2.516172
H 3.414741 -1.348966 -2.173754
H 3.388954 -3.053160 -1.652728
H -1.618474 -3.190015 0.616305
H -2.235709 -2.410682 -0.824679
H 0.955455 -2.433486 1.008367
H 1.622770 -3.710228 0.000445
H -0.250704 -3.676644 -1.349778
H -0.001149 -1.978766 -1.689667
H 1.561170 4.474610 -1.160628

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.622324763

Comp_17Z_c38

B3LYP/6-31G* Geometry

C -3.780237 0.115181 -0.244320
C -2.732569 0.294299 -1.356116
C -1.297643 0.499675 -0.825895
C -3.379508 -1.062303 0.669244
C -1.941785 -0.983208 1.167692
C -0.865591 -0.637872 0.137775
O -1.651205 -1.237331 2.323904
H -3.796479 1.026412 0.370651
C -5.188501 -0.082637 -0.816920
C -1.135630 1.899008 -0.178148
C 0.271001 2.248639 0.251554
C 1.367234 2.293203 -0.812396
C 2.362411 1.152061 -0.925972
O 1.330648 3.203504 -1.619636
N 0.436611 2.625056 1.464234
C 2.946247 0.547223 0.360463
C 3.563156 -0.837580 0.103580
N 2.583977 -1.824720 -0.368387
C 3.211624 -2.891329 -1.140574
C -0.432388 -1.928778 -0.612530
H -0.008327 -0.289835 0.719940
H -0.625458 0.468179 -1.694880
C 1.745476 -2.359142 0.712689
C 0.391094 -2.912986 0.235475
O 1.769135 3.025726 1.706605
H -2.752848 -0.594054 -2.004020
H -3.009873 1.144027 -1.994051
H -4.037019 -1.149781 1.540069
H -3.478859 -1.997668 0.094798
H -5.233071 -0.978408 -1.449912
H -5.490078 0.774924 -1.429760
H -5.929287 -0.201568 -0.017701
H -1.777632 2.008676 0.702261
H -1.450266 2.655940 -0.910516
H 3.151607 1.490802 -1.606865
H 1.825989 0.342023 -1.446019

H 2.172747 0.475238 1.131560
H 3.714977 1.208677 0.773843
H 4.332391 -0.738874 -0.672470
H 4.084953 -1.183530 1.015911
H 3.917721 -3.501673 -0.544176
H 2.448676 -3.564386 -1.543802
H 3.759390 -2.465108 -1.987454
H -1.313013 -2.448482 -1.012288
H 0.171036 -1.629035 -1.476849
H 1.560108 -1.556654 1.431835
H 2.279907 -3.151260 1.272593
H -0.173163 -3.215952 1.126010
H 0.546798 -3.826658 -0.352738
H 1.749979 3.239754 2.652520

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.627095240

Comp_17Z_c40

B3LYP/6-31G* Geometry

C 2.862820 -0.139750 -0.752619
C 2.825162 -0.019234 0.780870
C 1.443234 -0.388994 1.391917
C 2.610662 -1.613143 -1.127912
C 1.560942 -2.291426 -0.252051
C 0.607510 -1.348538 0.478835
O 1.507319 -3.504493 -0.147087
H 2.054087 0.474335 -1.169108
C 4.186239 0.367551 -1.335317
C 0.655435 0.876864 1.839568
C 0.438874 1.972961 0.819772
C -0.591025 1.826302 -0.295793
C -2.021384 2.131348 0.099187
O -0.247825 1.500870 -1.417770
N 1.110875 3.053730 0.978589
C -3.093711 1.695378 -0.907933
C -3.011537 0.213834 -1.322852
N -2.739447 -0.700579 -0.210332
C -3.899219 -0.859737 0.659332
C -0.487919 -2.092984 1.257852
H 0.148771 -0.731479 -0.303058
H 1.626004 -0.940968 2.323814
C -2.220160 -1.992052 -0.678694
C -1.535797 -2.835407 0.408693
O 0.773539 4.024174 0.010774
H 3.595928 -0.685011 1.195529
H 3.100798 0.997878 1.084014
H 2.282307 -1.701210 -2.173921
H 3.530588 -2.206721 -1.045724
H 5.038744 -0.186456 -0.920684
H 4.334243 1.430064 -1.109843
H 4.211132 0.250356 -2.425333
H 1.204759 1.336460 2.668501
H -0.321882 0.572512 2.234797
H -2.064697 3.219593 0.260797

H -2.201702 1.677948 1.081093
H -3.011248 2.297585 -1.820148
H -4.074448 1.927974 -0.474864
H -3.940818 -0.057748 -1.861804
H -2.189212 0.113219 -2.033830
H -3.645971 -1.480526 1.523757
H -4.226318 0.114445 1.037099
H -4.759088 -1.328351 0.141147
H -0.005461 -2.821935 1.920509
H -1.008746 -1.374791 1.900424
H -1.491532 -1.776407 -1.467902
H -3.015542 -2.599793 -1.154563
H -1.062505 -3.689463 -0.087032
H -2.288210 -3.258334 1.087414
H 1.335006 4.772520 0.266643

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623697658

Comp_17Z_c41

B3LYP/6-31G* Geometry

C -2.115426 -2.089574 1.286073
C -0.954492 -2.325142 0.303336
C -0.566474 -1.088714 -0.533827
C -3.331221 -1.523970 0.514910
C -2.951764 -0.321102 -0.335986
C -1.794877 -0.546803 -1.322532
O -3.545925 0.738942 -0.238004
H -2.409043 -3.064883 1.697480
C -1.722537 -1.191055 2.468018
C 0.640367 -1.451031 -1.445504
C 1.935666 -1.443713 -0.669607
C 2.525106 -0.075990 -0.336290
C 2.434846 0.415284 1.096883
O 2.996075 0.585674 -1.243550
N 2.475330 -2.558267 -0.347826
C 2.449620 1.944879 1.241207
C 1.381997 2.681578 0.413031
N 0.011305 2.175030 0.576450
C -0.560805 2.617472 1.846440
C -1.559060 0.670713 -2.251422
H -2.142386 -1.375121 -1.965423
H -0.255146 -0.274174 0.131083
C -0.849716 2.583722 -0.552404
C -0.576980 1.799766 -1.856976
O 3.663588 -2.361112 0.397542
H -0.074319 -2.688551 0.847531
H -1.236403 -3.132331 -0.390004
H -3.717246 -2.302699 -0.159524
H -4.143149 -1.230085 1.187209
H -1.427460 -0.187944 2.142010
H -0.879549 -1.624569 3.019353
H -2.558717 -1.078026 3.167739
H 0.741698 -0.734717 -2.266763
H 0.495752 -2.443835 -1.886901

H 3.286694 -0.029742 1.630450
H 1.538493 -0.014281 1.557081
H 3.426018 2.332107 0.928070
H 2.349866 2.184133 2.307151
H 1.429605 3.762165 0.653390
H 1.656263 2.587252 -0.638797
H -0.627658 3.720352 1.923736
H -1.568796 2.207682 1.962553
H 0.049685 2.261103 2.682755
H -1.214276 0.287253 -3.220403
H -2.541262 1.119110 -2.438203
H -0.728716 3.667189 -0.743135
H -1.889826 2.434671 -0.253371
H 0.447272 1.415181 -1.839499
H -0.599032 2.509873 -2.693823
H 3.969803 -3.270397 0.537884

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.620040725

Comp_17Z_c42

B3LYP/6-31G* Geometry

C 2.916497 0.981412 1.031183
C 1.428812 0.601547 1.104908
C 0.806955 0.216251 -0.256007
C 3.716743 -0.180005 0.405500
C 3.147865 -0.611922 -0.936958
C 1.639206 -0.859266 -1.002793
O 3.857334 -0.778442 -1.913051
H 3.023358 1.854842 0.371185
C 3.474809 1.366571 2.405837
C 0.516486 1.465175 -1.134000
C -0.730784 2.167044 -0.662874
C -2.018839 1.363639 -0.813738
C -2.767226 0.958583 0.443699
O -2.358491 1.015273 -1.930137
N -0.644235 3.350619 -0.184346
C -3.650446 -0.282811 0.263222
C -2.909514 -1.577382 -0.113278
N -1.782181 -1.943050 0.759113
C -2.224028 -2.194616 2.129870
C 1.313215 -2.286269 -0.478453
H 1.391827 -0.844911 -2.071137
H -0.156898 -0.256031 -0.032120
C -1.073194 -3.118047 0.220020
C -0.079687 -2.820835 -0.918642
O -1.907577 3.852021 0.209698
H 1.318060 -0.240652 1.803339
H 0.858164 1.433367 1.537787
H 4.772461 0.073512 0.265646
H 3.672266 -1.043413 1.089149
H 2.928370 2.217624 2.829019
H 4.533308 1.644478 2.341527
H 3.391542 0.530386 3.112373
H 0.339464 1.148768 -2.169581

H 1.351544 2.172966 -1.139807
H -3.376878 1.823614 0.737448
H -2.040498 0.819588 1.252738
H -4.377445 -0.091014 -0.533663
H -4.231634 -0.427948 1.181429
H -3.653254 -2.399422 -0.145099
H -2.523862 -1.466461 -1.130074
H -1.361274 -2.454149 2.751551
H -2.961294 -3.017794 2.202863
H -2.680574 -1.296492 2.555277
H 1.387621 -2.299522 0.616437
H 2.087382 -2.970630 -0.845584
H -1.802320 -3.876685 -0.124074
H -0.521134 -3.582525 1.045794
H -0.537438 -2.132421 -1.639053
H 0.066433 -3.758736 -1.468309
H -1.683740 4.741468 0.524513

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.624162728

Comp_17Z_c43

B3LYP/6-31G* Geometry

C -3.728559 0.457830 0.144683
C -2.801504 0.819437 -1.026525
C -1.301534 0.751127 -0.672869
C -3.380570 -0.957242 0.655654
C -1.902358 -1.104311 0.982518
C -0.903336 -0.628049 -0.070965
O -1.529342 -1.591118 2.038240
H -3.545153 1.166271 0.966690
C -5.208072 0.561199 -0.241799
C -0.879825 1.896385 0.289203
C 0.534973 2.399845 0.080413
C 1.693413 1.439815 -0.195319
C 2.542493 1.054073 1.001341
O 1.900054 1.077548 -1.336715
N 0.701880 3.669298 0.117151
C 3.591284 -0.041366 0.761991
C 3.055534 -1.477417 0.894961
N 2.105122 -1.860581 -0.149071
C 2.782466 -2.199637 -1.393698
C -0.662252 -1.702505 -1.158832
H 0.048865 -0.518924 0.452296
H -0.736595 0.880968 -1.603216
C 1.151174 -2.884021 0.283127
C -0.066625 -3.030120 -0.652360
O 2.063333 4.020685 -0.048467
H -3.006185 0.130991 -1.859495
H -3.040880 1.825094 -1.396712
H -3.957733 -1.228570 1.545337
H -3.630080 -1.683131 -0.134847
H -5.446688 -0.123227 -1.066168
H -5.460984 1.577101 -0.567423
H -5.859141 0.306711 0.602678

H -0.981319 1.559491 1.331907
H -1.535183 2.767801 0.181940
H 1.872386 0.787232 1.832001
H 3.025339 1.992698 1.311999
H 4.390443 0.078357 1.504613
H 4.054063 0.112212 -0.218575
H 3.915257 -2.176173 0.935339
H 2.545937 -1.563507 1.862786
H 3.367314 -1.346053 -1.745479
H 3.457434 -3.072194 -1.285713
H 2.052347 -2.432193 -2.173539
H -1.589035 -1.913923 -1.709307
H 0.031072 -1.253000 -1.877969
H 0.783010 -2.588818 1.270622
H 1.627187 -3.878423 0.402805
H -0.823321 -3.606067 -0.103848
H 0.191843 -3.638191 -1.528953
H 2.028214 4.989271 -0.019933

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623203568

Comp_17Z_c44

B3LYP/6-31G* Geometry

C 3.466385 1.270775 0.253808
C 2.163913 1.579231 -0.508552
C 1.130158 0.440194 -0.447845
C 4.080713 -0.042531 -0.285369
C 3.072912 -1.182865 -0.271690
C 1.735634 -0.901694 -0.969677
O 3.322593 -2.256280 0.248123
H 4.176154 2.082111 0.042340
C 3.269147 1.214451 1.777324
C -0.152947 0.810384 -1.230566
C -0.978595 1.918005 -0.616595
C -1.549532 1.712159 0.782238
C -3.020605 1.355795 0.902372
O -0.801752 1.770911 1.742112
N -1.167860 2.982191 -1.303353
C -3.346880 0.002223 0.227301
C -2.598625 -1.192378 0.860471
N -2.206123 -2.203811 -0.125957
C -3.366884 -2.928379 -0.632334
C 0.792082 -2.121878 -0.922233
H 1.998168 -0.726095 -2.028455
H 0.851023 0.302239 0.601239
C -1.176074 -3.122392 0.386595
C 0.224256 -2.494634 0.464218
O -1.989463 3.904817 -0.611783
H 1.712512 2.494631 -0.107945
H 2.404676 1.785048 -1.562841
H 4.396193 0.112656 -1.328179
H 4.960208 -0.350939 0.288425
H 2.791973 2.129744 2.144792
H 4.232726 1.102956 2.287803

H 2.640805 0.370362 2.083449
H -0.795169 -0.075020 -1.304025
H 0.102472 1.115453 -2.253054
H -3.605180 2.151438 0.425630
H -3.264641 1.333831 1.970083
H -3.085720 0.055635 -0.835943
H -4.431450 -0.147679 0.271747
H -1.687786 -0.828945 1.343294
H -3.213796 -1.633916 1.669926
H -3.894169 -3.505677 0.152623
H -4.085123 -2.229837 -1.073676
H -3.055182 -3.625800 -1.416650
H -0.043303 -1.943271 -1.606881
H 1.341129 -2.982298 -1.321334
H -1.137546 -3.977976 -0.299401
H -1.458417 -3.530156 1.376532
H 0.898206 -3.201630 0.957994
H 0.192938 -1.620520 1.124316
H -2.045195 4.640617 -1.241041

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.624033658**

Comp_17Z_c45

B3LYP/6-31G* Geometry

C -2.707623 -0.104470 0.904743
C -2.874064 0.000723 -0.620981
C -1.574347 -0.323931 -1.412180
C -2.365764 -1.563534 1.256164
C -1.437031 -2.225817 0.241848
C -0.611405 -1.276759 -0.626450
O -1.376406 -3.439257 0.145402
H -1.868361 0.537393 1.204659
C -3.952610 0.380367 1.654948
C -0.876716 0.965747 -1.934152
C -0.436222 1.972383 -0.888022
C 1.040964 2.002507 -0.496049
C 1.431286 1.948441 0.966913
O 1.850764 2.061907 -1.404688
N -1.311869 2.830020 -0.507713
C 2.896870 1.574576 1.231285
C 3.381044 0.304328 0.509478
N 2.421097 -0.802932 0.550630
C 2.336476 -1.394742 1.881874
C 0.353529 -2.044825 -1.545193
H -0.022720 -0.665492 0.072768
H -1.868461 -0.867036 -2.320756
C 2.713732 -1.814851 -0.476222
C 1.539995 -2.733676 -0.843433
O -0.814272 3.751143 0.437569
H -3.665846 -0.700977 -0.921672
H -3.227189 1.002558 -0.887867
H -1.889709 -1.633059 2.245384
H -3.272389 -2.179796 1.311445
H -4.837947 -0.198336 1.361516

H -4.155483 1.435771 1.439289
H -3.831419 0.274796 2.739895
H -1.582112 1.468534 -2.604467
H 0.002819 0.706778 -2.531250
H 0.747752 1.254507 1.471255
H 1.207669 2.934458 1.392412
H 3.025859 1.481944 2.316899
H 3.549797 2.397063 0.916598
H 3.538034 0.557620 -0.540492
H 4.365118 0.009139 0.924741
H 1.573178 -2.177946 1.904233
H 3.295416 -1.844113 2.206710
H 2.054370 -0.635448 2.618357
H 0.746104 -1.363642 -2.311797
H -0.229060 -2.809480 -2.072708
H 3.578719 -2.439695 -0.175204
H 3.020770 -1.277863 -1.381684
H 1.180705 -3.291976 0.026924
H 1.946237 -3.491828 -1.526579
H -1.575818 4.337368 0.567276

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.622727262**

Comp_17Z_c46

B3LYP/6-31G* Geometry

C 4.142114 0.371970 -0.150976
C 2.966134 1.228152 0.357695
C 1.776079 0.407311 0.897462
C 3.630502 -0.610597 -1.231084
C 2.471215 -1.437469 -0.698838
C 1.282722 -0.639253 -0.149822
O 2.498530 -2.655781 -0.692298
H 4.863562 1.048048 -0.629767
C 4.880491 -0.370095 0.974584
C 0.640665 1.336167 1.423914
C -0.272090 1.956822 0.375911
C -1.761890 1.606510 0.445684
C -2.579326 1.494241 -0.831107
O -2.249521 1.460501 1.552428
N 0.265327 2.817802 -0.412298
C -3.835609 0.617168 -0.727703
C -3.574997 -0.890158 -0.876689
N -2.829099 -1.483739 0.231183
C -3.669055 -1.709081 1.399872
C 0.171233 -1.556493 0.376721
H 0.897128 -0.059140 -1.005421
H 2.120783 -0.152129 1.779215
C -2.043263 -2.660380 -0.166041
C -0.663729 -2.256282 -0.708170
O -0.626056 3.398315 -1.330345
H 3.320467 1.902284 1.149497
H 2.610502 1.873448 -0.454838
H 3.275348 -0.034690 -2.098240
H 4.417324 -1.290450 -1.571949

H 4.242572 -1.111823 1.468763
H 5.234005 0.331297 1.739519
H 5.751896 -0.905631 0.580531
H 1.112117 2.144045 1.996280
H 0.001641 0.798467 2.126461
H -1.930728 1.172230 -1.654711
H -2.864723 2.523479 -1.086201
H -4.523349 0.911358 -1.530992
H -4.350016 0.832159 0.214501
H -4.544082 -1.408433 -1.025503
H -2.999892 -1.046985 -1.797595
H -3.061444 -2.105773 2.219185
H -4.096015 -0.761827 1.741288
H -4.500506 -2.416761 1.210591
H 0.617872 -2.311033 1.036169
H -0.522071 -0.966546 0.981454
H -2.582184 -3.284501 -0.902043
H -1.900823 -3.287305 0.722236
H -0.802289 -1.581651 -1.566054
H -0.137941 -3.137753 -1.090521
H -0.053561 4.031703 -1.790811

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.623432591**

Comp_17Z_c47

B3LYP/6-31G* Geometry

C -3.730365 0.655945 0.563226
C -3.055040 0.924309 -0.795767
C -1.516506 0.822271 -0.760490
C -3.086116 -0.595772 1.244979
C -2.249753 -1.390917 0.253349
C -1.060649 -0.623739 -0.332268
O -2.527411 -2.537790 -0.051295
H -3.557839 1.524160 1.211688
C -5.245628 0.485671 0.397971
C -0.906264 1.959309 0.101110
C 0.580120 2.176079 -0.117678
C 1.544063 1.495247 0.844809
C 2.975980 1.209615 0.438113
O 1.110509 1.176072 1.943269
N 0.864262 2.975135 -1.085504
C 3.652798 0.100820 1.255618
C 2.894778 -1.240021 1.263394
N 2.326720 -1.602302 -0.036428
C 3.355813 -1.952954 -1.007677
C -0.341129 -1.365403 -1.474766
H -0.361340 -0.512681 0.506897
H -1.159912 0.985305 -1.785402
C 1.301332 -2.646799 0.072546
C 0.334828 -2.702826 -1.119367
O 2.229820 3.206367 -1.282605
H -3.429142 0.188856 -1.523960
H -3.356363 1.910526 -1.171702
H -2.425178 -0.274390 2.060831

H -3.844764 -1.259016 1.669807
H -5.475199 -0.399762 -0.207881
H -5.689499 1.357008 -0.098831
H -5.739351 0.364158 1.369061
H -1.065597 1.772629 1.167026
H -1.416857 2.893096 -0.157096
H 3.536600 2.149082 0.540151
H 2.994492 0.983634 -0.630985
H 3.768467 0.420742 2.297271
H 4.667567 -0.028671 0.859094
H 2.063059 -1.152457 1.966732
H 3.567695 -2.028466 1.656506
H 3.937524 -2.847130 -0.707388
H 2.903422 -2.156256 -1.982622
H 4.057520 -1.123188 -1.137879
H -1.059132 -1.544780 -2.286323
H 0.419273 -0.682411 -1.872087
H 0.726703 -2.446502 0.983553
H 1.756370 -3.647114 0.214688
H -0.430540 -3.449399 -0.890283
H 0.861889 -3.063768 -2.012925
H 2.220353 3.834745 -2.021973

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.620690206**

Comp_17Z_c48

B3LYP/6-31G* Geometry

C 3.864132 0.253029 -0.456399
C 2.649195 1.154506 -0.109073
C 1.642668 0.462788 0.831319
C 3.465009 -1.250337 -0.455814
C 2.006969 -1.434430 -0.827701
C 1.003694 -0.750987 0.103635
O 1.648614 -2.088721 -1.792866
H 4.182953 0.504375 -1.475800
C 5.056404 0.495249 0.478775
C 0.603499 1.449611 1.428707
C -0.365178 2.081721 0.444215
C -1.817012 1.606878 0.470559
C -2.610929 1.514272 -0.822133
O -2.303959 1.356088 1.559851
N 0.093099 3.061941 -0.248512
C -3.726216 0.460264 -0.810215
C -3.225035 -0.971829 -1.045897
N -2.330540 -1.470298 0.000431
C -3.073554 -1.822398 1.207156
C 0.414989 -1.781662 1.101291
H 0.185092 -0.398670 -0.534655
H 2.201050 0.082799 1.701062
C -1.486307 -2.569516 -0.479554
C -0.360054 -2.961380 0.490589
O -0.853107 3.650480 -1.104871
H 3.001582 2.092722 0.336321
H 2.125822 1.439676 -1.029989

H 4.093015 -1.838639 -1.130307
H 3.597932 -1.651183 0.560687
H 4.780146 0.320457 1.526836
H 5.417984 1.526888 0.396400
H 5.891405 -0.174357 0.240184
H 1.156860 2.251918 1.929349
H 0.003793 0.951698 2.195073
H -1.927174 1.362988 -1.665264
H -3.040146 2.513303 -0.976954
H -4.435760 0.696337 -1.613377
H -4.285144 0.534625 0.128039
H -4.097075 -1.642442 -1.182559
H -2.670759 -0.988910 -1.992764
H -3.810111 -2.630178 1.027091
H -2.389437 -2.156671 1.991273
H -3.599564 -0.945711 1.591761
H 1.228800 -2.179565 1.725120
H -0.250121 -1.233729 1.776816
H -1.025163 -2.246968 -1.418342
H -2.083762 -3.474448 -0.711386
H 0.321104 -3.618943 -0.061398
H -0.758390 -3.563924 1.317258
H -0.338865 4.367598 -1.507579

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.623200820**

Comp_17Z_c49

B3LYP/6-31G* Geometry

C -3.595318 0.234768 -0.738238
C -2.406248 -0.489033 -1.401160
C -1.038681 -0.128176 -0.779917
C -3.572409 0.054997 0.797354
C -2.199475 0.254481 1.437139
C -1.023483 -0.435032 0.739716
O -2.061013 0.882125 2.470833
H -3.501470 1.309605 -0.944120
C -4.935054 -0.224388 -1.326848
C -0.690446 1.352361 -1.097142
C 0.539503 1.914928 -0.421425
C 1.892592 1.351622 -0.813505
C 3.022087 1.300743 0.203780
O 2.037047 0.970863 -1.965304
N 0.318684 2.908067 0.365421
C 3.943120 0.083773 0.050458
C 3.351203 -1.198910 0.648321
N 2.101196 -1.639942 0.017755
C 2.359560 -2.146735 -1.331422
C -1.089619 -1.946203 1.102235
H -0.112396 -0.024312 1.184319
H -0.266861 -0.743628 -1.251568
C 1.422790 -2.650467 0.843794
C -0.051158 -2.898375 0.480136
O 1.476516 3.477607 0.913033
H -2.564687 -1.574525 -1.327409

H -2.394623 -0.257233 -2.474835
H -4.278347 0.729394 1.292617
H -3.894835 -0.971275 1.034161
H -5.090361 -1.298449 -1.160723
H -4.974554 -0.044491 -2.407779
H -5.775310 0.309235 -0.867145
H -1.517231 2.012585 -0.821016
H -0.546990 1.437331 -2.181506
H 2.616252 1.362264 1.217881
H 3.595044 2.227729 0.062653
H 4.882582 0.285407 0.580159
H 4.205277 -0.049707 -1.003630
H 4.117059 -2.000141 0.615434
H 3.138308 -1.012474 1.708566
H 1.435739 -2.514642 -1.784405
H 2.731898 -1.343864 -1.969861
H 3.091662 -2.977799 -1.328997
H -1.016284 -2.016261 2.196478
H -2.079855 -2.343269 0.845980
H 1.472616 -2.318775 1.888398
H 1.969339 -3.613680 0.798031
H -0.307003 -3.907283 0.831102
H -0.174031 -2.933538 -0.608225
H 1.105722 4.168052 1.485057

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.626724840**

Comp_17Z_c50

B3LYP/6-31G* Geometry

C -4.115695 -0.903013 0.053129
C -2.857294 -1.553484 -0.552766
C -1.571104 -0.727524 -0.349555
C -4.292711 0.518724 -0.526736
C -3.028318 1.355988 -0.386809
C -1.743221 0.712533 -0.925166
O -3.051400 2.474602 0.094968
H -4.982964 -1.500742 -0.258572
C -4.097495 -0.885788 1.590162
C -0.351453 -1.456922 -0.977551
C 0.820477 -1.722418 -0.052855
C 2.150260 -2.033485 -0.732473
C 3.125793 -0.904830 -1.018960
O 2.338640 -3.173126 -1.115298
N 0.621170 -1.800412 1.206582
C 3.797141 -0.227257 0.201261
C 2.960422 0.853929 0.906178
N 2.447461 1.896700 0.012470
C 3.508929 2.788237 -0.443775
C -0.519523 1.638781 -0.792185
H -1.935766 0.580723 -2.005652
H -1.390664 -0.650096 0.726106
C 1.341247 2.653339 0.621721
C 0.000587 1.903233 0.628987
O 1.809065 -2.130083 1.901677

H -2.712130 -2.550496 -0.116546
H -3.017934 -1.705614 -1.631176
H -4.520811 0.440388 -1.600483
H -5.117799 1.056725 -0.049711
H -3.961031 -1.897152 1.990488
H -5.041305 -0.491637 1.983873
H -3.292499 -0.258183 1.989572
H 0.017361 -0.909744 -1.853707
H -0.657574 -2.438771 -1.367060
H 2.598113 -0.124484 -1.585044
H 3.890230 -1.342870 -1.668603
H 4.737380 0.209678 -0.155039
H 4.073802 -0.981062 0.945965
H 2.111434 0.376000 1.396416
H 3.578454 1.294714 1.714834
H 4.284953 2.221917 -0.967806
H 3.100121 3.519500 -1.148590
H 3.995582 3.342163 0.383379
H 0.303052 1.230301 -1.389340
H -0.780642 2.601106 -1.250035
H 1.217655 3.574781 0.039427
H 1.596437 2.970192 1.651713
H -0.728444 2.508450 1.177620
H 0.105755 0.964204 1.183825
H 1.510128 -2.145410 2.824365

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.620925652

Comp_17Z_c51

B3LYP/6-31G* Geometry

C -3.462498 0.443455 0.980611
C -2.917503 1.470118 -0.026603
C -1.464636 1.157834 -0.476693
C -3.611245 -0.903623 0.243378
C -2.532517 -1.126570 -0.813820
C -1.214424 -0.389886 -0.579084
O -2.729445 -1.850702 -1.773677
H -2.725099 0.326910 1.788401
C -4.784882 0.886906 1.614942
C -0.455051 1.865738 0.468910
C 0.966349 1.993004 -0.055072
C 2.078095 1.268041 0.691661
C 3.287381 0.731060 -0.059546
O 1.975885 1.175068 1.904349
N 1.114433 2.812762 -1.033125
C 3.842697 -0.577640 0.518306
C 3.022476 -1.813252 0.120960
N 1.639147 -1.792372 0.601431
C 1.568983 -2.037258 2.039807
C -0.141325 -0.768942 -1.611365
H -0.879557 -0.705409 0.419793
H -1.322033 1.588063 -1.475870
C 0.771234 -2.712524 -0.146151
C 0.376558 -2.218862 -1.546950

O 2.443120 2.966127 -1.460648
H -3.580686 1.470438 -0.904530
H -2.964843 2.483521 0.390701
H -3.577188 -1.747659 0.947879
H -4.580263 -0.968463 -0.266832
H -5.546380 1.068330 0.845652
H -4.658807 1.813790 2.186625
H -5.176367 0.122193 2.296472
H -0.414523 1.368030 1.442614
H -0.824953 2.881890 0.645551
H 4.049509 1.520615 -0.002858
H 3.056234 0.626479 -1.123663
H 3.924303 -0.489161 1.606236
H 4.862621 -0.723297 0.140745
H 2.998773 -1.868415 -0.973430
H 3.548022 -2.725331 0.469180
H 0.523765 -2.010460 2.365268
H 1.993755 -3.018182 2.328573
H 2.099511 -1.251175 2.581738
H -0.548020 -0.592059 -2.614537
H 0.704364 -0.087747 -1.492667
H -0.140616 -2.843659 0.447714
H 1.221526 -3.721208 -0.227902
H -0.390583 -2.900100 -1.929656
H 1.228787 -2.305683 -2.234116
H 2.349045 3.615486 -2.175152

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -999.623330230

Comp_17Z_c52

B3LYP/6-31G* Geometry

C 2.954356 0.349212 -0.738421
C 2.884134 0.427351 0.796467
C 1.567758 -0.149601 1.398476
C 2.907421 -1.132546 -1.156664
C 1.961318 -1.966728 -0.297314
C 0.879522 -1.184011 0.443831
O 2.089390 -3.175156 -0.206922
H 2.074393 0.861219 -1.148851
C 4.199474 1.050930 -1.291016
C 0.601085 0.963267 1.893225
C 0.026070 1.892030 0.836823
C -1.462022 1.773254 0.511415
C -1.949849 1.953327 -0.917132
O -2.222863 1.587366 1.445298
N 0.809286 2.813156 0.402610
C -3.230420 1.176638 -1.249474
C -2.988155 -0.311998 -1.535636
N -2.442748 -1.055068 -0.398743
C -3.468362 -1.305069 0.611102
C -0.112088 -2.094787 1.180272
H 0.342286 -0.601685 -0.319864
H 1.838766 -0.704474 2.306906
C -1.762742 -2.283452 -0.823640

C -0.990776 -2.998582 0.295716
O 0.212539 3.673991 -0.536473
H 3.739876 -0.134530 1.198745
H 3.013377 1.465390 1.119128
H 2.594480 -1.238148 -2.205994
H 3.899559 -1.596898 -1.087072
H 4.195984 2.116999 -1.035702
H 4.254503 0.965615 -2.383139
H 5.115405 0.610208 -0.876695
H 1.151267 1.572298 2.619181
H -0.243024 0.523650 2.429917
H -1.142611 1.712245 -1.618478
H -2.122462 3.031325 -1.035569
H -3.682823 1.615780 -2.147614
H -3.955009 1.311524 -0.440274
H -3.929094 -0.768551 -1.903263
H -2.266906 -0.387304 -2.359999
H -3.039491 -1.837302 1.463045
H -4.309136 -1.908129 0.216024
H -3.859487 -0.357431 0.987603
H -0.761856 -1.466710 1.797963
H 0.454193 -2.738245 1.865105
H -1.059757 -1.999740 -1.617108
H -2.468625 -3.005008 -1.282965
H -0.367575 -3.767115 -0.172100
H -1.691216 -3.534388 0.949065
H 0.926357 4.307767 -0.708467

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.623226428

Comp_17Z_c53

B3LYP/6-31G* Geometry

C -4.270953 0.432226 0.601828
C -2.992142 1.081045 1.164691
C -1.714034 0.775266 0.356865
C -4.069369 -1.097032 0.492384
C -2.816771 -1.427760 -0.304064
C -1.523003 -0.765764 0.187025
O -2.844875 -2.166454 -1.272463
H -5.080634 0.612066 1.322128
C -4.705557 1.037755 -0.742561
C -0.494238 1.439579 1.054733
C 0.648582 1.874487 0.145569
C 2.060530 1.473448 0.560019
C 3.169236 1.337184 -0.473910
O 2.264200 1.292095 1.750371
N 0.309930 2.635398 -0.832514
C 4.220581 0.274616 -0.118470
C 3.797710 -1.143950 -0.534753
N 2.543718 -1.577111 0.079162
C 2.726788 -1.967896 1.472536
C -0.319395 -1.151856 -0.683155
H -1.366181 -1.156863 1.207928
H -1.812765 1.226465 -0.638412

C 1.792758 -2.572975 -0.695893
C 0.284751 -2.536096 -0.388740
O 1.379388 3.104611 -1.607979
H -3.128767 2.169202 1.219304
H -2.845689 0.736637 2.199947
H -3.951941 -1.515619 1.502961
H -4.924428 -1.590126 0.019739
H -3.975132 0.848112 -1.537495
H -4.834834 2.123285 -0.659224
H -5.659437 0.609051 -1.070552
H -0.085186 0.780481 1.825731
H -0.845374 2.336342 1.580730
H 3.638906 2.328782 -0.541719
H 2.739394 1.153435 -1.462502
H 4.441470 0.325884 0.952392
H 5.156684 0.507567 -0.641558
H 3.657111 -1.149900 -1.622679
H 4.626056 -1.848124 -0.320741
H 3.422485 -2.822540 1.582834
H 3.110128 -1.124674 2.052239
H 1.768731 -2.254101 1.914715
H -0.608341 -1.089119 -1.738653
H 0.474912 -0.422453 -0.522565
H 2.182707 -3.596670 -0.537874
H 1.936409 -2.343023 -1.758521
H 0.123153 -2.799499 0.665434
H -0.219862 -3.313683 -0.972958
H 0.922332 3.645396 -2.271197

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.624958221

Comp_17Z_c54

B3LYP/6-31G* Geometry

C 3.177205 1.403374 0.233960
C 1.729486 1.237158 0.719972
C 0.889890 0.325500 -0.206803
C 3.873562 0.035633 0.328398
C 3.011261 -1.147710 -0.114055
C 1.731973 -0.808758 -0.877732
O 3.382824 -2.290316 0.088825
H 3.154963 1.715751 -0.821257
C 3.937897 2.476529 1.020475
C 0.160073 1.156550 -1.299818
C -1.023219 1.909608 -0.750740
C -2.310144 1.123578 -0.515704
C -2.869112 1.055618 0.897195
O -2.850202 0.597902 -1.471228
N -0.896040 3.167460 -0.541531
C -3.532769 -0.283405 1.247948
C -2.539344 -1.418517 1.538683
N -1.710864 -1.819945 0.397221
C -2.501888 -2.540323 -0.598885
C 0.912427 -2.044188 -1.309846
H 2.130272 -0.366702 -1.810281

H 0.113715 -0.158326 0.388482
 C -0.543490 -2.589595 0.852564
 C 0.427235 -3.053483 -0.245617
 O -2.078368 3.740204 -0.016839
 H 1.758284 0.810174 1.733958
 H 1.239798 2.214110 0.810504
 H 4.798211 0.009873 -0.265250
 H 4.179344 -0.167397 1.363923
 H 3.467692 3.459736 0.903741
 H 4.977863 2.557970 0.682101
 H 3.954692 2.238233 2.091881
 H -0.212526 0.493848 -2.088837
 H 0.855511 1.869298 -1.758038
 H -3.605093 1.868178 0.961825
 H -2.081937 1.308739 1.617889
 H -4.227034 -0.560406 0.448441
 H -4.140997 -0.144266 2.150520
 H -1.863020 -1.085173 2.337094
 H -3.096991 -2.285496 1.946840
 H -2.949414 -3.468249 -0.192242
 H -3.301203 -1.897706 -0.973112
 H -1.879541 -2.809257 -1.454586
 H 0.053472 -1.685739 -1.889705
 H 1.532890 -2.616109 -2.010424
 H -0.859681 -3.493218 1.412994
 H -0.005425 -1.961726 1.574453
 H -0.031773 -3.887125 -0.792772
 H 1.300940 -3.475254 0.258837
 H -1.834950 4.675898 0.057156

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.622593039

Comp_18E_c01

B3LYP/6-31G* Geometry

C -0.705627 1.702292 0.169169
 O -1.081618 -0.413860 1.273252
 C 0.936352 -0.206870 0.019957
 C -0.248752 -1.088131 0.348798
 C 0.586712 1.168187 -0.498855
 C -1.711936 0.576852 0.440360
 N 2.094791 -0.714650 0.199678
 C -2.062291 -0.264843 -0.800979
 O -1.041352 -1.271621 -0.827423
 O 3.126991 0.182361 -0.143701
 H -1.161378 2.481235 -0.454619
 H -0.458630 2.160443 1.133644
 H 0.049791 -2.055644 0.754861
 H 0.440316 1.087170 -1.584938
 H 1.423809 1.852890 -0.346640
 H -2.592749 0.943673 0.973225
 H -2.040727 0.311729 -1.733193
 H -3.042449 -0.745955 -0.700500
 H 3.919564 -0.332953 0.072685

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -514.320434603

Comp_18Z_c01

B3LYP/6-31G* Geometry

C -1.250582 1.530924 0.308853
 O -0.659033 -0.616280 1.254904
 C 0.929015 0.384873 -0.197052
 C 0.206525 -0.902430 0.170152
 C 0.006113 1.513215 -0.595436
 C -1.727159 0.103924 0.610432
 N 2.188216 0.598472 -0.164094
 O 2.917988 -0.554305 0.206946
 C -1.940464 -0.760009 -0.645646
 O -0.636974 -1.296736 -0.913673
 H -2.053137 2.111768 -0.162846
 H -1.014760 2.011496 1.265269
 H 0.874262 -1.717451 0.440658
 H -0.299650 1.354208 -1.638596
 H 0.542561 2.465403 -0.558396
 H -2.583708 0.096273 1.289044
 H 3.829444 -0.225297 0.188073
 H -2.289785 -0.186686 -1.511967
 H -2.639283 -1.583431 -0.455812

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -514.316891478

Comp_19E_c01

B3LYP/6-31G* Geometry

C -3.861418 0.733642 0.466495
 C -4.059722 -2.022782 -0.067477
 C -5.078124 0.061189 0.575783
 C -2.726215 -0.010006 0.077739
 C -2.823231 -1.379546 -0.185881
 C -5.190596 -1.307928 0.312245
 C -3.737286 2.209442 0.749233
 O -1.563013 0.709296 -0.008597
 C -0.374823 0.032428 -0.410944
 C 0.757199 1.033056 -0.478085
 C 2.812748 2.947719 -0.635318
 C 2.081537 0.680750 -0.146912
 C 0.489436 2.343881 -0.888754
 C 1.503807 3.294558 -0.971774
 C 3.093763 1.650983 -0.217625
 C 2.454919 -0.692162 0.292650
 C 3.115208 -0.851379 1.633668
 O 3.316834 -2.138025 1.991505
 O 3.440944 0.083498 2.335400
 N 2.314267 -1.788906 -0.373921
 O 1.755952 -1.595713 -1.618944
 C 1.697130 -2.850489 -2.307282
 H -4.125798 -3.087836 -0.273878
 H -5.958094 0.626070 0.875661
 H -1.950430 -1.951684 -0.478523

H -6.152034 -1.804589 0.406272
H -4.694475 2.623314 1.080906
H -3.416976 2.763059 -0.142263
H -2.987308 2.407124 1.523847
H -0.145575 -0.773668 0.297090
H -0.527690 -0.431018 -1.395182
H 3.609881 3.683746 -0.689233
H -0.533203 2.615069 -1.127341
H 1.270480 4.306240 -1.292805
H 4.105617 1.380386 0.064063
H 3.747329 -2.094784 2.865975
H 1.248015 -2.623654 -3.276135
H 1.076664 -3.566169 -1.758643
H 2.702007 -3.261858 -2.443838

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45758177

Comp_19E_c03
B3LYP/6-31G* Geometry

C 3.890249 0.646750 0.578421
C 4.151574 -2.025272 -0.265787
C 5.104811 -0.029977 0.685345
C 2.790163 -0.049015 0.032265
C 2.918007 -1.376945 -0.385867
C 5.248212 -1.357521 0.268905
C 3.732295 2.077865 1.026053
O 1.626682 0.671567 -0.041982
C 0.464795 0.029097 -0.559344
C -0.674772 1.023945 -0.584383
C -2.759548 2.909684 -0.695888
C -2.007681 0.619555 -0.380932
C -0.409796 2.373446 -0.842286
C -1.438839 3.311004 -0.899074
C -3.036860 1.571246 -0.434449
C -2.384320 -0.799432 -0.112235
C -2.145805 -1.820258 -1.182167
O -2.665506 -3.036280 -0.913208
O -1.535689 -1.580071 -2.206175
N -2.951631 -1.248254 0.957550
O -3.137138 -0.282661 1.915859
C -3.735489 -0.874609 3.074567
H 4.242577 -3.057179 -0.594606
H 5.957879 0.497840 1.106161
H 2.073012 -1.911241 -0.804507
H 6.207068 -1.858917 0.364584
H 4.660148 2.450630 1.470811
H 2.928571 2.179877 1.764455
H 3.469082 2.734187 0.187115
H 0.659430 -0.342318 -1.573982
H 0.214050 -0.837944 0.065936
H -3.568845 3.633309 -0.737388
H 0.619576 2.683620 -0.985055
H -1.208320 4.353710 -1.100644
H -4.060475 1.250909 -0.266188

H -2.434081 -3.589849 -1.682650
H -3.849540 -0.053853 3.785205
H -3.085063 -1.649211 3.492784
H -4.712432 -1.303620 2.830292

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45720107

Comp_19E_c04
B3LYP/6-31G* Geometry

C -3.810124 -0.357743 -0.577787
C -2.866356 2.168565 0.222403
C -4.688338 0.701330 -0.345263
C -2.430439 -0.123921 -0.402163
C -1.958565 1.128328 0.000746
C -4.231594 1.962069 0.050028
C -4.298453 -1.717277 -1.011171
O -1.625739 -1.211833 -0.655479
C -0.215247 -1.031880 -0.732047
C 0.468439 -0.971340 0.622548
C 1.687272 -0.905894 3.156695
C 1.662089 -0.250072 0.817039
C -0.090811 -1.657319 1.705827
C 0.511342 -1.631805 2.961727
C 2.251110 -0.213322 2.089575
C 2.325809 0.501550 -0.285353
C 2.435467 1.991192 -0.144339
O 3.206760 2.578325 -1.083507
O 1.873290 2.615999 0.732403
N 2.827983 0.011811 -1.368340
O 2.694268 -1.356346 -1.449416
C 3.303984 -1.818324 -2.660961
H -2.491075 3.137892 0.539235
H -5.754310 0.531904 -0.481445
H -0.902272 1.302520 0.169728
H -4.938231 2.768720 0.223549
H -5.386718 -1.720504 -1.126779
H -4.029319 -2.492962 -0.283728
H -3.848852 -2.018040 -1.964911
H 0.143764 -1.904490 -1.286001
H 0.018103 -0.144665 -1.332994
H 2.158507 -0.871746 4.134843
H -1.017583 -2.201371 1.554088
H 0.058097 -2.171247 3.789060
H 3.157629 0.366070 2.238180
H 3.164681 3.533758 -0.890119
H 3.166670 -2.901297 -2.653810
H 4.370183 -1.572273 -2.672767
H 2.812700 -1.378913 -3.534760

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45754953

Comp_19E_c06
B3LYP/6-31G* Geometry

C 3.839443 -0.224710 0.885939
 C 3.277327 1.204647 -1.471665
 C 4.864092 0.294425 0.093353
 C 2.509369 -0.008543 0.470376
 C 2.225870 0.696311 -0.702752
 C 4.597963 1.008214 -1.078812
 C 4.121783 -0.990649 2.153996
 O 1.551143 -0.551143 1.295062
 C 0.185630 -0.196866 1.106168
 C -0.528289 -1.017661 0.042824
 C -1.883554 -2.628317 -1.823670
 C -1.831934 -0.679383 -0.373138
 C 0.071423 -2.165166 -0.483040
 C -0.592583 -2.960948 -1.416015
 C -2.501060 -1.498770 -1.292144
 C -2.556038 0.514743 0.155575
 C -3.789099 0.270428 0.979228
 O -4.357592 1.396791 1.461244
 O -4.236359 -0.836678 1.195166
 N -2.276685 1.756643 -0.052141
 O -1.160435 1.936188 -0.839766
 C -0.951583 3.339265 -1.048902
 H 3.051910 1.747542 -2.386115
 H 5.893846 0.136524 0.406498
 H 1.201720 0.834663 -1.029409
 H 5.415942 1.400908 -1.676115
 H 5.198272 -1.046266 2.342951
 H 3.729502 -2.013574 2.102719
 H 3.642905 -0.518937 3.020218
 H -0.279971 -0.379636 2.081778
 H 0.103294 0.873358 0.891726
 H -2.412225 -3.246816 -2.543361
 H 1.068822 -2.431298 -0.150818
 H -0.102444 -3.844413 -1.816186
 H -3.513206 -1.243433 -1.590676
 H -5.135120 1.094058 1.966900
 H -0.035438 3.406443 -1.638197
 H -0.826588 3.857714 -0.093744
 H -1.791024 3.773263 -1.600748

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45668406**

Comp_19E_c07

B3LYP/6-31G* Geometry

C -3.822133 -0.205964 -0.558337
 C -2.713433 2.103095 0.602855
 C -4.632984 0.832713 -0.099952
 C -2.424936 -0.063772 -0.425052
 C -1.870878 1.080002 0.156793
 C -4.094176 1.986775 0.476533
 C -4.398739 -1.449326 -1.187482
 O -1.691837 -1.122725 -0.906751
 C -0.276474 -1.004203 -1.010679
 C 0.455233 -1.228698 0.301854

C 1.796157 -1.717872 2.724231
 C 1.709660 -0.642341 0.548546
 C -0.106940 -2.058807 1.276799
 C 0.554482 -2.305112 2.478466
 C 2.366131 -0.887696 1.762527
 C 2.379075 0.246029 -0.447323
 C 2.912490 -0.369901 -1.704223
 O 3.686740 0.454713 -2.439267
 O 2.664495 -1.512360 -2.036298
 N 2.562432 1.517255 -0.327128
 O 2.004592 2.028664 0.822602
 C 2.240825 3.440707 0.875299
 H -2.276183 2.988567 1.056880
 H -5.711558 0.733693 -0.201753
 H -0.799484 1.177698 0.288957
 H -4.749566 2.780463 0.823869
 H -5.490488 -1.390202 -1.235225
 H -4.128875 -2.349302 -0.621494
 H -4.015614 -1.597044 -2.204098
 H 0.015450 -1.775966 -1.728913
 H -0.014230 -0.032448 -1.447277
 H 2.317397 -1.901593 3.659545
 H -1.078780 -2.502463 1.085333
 H 0.098895 -2.952719 3.222731
 H 3.329167 -0.420623 1.947773
 H 3.947416 -0.065797 -3.222395
 H 1.764010 3.773395 1.799203
 H 1.789025 3.941547 0.013449
 H 3.314308 3.651906 0.905902

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45695476**

Comp_19E_c09

B3LYP/6-31G* Geometry

C -2.817930 0.689669 -0.759731
 C -4.390873 -1.485488 0.094187
 C -4.208933 0.777355 -0.706016
 C -2.219166 -0.528935 -0.374279
 C -2.998285 -1.609206 0.049609
 C -5.001759 -0.294622 -0.283252
 C -1.963400 1.850371 -1.203365
 O -0.847910 -0.559960 -0.457586
 C -0.176295 -1.760481 -0.080633
 C 1.318558 -1.589835 -0.227344
 C 4.124341 -1.496131 -0.442854
 C 2.019854 -0.431237 0.170752
 C 2.043701 -2.672432 -0.737675
 C 3.433037 -2.639026 -0.840431
 C 3.417228 -0.401937 0.047863
 C 1.342588 0.777150 0.721783
 C 0.469958 0.619376 1.928815
 O -0.250857 1.718312 2.235747
 O 0.413686 -0.403776 2.582901
 N 1.473285 1.990975 0.305488

O 2.283573 2.109769 -0.803167
C 2.337023 3.483565 -1.197318
H -4.988435 -2.330415 0.426098
H -4.680830 1.711310 -1.003369
H -2.537137 -2.543619 0.347405
H -6.083011 -0.194673 -0.252369
H -2.588821 2.678442 -1.551653
H -1.287036 1.560166 -2.015724
H -1.332320 2.214869 -0.384680
H -0.421137 -2.004380 0.961138
H -0.514089 -2.589184 -0.717052
H 5.207111 -1.451214 -0.519063
H 1.504824 -3.560309 -1.059837
H 3.968375 -3.497494 -1.236704
H 3.950428 0.494020 0.346587
H -0.763470 1.475357 3.029585
H 2.979065 3.501786 -2.080394
H 2.769449 4.100875 -0.402911
H 1.338209 3.853944 -1.449303

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45713890**

Comp_19E_c11
B3LYP/6-31G* Geometry

C 2.759178 0.193447 -0.545346
C 2.623453 -2.502967 0.254325
C 3.805942 -0.408540 0.154708
C 1.626155 -0.593883 -0.841864
C 1.555407 -1.930893 -0.443389
C 3.751661 -1.746914 0.556402
C 2.823371 1.633577 -0.989677
O 0.640056 0.058800 -1.543361
C -0.520171 -0.648793 -1.974455
C -1.532786 -0.954464 -0.884690
C -3.516063 -1.593098 1.006471
C -1.799899 -0.075467 0.183253
C -2.269813 -2.140208 -0.982233
C -3.260020 -2.460246 -0.054844
C -2.782912 -0.414831 1.123546
C -1.074155 1.216199 0.362187
C -1.221731 2.262485 -0.696309
O -0.511901 3.388346 -0.465917
O -1.921469 2.121257 -1.680165
N -0.348598 1.546764 1.375505
O -0.245719 0.545771 2.314683
C 0.697450 0.936029 3.317424
H 2.559176 -3.543282 0.562222
H 4.686681 0.187632 0.383806
H 0.672942 -2.524224 -0.650040
H 4.583312 -2.188259 1.098413
H 3.775799 2.085347 -0.694903
H 2.010849 2.226095 -0.554515
H 2.726679 1.717653 -2.078993
H -0.974058 0.019853 -2.710953

H -0.228932 -1.575441 -2.485932
H -4.278752 -1.832450 1.742113
H -2.061775 -2.824286 -1.802450
H -3.819743 -3.386046 -0.156490
H -2.972096 0.260754 1.951766
H -0.698057 3.966781 -1.229165
H 0.667364 0.138179 4.062185
H 0.410474 1.890585 3.769893
H 1.702181 1.011768 2.889524

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45675377**

Comp_19Z_c02
B3LYP/6-31G* Geometry

C -4.116928 0.581071 0.247705
C -4.005324 -2.211619 -0.079591
C -5.271913 -0.199072 0.292286
C -2.884047 -0.071738 0.032744
C -2.827154 -1.459451 -0.129020
C -5.230454 -1.587673 0.130369
C -4.159601 2.078205 0.420819
O -1.788222 0.750230 0.002026
C -0.511875 0.160512 -0.218717
C 0.544522 1.244645 -0.244444
C 2.446816 3.327445 -0.301086
C 1.930989 0.945212 -0.173287
C 0.152785 2.582890 -0.344086
C 1.086386 3.618147 -0.372199
C 2.859444 2.003319 -0.200587
C 2.460050 -0.429657 -0.061088
C 3.855744 -0.631874 0.502227
O 3.811685 -0.972999 1.804431
O 4.880200 -0.485233 -0.123129
N 1.771651 -1.444275 -0.455551
O 2.458805 -2.638913 -0.250289
C 1.676329 -3.726846 -0.735743
H -3.952168 -3.289765 -0.206479
H -6.226365 0.295751 0.458308
H -1.879710 -1.960354 -0.291485
H -6.146979 -2.169294 0.169936
H -5.181563 2.418407 0.614190
H -3.792330 2.595721 -0.474326
H -3.524805 2.403311 1.253619
H -0.292650 -0.570603 0.569458
H -0.513920 -0.393124 -1.166328
H 3.186139 4.122806 -0.326976
H -0.905706 2.806728 -0.390648
H 0.746931 4.647513 -0.449529
H 3.919719 1.778567 -0.166602
H 4.738553 -1.100533 2.087068
H 2.287994 -4.616103 -0.569638
H 1.465187 -3.611970 -1.804441
H 0.735766 -3.812910 -0.179388

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45469852

Comp_19Z_c03

B3LYP/6-31G* Geometry

C 2.703645 -0.284925 1.264437
C 4.189047 -0.956759 -1.034390
C 4.065418 0.001134 1.171643
C 2.088101 -0.923894 0.165573
C 2.824309 -1.261077 -0.974363
C 4.814300 -0.325121 0.035435
C 1.890923 0.065310 2.485235
O 0.752868 -1.182527 0.322492
C 0.012398 -1.684013 -0.790339
C -1.458279 -1.593400 -0.449827
C -4.187336 -1.551064 0.249464
C -2.110637 -0.359254 -0.211234
C -2.196781 -2.773064 -0.337799
C -3.551357 -2.764106 0.000844
C -3.467142 -0.361659 0.148365
C -1.429422 0.955299 -0.315531
C -1.754261 2.017955 0.716673
O -2.723317 2.859465 0.294509
O -1.225940 2.095970 1.800117
N -0.553977 1.169246 -1.228834
O -0.040490 2.459612 -1.159126
C 1.017188 2.598558 -2.108522
H 4.754514 -1.224087 -1.923409
H 4.549441 0.494960 2.011483
H 2.351904 -1.766031 -1.809631
H 5.873687 -0.088057 -0.006268
H 2.510863 0.576514 3.228519
H 1.468664 -0.833438 2.951574
H 1.042181 0.712172 2.235500
H 0.241283 -1.096544 -1.683838
H 0.285450 -2.731180 -0.980699
H -5.238808 -1.524136 0.521068
H -1.693955 -3.721925 -0.507515
H -4.097319 -3.699902 0.080992
H -3.969061 0.584232 0.328838
H -2.852517 3.510932 1.012112
H 1.360517 3.629912 -2.003831
H 0.650826 2.426880 -3.126742
H 1.834513 1.905306 -1.884230

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45214767

Comp_19Z_c05

B3LYP/6-31G* Geometry

C 2.764718 -0.273715 1.254776
C 4.212955 -0.952587 -1.063136
C 4.133799 -0.027759 1.158171
C 2.120931 -0.875778 0.151252
C 2.839953 -1.215426 -0.999214

C 4.865096 -0.358748 0.012120
C 1.971064 0.083881 2.485674
O 0.779672 -1.096377 0.313528
C 0.036221 -1.623432 -0.787219
C -1.433309 -1.584005 -0.432308
C -4.162716 -1.655338 0.258926
C -2.139950 -0.376632 -0.205967
C -2.119275 -2.794128 -0.307924
C -3.473428 -2.842208 0.027952
C -3.497377 -0.435063 0.148040
C -1.505034 0.962440 -0.319379
C -1.938298 2.049907 0.643933
O -1.017576 2.265300 1.603120
O -2.993822 2.639569 0.585361
N -0.647059 1.195816 -1.245255
O -0.173349 2.501617 -1.201428
C 0.844137 2.666388 -2.189376
H 4.763740 -1.221774 -1.960722
H 4.638153 0.436497 2.002955
H 2.347572 -1.688783 -1.841101
H 5.931088 -0.154493 -0.032986
H 2.614921 0.545645 3.240970
H 1.502711 -0.803298 2.929096
H 1.157845 0.779044 2.247846
H 0.235382 -1.031619 -1.684747
H 0.341611 -2.661351 -0.977905
H -5.216026 -1.671249 0.524443
H -1.574931 -3.721364 -0.468866
H -3.977564 -3.800503 0.116515
H -4.037626 0.490065 0.317357
H -1.370246 2.979959 2.168878
H 1.154088 3.710395 -2.108703
H 0.448906 2.469101 -3.191973
H 1.693466 2.005346 -1.986846

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45256283

Comp_19Z_c06

B3LYP/6-31G* Geometry

C -4.107388 0.341145 -0.387456
C -3.848876 -2.397206 0.206997
C -5.213404 -0.508419 -0.397795
C -2.850236 -0.214170 -0.068283
C -2.717659 -1.574709 0.225858
C -5.098431 -1.870720 -0.103301
C -4.228369 1.810441 -0.704157
O -1.802963 0.672780 -0.078218
C -0.513231 0.179094 0.257499
C 0.489109 1.313164 0.206143
C 2.319857 3.449534 0.055485
C 1.872306 1.058097 0.071694
C 0.054074 2.640217 0.275607
C 0.956503 3.701015 0.203181
C 2.770618 2.133999 -0.007243

C 2.442389 -0.313928 -0.005331
C 2.156717 -1.333073 1.082501
O 3.027323 -1.202157 2.101806
O 1.261468 -2.147328 1.065889
N 3.248350 -0.585268 -0.968299
O 3.795827 -1.860037 -0.834340
C 4.604060 -2.147706 -1.974178
H -3.738537 -3.453772 0.436306
H -6.187138 -0.090190 -0.643531
H -1.750478 -2.002377 0.464801
H -5.977805 -2.508275 -0.119555
H -5.257021 2.065633 -0.976947
H -3.570427 2.097335 -1.532846
H -3.940497 2.431347 0.153728
H -0.543718 -0.268236 1.261150
H -0.222320 -0.620368 -0.434580
H 3.029657 4.269571 -0.007134
H -1.008495 2.833205 0.364949
H 0.590857 4.722921 0.257912
H 3.828623 1.918847 -0.115066
H 2.794280 -1.890120 2.755951
H 5.018956 -3.140607 -1.788031
H 5.412236 -1.415128 -2.074290
H 4.001914 -2.159610 -2.889146

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45177157

Comp_19Z_c07

B3LYP/6-31G* Geometry

C 4.052541 -0.510074 -0.339424
C 3.082168 -0.374753 2.298611
C 4.917735 -0.574034 0.753591
C 2.672061 -0.377565 -0.082973
C 2.188256 -0.303590 1.226013
C 4.447929 -0.510613 2.068780
C 4.554807 -0.586557 -1.759386
O 1.878429 -0.323661 -1.205328
C 0.463689 -0.428643 -1.066979
C -0.211282 0.899468 -0.759247
C -1.356503 3.421880 -0.216568
C -1.543005 0.989175 -0.279449
C 0.504761 2.082432 -0.966167
C -0.052876 3.332331 -0.701872
C -2.088128 2.258292 -0.008167
C -2.408502 -0.183727 -0.048726
C -3.506050 -0.077690 0.994753
O -4.708552 0.193287 0.444758
O -3.319102 -0.204775 2.180611
N -2.209009 -1.291074 -0.674679
O -3.133294 -2.263261 -0.300831
C -2.871990 -3.467320 -1.019027
H 2.697737 -0.315993 3.313372
H 5.984124 -0.680313 0.566414
H 1.129847 -0.173159 1.419786

H 5.144802 -0.564604 2.900321
H 5.641685 -0.712651 -1.780676
H 4.304484 0.318993 -2.325592
H 4.099016 -1.424705 -2.299722
H 0.115779 -0.813153 -2.030235
H 0.209247 -1.186018 -0.318961
H -1.803752 4.388570 -0.003964
H 1.522875 2.009310 -1.331787
H 0.533287 4.231326 -0.871573
H -3.109956 2.331157 0.351643
H -5.348942 0.215824 1.183045
H -3.641355 -4.169120 -0.690406
H -1.878825 -3.861074 -0.775881
H -2.950521 -3.303656 -2.099300

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1013.45413513

Comp_19Z_c09

B3LYP/6-31G* Geometry

C -3.979797 -0.068915 0.533309
C -2.930226 -1.494830 -1.651814
C -4.817731 -0.669531 -0.406976
C -2.586613 -0.199264 0.356663
C -2.060688 -0.904001 -0.729632
C -4.308479 -1.381382 -1.497008
C -4.525260 0.694344 1.714098
O -1.824548 0.411021 1.326507
C -0.407559 0.261690 1.289737
C 0.273672 1.220555 0.318015
C 1.519105 3.177770 -1.286100
C 1.555765 0.983350 -0.229505
C -0.355712 2.437945 0.039150
C 0.248816 3.406912 -0.760026
C 2.167638 1.976231 -1.015086
C 2.312203 -0.280804 -0.020373
C 3.789799 -0.183668 0.304529
O 4.018395 -0.357258 1.620139
O 4.655343 0.055465 -0.505983
N 1.733978 -1.416352 -0.176945
O 2.605403 -2.478603 0.053948
C 1.930601 -3.709270 -0.203509
H -2.515350 -2.040176 -2.495533
H -5.894003 -0.577240 -0.277902
H -0.989608 -0.997162 -0.869065
H -4.984338 -1.838632 -2.214129
H -5.619574 0.681844 1.713005
H -4.195234 1.740512 1.705647
H -4.176218 0.267738 2.661999
H -0.086990 0.501915 2.310453
H -0.140197 -0.776321 1.092641
H 2.004414 3.925821 -1.906501
H -1.338273 2.618048 0.462558
H -0.270323 4.339621 -0.963459
H 3.152550 1.785094 -1.428554

H 4.984818 -0.281173 1.745269
H 2.667055 -4.487842 0.005942
H 1.609874 -3.769156 -1.249190
H 1.063588 -3.826215 0.455716
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45133115**

Comp_19Z_c10
B3LYP/6-31G* Geometry

C -4.011720 -0.516558 -0.325847
C -2.978539 -0.486370 2.291397
C -4.849570 -0.633880 0.783836
C -2.626126 -0.384474 -0.097509
C -2.111454 -0.362870 1.201651
C -4.348503 -0.622846 2.088963
C -4.547920 -0.536032 -1.735237
O -1.860733 -0.278582 -1.234879
C -0.441263 -0.370687 -1.134530
C 0.223713 0.950659 -0.777358
C 1.346839 3.460367 -0.146336
C 1.549151 1.034127 -0.279894
C -0.498350 2.134680 -0.956368
C 0.048936 3.378947 -0.648161
C 2.085852 2.296551 0.036966
C 2.404812 -0.154351 -0.074218
C 3.470666 -0.108991 1.004389
O 3.059037 -0.735000 2.123932
O 4.542687 0.439762 0.893547
N 2.267402 -1.195482 -0.818480
O 3.156461 -2.205409 -0.459398
C 2.997507 -3.312950 -1.343995
H -2.570291 -0.468030 3.298438
H -5.919457 -0.740274 0.617949
H -1.049403 -0.233252 1.374785
H -5.024622 -0.717578 2.933885
H -5.633883 -0.671298 -1.735820
H -4.098318 -1.345445 -2.322462
H -4.319066 0.395678 -2.267036
H -0.161383 -1.160863 -0.430936
H -0.113823 -0.701488 -2.124240
H 1.786551 4.423155 0.097853
H -1.512575 2.066207 -1.334016
H -0.540541 4.279478 -0.797395
H 3.103091 2.359818 0.408062
H 3.797491 -0.674022 2.761332
H 3.730772 -4.051133 -1.012585
H 3.202635 -3.019956 -2.379327
H 1.987220 -3.730717 -1.271225

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45412847**

Comp_19Z_c11
B3LYP/6-31G* Geometry

C -4.001117 -0.071538 0.490529
C -2.914982 -1.519271 -1.662174
C -4.823024 -0.678457 -0.459721
C -2.605114 -0.206426 0.340818
C -2.061227 -0.922315 -0.729277
C -4.295549 -1.401040 -1.533961
C -4.566176 0.703366 1.654348
O -1.859737 0.410985 1.318682
C -0.441966 0.262826 1.305795
C 0.252401 1.215297 0.337426
C 1.519921 3.167434 -1.258164
C 1.542714 0.976554 -0.188583
C -0.373962 2.430260 0.041157
C 0.241008 3.396436 -0.753385
C 2.163127 1.967585 -0.969512
C 2.309638 -0.277829 0.029348
C 3.774566 -0.154520 0.402308
O 4.589859 -0.328899 -0.659755
O 4.162143 0.098549 1.517325
N 1.737398 -1.423208 -0.065103
O 2.629368 -2.467584 0.166764
C 1.948453 -3.713384 0.025018
H -2.486054 -2.073540 -2.492971
H -5.901256 -0.582681 -0.351264
H -0.987980 -1.020110 -0.847317
H -4.959218 -1.863158 -2.259307
H -5.660327 0.691052 1.635007
H -4.235727 1.749369 1.641190
H -4.233062 0.286112 2.612038
H -0.136583 0.512669 2.328649
H -0.169490 -0.775885 1.120881
H 2.014374 3.913312 -1.873861
H -1.362963 2.611288 0.448788
H -0.276117 4.327413 -0.969123
H 3.153429 1.777619 -1.373533
H 5.503088 -0.239310 -0.322306
H 2.704641 -4.476000 0.222500
H 1.554016 -3.830994 -0.990101
H 1.132107 -3.798972 0.750507

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45113920**

Comp_19Z_c12
B3LYP/6-31G* Geometry

C -2.754686 0.381782 -0.943709
C -4.270334 -1.472804 0.541337
C -4.140346 0.499281 -0.833937
C -2.132549 -0.700521 -0.284541
C -2.882480 -1.622388 0.451163
C -4.904268 -0.413338 -0.099040
C -1.931193 1.369289 -1.731560
O -0.768459 -0.765862 -0.429763
C -0.066881 -1.856758 0.167802
C 1.411970 -1.703167 -0.099607

C 4.181397 -1.603199 -0.590936
 C 2.107805 -0.479871 0.035811
 C 2.124036 -2.846563 -0.476409
 C 3.496987 -2.810397 -0.714811
 C 3.487633 -0.454069 -0.221551
 C 1.450587 0.810554 0.397542
 C 0.493088 0.813338 1.561754
 O -0.478631 1.741375 1.503975
 O 0.593001 0.024537 2.480840
 N 1.867029 1.842532 -0.255147
 O 1.331801 3.047986 0.148764
 C 1.883334 4.090512 -0.657496
 H -4.846130 -2.194114 1.115153
 H -4.631575 1.327649 -1.339668
 H -2.401940 -2.453514 0.954035
 H -5.982115 -0.294639 -0.034093
 H -2.578924 2.076871 -2.258741
 H -1.298754 0.862392 -2.469261
 H -1.261057 1.937440 -1.076469
 H -0.258577 -1.871271 1.248467
 H -0.424952 -2.803921 -0.256404
 H 5.250724 -1.553240 -0.776531
 H 1.585628 -3.783988 -0.594082
 H 4.022168 -3.716781 -1.003109
 H 4.012243 0.489647 -0.119624
 H -1.029891 1.593592 2.296692
 H 1.423890 5.009383 -0.287455
 H 1.632227 3.942550 -1.712924
 H 2.971536 4.139850 -0.541351

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1013.45215083**

Comp_20E_c01

B3LYP/6-31G* Geometry

C 1.821823 1.154063 0.128537
 C 0.596843 1.351334 -0.829478
 N 0.540607 0.206171 -1.762721
 C 0.509430 -1.170562 -1.237462
 C 1.727557 -1.354337 -0.296349
 C 3.072084 -1.305376 -1.101640
 C 3.942575 -0.105510 -0.705480
 C 3.132943 1.196039 -0.758215
 C 1.744508 -0.241827 0.730779
 C -0.842113 -1.665375 -0.689759
 C -1.947992 -1.633156 -1.554351
 C -3.197374 -2.102581 -1.156887
 C -3.368616 -2.631883 0.124315
 C -2.277946 -2.685048 0.989579
 C -1.025465 -2.209696 0.587859
 C -0.746820 1.753184 -0.207660
 C -1.507644 2.711401 -0.895409
 C -2.767268 3.107157 -0.443903
 C -3.290997 2.554565 0.724518
 C -2.542029 1.610849 1.429398

C -1.285854 1.213917 0.970096
 C 1.890346 2.267417 1.183378
 N 1.789721 -0.362817 2.004810
 O 1.779791 -1.721997 2.421544
 H 0.875366 2.203763 -1.464117
 H -0.209927 0.349589 -2.432681
 H 0.711089 -1.803718 -2.114169
 H 1.645343 -2.317010 0.205912
 H 3.624864 -2.238305 -0.943424
 H 2.842730 -1.238840 -2.170994
 H 4.810269 -0.033337 -1.373154
 H 4.339524 -0.254648 0.307714
 H 2.854780 1.390274 -1.799245
 H 3.756537 2.033864 -0.425353
 H -1.831593 -1.239230 -2.562982
 H -4.034937 -2.062442 -1.848682
 H -4.340288 -3.003205 0.439241
 H -2.395238 -3.099762 1.987929
 H -0.199592 -2.264617 1.289920
 H -1.103467 3.159239 -1.802109
 H -3.332310 3.850994 -1.000111
 H -4.270008 2.858930 1.085386
 H -2.937110 1.176377 2.344099
 H -0.725175 0.482232 1.538443
 H 1.920840 3.243898 0.684943
 H 1.036840 2.256809 1.863305
 H 2.797968 2.161598 1.785397
 H 1.784914 -1.627394 3.386563

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -999.196731800**

Comp_20E_c02

B3LYP/6-31G* Geometry

C -1.177882 1.466474 -0.359348
 C -1.159466 -0.020487 -0.928786
 N 0.091745 -0.671761 -0.508533
 C 1.313947 0.127565 -0.639282
 C 1.225215 1.326724 0.379067
 C 1.660030 2.678694 -0.254110
 C 0.450344 3.425419 -0.863103
 C -0.590648 2.455648 -1.444517
 C -0.212441 1.472452 0.812205
 C 2.529341 -0.745253 -0.379111
 C 3.612121 -0.743530 -1.265486
 C 4.741000 -1.528603 -1.018632
 C 4.795961 -2.334139 0.118545
 C 3.716952 -2.348886 1.006688
 C 2.593957 -1.560577 0.761129
 C -2.326256 -0.896150 -0.496732
 C -3.380504 -1.146600 -1.383391
 C -4.463392 -1.943156 -1.006107
 C -4.503451 -2.505383 0.270000
 C -3.453660 -2.267690 1.160847
 C -2.372299 -1.473088 0.780842

C -2.587687 1.934287 0.025633
 N -0.655254 1.643616 1.999030
 O 0.385650 1.636914 2.963565
 H -1.222594 0.075966 -2.028074
 H 0.194704 -1.563783 -0.986646
 H 1.428220 0.541194 -1.656432
 H 1.847693 1.099005 1.244094
 H 2.132289 3.306358 0.508934
 H 2.422989 2.487226 -1.019638
 H 0.784039 4.127847 -1.636421
 H -0.029556 4.029790 -0.082422
 H -0.138204 1.895196 -2.270447
 H -1.419859 3.020795 -1.885930
 H 3.570955 -0.123957 -2.158894
 H 5.572944 -1.513127 -1.718017
 H 5.671584 -2.948242 0.311929
 H 3.751519 -2.976055 1.893917
 H 1.753871 -1.573395 1.449353
 H -3.350755 -0.717137 -2.382985
 H -5.269823 -2.128780 -1.711016
 H -5.342742 -3.128913 0.567067
 H -3.476025 -2.705760 2.155626
 H -1.551363 -1.294741 1.466873
 H -3.264593 1.843403 -0.831241
 H -3.000213 1.357757 0.854794
 H -2.559961 2.986196 0.330143
 H -0.112846 1.762537 3.785336

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-
 31+G**) = -999.201211014

Comp_20E_c03

B3LYP/6-31G* Geometry

C 1.796644 1.177044 0.156654
 C 0.564051 1.357209 -0.816187
 N 0.431524 0.246337 -1.787239
 C 0.531026 -1.128561 -1.263283
 C 1.759585 -1.320039 -0.318319
 C 3.104576 -1.229962 -1.118418
 C 3.950113 -0.019661 -0.700156
 C 3.116397 1.267924 -0.714710
 C 1.751577 -0.231014 0.731171
 C -0.813534 -1.626584 -0.718022
 C -1.951400 -1.437114 -1.518031
 C -3.193922 -1.928967 -1.128734
 C -3.327596 -2.623913 0.076596
 C -2.206615 -2.815066 0.880701
 C -0.957230 -2.323631 0.487357
 C -0.790211 1.702768 -0.187923
 C -1.619484 2.578690 -0.904252
 C -2.882425 2.934557 -0.434094
 C -3.344026 2.419987 0.778358
 C -2.530190 1.551697 1.505135
 C -1.266743 1.196023 1.028199
 C 1.841877 2.276503 1.228223

N 1.786189 -0.379178 2.003253
 O 1.805501 -1.746532 2.388638
 H 0.818167 2.227876 -1.432970
 H 1.133904 0.365361 -2.512522
 H 0.736205 -1.747651 -2.148291
 H 1.702066 -2.296014 0.160968
 H 3.676649 -2.153103 -0.975214
 H 2.889621 -1.164044 -2.194203
 H 4.817840 0.085677 -1.363252
 H 4.346494 -0.184427 0.310190
 H 2.862039 1.513945 -1.754602
 H 3.723521 2.102989 -0.348071
 H -1.850179 -0.877564 -2.442938
 H -4.061000 -1.767621 -1.764439
 H -4.296842 -3.008258 0.384001
 H -2.296932 -3.347792 1.824335
 H -0.109396 -2.472826 1.147560
 H -1.269603 2.982573 -1.852077
 H -3.502267 3.615645 -1.011895
 H -4.326879 2.694311 1.152793
 H -2.877863 1.141643 2.449803
 H -0.658227 0.515643 1.611278
 H 1.854186 3.260878 0.744103
 H 0.988483 2.241728 1.906180
 H 2.750575 2.180612 1.831087
 H 1.786638 -1.674772 3.355391

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-
 31+G**) = -999.196076985

Comp_20E_c04

B3LYP/6-31G* Geometry

C -1.115217 1.354243 0.443098
 C -1.234198 0.075021 -0.516530
 N -0.012294 -0.725628 -0.375847
 C 1.178089 -0.101971 -0.972084
 C 1.205788 1.412085 -0.548797
 C 0.616965 2.365828 -1.645748
 C -0.415747 3.345543 -1.065412
 C -1.577361 2.632392 -0.336669
 C 0.371673 1.532378 0.704925
 C 2.430288 -0.857886 -0.557318
 C 3.449119 -1.086254 -1.489900
 C 4.620552 -1.751485 -1.123410
 C 4.784941 -2.202722 0.186582
 C 3.772079 -1.983139 1.123285
 C 2.603867 -1.316003 0.755753
 C -2.458976 -0.792434 -0.278603
 C -3.630586 -0.565891 -1.013595
 C -4.767785 -1.349787 -0.813681
 C -4.746750 -2.387377 0.119326
 C -3.581415 -2.632243 0.848302
 C -2.449143 -1.840789 0.653425
 C -1.918165 1.207852 1.740988
 N 0.775710 1.799250 1.887770

O 2.178712 1.994534 1.947554
H -1.333203 0.459741 -1.545457
H -0.149054 -1.651296 -0.776083
H 1.131929 -0.121727 -2.076295
H 2.234805 1.695706 -0.332259
H 1.434996 2.925953 -2.113078
H 0.155593 1.778640 -2.449132
H -0.808714 3.992802 -1.859056
H 0.095797 4.006187 -0.353617
H -2.365250 2.353549 -1.048245
H -2.036188 3.334568 0.368549
H 3.322731 -0.743429 -2.515245
H 5.399100 -1.922804 -1.862520
H 5.693225 -2.725551 0.475032
H 3.892546 -2.333812 2.145355
H 1.813038 -1.149023 1.479080
H -3.649708 0.226828 -1.758300
H -5.665215 -1.156582 -1.395748
H -5.628215 -3.004520 0.271696
H -3.552482 -3.442518 1.572362
H -1.544327 -2.034983 1.221262
H -2.990895 1.161151 1.529002
H -1.636158 0.304880 2.289262
H -1.725949 2.063483 2.393593
H 2.309877 2.166982 2.892334

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.199177459

Comp_20Z_c01

B3LYP/6-31G* Geometry

C 1.945092 0.881906 -0.091030
C 0.719710 1.013392 -1.064299
N 0.524477 -0.264733 -1.778768
C 0.353056 -1.508404 -1.007041
C 1.559723 -1.633586 -0.045541
C 2.881508 -1.910437 -0.836094
C 3.888272 -0.766621 -0.670668
C 3.226702 0.581536 -0.975424
C 1.714694 -0.359499 0.774055
C -1.036734 -1.747593 -0.389265
C -2.134346 -1.810775 -1.262595
C -3.421139 -2.071954 -0.797992
C -3.639796 -2.290341 0.564114
C -2.559450 -2.245126 1.442976
C -1.270336 -1.978010 0.972437
C -0.565023 1.645338 -0.511043
C -1.309591 2.446930 -1.390288
C -2.518340 3.026962 -1.004972
C -3.005314 2.824037 0.286289
C -2.270110 2.042408 1.178463
C -1.064726 1.458857 0.785920
C 2.175810 2.219405 0.636785
N 1.677704 -0.547173 2.041774
O 1.826015 0.620309 2.826294

H 1.064131 1.708214 -1.842873
H -0.224105 -0.161408 -2.458842
H 0.473554 -2.311553 -1.749016
H 1.376647 -2.457817 0.646413
H 3.322406 -2.854189 -0.494999
H 2.647968 -2.027177 -1.900481
H 4.748565 -0.918100 -1.334539
H 4.281216 -0.764042 0.355170
H 2.938968 0.597357 -2.031698
H 3.950971 1.389238 -0.820533
H -1.980090 -1.663462 -2.330646
H -4.251011 -2.113923 -1.498906
H -4.640767 -2.498858 0.932556
H -2.714603 -2.418007 2.505210
H -0.451571 -1.935824 1.682230
H -0.931198 2.624559 -2.396075
H -3.071442 3.643672 -1.708992
H -3.943670 3.275997 0.596869
H -2.634973 1.883316 2.189967
H -0.510137 0.869537 1.506139
H 2.317839 3.001963 -0.120049
H 1.345665 2.511690 1.278029
H 3.077120 2.174777 1.252629
H 1.767141 0.254366 3.722321

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.189670686

Comp_20Z_c02

B3LYP/6-31G* Geometry

C -1.126108 1.452400 -0.340045
C -1.032036 -0.021224 -0.941057
N 0.221329 -0.648730 -0.493010
C 1.422998 0.185974 -0.560650
C 1.253270 1.363385 0.474851
C 1.686405 2.734700 -0.107119
C 0.478770 3.466862 -0.729613
C -0.501678 2.477976 -1.374680
C -0.205431 1.441962 0.880390
C 2.655264 -0.651837 -0.268085
C 3.792847 -0.551171 -1.077104
C 4.939393 -1.298024 -0.796758
C 4.958001 -2.164875 0.295822
C 3.824888 -2.278629 1.105788
C 2.683909 -1.527132 0.828195
C -2.183792 -0.948593 -0.581495
C -3.164846 -1.248274 -1.533727
C -4.226831 -2.102119 -1.227790
C -4.318178 -2.672127 0.041847
C -3.341476 -2.383589 0.998857
C -2.281161 -1.532519 0.690019
C -2.585523 1.877814 -0.101602
N -0.412678 1.475205 2.142912
O -1.772848 1.560022 2.522422
H -1.057295 0.106728 -2.038562

H 0.364128 -1.525564 -0.988633
H 1.565253 0.623127 -1.564308
H 1.840965 1.130737 1.365129
H 2.124662 3.351016 0.685313
H 2.473817 2.581668 -0.856692
H 0.812966 4.204132 -1.469522
H -0.047774 4.029817 0.052506
H 0.008620 1.944593 -2.184818
H -1.322562 3.026403 -1.850157
H 3.780292 0.115762 -1.936599
H 5.813713 -1.205704 -1.435968
H 5.847275 -2.750292 0.514268
H 3.830969 -2.954486 1.957216
H 1.801260 -1.616261 1.454721
H -3.093904 -0.812744 -2.528550
H -4.976197 -2.325413 -1.982946
H -5.140795 -3.340136 0.283789
H -3.404975 -2.826197 1.989831
H -1.519554 -1.312426 1.430245
H -3.126726 1.845550 -1.055276
H -3.103843 1.242211 0.612530
H -2.622191 2.906275 0.272649
H -1.697981 1.569937 3.488893

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.194108843

Comp_20Z_c03

B3LYP/6-31G* Geometry

C 1.911226 0.935300 -0.043907
C 0.683684 1.046420 -1.039549
N 0.432903 -0.187394 -1.814520
C 0.405405 -1.456510 -1.064055
C 1.623862 -1.587991 -0.101580
C 2.954828 -1.783038 -0.899969
C 3.923655 -0.617278 -0.675330
C 3.222824 0.724957 -0.911569
C 1.723017 -0.345963 0.769990
C -0.973387 -1.723434 -0.445950
C -2.103391 -1.526091 -1.255044
C -3.380751 -1.832778 -0.794333
C -3.559051 -2.345966 0.493225
C -2.446478 -2.542894 1.307779
C -1.163664 -2.236562 0.842653
C -0.627504 1.602641 -0.472569
C -1.434952 2.341873 -1.349897
C -2.659939 2.867148 -0.943493
C -3.104845 2.664467 0.364127
C -2.311730 1.935506 1.249136
C -1.085088 1.409628 0.836658
C 2.082763 2.258130 0.727714
N 1.669621 -0.582801 2.029286
O 1.749736 0.563558 2.854776
H 1.004907 1.780242 -1.789496
H 1.134128 -0.261137 -2.546626

H 0.537719 -2.235256 -1.828973
H 1.480965 -2.449755 0.552543
H 3.425683 -2.727742 -0.606247
H 2.738024 -1.868929 -1.974136
H 4.794967 -0.707804 -1.335920
H 4.305090 -0.653078 0.353564
H 2.978761 0.814309 -1.978965
H 3.917449 1.542643 -0.691440
H -1.965813 -1.109223 -2.247849
H -4.240082 -1.668712 -1.439798
H -4.555381 -2.585176 0.856129
H -2.569615 -2.934157 2.314747
H -0.321743 -2.378498 1.510982
H -1.097888 2.499294 -2.372341
H -3.263431 3.437378 -1.645345
H -4.058038 3.073110 0.689498
H -2.646029 1.769250 2.269942
H -0.490883 0.853603 1.551804
H 2.201241 3.068653 -0.003896
H 1.236714 2.499980 1.367673
H 2.979592 2.231609 1.351882
H 1.675207 0.166923 3.736474

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -999.189215328

Comp_21E_c01

B3LYP/6-31G* Geometry

C -0.097820 -0.952289 -0.466085
C 2.243391 -0.799554 0.388676
C 0.810438 1.201741 0.427814
N 2.140686 0.648487 0.156282
C -0.195392 0.549765 -0.551763
C 1.294361 -1.541811 -0.606231
N -1.068426 -1.762769 -0.252845
O -2.309489 -1.105901 -0.141791
C -3.312103 -2.076184 0.181801
C -4.663693 -1.414594 0.074467
C -7.202523 -0.237331 -0.156544
C -5.022554 -0.719636 -1.088786
C -5.588379 -1.506850 1.119303
C -6.854105 -0.927506 1.004298
C -6.281069 -0.131892 -1.202225
H 1.902231 -1.070157 1.407146
H 0.470743 0.950064 1.450934
H 0.063544 0.872304 -1.568932
H -1.209569 0.886062 -0.334702
H 1.652203 -1.276677 -1.612829
H -3.145813 -2.465344 1.195023
H -3.223061 -2.918687 -0.517051
H -8.184941 0.218679 -0.246869
H -4.303773 -0.633270 -1.898742
H -5.316200 -2.035130 2.030347
H -7.562567 -1.009584 1.824466
H -6.545686 0.407459 -2.108075

C 1.340402 -3.063219 -0.444744
H 2.349840 -3.437343 -0.636590
H 0.648691 -3.543964 -1.141198
H 1.043542 -3.364707 0.565524
C 3.693859 -1.228276 0.248983
C 6.375037 -2.036544 -0.018819
C 4.291942 -2.052885 1.209248
C 4.461273 -0.807075 -0.846871
C 5.790554 -1.207941 -0.979673
C 5.621681 -2.457778 1.077422
H 3.710753 -2.380115 2.068501
H 4.011051 -0.150166 -1.585258
H 6.372352 -0.871117 -1.833955
H 6.068658 -3.097388 1.834073
H 7.411249 -2.347561 -0.122263
C 0.812323 2.714353 0.293829
C 0.734912 5.510994 0.014448
C 0.025042 3.496383 1.147785
C 1.564150 3.352280 -0.702317
C 1.527336 4.740424 -0.838869
C -0.017714 4.884293 1.009054
H -0.558933 3.013086 1.928354
H 2.184203 2.750447 -1.359888
H 2.119222 5.221289 -1.613655
H -0.633780 5.475462 1.681669
H 0.706957 6.592180 -0.092650
H 2.831090 1.128141 0.731669

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1152.80980885

Comp_21E_c02

B3LYP/6-31G* Geometry

C -0.422047 -0.176898 -1.362667
C 1.357719 -1.076412 0.139731
C 0.888093 1.341341 0.130160
N 1.907522 0.287636 0.158717
C 0.108977 1.224760 -1.202125
C 0.590216 -1.296766 -1.203328
N -1.642589 -0.503193 -1.580887
O -2.485986 0.614321 -1.732250
C -3.847464 0.163690 -1.800841
C -4.416600 -0.215585 -0.452817
C -5.428091 -0.903465 2.075486
C -4.855510 0.776229 0.434019
C -4.488845 -1.555643 -0.055437
C -4.992720 -1.899720 1.200125
C -5.357539 0.437524 1.690178
H 0.617545 -1.225241 0.949822
H 0.150793 1.211823 0.945486
H 0.803263 1.446825 -2.023242
H -0.701723 1.953056 -1.233453
H 1.339003 -1.165731 -1.999537
H -3.910706 -0.673859 -2.504113
H -4.382057 1.021494 -2.221372

H -5.823399 -1.169794 3.052346
H -4.801972 1.821043 0.135413
H -4.142225 -2.330198 -0.734505
H -5.045920 -2.944821 1.494207
H -5.698404 1.217391 2.366364
C -0.016074 -2.697796 -1.313422
H 0.768021 -3.458720 -1.268193
H -0.558392 -2.807453 -2.256146
H -0.730460 -2.885084 -0.504630
C 2.485020 -2.073799 0.343704
C 4.564891 -3.932371 0.709461
C 2.363150 -3.109514 1.277644
C 3.669466 -1.976798 -0.401228
C 4.700354 -2.898670 -0.220395
C 3.392765 -4.035037 1.459270
H 1.453422 -3.191291 1.868287
H 3.781176 -1.162692 -1.111197
H 5.612647 -2.808764 -0.804684
H 3.279660 -4.831969 2.189724
H 5.369133 -4.649622 0.850754
C 1.521820 2.712314 0.285982
C 2.639094 5.281301 0.527344
C 0.882430 3.701706 1.042710
C 2.732695 3.025620 -0.347077
C 3.287689 4.299836 -0.225194
C 1.433129 4.978653 1.161450
H -0.054297 3.468148 1.544588
H 3.238845 2.258045 -0.924821
H 4.229384 4.526800 -0.718699
H 0.923513 5.733689 1.754495
H 3.072575 6.273476 0.621878
H 2.488221 0.400786 0.988020

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1152.81015933

Comp_21E_c03

B3LYP/6-31G* Geometry

C 0.608250 -0.104579 -0.208872
C -1.645043 -1.126558 -0.529269
C -1.414799 1.327231 -0.529637
N -2.195568 0.165444 -0.092686
C -0.008793 1.232754 0.112314
C -0.236734 -1.322458 0.118012
N 1.743931 -0.300697 -0.770348
O 2.420944 0.898083 -1.065001
C 3.724036 0.580263 -1.577684
C 4.693334 0.129593 -0.509282
C 6.461991 -0.698833 1.508525
C 4.980780 -1.227926 -0.328093
C 5.301198 1.067512 0.335406
C 6.179265 0.658734 1.338532
C 5.860889 -1.641784 0.673291
H -1.490973 -1.150790 -1.625767
H -1.268038 1.325517 -1.626794

H -0.125009 1.325738 1.200116
 H 0.624697 2.049022 -0.235447
 H -0.404904 -1.311900 1.205685
 H 4.055477 1.518898 -2.033385
 H 3.624132 -0.178491 -2.361851
 H 7.149321 -1.018992 2.287310
 H 4.506194 -1.962159 -0.973855
 H 5.081832 2.125039 0.204792
 H 6.646296 1.397670 1.984580
 H 6.076735 -2.699401 0.801169
 C 0.417452 -2.650045 -0.272304
 H -0.202144 -3.491574 0.049839
 H 1.402994 -2.740685 0.191778
 H 0.561971 -2.718579 -1.355843
 C -2.618774 -2.234797 -0.166947
 C -4.406275 -4.299532 0.508973
 C -2.967251 -3.215045 -1.103686
 C -3.185167 -2.298879 1.114575
 C -4.071093 -3.322733 1.449642
 C -3.851906 -4.242571 -0.770200
 H -2.542061 -3.172449 -2.103996
 H -2.936783 -1.530226 1.840318
 H -4.502640 -3.357130 2.446815
 H -4.110646 -4.993978 -1.511728
 H -5.097580 -5.096299 0.770595
 C -2.113943 2.621281 -0.153174
 C -3.340758 5.050636 0.553768
 C -2.097061 3.712339 -1.030309
 C -2.757337 2.761699 1.084302
 C -3.367645 3.966583 1.433811
 C -2.702581 4.920282 -0.680640
 H -1.606769 3.613485 -1.996638
 H -2.784481 1.914103 1.762570
 H -3.866028 4.058977 2.395532
 H -2.680937 5.756145 -1.375156
 H -3.816984 5.988695 0.826659
 H -3.151979 0.252487 -0.432387
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1152.80994890**

Comp_21Z_c03

B3LYP/6-31G* Geometry

C 0.124741 -0.899787 -0.597139
 C -1.014962 1.093878 0.352695
 C -2.185262 -1.079633 0.349467
 N -2.282362 0.371539 0.171425
 C -1.200101 -1.620370 -0.713625
 C 0.012553 0.614313 -0.733491
 N 1.113486 -1.675337 -0.334982
 O 2.353349 -1.032518 -0.178913
 C 3.326698 -2.021268 0.185274
 C 4.691250 -1.383191 0.118524
 C 7.240706 -0.216256 -0.028304
 C 5.497213 -1.289587 1.257105

C 5.175755 -0.881086 -1.097442
 C 6.439467 -0.298758 -1.170857
 C 6.768009 -0.713974 1.185732
 H -0.553936 0.870942 1.334199
 H -1.762096 -1.341335 1.338437
 H -1.639863 -1.449903 -1.705140
 H -1.049211 -2.694340 -0.579934
 H -0.492252 0.781057 -1.697112
 H 3.244641 -2.866283 -0.510368
 H 3.117288 -2.396749 1.195460
 H 8.228034 0.234397 -0.086247
 H 5.127591 -1.669961 2.206677
 H 4.552036 -0.944709 -1.985372
 H 6.802953 0.087912 -2.119411
 H 7.384164 -0.650833 2.078835
 C 1.303200 1.443001 -0.723727
 H 1.065929 2.485856 -0.954431
 H 2.010234 1.074909 -1.469222
 H 1.806462 1.408126 0.245598
 C -1.286394 2.587514 0.292516
 C -1.778351 5.354753 0.177751
 C -0.760927 3.448509 1.263168
 C -2.070424 3.131771 -0.735129
 C -2.313607 4.503927 -0.792437
 C -1.001415 4.822737 1.207270
 H -0.157797 3.038674 2.070296
 H -2.500217 2.467711 -1.479118
 H -2.924488 4.910037 -1.594715
 H -0.585253 5.474937 1.970703
 H -1.969470 6.423703 0.133122
 C -3.551735 -1.731590 0.236304
 C -6.048845 -3.001964 -0.003163
 C -3.891323 -2.803665 1.070425
 C -4.482092 -1.301124 -0.719757
 C -5.721775 -1.930359 -0.836773
 C -5.128815 -3.437975 0.951623
 H -3.180048 -3.142513 1.820974
 H -4.228151 -0.462035 -1.360496
 H -6.434472 -1.582567 -1.580388
 H -5.375880 -4.267483 1.609160
 H -7.015096 -3.491072 -0.094610
 H -2.977163 0.749374 0.813238

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1152.80254209**

Comp_21Z_c04

B3LYP/6-31G* Geometry

C 0.410754 0.098197 1.484995
 C -1.033391 -1.141601 -0.109278
 C -1.163451 1.321330 -0.024712
 N -1.887176 0.054347 -0.163499
 C -0.470123 1.320967 1.358768
 C -0.339772 -1.214873 1.297328
 N 1.654389 0.367278 1.652413

O	2.501160	-0.749877	1.739745	C	0.845833	1.138469	0.443833
C	3.862913	-0.292409	1.770784	O	2.128025	0.577160	0.187045
C	4.385841	0.100576	0.408107	C	-0.201834	0.528757	-0.518342
C	5.306381	0.811171	-2.148554	C	1.235280	-1.588601	-0.564456
C	4.362995	1.436225	-0.011022	N	-1.134787	-1.761654	-0.219257
C	4.874482	-0.874510	-0.470871	O	-2.358793	-1.074391	-0.116179
C	5.331795	-0.524639	-1.741243	C	-3.389173	-2.017940	0.203973
C	4.820937	1.791181	-1.280756	C	-4.721993	-1.323652	0.074431
H	-0.216675	-1.093868	-0.854682	C	-7.225265	-0.081572	-0.197362
H	-0.360874	1.415868	-0.780935	C	-5.059178	-0.654155	-1.110145
H	-1.248866	1.311455	2.132584	C	-5.649989	-1.357768	1.119727
H	0.131429	2.224943	1.481204	C	-6.898361	-0.745905	0.984589
H	-1.164635	-1.183763	2.025066	C	-6.300073	-0.034315	-1.244062
H	4.416533	-1.149654	2.166608	H	1.874354	-1.052908	1.436982
H	3.940658	0.540034	2.478464	H	0.546966	0.887685	1.476059
H	5.666623	1.086764	-3.136345	H	0.051447	0.850372	-1.537441
H	3.976781	2.196543	0.662497	H	-1.201724	0.897031	-0.285090
H	4.896495	-1.915439	-0.154982	H	1.595110	-1.356052	-1.578826
H	5.712258	-1.291598	-2.411029	H	-3.243536	-2.401415	1.222393
H	4.800637	2.832516	-1.591929	H	-3.311772	-2.867742	-0.487015
C	0.426356	-2.526966	1.507022	H	-8.194154	0.399232	-0.303592
H	-0.275310	-3.365754	1.472191	H	-4.337556	-0.613617	-1.921294
H	0.928272	-2.534433	2.476384	H	-5.394352	-1.866249	2.046655
H	1.190210	-2.682838	0.741168	H	-7.610042	-0.782877	1.805190
C	-1.878360	-2.365624	-0.418019	H	-6.548281	0.484324	-2.166467
C	-3.434882	-4.638935	-0.985393	C	1.264893	-3.105608	-0.361285
C	-1.442275	-3.317732	-1.346952	H	2.268247	-3.497619	-0.548948
C	-3.112112	-2.564016	0.219102	H	0.562077	-3.595887	-1.039657
C	-3.883258	-3.691736	-0.061579	H	0.970452	-3.375127	0.658842
C	-2.211734	-4.448168	-1.628926	C	3.647268	-1.242327	0.243306
H	-0.491763	-3.171479	-1.855041	C	6.322924	-2.033323	-0.082980
H	-3.468267	-1.818571	0.923849	C	4.267484	-2.064328	1.189862
H	-4.837878	-3.830383	0.439662	C	4.385413	-0.814674	-0.868562
H	-1.856907	-5.175580	-2.354459	C	5.714067	-1.205313	-1.029372
H	-4.037324	-5.516562	-1.204591	C	5.596125	-2.462177	1.027771
C	-2.102953	2.503150	-0.185027	H	3.708206	-2.393527	2.062595
C	-3.796296	4.734872	-0.429115	H	3.918339	-0.160264	-1.598548
C	-1.670341	3.660261	-0.844289	H	6.276516	-0.861320	-1.893534
C	-3.398587	2.476988	0.349099	H	6.063167	-3.100323	1.773300
C	-4.239182	3.583785	0.225835	H	7.358622	-2.337438	-0.209079
C	-2.507584	4.770352	-0.964203	C	0.926609	2.645795	0.307986
H	-0.669108	3.689632	-1.269337	C	0.977437	5.437470	0.010513
H	-3.742873	1.577371	0.850239	C	-0.050416	3.444869	0.914938
H	-5.242892	3.546928	0.641860	C	1.932768	3.258974	-0.446081
H	-2.155345	5.659265	-1.481210	C	1.957827	4.647335	-0.591015
H	-4.452044	5.596269	-0.525207	C	-0.028579	4.831300	0.765937
H	-2.407820	0.052890	-1.039000	H	-0.832149	2.979127	1.511903
Number of Imaginary Frequencies= 0				H	2.701559	2.644955	-0.902022
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1152.80261054				H	2.748731	5.112066	-1.174303
Comp_22E_c01				H	-0.792721	5.437706	1.245171
B3LYP/6-31G* Geometry				H	0.999363	6.518086	-0.103116
C	-0.145209	-0.974431	-0.432275	Number of Imaginary Frequencies= 0			
C	2.198273	-0.833347	0.405356	SCF Energy (PCM/mPW1PW91/6-31+G**) = -1172.66576831			

Comp_22E_c02
B3LYP/6-31G* Geometry

C	0.636955	-0.107564	-0.222889
C	-1.622802	-1.099437	-0.556213
C	-1.400086	1.283861	-0.545425
O	-2.168689	0.155644	-0.143264
C	0.005771	1.221529	0.099977
C	-0.215136	-1.324441	0.080889
N	1.778485	-0.295292	-0.775218
O	2.453024	0.908468	-1.049985
C	3.763517	0.602578	-1.553307
C	4.722853	0.141373	-0.480829
C	6.473175	-0.707853	1.543932
C	5.021293	-1.216458	-0.321546
C	5.310347	1.069181	0.389135
C	6.179219	0.649936	1.395860
C	5.892461	-1.640659	0.683318
H	-1.496288	-1.092465	-1.652170
H	-1.272892	1.256889	-1.641198
H	-0.119264	1.317482	1.186744
H	0.627789	2.048108	-0.245544
H	-0.381618	-1.338769	1.169216
H	4.094940	1.548819	-1.992869
H	3.674389	-0.145737	-2.348606
H	7.153547	-1.035983	2.325466
H	4.562810	-1.942976	-0.987410
H	5.082358	2.126830	0.275447
H	6.630540	1.380945	2.061740
H	6.117302	-2.698312	0.794006
C	0.419801	-2.651163	-0.343078
H	-0.207751	-3.492137	-0.035436
H	1.407467	-2.763094	0.111647
H	0.556275	-2.696592	-1.429011
C	-2.624911	-2.170618	-0.180003
C	-4.451692	-4.181309	0.535959
C	-3.001029	-3.152642	-1.102180
C	-3.179839	-2.203002	1.106488
C	-4.087964	-3.199627	1.461152
C	-3.905652	-4.155567	-0.747502
H	-2.585617	-3.131313	-2.107122
H	-2.909098	-1.433103	1.822902
H	-4.514660	-3.209370	2.460816
H	-4.187506	-4.910568	-1.476685
H	-5.159583	-4.957813	0.813440
C	-2.142237	2.550187	-0.168243
C	-3.427056	4.941499	0.550058
C	-1.833185	3.749547	-0.822209
C	-3.104986	2.559128	0.846677
C	-3.744365	3.748581	1.201023
C	-2.467984	4.938771	-0.464975
H	-1.093663	3.751801	-1.620645
H	-3.360799	1.628868	1.341677
H	-4.495382	3.740987	1.986915
H	-2.219216	5.860719	-0.984101
H	-3.926959	5.865938	0.826890

Number of Imaginary Frequencies= 0
 SCF Energy (PCM/mPW1PW91/6-31+G**) = -1172.66583553

Comp_22Z_c03
B3LYP/6-31G* Geometry

C	0.179295	-0.904538	-0.575955
C	-1.050798	1.037509	0.368590
C	-2.125801	-1.103428	0.357353
O	-2.263820	0.303792	0.196375
C	-1.132102	-1.647234	-0.694008
C	0.027702	0.606791	-0.688140
N	1.187827	-1.661282	-0.334971
O	2.413143	-0.992928	-0.181959
C	3.414636	-1.965006	0.154313
C	4.759979	-1.286738	0.103011
C	7.270867	-0.036538	-0.013644
C	5.541625	-1.152553	1.254477
C	5.249053	-0.783095	-1.110429
C	6.493872	-0.159689	-1.169159
C	6.793361	-0.535168	1.198203
H	-0.637529	0.823553	1.368543
H	-1.708929	-1.311951	1.357723
H	-1.575030	-1.492825	-1.687169
H	-0.967150	-2.718507	-0.552082
H	-0.446585	0.781888	-1.666372
H	3.354435	-2.792390	-0.564096
H	3.216466	-2.372074	1.154235
H	8.243633	0.445958	-0.059894
H	5.168167	-1.534576	2.201849
H	4.644428	-0.879066	-2.008760
H	6.861622	0.226999	-2.116021
H	7.391193	-0.440933	2.100924
C	1.288537	1.477384	-0.608054
H	1.022428	2.519648	-0.806793
H	2.030561	1.160864	-1.342512
H	1.762102	1.421678	0.375568
C	-1.410856	2.506730	0.288142
C	-2.053155	5.235901	0.118664
C	-0.962802	3.405543	1.261480
C	-2.191825	2.989521	-0.770569
C	-2.512014	4.343851	-0.853905
C	-1.277579	4.763333	1.177441
H	-0.364486	3.040464	2.093054
H	-2.561096	2.295777	-1.520017
H	-3.122811	4.704043	-1.677711
H	-0.921828	5.448255	1.942592
H	-2.303255	6.291458	0.052868
C	-3.491208	-1.751056	0.247144
C	-5.976568	-3.033296	-0.006809
C	-3.700112	-3.017745	0.806926
C	-4.541639	-1.130172	-0.437299
C	-5.777316	-1.767964	-0.560733
C	-4.932683	-3.657605	0.679125
H	-2.893801	-3.504992	1.351750

H -4.389896 -0.140722 -0.854427
H -6.587367 -1.271883 -1.089345
H -5.079830 -4.639391 1.121647
H -6.939644 -3.527627 -0.103078
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1172.65843025**

Comp_22Z_c05
B3LYP/6-31G* Geometry
C -0.478262 0.025197 -1.399165
C 1.128381 -1.076086 0.151635
C 1.093070 1.316026 0.047096
O 1.881402 0.136968 0.167908
C 0.340483 1.292341 -1.301961
C 0.343950 -1.241536 -1.197938
N -1.733224 0.226275 -1.577736
O -2.520441 -0.932333 -1.655332
C -3.902588 -0.544117 -1.736056
C -4.479223 -0.121915 -0.404631
C -5.503455 0.648516 2.094371
C -4.555985 1.230999 -0.053176
C -4.920754 -1.084078 0.512805
C -5.429212 -0.704345 1.754770
C -5.065705 1.615732 1.187877
H 0.384855 -1.051128 0.965638
H 0.342130 1.331594 0.855326
H 1.089413 1.329135 -2.104718
H -0.311154 2.164844 -1.397222
H 1.116664 -1.216343 -1.982077
H -4.401863 -1.443904 -2.108896
H -4.002880 0.253264 -2.480235
H -5.903717 0.946953 3.059823
H -4.207360 1.982441 -0.756574
H -4.865421 -2.138269 0.249507
H -5.772063 -1.461683 2.455041
H -5.122515 2.669971 1.446511
C -0.370609 -2.597134 -1.277424
H -1.098491 -2.721212 -0.471058
H 0.367078 -3.401745 -1.204588
H -0.907909 -2.701002 -2.221291
C 2.108334 -2.201738 0.411800
C 3.917933 -4.300481 0.871887
C 1.847349 -3.165104 1.391509
C 3.291985 -2.297162 -0.332411
C 4.190802 -3.337864 -0.103414
C 2.743583 -4.211467 1.619463
H 0.937284 -3.094726 1.982956
H 3.513603 -1.542138 -1.080900
H 5.107392 -3.396824 -0.684652
H 2.525897 -4.951237 2.385327
H 4.619127 -5.111425 1.050143
C 1.991352 2.528292 0.184198
C 3.596299 4.825448 0.366602
C 1.440798 3.752525 0.583360

C 3.355881 2.464712 -0.118713
C 4.152835 3.606985 -0.025210
C 2.235428 4.895322 0.671435
H 0.383020 3.810630 0.832671
H 3.790159 1.514142 -0.408535
H 5.213046 3.542694 -0.256595
H 1.793660 5.837348 0.985795
H 4.218911 5.713216 0.439905
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1172.65852746**

Comp_23E_c01
B3LYP/6-31G* Geometry
C -3.435447 1.782449 -0.000614
N -3.176935 -0.996744 0.000621
C -4.569620 0.966916 0.000220
C -2.178791 1.191874 -0.000802
C -2.084431 -0.211945 -0.000132
C -4.379573 -0.413626 0.000796
C -0.771411 -0.907286 -0.000204
N 0.286213 -0.158834 -0.000139
N 1.500431 -0.754342 -0.000195
C 2.673308 -0.020863 0.000031
N 2.506649 1.311926 0.000292
S 4.147430 -0.824643 -0.000049
C 3.603921 2.262318 0.000481
C -0.728747 -2.414076 -0.000315
H -3.531491 2.864949 -0.001137
H -5.570832 1.386562 0.000398
H -1.276435 1.791065 -0.001487
H -5.233886 -1.088698 0.001414
H 1.613440 -1.763153 -0.000215
H 1.549014 1.641259 0.000352
H 4.234020 2.132014 0.886183
H 3.180083 3.269525 0.000587
H 4.234132 2.132243 -0.885176
H -1.741967 -2.813079 -0.000595
H -0.202636 -2.793579 0.886419
H -0.202086 -2.793426 -0.886779
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -967.282828343**

Comp_23E_c02
B3LYP/6-31G* Geometry
C 3.416761 1.565613 -0.350492
N 2.968880 -1.145239 0.142110
C 4.492398 0.688403 -0.192792
C 2.122492 1.071098 -0.257790
C 1.933307 -0.299902 -0.005317
C 4.208726 -0.654233 0.049938
C 0.573344 -0.890048 0.109141
N -0.422666 -0.064972 0.039743
N -1.674748 -0.586612 0.130413

C -2.832918 0.135609 -0.048964
N -2.807399 1.483027 0.040784
S -4.261227 -0.710311 -0.354622
C -1.787345 2.379197 0.579470
C 0.427934 -2.379770 0.295129
H 3.586933 2.621012 -0.546183
H 5.519988 1.032416 -0.258644
H 1.261501 1.716827 -0.379937
H 5.015018 -1.374957 0.176574
H -1.817918 -1.590990 0.069767
H -3.720798 1.881133 -0.126257
H -1.300754 1.945104 1.455114
H -2.291443 3.302321 0.878493
H -1.018794 2.618362 -0.160819
H 1.412217 -2.838079 0.379917
H -0.094264 -2.838410 -0.556376
H -0.148708 -2.608988 1.201012

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -967.272372761**

Comp_23E_c03

B3LYP/6-31G* Geometry

C -4.454276 -0.217999 0.328998
N -2.051806 1.065452 -0.300566
C -4.435483 1.147192 0.060082
C -3.259342 -0.933307 0.274850
C -2.069205 -0.259423 -0.047130
C -3.202800 1.732940 -0.245116
C -0.766893 -0.976562 -0.100207
N 0.291029 -0.238289 -0.021750
N 1.513427 -0.802268 -0.037084
C 2.652000 -0.011311 0.023732
N 2.409873 1.307358 0.049783
S 4.161782 -0.745033 0.052684
C 3.450790 2.316304 0.111108
C -0.712283 -2.482066 -0.228461
H -5.382226 -0.723670 0.582116
H -5.340987 1.745562 0.085341
H -3.256562 -1.993696 0.502339
H -3.142893 2.799164 -0.461080
H 1.674123 -1.805042 -0.042771
H 1.431537 1.578619 0.022564
H 4.056046 2.200079 1.016128
H 2.971099 3.297881 0.117777
H 4.118534 2.242722 -0.753499
H -1.665600 -2.898683 -0.555850
H -0.439634 -2.965507 0.719945
H 0.035346 -2.777280 -0.975775

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -967.277437946**

Comp_23Z_c01

B3LYP/6-31G* Geometry

C -4.253084 -0.202427 0.000027
N -1.569245 -0.941342 0.000023
C -3.893903 -1.549936 -0.000064
C -3.255978 0.766997 0.000106
C -1.903945 0.369993 0.000096
C -2.535085 -1.862013 -0.000038
C -0.817041 1.375219 0.000045
N 0.463080 1.141782 -0.000029
N 0.969393 -0.102993 -0.000058
C 2.338785 -0.300140 -0.000078
N 3.074746 0.824595 -0.000192
S 2.952027 -1.863908 0.000032
C 4.524956 0.842207 0.000119
H -5.298993 0.092129 0.000035
H -4.640178 -2.337904 -0.000175
H -3.521805 1.817170 0.000210
H -2.201208 -2.897498 -0.000051
H 0.338611 -0.908430 0.000039
H 2.552229 1.693024 0.000022
H 4.923252 0.336058 0.885667
H 4.851759 1.885171 -0.000517
H 4.923518 0.334883 -0.884617
C -1.187434 2.841152 -0.000067
H -1.777366 3.114602 0.884318
H -1.777837 3.114391 -0.884186
H -0.273849 3.438337 -0.000353

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -967.284099143**

Comp_23Z_c02

B3LYP/6-31G* Geometry

C -2.895873 -1.700270 0.772840
N -2.930355 0.674905 -0.704185
C -3.974984 -1.396887 -0.053604
C -1.826493 -0.808278 0.839894
C -1.873222 0.367782 0.073151
C -3.941110 -0.194613 -0.764446
C -0.789645 1.397308 0.116638
N 0.481302 1.166819 0.112727
N 0.967630 -0.100320 0.009702
C 2.330842 -0.325032 -0.068644
N 3.094224 0.762412 0.125452
S 2.895076 -1.881397 -0.357945
C 4.544980 0.747757 0.090358
H -2.883711 -2.613281 1.361488
H -4.826961 -2.064002 -0.141108
H -0.983485 -1.007618 1.493849
H -4.771408 0.086369 -1.410368
H 0.381472 -0.885048 -0.260404
H 2.595382 1.636981 0.243491
H 4.943149 0.052202 0.835428
H 4.899691 1.757837 0.309800
H 4.914474 0.437407 -0.892979
C -1.219135 2.840348 0.147321

H -1.847646 3.044804 1.023265
H -1.822412 3.071359 -0.736567
H -0.341544 3.489947 0.174328
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -967.275968185**

Comp_23Z_c03
B3LYP/6-31G* Geometry
C 4.128175 -0.121494 0.029309
N 1.471285 -0.945864 0.060743
C 3.813034 -1.477741 0.107125
C 3.100356 0.813502 -0.033877
C 1.761926 0.373261 -0.016333
C 2.465199 -1.833896 0.118676
C 0.641049 1.340804 -0.085968
N -0.633133 1.078387 -0.069235
N -1.089231 -0.186876 0.025655
C -2.419745 -0.518911 -0.029489
N -3.376166 0.437766 -0.001867
S -2.827527 -2.156530 -0.133239
C -3.312066 1.862951 0.316631
H 5.164027 0.206501 0.017266
H 4.584611 -2.239310 0.157351
H 3.332251 1.869744 -0.095914
H 2.163672 -2.877524 0.177281
H -0.409882 -0.954122 0.037039
H -4.298031 0.028040 -0.056200
H -2.738361 2.047556 1.228375
H -4.340639 2.199334 0.474081
H -2.865640 2.444676 -0.492872
C 0.970712 2.813101 -0.196808
H 1.563025 3.033073 -1.094282
H 1.543256 3.171218 0.668696
H 0.041029 3.381945 -0.251672

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -967.273110127**

Comp_24E_c01
B3LYP/6-31G* Geometry
C 0.413700 -0.799823 0.000520
C 1.802824 -0.332870 0.000197
C 4.453643 0.354073 -0.000485
C 2.149916 1.028294 0.000286
N 2.720728 -1.319240 -0.000184
C 4.009875 -0.969373 -0.000522
C 3.496509 1.371136 -0.000065
N -0.585046 0.012114 0.000622
N -1.827278 -0.523837 0.001179
C -2.960753 0.256229 0.000096
S -4.474194 -0.464317 -0.000642
N -2.737860 1.583710 -0.000037
H 0.286854 -1.887462 0.000754
H 5.515988 0.577747 -0.000764

H 1.371384 1.783196 0.000637
H 4.724904 -1.790341 -0.000824
H 3.797558 2.415230 -0.000001
H -1.972043 -1.531498 0.000378
H -1.793234 1.944031 -0.000162
H -3.532392 2.202949 -0.000969

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -888.669103714**

Comp_24E_c02
B3LYP/6-31G* Geometry
C -0.411196 -0.836899 0.000254
C -1.798037 -0.358141 0.000025
C -4.394990 0.521837 -0.000669
C -2.839520 -1.300352 0.000942
N -2.023285 0.970942 -0.001268
C -3.290578 1.381645 -0.001565
C -4.157366 -0.850623 0.000591
N 0.589475 -0.029376 0.000366
N 1.831745 -0.551792 0.000951
C 2.946635 0.259474 0.000834
S 4.477871 -0.423381 -0.001923
N 2.680716 1.576986 0.004457
H -0.263899 -1.924142 0.000929
H -5.403886 0.922686 -0.000986
H -2.614190 -2.363365 0.001903
H -3.439292 2.460689 -0.002606
H -4.980920 -1.559353 0.001297
H 2.001283 -1.556049 0.000177
H 1.721170 1.901670 -0.000926
H 3.453546 2.223004 -0.003024

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -888.666573237**

Comp_25Z_c01
B3LYP/6-31G* Geometry
C 0.551855 -1.631058 0.000108
C 1.618986 -0.627036 0.000062
C 3.625190 1.255123 -0.000039
C 2.960747 -1.050755 0.000046
N 1.288489 0.684413 0.000020
C 2.270789 1.589295 -0.000026
C 3.971788 -0.097301 -0.000005
N -0.734787 -1.479693 -0.000003
N -1.276853 -0.247496 -0.000267
C -2.645908 -0.090474 -0.000077
S -3.319685 1.444962 0.000105
N -3.351906 -1.236397 -0.000228
H 0.873128 -2.670581 0.000269
H 4.381549 2.033401 -0.000082
H 3.192812 -2.111734 0.000075
H 1.955462 2.630450 -0.000035
H 5.014617 -0.402161 -0.000020

H -0.669874 0.576758 -0.000047
H -2.870486 -2.126221 0.000501
H -4.357530 -1.181851 0.000591
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -888.672249921**

Comp_25Z_c02
B3LYP/6-31G* Geometry
C 0.521881 -1.578696 0.162160
C 1.616050 -0.585880 0.098621
C 3.809746 1.057681 -0.094041
C 1.538562 0.721672 0.609416
N 2.748399 -1.075565 -0.450011
C 3.802370 -0.265473 -0.546342
C 2.655165 1.550480 0.508125
N -0.759043 -1.433276 0.159661
N -1.320770 -0.202033 0.045841
C -2.693845 -0.065532 -0.015743
S -3.370105 1.432963 -0.343938
N -3.385934 -1.190290 0.234793
H 0.858206 -2.612620 0.178571
H 4.700091 1.669936 -0.198300
H 0.646892 1.073011 1.117940
H 4.693210 -0.696274 -1.000575
H 2.620245 2.562442 0.901593
H -0.790877 0.607733 -0.263333
H -2.893840 -2.068763 0.339755
H -4.390389 -1.160245 0.162193
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -888.660738776**

Comp_26E_c01
B3LYP/6-31G* Geometry
C 4.518319 -1.720860 0.001483
C 4.021893 -0.299125 -0.035589
C 3.107756 2.329147 0.007276
C 4.941898 0.752860 -0.024883
C 2.652054 -0.045969 -0.026727
C 2.175424 1.275505 -0.005103
C 4.473986 2.066913 -0.003429
F 3.631724 -2.581750 -0.544234
F 4.741470 -2.136546 1.270134
F 5.685090 -1.860068 -0.666652
C 0.746540 1.550416 -0.000803
O -0.099868 0.476204 -0.005554
C -1.384772 0.952947 0.000039
C -1.362490 2.328548 0.008543
C 0.002656 2.709972 0.007878
C -2.419671 -0.044799 -0.003794
N -3.668828 0.282454 0.000872
N -4.576921 -0.720627 -0.003016
C -5.930314 -0.475086 0.001108
N -6.269748 0.827474 0.009593

S -7.015504 -1.753315 -0.004242
H 2.760055 3.357761 0.023086
H 6.006411 0.545092 -0.040728
H 1.949496 -0.870265 -0.043593
H 5.180101 2.892050 0.001754
H -2.228016 2.974868 0.014190
H 0.389389 3.719217 0.012541
H -2.088386 -1.088868 -0.010715
H -4.296068 -1.699180 -0.009293
H -7.247754 1.068363 0.012193
H -5.553957 1.541737 0.011499
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41769924**

Comp_26E_c02
B3LYP/6-31G* Geometry
C 5.606777 -0.521946 0.002816
C 4.346054 0.301018 -0.033208
C 2.014681 1.824237 0.009289
C 4.431096 1.697016 -0.016997
C 3.107212 -0.333582 -0.029478
C 1.921725 0.420872 -0.007785
C 3.258381 2.450331 0.003838
F 5.432665 -1.739937 -0.557074
F 6.029967 -0.730145 1.271504
F 6.619545 0.086161 -0.653180
C 0.628149 -0.245423 -0.007706
O -0.486535 0.547199 -0.005489
C -1.585038 -0.272826 -0.004236
C -1.175773 -1.586395 -0.005589
C 0.241385 -1.567647 -0.007461
C -2.859501 0.391925 -0.002885
N -3.965573 -0.274499 -0.000074
N -5.120037 0.431336 0.000297
C -6.349068 -0.186306 0.003685
N -6.307373 -1.531594 0.005745
S -7.750703 0.734429 0.004190
H 1.106652 2.416990 0.024111
H 5.401180 2.182126 -0.029234
H 3.065092 -1.416934 -0.052148
H 3.313652 3.534969 0.012481
H -1.823773 -2.450689 -0.005001
H 0.896984 -2.426839 -0.007535
H -2.836888 1.487139 -0.004581
H -5.127435 1.449327 -0.002317
H -7.177821 -2.038370 0.012799
H -5.419318 -2.015236 0.009573
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41761838**

Comp_26E_c03
B3LYP/6-31G* Geometry
C 3.289829 -2.193745 0.016055

C 3.300259 -0.688581 -0.038570
 C 3.328764 2.094680 -0.026661
 C 4.521822 -0.009182 -0.053330
 C 2.097226 0.012679 -0.019744
 C 2.095856 1.417729 -0.013534
 C 4.525907 1.385748 -0.047052
 F 2.133810 -2.711415 -0.454774
 F 3.437179 -2.645656 1.283322
 F 4.298920 -2.726895 -0.708220
 C 0.841929 2.155879 0.002071
 O -0.313280 1.421462 0.001324
 C -1.363189 2.295193 0.018687
 C -0.886555 3.586751 0.031045
 C 0.529336 3.496105 0.020219
 C -2.705772 1.786550 0.020225
 N -2.965336 0.521811 0.003184
 N -4.264949 0.149600 0.006275
 C -4.637034 -1.175412 -0.013507
 N -3.614540 -2.049084 -0.034979
 S -6.262907 -1.587571 -0.009582
 H 3.349212 3.180413 -0.024185
 H 5.453463 -0.564571 -0.076740
 H 1.156642 -0.524136 -0.015972
 H 5.469327 1.923503 -0.061827
 H -1.485468 4.486989 0.045869
 H 1.229093 4.319494 0.026032
 H -3.499242 2.542034 0.036305
 H -5.022428 0.829559 0.021736
 H -3.824667 -3.034104 -0.051165
 H -2.658848 -1.716690 -0.037069

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41891882**

Comp_26E_c04

B3LYP/6-31G* Geometry

C -5.369512 -0.174710 0.022070
 C -3.918784 -0.574709 -0.034048
 C -1.239172 -1.334275 -0.032669
 C -3.583594 -1.933292 -0.044180
 C -2.926013 0.399824 -0.024694
 C -1.569143 0.032462 -0.024624
 C -2.240071 -2.302939 -0.042996
 F -5.563892 1.098805 -0.386097
 F -5.861594 -0.266711 1.279464
 F -6.135615 -0.972331 -0.755088
 C -0.532577 1.053632 -0.020081
 O 0.767260 0.624310 -0.014220
 C 1.570794 1.729518 -0.010344
 C 0.791774 2.864702 -0.013918
 C -0.558400 2.429792 -0.019981
 C 2.997086 1.568147 -0.003153
 N 3.562619 0.407347 0.000437
 N 4.914826 0.370309 0.007475
 C 5.603504 -0.820750 0.012477

N 4.828295 -1.920636 0.009340
 S 7.280602 -0.820800 0.021440
 H -0.195255 -1.628020 -0.033617
 H -4.365332 -2.685508 -0.059489
 H -3.209522 1.446256 -0.023563
 H -1.969502 -3.354738 -0.053654
 H 1.151588 3.884469 -0.012263
 H -1.439083 3.055908 -0.024337
 H 3.578412 2.496937 -0.000598
 H 5.479385 1.217461 0.009509
 H 5.275567 -2.823057 0.014621
 H 3.820415 -1.832798 0.005688

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41885740**

Comp_26Z_c01

B3LYP/6-31G* Geometry

C -4.839510 -0.256331 0.021192
 C -3.362238 -0.541996 -0.039763
 C -0.628794 -1.086189 -0.038996
 C -2.918822 -1.868868 -0.053465
 C -2.449997 0.508297 -0.027547
 C -1.067995 0.250077 -0.027693
 C -1.550268 -2.130737 -0.052605
 F -5.138996 0.976914 -0.444181
 F -5.306581 -0.323056 1.289656
 F -5.549978 -1.148088 -0.704051
 C -0.125319 1.359456 -0.020362
 O 1.210738 1.052412 -0.011359
 C 1.922509 2.230459 -0.005084
 C 1.036875 3.284634 -0.010359
 C -0.267115 2.728471 -0.019931
 C 3.361763 2.206808 0.005884
 N 4.193699 1.212710 0.012394
 N 3.723350 -0.057315 0.008869
 C 4.579226 -1.132284 0.015657
 N 5.887692 -0.823382 0.025863
 S 3.957097 -2.693033 0.010764
 H 0.432247 -1.313015 -0.040178
 H -3.638019 -2.680865 -0.072113
 H -2.815658 1.529041 -0.024268
 H -1.193938 -3.156247 -0.066047
 H 1.299938 4.333378 -0.007627
 H -1.199825 3.273831 -0.026555
 H 3.831817 3.187227 0.009565
 H 2.730044 -0.263749 0.002435
 H 6.560405 -1.572944 0.030941
 H 6.178437 0.145797 0.028207

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41850129**

Comp_26Z_c02

B3LYP/6-31G* Geometry

C -2.937355 -1.752026 0.008051
 C -2.781493 -0.252421 -0.035663
 C -2.510490 2.516699 -0.003686
 C -3.921674 0.555068 -0.032317
 C -1.508083 0.313651 -0.025291
 C -1.356554 1.710998 -0.008876
 C -3.776856 1.942235 -0.016303
 F -1.875945 -2.388971 -0.519672
 F -4.037647 -2.152776 -0.671153
 F -3.081325 -2.193525 1.279073
 C -0.038750 2.329955 -0.001709
 O 1.054353 1.501749 0.000106
 C 2.186057 2.285175 0.008008
 C 1.810439 3.609642 0.011431
 C 0.393328 3.636689 0.005134
 C 3.492121 1.679796 0.010917
 N 3.851753 0.434575 0.007365
 N 2.912422 -0.538910 0.000008
 C 3.266059 -1.868527 -0.005696
 N 4.589673 -2.107589 -0.002941
 S 2.070310 -3.045617 -0.015572
 H -2.414447 3.598194 0.007977
 H -4.906919 0.101781 -0.049752
 H -0.639241 -0.334564 -0.036200
 H -4.656823 2.578692 -0.016681
 H 2.480727 4.458026 0.017505
 H -0.233514 4.516686 0.005104
 H 4.317997 2.386999 0.017057
 H 1.919052 -0.331680 -0.002363
 H 4.906782 -3.063531 -0.006583
 H 5.243418 -1.335424 0.002991

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41741271**

Comp_26Z_c03
B3LYP/6-31G* Geometry
 C 4.798108 -1.241106 0.177613
 C 4.001611 0.032085 0.059136
 C 2.527377 2.391039 -0.046840
 C 4.660322 1.263486 0.118951
 C 2.614802 -0.026629 -0.055739
 C 1.858441 1.155746 -0.110991
 C 3.913505 2.440309 0.065461
 F 4.153444 -2.296019 -0.366198
 F 5.045332 -1.552315 1.471143
 F 5.998435 -1.136979 -0.435135
 C 0.408465 1.103690 -0.238027
 O -0.173627 -0.130335 -0.263839
 C -1.532625 0.036918 -0.379980
 C -1.810577 1.388351 -0.434697
 C -0.568137 2.066960 -0.343762
 C -2.279361 -1.195820 -0.467875
 N -3.551185 -1.399917 -0.344127
 N -4.360660 -0.355732 -0.032668

C -5.718908 -0.544889 0.128227
 N -6.167674 -1.756469 -0.242898
 S -6.673044 0.705352 0.708775
 H 1.960145 3.316152 -0.085992
 H 5.741676 1.298541 0.199203
 H 2.116798 -0.986948 -0.109645
 H 4.415940 3.402031 0.109435
 H -2.776838 1.850526 -0.579000
 H -0.419616 3.137030 -0.362798
 H -1.689678 -2.087645 -0.665218
 H -3.993217 0.501142 0.371180
 H -7.145490 -1.964493 -0.118190
 H -5.508425 -2.477470 -0.507956

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41435545**

Comp_26Z_c04
B3LYP/6-31G* Geometry
 C -4.797123 -1.239799 0.166192
 C -4.001630 0.039093 0.128997
 C -2.528914 2.394146 -0.056666
 C -4.659654 1.270980 0.164274
 C -2.615201 -0.022501 0.002835
 C -1.859932 1.157172 -0.093558
 C -3.913049 2.446290 0.071629
 F -4.106947 -2.245024 0.748214
 F -5.123379 -1.657082 -1.079224
 F -5.954628 -1.092144 0.847163
 C -0.410588 1.101934 -0.226524
 O 0.170639 -0.132719 -0.232382
 C 1.528830 0.031283 -0.361194
 C 1.807131 1.381196 -0.444645
 C 0.565729 2.062302 -0.358057
 C 2.274029 -1.203608 -0.429697
 N 3.546708 -1.406381 -0.313090
 N 4.359814 -0.356435 -0.030966
 C 5.719201 -0.543835 0.121891
 N 6.163768 -1.762969 -0.229025
 S 6.679561 0.716761 0.668981
 H -1.962157 3.317834 -0.125190
 H -5.738392 1.308486 0.270466
 H -2.115857 -0.983769 -0.014767
 H -4.414638 3.408950 0.103208
 H 2.772585 1.839823 -0.604778
 H 0.417612 3.131908 -0.396554
 H 1.681915 -2.098790 -0.603167
 H 3.996589 0.508438 0.359367
 H 7.142297 -1.969602 -0.107499
 H 5.501550 -2.488874 -0.472394

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1438.41432035**

Comp_26Z_c05

B3LYP/6-31G* Geometry

C 5.258674 -0.950468 -0.000801
C 4.151846 0.063834 -0.122374
C 2.125813 1.971087 -0.250832
C 4.474227 1.402568 -0.370306
C 2.827809 -0.323702 0.059027
C 1.795196 0.627474 -0.003133
C 3.453924 2.349597 -0.432489
F 4.817309 -2.212009 -0.198249
F 5.829423 -0.918055 1.225671
F 6.244543 -0.719125 -0.895833
C 0.409601 0.218694 0.182086
O -0.545694 1.190124 0.100677
C -1.773431 0.602988 0.293517
C -1.590764 -0.749193 0.505397
C -0.194952 -0.991218 0.433738
C -2.883954 1.525565 0.281482
N -4.152815 1.288192 0.190200
N -4.575190 0.008822 0.025027
C -5.920658 -0.275999 -0.097609
N -6.741882 0.756495 0.160825
S -6.412186 -1.827048 -0.501049
H 1.335967 2.712338 -0.303228
H 5.508927 1.692578 -0.519995
H 2.600190 -1.367990 0.241018
H 3.694001 3.390538 -0.627959
H -2.350247 -1.481444 0.740173
H 0.297626 -1.944636 0.559326
H -2.619932 2.577466 0.358339
H -3.947847 -0.721769 -0.299056
H -7.734359 0.617094 0.058354
H -6.356032 1.678381 0.321504

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1438.41421738

Comp_26Z_c06**B3LYP/6-31G* Geometry**

C 5.251569 -0.957961 0.012768
C 4.157476 0.076441 0.056438
C 2.129078 1.975911 0.249904
C 4.480796 1.411595 0.320234
C 2.831320 -0.310985 -0.111623
C 1.797769 0.636098 -0.017876
C 3.458990 2.354718 0.415465
F 4.898889 -2.038096 -0.718736
F 5.562201 -1.404533 1.251733
F 6.388781 -0.459144 -0.519976
C 0.411378 0.228814 -0.200531
O -0.544665 1.197274 -0.096022
C -1.772869 0.611591 -0.290241
C -1.589791 -0.736564 -0.526198
C -0.193238 -0.977676 -0.468032
C -2.884564 1.532119 -0.254980
N -4.152630 1.291335 -0.161700

N -4.572119 0.008186 -0.018248
C -5.916509 -0.281091 0.105044
N -6.740682 0.754121 -0.132510
S -6.403728 -1.839731 0.483844
H 1.338629 2.714621 0.324495
H 5.518230 1.704925 0.440769
H 2.604333 -1.350027 -0.322687
H 3.700413 3.394155 0.617228
H -2.349814 -1.465917 -0.768119
H 0.299845 -1.928151 -0.612638
H -2.622308 2.585638 -0.313736
H -3.942239 -0.726598 0.291015
H -7.732262 0.611521 -0.025638
H -6.357113 1.679756 -0.276215

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1438.41417850

Comp_27E_c01**B3LYP/6-31G* Geometry**

C -2.184389 -1.830105 0.091241
C -4.545795 -0.342258 0.017031
C -3.411917 -2.460535 0.124906
C -2.078612 -0.416043 0.006200
C -3.299908 0.333021 -0.019453
C -4.609495 -1.716118 0.083766
C -3.243128 1.754086 -0.074271
C -2.047567 2.419516 -0.100165
C -0.827916 1.698520 -0.078911
C -0.816697 0.291363 -0.039375
C 0.435970 -0.435559 -0.090752
N 1.593058 0.144412 0.014433
N 2.705544 -0.630094 -0.125006
C 3.973477 -0.158347 0.088792
N 4.057275 1.128990 0.497133
S 5.295420 -1.156341 -0.177152
O 0.293570 2.442399 -0.118327
H -1.292861 -2.444992 0.147975
H -5.456186 0.252100 -0.006050
H -3.453098 -3.544455 0.190210
H -5.569073 -2.223982 0.111817
H -4.176220 2.311705 -0.092441
H -1.992166 3.502351 -0.141008
H 0.400625 -1.515272 -0.253594
H 2.629654 -1.601340 -0.416362
H 3.241120 1.607539 0.853584
H 4.970988 1.460362 0.766572
H 1.066667 1.829831 -0.139632

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1101.46671687

Comp_27E_c02**B3LYP/6-31G* Geometry**

C 1.008781 -1.617968 -0.246642

C 3.787921 -1.597930 0.076142
 C 1.726625 -2.796169 -0.243589
 C 1.652506 -0.361433 -0.079202
 C 3.081309 -0.367038 0.065705
 C 3.128001 -2.795962 -0.069526
 C 3.777523 0.863577 0.183799
 C 3.105663 2.058733 0.151048
 C 1.699380 2.077093 0.017540
 C 0.948848 0.899563 -0.080882
 C -0.496235 1.070814 -0.193400
 N -1.372286 0.146084 0.018095
 N -2.676849 0.497063 -0.141832
 C -3.700019 -0.377444 0.114188
 N -3.315584 -1.604333 0.526174
 S -5.295771 0.097599 -0.105079
 O 1.031622 3.271642 0.006367
 H -0.062157 -1.640739 -0.390061
 H 4.868700 -1.572322 0.194585
 H 1.203787 -3.738934 -0.382457
 H 3.677682 -3.732881 -0.062574
 H 4.858503 0.848450 0.296297
 H 3.643967 3.000571 0.240073
 H -0.827694 2.081252 -0.449742
 H -2.942574 1.432320 -0.443519
 H -2.349566 -1.771245 0.775449
 H -4.036059 -2.242947 0.823780
 H 1.675981 3.995046 0.040352

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1101.45901590**

Comp_27Z_c01

B3LYP/6-31G* Geometry

C -2.291598 -1.720485 -0.032442
 C -4.201549 0.201454 0.657966
 C -3.555425 -2.102655 0.370825
 C -1.933975 -0.349802 -0.127313
 C -2.915053 0.624118 0.240321
 C -4.524384 -1.136892 0.717670
 C -2.567658 2.003455 0.182938
 C -1.319820 2.404169 -0.208153
 C -0.337017 1.450232 -0.588584
 C -0.624627 0.079578 -0.558862
 C 0.293275 -0.922661 -1.124586
 N 1.565270 -1.072256 -0.972220
 N 2.203807 -0.224707 -0.076836
 C 3.559705 -0.441924 0.183516
 N 4.183022 -1.196482 -0.736409
 S 4.283048 0.269238 1.510150
 O 0.824127 1.988501 -1.030279
 H -1.554630 -2.484476 -0.259458
 H -4.932178 0.958138 0.934072
 H -3.801985 -3.159169 0.432544
 H -5.513579 -1.450125 1.038769
 H -3.314011 2.742942 0.462459

H -1.041720 3.451855 -0.255042
 H -0.144061 -1.661508 -1.794810
 H 1.682496 0.083089 0.746031
 H 3.632258 -1.691749 -1.427650
 H 5.154704 -1.421320 -0.589553
 H 1.554995 1.339100 -0.989063

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1101.45537426**

Comp_27Z_c02

B3LYP/6-31G* Geometry

C 0.537286 1.338936 -1.107524
 C 2.799469 2.141684 0.338510
 C 0.909741 2.664749 -1.066796
 C 1.278496 0.347549 -0.405183
 C 2.448455 0.766282 0.313102
 C 2.044908 3.077194 -0.330940
 C 3.242603 -0.211648 0.965689
 C 2.917015 -1.544347 0.907301
 C 1.759313 -1.960319 0.207389
 C 0.922202 -1.043394 -0.420598
 C -0.265703 -1.571548 -1.132518
 N -1.506949 -1.258942 -0.979047
 N -1.856579 -0.343845 -0.036510
 C -3.175740 -0.017678 0.172120
 N -4.045147 -0.595344 -0.679446
 S -3.603812 1.045390 1.398292
 O 1.411274 -3.279884 0.144025
 H -0.327477 1.040997 -1.690287
 H 3.684551 2.440897 0.895087
 H 0.323887 3.401829 -1.608772
 H 2.321198 4.127218 -0.303880
 H 4.126671 0.107912 1.511477
 H 3.536241 -2.288030 1.405468
 H -0.100685 -2.369219 -1.854120
 H -1.178758 0.058203 0.605164
 H -3.715412 -1.289584 -1.337785
 H -5.029583 -0.445875 -0.527128
 H 2.082625 -3.809361 0.601605

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1101.45575206**

Comp_28E_c01

B3LYP/6-31G* Geometry

C 2.302903 0.339570 -0.806194
 C 2.366602 1.393197 1.826283
 C 2.089835 -0.510413 0.307805
 C 2.536096 1.674069 -0.563334
 C 2.569115 2.195077 0.726592
 C 2.127293 0.017619 1.609362
 O 2.794093 3.551365 0.675246
 C 3.100643 3.831453 -0.696077
 O 2.740086 2.687465 -1.475008

C 1.933528 -0.886017 2.808295
 C 1.198524 -2.152370 2.396092
 O 1.861843 -2.757953 1.296547
 C 1.855406 -2.011337 0.066586
 C 3.005388 -2.632174 -0.737176
 C 0.469923 -2.307971 -0.599748
 C 0.204757 -1.662611 -1.945046
 N -0.953176 -0.915429 -2.079421
 O 0.933634 -1.774345 -2.924512
 N -1.871342 -0.717397 -1.101514
 C -2.898194 -0.000749 -1.392474
 C -3.959400 0.279640 -0.424938
 C -6.037872 0.857016 1.372789
 C -3.924530 -0.220739 0.889563
 C -5.049487 1.071265 -0.820848
 C -6.081555 1.358205 0.071403
 C -4.955386 0.067185 1.776801
 H 2.289583 -0.039052 -1.820739
 H 2.389814 1.801220 2.832103
 H 2.519461 4.696297 -1.028196
 H 4.179187 4.021120 -0.797636
 H 1.380089 -0.361835 3.598488
 H 2.908675 -1.164021 3.232584
 H 0.148900 -1.922518 2.155473
 H 1.202443 -2.901787 3.193469
 H 3.022607 -2.260439 -1.762377
 H 3.958234 -2.413424 -0.246161
 H 2.871718 -3.718660 -0.767156
 H -0.328192 -2.042035 0.093223
 H 0.429447 -3.392269 -0.758524
 H -1.093682 -0.513167 -3.007862
 H -3.019004 0.432476 -2.394959
 H -6.840939 1.078841 2.070244
 H -3.083122 -0.832782 1.197562
 H -5.085571 1.462661 -1.835188
 H -6.918341 1.972177 -0.250123
 H -4.918455 -0.324773 2.789723

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32963394

Comp_28E_c02

B3LYP/6-31G* Geometry

C -1.872988 1.117242 0.009259
 C -4.540187 0.169054 0.154812
 C -2.133020 -0.244416 0.292301
 C -2.949014 1.954902 -0.178199
 C -4.259499 1.491509 -0.104754
 C -3.455027 -0.713573 0.355382
 O -5.131622 2.524470 -0.359854
 C -4.320598 3.703070 -0.426543
 O -2.948428 3.297969 -0.481872
 C -3.735402 -2.174315 0.645985
 C -2.513039 -3.025871 0.325571
 O -1.373669 -2.476865 0.976818

C -0.949046 -1.202057 0.498139
 C -0.008451 -0.699567 1.602648
 C -0.200023 -1.355163 -0.874857
 C 0.761033 -2.525961 -0.917762
 N 2.102480 -2.279859 -0.656947
 O 0.417077 -3.670097 -1.172105
 N 2.634219 -1.048959 -0.462138
 C 3.904307 -0.975406 -0.273715
 C 4.596633 0.295665 -0.059591
 C 5.999480 2.692832 0.360998
 C 3.919782 1.529111 -0.066009
 C 5.983792 0.285642 0.159034
 C 6.680350 1.475022 0.368086
 C 4.617151 2.713617 0.142986
 H -0.861124 1.501760 -0.056935
 H -5.564017 -0.189479 0.198532
 H -4.570418 4.265069 -1.331174
 H -4.487175 4.313468 0.472536
 H -4.603146 -2.517595 0.067619
 H -3.990174 -2.303484 1.707455
 H -2.347881 -3.101114 -0.757414
 H -2.614339 -4.042378 0.715568
 H 0.468215 0.246852 1.336206
 H -0.576482 -0.564432 2.527519
 H 0.775970 -1.439578 1.784009
 H 0.309957 -0.418447 -1.107518
 H -0.935135 -1.546670 -1.660357
 H 2.706202 -3.102345 -0.704050
 H 4.526257 -1.881151 -0.267138
 H 6.539810 3.621423 0.523168
 H 2.848507 1.540624 -0.238317
 H 6.516805 -0.662650 0.165681
 H 7.753535 1.449744 0.536196
 H 4.083487 3.660288 0.135498

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.33000932

Comp_28E_c04

B3LYP/6-31G* Geometry

C 2.622673 -0.587099 0.689997
 C 3.720421 0.162542 -1.816278
 C 2.289673 0.661739 0.110218
 C 3.468481 -1.416329 -0.010702
 C 4.006367 -1.054982 -1.241995
 C 2.846155 1.032335 -1.126798
 O 4.839289 -2.050737 -1.697700
 C 4.654398 -3.143157 -0.788752
 O 3.947360 -2.656864 0.354278
 C 2.544442 2.389880 -1.723634
 C 2.141524 3.349067 -0.613791
 O 1.050223 2.800271 0.106903
 C 1.327248 1.598930 0.863097
 C 1.892354 2.019774 2.231305
 C -0.105553 1.011932 0.960206

C -0.389555 -0.113597 1.938001
N -1.641226 -0.695076 1.820359
O 0.350861 -0.529107 2.821434
N -2.569500 -0.323404 0.905094
C -3.699859 -0.935635 0.925509
C -4.776353 -0.625711 -0.015548
C -6.887261 -0.088147 -1.786635
C -4.638869 0.361479 -1.008740
C -5.984528 -1.335544 0.074320
C -7.033037 -1.068894 -0.804943
C -5.686606 0.624618 -1.883891
H 2.216839 -0.884742 1.648701
H 4.159252 0.453741 -2.765683
H 4.063907 -3.930180 -1.280488
H 5.631020 -3.525437 -0.478265
H 1.721407 2.324992 -2.449512
H 3.419724 2.770692 -2.265859
H 1.784268 4.305165 -1.009003
H 2.997522 3.553740 0.047715
H 2.064558 1.159177 2.878194
H 2.837957 2.555277 2.097852
H 1.182828 2.691963 2.726189
H -0.428482 0.707869 -0.039378
H -0.768253 1.844446 1.231326
H -1.840929 -1.432799 2.497715
H -3.901093 -1.726480 1.661541
H -7.702632 0.121686 -2.473470
H -3.705680 0.910766 -1.079400
H -6.099711 -2.100533 0.839160
H -7.961909 -1.626611 -0.722902
H -5.570047 1.388911 -2.647584

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32845673**

Comp_28E_c06
B3LYP/6-31G* Geometry
C -2.304942 0.901005 0.883875
C -4.435159 -0.091273 -0.700750
C -2.323577 -0.453420 0.478549
C -3.338372 1.712339 0.471005
C -4.385231 1.227188 -0.305776
C -3.379943 -0.940320 -0.304990
O -5.295313 2.234871 -0.538008
C -4.669303 3.426535 -0.051708
O -3.550760 3.044438 0.755396
C -3.372798 -2.386928 -0.738855
C -2.602691 -3.222009 0.275860
O -1.286670 -2.712534 0.431805
C -1.184266 -1.374713 0.939560
C -1.156487 -1.454982 2.482896
C 0.193969 -0.894525 0.444126
C 0.335029 -0.790304 -1.067490
N 1.602943 -0.443919 -1.518319
O -0.544639 -0.972421 -1.891924

N 2.654984 -0.208936 -0.699333
C 3.776255 0.107996 -1.243566
C 4.979635 0.382101 -0.457536
C 7.328788 0.923057 0.983864
C 4.987936 0.305784 0.947435
C 6.164713 0.732294 -1.124423
C 7.330906 1.001086 -0.409188
C 6.152598 0.574298 1.657617
H -1.506139 1.305251 1.496698
H -5.257199 -0.467956 -1.301483
H -4.319047 4.029743 -0.902377
H -5.382124 3.988426 0.558167
H -2.877130 -2.477168 -1.713542
H -4.397811 -2.764867 -0.845686
H -2.476732 -4.255218 -0.061911
H -3.136993 -3.243268 1.239697
H -1.007260 -0.473016 2.943212
H -2.102987 -1.856701 2.858288
H -0.346793 -2.119107 2.802885
H 0.954676 -1.592478 0.810972
H 0.447194 0.075730 0.885335
H 1.702152 -0.373134 -2.532101
H 3.871915 0.185371 -2.335508
H 8.236373 1.131725 1.543648
H 4.073131 0.034277 1.464074
H 6.168802 0.793562 -2.210559
H 8.239843 1.270771 -0.940028
H 6.147318 0.511950 2.742596

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32911458**

Comp_28E_c07
B3LYP/6-31G* Geometry
C 3.472959 -0.951085 0.344512
C 4.547464 1.564141 -0.398684
C 2.620451 0.167035 0.176058
C 4.819624 -0.777279 0.122454
C 5.349769 0.456536 -0.247132
C 3.158886 1.412679 -0.182950
O 6.713498 0.355632 -0.376086
C 7.012385 -1.038847 -0.230481
O 5.832247 -1.699427 0.240428
C 2.257190 2.620447 -0.321848
C 0.990093 2.410740 0.493043
O 0.377108 1.186209 0.101204
C 1.113148 -0.020733 0.408392
C 0.825109 -0.425240 1.866847
C 0.564836 -1.073457 -0.590315
C -0.893710 -1.518650 -0.417502
N -1.803020 -0.476092 -0.437804
O -1.204425 -2.691357 -0.319435
N -3.134967 -0.704419 -0.309917
C -3.901344 0.325749 -0.268260
C -5.354625 0.203605 -0.135622

C -8.145530 0.033941 0.120258
 C -5.986129 -1.050525 -0.043040
 C -6.141700 1.365308 -0.098027
 C -7.527870 1.281719 0.029169
 C -7.368463 -1.129819 0.083497
 H 3.090218 -1.922718 0.637063
 H 4.966329 2.528639 -0.668354
 H 7.301501 -1.454395 -1.205684
 H 7.815413 -1.163296 0.501587
 H 1.980580 2.780693 -1.373414
 H 2.778290 3.526683 0.012295
 H 0.246334 3.189995 0.302734
 H 1.214814 2.408819 1.569426
 H 1.300850 -1.379270 2.112526
 H 1.210211 0.326846 2.562559
 H -0.252510 -0.528732 2.024861
 H 1.149616 -1.991449 -0.518816
 H 0.701671 -0.670622 -1.601563
 H -1.432073 0.475358 -0.411019
 H -3.495854 1.346203 -0.330498
 H -9.225561 -0.034385 0.219388
 H -5.374695 -1.946633 -0.071994
 H -5.661443 2.339070 -0.169326
 H -8.123908 2.190036 0.056780
 H -7.846552 -2.103301 0.154401

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.33219241**

Comp_28E_c09
B3LYP/6-31G* Geometry
 C 3.045553 0.118629 -0.754606
 C 2.257599 1.214484 1.739884
 C 2.262043 -0.642231 0.145895
 C 3.394054 1.396545 -0.383744
 C 3.006275 1.937824 0.840211
 C 1.878543 -0.098617 1.381219
 O 3.511462 3.209124 0.964451
 C 4.060598 3.525523 -0.321520
 O 4.159040 2.309538 -1.070099
 C 1.040754 -0.910410 2.346649
 C 1.179007 -2.396523 2.048559
 O 0.914201 -2.646343 0.668785
 C 1.866489 -2.069540 -0.256868
 C 3.102933 -2.988078 -0.322356
 C 1.145012 -2.109019 -1.627870
 C -0.011692 -1.126469 -1.839063
 N -1.014618 -1.258486 -0.895358
 O -0.049680 -0.349925 -2.774477
 N -2.127765 -0.484898 -0.933119
 C -2.983568 -0.646494 0.011381
 C -4.225715 0.126584 0.071336
 C -6.625159 1.575499 0.236445
 C -4.542815 1.092255 -0.901910
 C -5.126813 -0.098882 1.123866

C -6.318667 0.620387 1.206335
 C -5.732224 1.807106 -0.816418
 H 3.354655 -0.274204 -1.716620
 H 1.965752 1.637279 2.696186
 H 3.391342 4.224463 -0.842563
 H 5.057428 3.955565 -0.193963
 H -0.017300 -0.621468 2.268425
 H 1.344073 -0.706926 3.381718
 H 0.449082 -2.994891 2.601840
 H 2.182429 -2.753987 2.318762
 H 3.831974 -2.611606 -1.046189
 H 3.604300 -3.044511 0.648719
 H 2.802388 -3.998241 -0.619673
 H 0.778097 -3.134201 -1.767828
 H 1.856745 -1.903268 -2.429379
 H -0.836247 -1.883274 -0.106862
 H -2.819559 -1.379022 0.815638
 H -7.553367 2.137261 0.298022
 H -3.843862 1.264183 -1.714068
 H -4.889982 -0.844504 1.880187
 H -7.006626 0.434165 2.026765
 H -5.968058 2.550288 -1.573597

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.33268476**

Comp_28E_c10
B3LYP/6-31G* Geometry
 C 2.806482 0.413162 -0.898632
 C 2.228990 1.215661 1.759466
 C 2.308057 -0.522579 0.039409
 C 2.986287 1.711212 -0.480217
 C 2.701606 2.107923 0.824541
 C 2.027717 -0.123108 1.355029
 O 2.998109 3.440396 0.978239
 C 3.305369 3.917479 -0.338056
 O 3.474129 2.781085 -1.192506
 C 1.500401 -1.125837 2.359421
 C 1.875286 -2.538660 1.935501
 O 1.449056 -2.774069 0.593539
 C 2.104755 -1.973673 -0.417125
 C 3.451083 -2.639712 -0.763643
 C 1.167963 -2.066044 -1.648745
 C -0.163806 -1.310970 -1.565590
 N -0.923304 -1.662572 -0.473772
 O -0.508126 -0.509421 -2.426070
 N -2.122257 -1.174886 -0.023158
 C -2.803692 -0.340365 -0.731771
 C -4.086829 0.166750 -0.228989
 C -6.551889 1.190681 0.649558
 C -4.621240 -0.224582 1.012003
 C -4.807641 1.076897 -1.018355
 C -6.031140 1.585690 -0.583084
 C -5.841352 0.283423 1.444204
 H 3.032075 0.133175 -1.921536

H 2.017651 1.527635 2.777468
H 2.473749 4.534136 -0.706630
H 4.235986 4.490723 -0.307832
H 0.406442 -1.049551 2.436989
H 1.902977 -0.914709 3.358368
H 1.369553 -3.296373 2.540777
H 2.958962 -2.697462 2.027905
H 3.968831 -2.093889 -1.558165
H 4.113553 -2.659352 0.107294
H 3.282473 -3.669032 -1.096937
H 0.969136 -3.131009 -1.824947
H 1.673955 -1.674870 -2.533392
H -0.474068 -2.280043 0.193423
H -2.464430 0.015342 -1.701325
H -7.505144 1.585168 0.991477
H -4.063980 -0.928877 1.621173
H -4.401359 1.384501 -1.979284
H -6.576504 2.289483 -1.206332
H -6.244718 -0.026810 2.404858

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.33198486**

Comp_28E_c11
B3LYP/6-31G* Geometry
C 3.347029 -0.993513 0.384137
C 4.778503 1.305456 -0.451436
C 2.668114 0.229959 0.167408
C 4.704466 -1.028501 0.161832
C 5.409349 0.098629 -0.253188
C 3.383056 1.368501 -0.237036
O 6.743314 -0.205711 -0.371682
C 6.837565 -1.620570 -0.160813
O 5.570666 -2.084085 0.320493
C 2.668112 2.689788 -0.425780
C 1.384594 2.700010 0.389938
O 0.600692 1.563711 0.039665
C 1.149766 0.276214 0.399032
C 0.807157 -0.023232 1.871411
C 0.450957 -0.721382 -0.561003
C -1.062693 -0.930331 -0.401191
N -1.800511 0.230079 -0.406606
O -1.541997 -2.056725 -0.328216
N -3.150912 0.429788 -0.278008
C -3.970295 -0.565692 -0.257515
C -5.412188 -0.320385 -0.124480
C -8.186137 0.049293 0.128088
C -5.952441 0.973279 -0.008630
C -6.283959 -1.420761 -0.111345
C -7.660947 -1.238268 0.013837
C -7.325591 1.153287 0.116073
H 2.825931 -1.885482 0.714191
H 5.334720 2.186578 -0.755826
H 7.072787 -2.117051 -1.112247
H 7.608135 -1.825363 0.588129

H 2.416519 2.847406 -1.483910
H 3.317636 3.521627 -0.124810
H 0.762368 3.570921 0.165883
H 1.606072 2.705371 1.466896
H 1.137023 -1.026616 2.157526
H 1.300780 0.690656 2.538166
H -0.273359 0.042560 2.029117
H 0.884684 -1.715758 -0.444393
H 0.655453 -0.390178 -1.586692
H -1.273051 1.095863 -0.380577
H -3.639215 -1.598323 -0.332091
H -9.258717 0.194928 0.226004
H -5.277551 1.823007 -0.018381
H -5.874262 -2.424429 -0.199961
H -8.322179 -2.100753 0.022205
H -7.731722 2.157746 0.204967

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.33092493**

Comp_28E_c12
B3LYP/6-31G* Geometry
C -1.569977 1.008851 -0.057985
C -4.367045 0.591294 0.129235
C -2.083629 -0.289316 0.174676
C -2.466403 2.042528 -0.204941
C -3.840964 1.839060 -0.117374
C -3.469411 -0.490202 0.275498
O -4.497453 3.038422 -0.268806
C -3.487040 3.980015 -0.647608
O -2.208841 3.379120 -0.413679
C -4.011743 -1.872906 0.567893
C -2.941647 -2.704369 1.263247
O -1.763922 -2.718119 0.472188
C -1.096789 -1.459813 0.321425
C -0.169751 -1.242582 1.533811
C -0.303101 -1.606424 -1.010831
C 0.697951 -2.749724 -1.034674
N 2.023555 -2.441885 -0.736736
O 0.422256 -3.903625 -1.313825
N 2.491962 -1.194593 -0.494279
C 3.752436 -1.065706 -0.272263
C 4.377348 0.230103 -0.004854
C 5.652426 2.677822 0.521642
C 3.644134 1.430935 -0.000811
C 5.756415 0.278829 0.256300
C 6.389404 1.493093 0.517931
C 4.277908 2.640429 0.260872
H -0.503389 1.195657 -0.121811
H -5.438559 0.439992 0.215965
H -3.590843 4.218093 -1.716051
H -3.582629 4.881019 -0.035322
H -4.300468 -2.379929 -0.363253
H -4.913609 -1.805167 1.190021
H -3.241603 -3.751507 1.362827

H -2.743890 -2.309576 2.272274
H 0.451726 -0.350655 1.416707
H -0.761919 -1.124265 2.446904
H 0.487586 -2.107786 1.658894
H 0.202896 -0.666999 -1.236565
H -1.030015 -1.821233 -1.797901
H 2.666170 -3.234291 -0.785466
H 4.416973 -1.940656 -0.275106
H 6.143204 3.625639 0.724946
H 2.579496 1.398544 -0.208285
H 6.333310 -0.643444 0.254579
H 7.457096 1.512995 0.718670
H 3.700399 3.561035 0.260908

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32848701

Comp_28E_c14

B3LYP/6-31G* Geometry

C -3.026183 0.420015 -0.692646
C -2.739167 -1.713057 1.152266
C -2.031089 0.474105 0.312377
C -3.827538 -0.697376 -0.748905
C -3.687195 -1.747045 0.154873
C -1.894925 -0.582191 1.226994
O -4.630740 -2.713202 -0.106408
C -5.264144 -2.310216 -1.326558
O -4.864578 -0.965817 -1.613304
C -0.848116 -0.506633 2.317877
C -0.492424 0.949369 2.587196
O -0.091394 1.570632 1.375889
C -1.110863 1.702715 0.372308
C -1.916156 2.987805 0.642690
C -0.303480 1.794141 -0.955480
C 0.798935 2.836409 -0.893138
N 2.102538 2.384055 -0.781800
O 0.601749 4.042556 -0.953575
N 2.461084 1.084382 -0.665486
C 3.705499 0.827500 -0.471896
C 4.210791 -0.539887 -0.341415
C 5.252592 -3.135240 -0.076487
C 3.363485 -1.660398 -0.422282
C 5.583402 -0.742549 -0.126111
C 6.100891 -2.030548 0.005493
C 3.882817 -2.943483 -0.290768
H -3.161946 1.227220 -1.404147
H -2.644906 -2.526068 1.865590
H -4.940167 -2.971500 -2.142836
H -6.350147 -2.348029 -1.201545
H 0.063818 -1.040234 2.015557
H -1.214415 -0.989271 3.233304
H 0.362192 1.040152 3.264112
H -1.345082 1.476146 3.042835
H -2.690410 3.140283 -0.115871
H -2.414687 2.924862 1.615598

H -1.250136 3.852896 0.631156
H -0.972756 2.090403 -1.768249
H 0.113771 0.811627 -1.176869
H 2.804377 3.122193 -0.705876
H 4.445141 1.636420 -0.392469
H 5.653369 -4.140088 0.025295
H 2.302295 -1.505478 -0.588277
H 6.246838 0.117203 -0.061525
H 7.165614 -2.170308 0.171695
H 3.218807 -3.801459 -0.355613

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.33060128

Comp_28E_c16

B3LYP/6-31G* Geometry

C -3.093118 0.450215 -0.677717
C -2.938382 -1.714015 1.146789
C -2.123044 0.453200 0.352954
C -3.952705 -0.621966 -0.752961
C -3.880248 -1.684681 0.143559
C -2.045732 -0.623461 1.250417
O -4.828864 -2.627814 -0.177653
C -5.630280 -2.028261 -1.202422
O -4.951475 -0.858394 -1.670792
C -0.992884 -0.625228 2.337894
C 0.172750 0.264599 1.928944
O -0.308334 1.564053 1.607273
C -1.168172 1.652079 0.463307
C -1.955519 2.951124 0.689953
C -0.288455 1.718035 -0.831004
C 0.781546 2.789843 -0.758046
N 2.099274 2.379750 -0.624096
O 0.552955 3.989752 -0.818892
N 2.512104 1.091621 -0.567793
C 3.770633 0.878598 -0.409722
C 4.338806 -0.468369 -0.347175
C 5.505044 -3.020102 -0.203406
C 3.555172 -1.622633 -0.530652
C 5.712816 -0.615514 -0.096659
C 6.291656 -1.881691 -0.024079
C 4.135586 -2.884075 -0.457643
H -3.171435 1.265378 -1.388643
H -2.876433 -2.550821 1.835679
H -5.750372 -2.734284 -2.028963
H -6.606457 -1.743796 -0.784059
H -0.644370 -1.648185 2.530952
H -1.413964 -0.247405 3.280199
H 0.723777 -0.173918 1.085099
H 0.879096 0.408977 2.751942
H -2.618774 3.169001 -0.152037
H -2.559888 2.850365 1.596229
H -1.266397 3.789583 0.805710
H -0.926696 1.967546 -1.684083
H 0.159353 0.741254 -1.018004

H 2.776435 3.141510 -0.559034
H 4.475777 1.715377 -0.311350
H 5.954008 -4.008016 -0.148473
H 2.495111 -1.513146 -0.735256
H 6.328162 0.270381 0.044322
H 7.356035 -1.978249 0.171927
H 3.520303 -3.768109 -0.602397

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.33130208

Comp_28E_c17

B3LYP/6-31G* Geometry

C 2.619202 -0.612963 0.658470
C 3.709927 0.229740 -1.821168
C 2.277937 0.653140 0.122486
C 3.474935 -1.409283 -0.067815
C 4.009637 -1.002208 -1.285950
C 2.830711 1.069631 -1.101501
O 4.813413 -1.994199 -1.798164
C 4.904190 -2.981854 -0.763377
O 3.922005 -2.679085 0.230111
C 2.523981 2.447089 -1.648231
C 2.121471 3.364519 -0.503451
O 1.033171 2.787536 0.199372
C 1.313853 1.559487 0.910108
C 1.878696 1.931379 2.292560
C -0.117477 0.965869 0.986150
C -0.398064 -0.195996 1.921394
N -1.648949 -0.774615 1.784535
O 0.344998 -0.643188 2.787037
N -2.580598 -0.368327 0.887606
C -3.709921 -0.982787 0.886937
C -4.790167 -0.636420 -0.036972
C -6.908318 -0.029731 -1.776867
C -4.657872 0.391227 -0.988977
C -5.996863 -1.351482 0.027690
C -7.048954 -1.050476 -0.836048
C -5.709163 0.688541 -1.848775
H 2.210277 -0.949154 1.603017
H 4.141247 0.553653 -2.763369
H 4.702086 -3.969997 -1.187166
H 5.907042 -2.947124 -0.313343
H 1.699079 2.405989 -2.373716
H 3.396643 2.849962 -2.178512
H 1.761101 4.333485 -0.862913
H 2.978601 3.547147 0.163076
H 2.053007 1.048420 2.908043
H 2.823299 2.473149 2.178313
H 1.168156 2.583967 2.811618
H -0.440117 0.698347 -0.023944
H -0.781985 1.786153 1.288276
H -1.845609 -1.538465 2.433219
H -3.907502 -1.803051 1.591069
H -7.726515 0.206909 -2.451517

H -3.725859 0.944660 -1.040044
H -6.108135 -2.147796 0.760450
H -7.976616 -1.612767 -0.773869
H -5.596542 1.484052 -2.580506

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32845278

Comp_28E_c18

B3LYP/6-31G* Geometry

C -0.985640 0.758751 0.627617
C -3.485467 1.693495 -0.332449
C -2.088357 -0.122802 0.523247
C -1.175980 2.072552 0.263469
C -2.403296 2.534517 -0.203555
C -3.322020 0.341206 0.041366
O -2.303804 3.868915 -0.526353
C -1.015384 4.277598 -0.054249
O -0.259475 3.101607 0.250911
C -4.480579 -0.620930 -0.103135
C -3.950176 -2.037206 -0.282997
O -3.091594 -2.366970 0.808687
C -1.912975 -1.575019 0.983209
C -1.680411 -1.619731 2.506412
C -0.691182 -2.280608 0.297614
C -0.486044 -1.995987 -1.177717
N 0.746135 -1.487002 -1.561710
O -1.313084 -2.206994 -2.054461
N 1.765025 -1.184615 -0.720324
C 2.840297 -0.708128 -1.240458
C 4.010387 -0.347905 -0.439427
C 6.297344 0.367230 1.025654
C 4.043827 -0.514834 0.957171
C 5.139416 0.180325 -1.086117
C 6.274677 0.535661 -0.359199
C 5.177455 -0.159385 1.679295
H -0.014089 0.420829 0.971824
H -4.434393 2.052986 -0.718206
H -0.505009 4.844984 -0.837582
H -1.134251 4.884460 0.855347
H -5.105970 -0.335974 -0.958983
H -5.122750 -0.587777 0.788777
H -3.421168 -2.142344 -1.235528
H -4.758254 -2.774041 -0.240711
H -0.779409 -1.070055 2.795019
H -2.540264 -1.179962 3.019394
H -1.579215 -2.660715 2.832646
H -0.872568 -3.356532 0.395113
H 0.225298 -2.046967 0.840433
H 0.841043 -1.320825 -2.564958
H 2.920196 -0.552684 -2.325084
H 7.180863 0.643224 1.594667
H 3.174394 -0.925783 1.459808
H 5.123954 0.312557 -2.165759
H 7.140007 0.943453 -0.874461

H 5.191782 -0.292777 2.757701
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1184.32804185

Comp_28E_c20
B3LYP/6-31G* Geometry
C 2.971811 -0.744363 0.979970
C 4.309399 0.946109 -0.859776
C 2.315020 0.385577 0.441093
C 4.260068 -0.999495 0.568394
C 4.918623 -0.171441 -0.335407
C 2.982718 1.222254 -0.464947
O 6.199289 -0.634576 -0.539620
C 6.246612 -1.908841 0.111027
O 5.103162 -2.014866 0.965134
C 2.269882 2.430721 -1.027587
C 1.208386 2.901906 -0.043252
O 0.312585 1.837602 0.246256
C 0.882685 0.692580 0.902026
C 0.853800 0.942735 2.425027
C -0.112210 -0.443757 0.557261
C -0.337129 -0.584386 -0.939103
N -1.652516 -0.617738 -1.380426
O 0.553091 -0.694161 -1.767546
N -2.745097 -0.504544 -0.588931
C -3.896515 -0.534645 -1.160410
C -5.148668 -0.422408 -0.411577
C -7.593959 -0.213920 0.955009
C -5.173404 -0.262754 0.986147
C -6.366253 -0.474609 -1.109186
C -7.580127 -0.371382 -0.431280
C -6.385645 -0.160148 1.659195
H 2.485812 -1.404520 1.690477
H 4.829728 1.596033 -1.556449
H 6.215489 -2.707417 -0.644674
H 7.157019 -1.975498 0.713075
H 1.779761 2.169959 -1.975134
H 2.983688 3.237746 -1.237336
H 0.588152 3.699571 -0.463340
H 1.678550 3.285396 0.876054
H 1.178969 0.062041 2.988131
H 1.521423 1.768873 2.689963
H -0.163299 1.202065 2.735889
H -1.061739 -0.245780 1.056505
H 0.269994 -1.400975 0.928953
H -1.756463 -0.714697 -2.391906
H -3.983069 -0.647168 -2.250107
H -8.538569 -0.132765 1.485832
H -4.233745 -0.219905 1.527095
H -6.358051 -0.597069 -2.190118
H -8.513603 -0.413728 -0.985869
H -6.392324 -0.036586 2.738925
Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1184.32922937

Comp_28E_c21
B3LYP/6-31G* Geometry
C -2.058676 0.921332 0.637091
C -4.570136 0.049274 -0.346435
C -2.323157 -0.458519 0.475874
C -3.055335 1.811864 0.306461
C -4.289369 1.386264 -0.174451
C -3.568406 -0.886006 -0.007932
O -5.080120 2.478506 -0.453829
C -4.359851 3.607889 0.050838
O -3.024338 3.188702 0.350185
C -3.820980 -2.364755 -0.196261
C -2.500652 -3.070044 -0.479355
O -1.576076 -2.830250 0.580170
C -1.261809 -1.471241 0.918598
C -1.195490 -1.482725 2.461645
C 0.160340 -1.145429 0.392855
C 0.311644 -0.953169 -1.106090
N 1.564589 -0.535691 -1.530971
O -0.552794 -1.133385 -1.950361
N 2.609006 -0.306814 -0.698619
C 3.719722 0.066311 -1.228533
C 4.915016 0.344784 -0.432108
C 7.248402 0.898925 1.028648
C 4.927862 0.211055 0.968487
C 6.087287 0.758615 -1.085028
C 7.245811 1.034069 -0.360038
C 6.084958 0.486336 1.688368
H -1.106730 1.282866 1.010707
H -5.528145 -0.278585 -0.737857
H -4.332525 4.391607 -0.711704
H -4.844556 3.971275 0.968847
H -4.523168 -2.528833 -1.023615
H -4.277767 -2.801705 0.703806
H -2.088550 -2.735637 -1.436328
H -2.626112 -4.157344 -0.500235
H -0.899217 -0.507457 2.861279
H -2.178362 -1.740048 2.866406
H -0.475912 -2.237480 2.797535
H 0.815085 -1.972348 0.692980
H 0.568455 -0.261759 0.894155
H 1.664979 -0.416936 -2.540220
H 3.811883 0.191934 -2.316293
H 8.150011 1.112784 1.596048
H 4.022966 -0.109899 1.474138
H 6.087410 0.864426 -2.167729
H 8.144936 1.353555 -0.879769
H 6.083703 0.379545 2.769848
Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1184.32772533

Comp_29Z_c01**B3LYP/6-31G* Geometry**

C 1.453401 0.758556 -1.171277
 C 2.355812 1.808953 1.304306
 C 2.182905 -0.054783 -0.271728
 C 1.202136 2.060912 -0.802840
 C 1.644988 2.578786 0.410895
 C 2.625055 0.467725 0.953647
 O 1.239478 3.888778 0.531520
 C 0.691368 4.234341 -0.745614
 O 0.496844 3.026908 -1.488004
 C 3.411749 -0.415522 1.894658
 C 4.142994 -1.480032 1.087741
 O 3.210326 -2.231564 0.328621
 C 2.464710 -1.513933 -0.661900
 C 3.250502 -1.593526 -1.987448
 C 1.142567 -2.317647 -0.806679
 C 0.180125 -2.109606 0.349949
 N -1.079465 -1.602570 0.043787
 O 0.437542 -2.342417 1.520284
 N -1.524509 -1.392708 -1.220357
 C -2.707973 -0.923718 -1.420345
 C -3.746894 -0.494045 -0.459503
 C -5.819230 0.322859 1.262049
 C -3.461672 0.216667 0.721563
 C -5.091874 -0.760112 -0.772357
 C -6.117218 -0.364490 0.082846
 C -4.491064 0.619438 1.572243
 H 1.081927 0.375419 -2.115189
 H 2.701083 2.217295 2.248993
 H -0.271223 4.733715 -0.604307
 H 1.396515 4.886251 -1.281902
 H 2.734013 -0.919652 2.595456
 H 4.120913 0.181026 2.482642
 H 4.644296 -2.206202 1.734440
 H 4.905490 -1.015209 0.441033
 H 2.727692 -1.094557 -2.809298
 H 4.230313 -1.117719 -1.874635
 H 3.406053 -2.643213 -2.257446
 H 1.417753 -3.377958 -0.819623
 H 0.652176 -2.077111 -1.750399
 H -1.703263 -1.515383 0.844531
 H -2.977599 -0.864793 -2.474386
 H -6.618133 0.634619 1.929092
 H -2.438582 0.496903 0.954492
 H -5.326993 -1.290139 -1.692230
 H -7.149518 -0.588483 -0.171903
 H -4.252950 1.173547 2.476028

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32170941

Comp_29Z_c03**B3LYP/6-31G* Geometry**

C -3.134995 0.861691 0.263412

C -3.463780 -1.911543 -0.217957
 C -2.007586 0.006123 0.224144
 C -4.375866 0.307769 0.047583
 C -4.539695 -1.054003 -0.193158
 C -2.176241 -1.368725 -0.005677
 O -5.874079 -1.341236 -0.346922
 C -6.545749 -0.074677 -0.341148
 O -5.602758 0.927786 0.054847
 C -0.978703 -2.295761 -0.011976
 C 0.163741 -1.671797 0.775128
 O 0.424015 -0.368454 0.263645
 C -0.616620 0.614618 0.458425
 C -0.503136 1.198198 1.880368
 C -0.327931 1.694722 -0.616549
 C 0.965926 2.508820 -0.467127
 N 2.112942 1.729638 -0.399620
 O 0.965371 3.724683 -0.475906
 N 3.320851 2.322011 -0.187428
 C 4.371668 1.589280 -0.059183
 C 4.566882 0.124238 -0.135576
 C 5.106494 -2.641870 -0.219841
 C 3.841839 -0.725422 -0.992719
 C 5.584257 -0.440934 0.655207
 C 5.845661 -1.808222 0.622839
 C 4.112441 -2.093437 -1.032353
 H -3.038957 1.924737 0.455210
 H -3.597670 -2.975359 -0.387876
 H -6.915388 0.147583 -1.351578
 H -7.369102 -0.103919 0.378600
 H -0.640336 -2.482184 -1.041061
 H -1.248000 -3.269960 0.415825
 H 1.098720 -2.226273 0.656154
 H -0.076802 -1.630413 1.847134
 H -1.222653 2.008710 2.030439
 H -0.704813 0.431723 2.635156
 H 0.501794 1.597588 2.047341
 H -1.129016 2.435146 -0.624569
 H -0.326586 1.195916 -1.593738
 H 1.977947 0.733303 -0.227119
 H 5.269351 2.164862 0.168469
 H 5.312286 -3.708314 -0.251841
 H 3.091042 -0.314226 -1.659350
 H 6.167981 0.206541 1.305272
 H 6.630248 -2.223301 1.249763
 H 3.551364 -2.730331 -1.711237

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32473669

Comp_29Z_c04**B3LYP/6-31G* Geometry**

C -3.323514 0.868382 -0.494411
 C -3.904465 -1.613299 0.745659
 C -2.391851 0.278309 0.392696
 C -4.509419 0.207581 -0.719984

C -4.798198 -1.010138 -0.109805
 C -2.680762 -0.953775 0.999719
 O -6.028189 -1.459708 -0.532057
 C -6.590713 -0.376569 -1.281626
 O -5.548959 0.567783 -1.548284
 C -1.673912 -1.590534 1.933309
 C -0.278242 -1.065591 1.626035
 O -0.282074 0.356569 1.672674
 C -1.071924 1.013945 0.672976
 C -1.343125 2.403279 1.269200
 C -0.248977 1.098118 -0.656725
 C 1.122468 1.714719 -0.465789
 N 2.224453 0.870318 -0.489393
 O 1.313421 2.909062 -0.284808
 N 2.158391 -0.447070 -0.804620
 C 3.231436 -1.160990 -0.827713
 C 4.631981 -0.808408 -0.512266
 C 7.343424 -0.266119 0.019259
 C 5.000057 0.057443 0.535263
 C 5.651541 -1.417249 -1.266109
 C 6.992425 -1.142877 -1.010241
 C 6.344342 0.323681 0.795174
 H -3.124552 1.816262 -0.982336
 H -4.127860 -2.569570 1.208689
 H -6.987530 -0.756832 -2.226953
 H -7.381288 0.106454 -0.689220
 H -1.701714 -2.683752 1.836677
 H -1.919518 -1.355476 2.978597
 H 0.072921 -1.427787 0.649764
 H 0.446763 -1.381671 2.382329
 H -1.890977 3.039725 0.568520
 H -1.936104 2.293077 2.181861
 H -0.400067 2.897911 1.509341
 H -0.783268 1.739371 -1.363971
 H -0.163255 0.103506 -1.095978
 H 3.120657 1.346553 -0.402096
 H 3.061973 -2.183362 -1.164157
 H 8.389236 -0.052937 0.222098
 H 4.239702 0.488395 1.179927
 H 5.381517 -2.104380 -2.064448
 H 7.764530 -1.615867 -1.610891
 H 6.609906 0.988541 1.612416

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32449616**

Comp_29Z_c05

B3LYP/6-31G* Geometry

C 2.630681 -1.084918 0.086557
 C 4.797096 0.742373 0.025207
 C 2.406666 0.296538 0.294437
 C 3.923826 -1.503793 -0.130264
 C 4.989142 -0.608249 -0.158805
 C 3.480255 1.200743 0.255235
 O 6.157438 -1.285615 -0.422797

C 5.811544 -2.674583 -0.377025
 O 4.383885 -2.778673 -0.375043
 C 3.240813 2.682033 0.468211
 C 1.783085 3.031647 0.193738
 O 0.941335 2.159318 0.935999
 C 0.971697 0.790041 0.536593
 C 0.321248 0.056538 1.718195
 C 0.156123 0.587804 -0.789667
 C -1.192422 1.279385 -0.792751
 N -2.321464 0.510826 -0.528071
 O -1.340559 2.465019 -1.043716
 N -2.266497 -0.803205 -0.196879
 C -3.348748 -1.457257 0.051679
 C -4.764130 -1.030919 0.012693
 C -7.494849 -0.342429 0.017156
 C -5.291410 -0.173498 -0.971342
 C -5.640033 -1.557010 0.979181
 C -6.988550 -1.210168 0.987943
 C -6.644393 0.165664 -0.965896
 H 1.817275 -1.802062 0.099726
 H 5.629911 1.437999 -0.010315
 H 6.211539 -3.177732 -1.261975
 H 6.213597 -3.121704 0.543600
 H 3.904089 3.271812 -0.178076
 H 3.482551 2.955564 1.505097
 H 1.555140 2.980726 -0.879642
 H 1.537704 4.040915 0.535606
 H 0.181545 -1.007095 1.512329
 H 0.949539 0.171714 2.606173
 H -0.657816 0.496094 1.929583
 H 0.048992 -0.481365 -0.979149
 H 0.718404 1.026171 -1.618252
 H -3.195168 1.033128 -0.492116
 H -3.169152 -2.484703 0.366760
 H -8.547300 -0.072980 0.020852
 H -4.656435 0.193860 -1.772278
 H -5.250363 -2.236755 1.733119
 H -7.646276 -1.619923 1.749612
 H -7.034674 0.822945 -1.738007

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32300456**

Comp_29Z_c06

B3LYP/6-31G* Geometry

C -1.267407 0.680999 1.044564
 C -2.767004 1.887784 -1.038511
 C -2.212145 -0.075869 0.310548
 C -1.117584 2.010435 0.721289
 C -1.856347 2.606247 -0.297234
 C -2.947514 0.522219 -0.724405
 O -1.483301 3.925174 -0.429211
 C -0.635041 4.189605 0.693400
 O -0.251660 2.935510 1.265299
 C -3.930949 -0.304471 -1.523984

C -3.534984 -1.774252 -1.469062
 O -3.426880 -2.187302 -0.106949
 C -2.433105 -1.543863 0.695274
 C -3.017210 -1.635588 2.118238
 C -1.102808 -2.379088 0.673436
 C -0.137030 -2.087120 -0.458772
 N 1.113769 -1.587376 -0.120995
 O -0.377512 -2.264186 -1.645551
 N 1.549334 -1.427777 1.154928
 C 2.726320 -0.953526 1.379213
 C 3.762041 -0.472580 0.439400
 C 5.825442 0.433588 -1.246046
 C 3.470203 0.295516 -0.703397
 C 5.108362 -0.750624 0.734856
 C 6.129550 -0.310632 -0.103504
 C 4.495587 0.742419 -1.536618
 H -0.666302 0.235151 1.829532
 H -3.325922 2.351119 -1.845655
 H 0.257478 4.723603 0.356121
 H -1.187799 4.780268 1.438906
 H -3.961595 0.043952 -2.564447
 H -4.946270 -0.189819 -1.117885
 H -2.595778 -1.952131 -2.002700
 H -4.313120 -2.412409 -1.899119
 H -2.344649 -1.196254 2.860766
 H -3.974634 -1.108279 2.153832
 H -3.191049 -2.685885 2.376672
 H -1.408157 -3.425619 0.572284
 H -0.582282 -2.267799 1.625271
 H 1.740142 -1.450237 -0.912673
 H 2.991658 -0.936511 2.435770
 H 6.621228 0.780077 -1.899503
 H 2.445423 0.584993 -0.917259
 H 5.347983 -1.325084 1.626419
 H 7.163293 -0.544311 0.136040
 H 4.253182 1.340466 -2.410717

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32139881**

Comp_29Z_c07

B3LYP/6-31G* Geometry

C 2.580754 0.442244 -1.128585
 C 3.868341 0.473456 1.396007
 C 2.393028 -0.622516 -0.217440
 C 3.388693 1.488255 -0.741413
 C 4.022549 1.504847 0.496412
 C 3.032730 -0.603141 1.030505
 O 4.796029 2.639631 0.606033
 C 4.458980 3.436925 -0.533803
 O 3.738890 2.613630 -1.456851
 C 2.807377 -1.743419 1.994985
 C 2.479138 -3.013339 1.220131
 O 1.354171 -2.799772 0.380987
 C 1.507659 -1.803966 -0.640404

C 2.103838 -2.493580 -1.888512
 C 0.062269 -1.372040 -0.955439
 C -0.673893 -0.702192 0.195062
 N -2.007600 -0.388932 -0.053960
 O -0.201142 -0.400187 1.277329
 N -2.654186 -0.799735 -1.173848
 C -3.905657 -0.537428 -1.334373
 C -4.849508 0.217099 -0.482491
 C -6.759847 1.592225 1.063952
 C -4.497515 1.380190 0.228401
 C -6.184127 -0.223175 -0.423896
 C -7.127379 0.450420 0.347688
 C -5.446345 2.058671 0.993167
 H 2.107245 0.451519 -2.104677
 H 4.369960 0.486662 2.358680
 H 3.823165 4.277299 -0.218002
 H 5.375654 3.798438 -1.008248
 H 1.962359 -1.507235 2.653882
 H 3.692633 -1.898705 2.625175
 H 2.193168 -3.832080 1.887523
 H 3.353962 -3.342602 0.635818
 H 2.189789 -1.806269 -2.736086
 H 3.106097 -2.874707 -1.668438
 H 1.469300 -3.335921 -2.183208
 H -0.507471 -2.258137 -1.255156
 H 0.037312 -0.702271 -1.822325
 H -2.513516 -0.005624 0.742872
 H -4.326124 -0.975911 -2.238959
 H -7.495149 2.120495 1.664429
 H -3.492626 1.784225 0.149580
 H -6.474714 -1.108520 -0.984304
 H -8.150825 0.087579 0.387441
 H -5.157823 2.958800 1.528953

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32210038**

Comp_29Z_c09

B3LYP/6-31G* Geometry

C -1.620947 0.614931 1.062706
 C -2.960065 1.658571 -1.208765
 C -2.272171 -0.257561 0.155357
 C -1.661604 1.965447 0.800577
 C -2.317490 2.481752 -0.312737
 C -2.938284 0.266961 -0.964989
 O -2.176962 3.850496 -0.342275
 C -1.578783 4.194391 0.913358
 O -1.085157 2.994337 1.514179
 C -3.668333 -0.651553 -1.921474
 C -3.123600 -2.067432 -1.808493
 O -3.141451 -2.483367 -0.450525
 C -2.264553 -1.769461 0.438188
 C -2.832707 -2.077196 1.829884
 C -0.849707 -2.412601 0.247224
 C 0.272761 -1.845086 1.092400

N 1.398649 -1.370980 0.435374
O 0.265694 -1.811559 2.317524
N 1.485618 -1.245423 -0.914461
C 2.546124 -0.744932 -1.447301
C 3.804147 -0.269989 -0.831769
C 6.227389 0.710293 0.214058
C 4.431266 -0.912275 0.252429
C 4.432465 0.853699 -1.397837
C 5.626028 1.345032 -0.875513
C 5.631565 -0.423564 0.768309
H -1.108831 0.242855 1.941584
H -3.470736 2.062405 -2.077631
H -0.747921 4.884547 0.742306
H -2.337833 4.648402 1.567203
H -3.572926 -0.286329 -2.952458
H -4.741939 -0.664211 -1.685829
H -2.109003 -2.120774 -2.232109
H -3.749056 -2.786560 -2.346228
H -2.168926 -1.723822 2.620117
H -3.817803 -1.613634 1.937669
H -2.945862 -3.161248 1.935488
H -0.571755 -2.362215 -0.805180
H -0.949957 -3.468376 0.524536
H 2.099493 -0.957703 1.048906
H 2.473077 -0.633962 -2.528765
H 7.160069 1.090720 0.621075
H 4.007714 -1.822569 0.666648
H 3.969391 1.347171 -2.248895
H 6.090091 2.220866 -1.320668
H 6.104837 -0.936563 1.600939

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32278213**

Comp_29Z_c10

B3LYP/6-31G* Geometry

C -3.280747 0.656898 -0.752790
C -3.806081 -1.339930 1.189241
C -2.345184 0.399804 0.277626
C -4.430890 -0.098141 -0.784789
C -4.690108 -1.081009 0.166578
C -2.611702 -0.586515 1.240290
O -5.915602 -1.654781 -0.081428
C -6.343375 -1.115092 -1.337493
O -5.484687 -0.018297 -1.667100
C -1.622086 -0.839694 2.357123
C -0.763840 0.399637 2.573603
O -0.152513 0.773205 1.348572
C -1.046050 1.218952 0.314850
C -1.342758 2.716936 0.519277
C -0.246171 0.957861 -0.994476
C 1.146230 1.562163 -0.959213
N 2.218945 0.699643 -0.802117
O 1.372078 2.760999 -1.057230
N 2.106604 -0.651811 -0.791717

C 3.152184 -1.381358 -0.606631
C 4.554184 -1.000854 -0.328296
C 7.261653 -0.412326 0.173548
C 4.913323 0.068466 0.514052
C 5.579033 -1.783960 -0.888827
C 6.918546 -1.488548 -0.648509
C 6.255591 0.357126 0.760035
H -3.107170 1.421884 -1.501704
H -4.019449 -2.095720 1.938834
H -6.264904 -1.889297 -2.114153
H -7.372720 -0.756453 -1.246731
H -0.964293 -1.683006 2.104469
H -2.149357 -1.108903 3.281626
H 0.058557 0.207380 3.269275
H -1.370621 1.221496 2.984181
H -2.003098 3.102461 -0.264049
H -1.842334 2.876640 1.480521
H -0.412227 3.287067 0.493442
H -0.769491 1.420563 -1.836300
H -0.187467 -0.118423 -1.157752
H 3.130740 1.154040 -0.804966
H 2.955861 -2.449381 -0.696394
H 8.306198 -0.181914 0.363924
H 4.143650 0.648670 1.014478
H 5.314962 -2.625410 -1.524918
H 7.695639 -2.099954 -1.099132
H 6.513964 1.181920 1.418479

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32366847**

Comp_29Z_c11

B3LYP/6-31G* Geometry

C -2.454524 -1.024505 -0.113599
C -4.793975 0.576326 -0.073981
C -2.354680 0.387245 -0.136480
C -3.711372 -1.582101 -0.055984
C -4.861552 -0.797756 -0.032698
C -3.515544 1.176347 -0.124494
O -5.973956 -1.606653 -0.007511
C -5.473969 -2.936718 0.172724
O -4.059763 -2.914383 -0.046757
C -3.403622 2.684356 -0.190790
C -2.075935 3.070335 -0.829878
O -1.010501 2.457762 -0.120925
C -0.957372 1.027390 -0.184361
C -0.216650 0.617124 -1.472408
C -0.183042 0.618516 1.103748
C 1.199979 1.232412 1.243525
N 2.278978 0.503931 0.738298
O 1.425422 2.309281 1.766885
N 2.174185 -0.789203 0.338082
C 3.221739 -1.441980 -0.033090
C 4.632449 -1.019347 -0.156233
C 7.361866 -0.368785 -0.402967

C 5.630662 -1.970758 0.122384
 C 5.031013 0.259641 -0.589514
 C 6.383581 0.577778 -0.710925
 C 6.980214 -1.647751 0.009880
 H -1.574386 -1.658104 -0.138531
 H -5.693859 1.183599 -0.074483
 H -5.681072 -3.269261 1.200089
 H -5.944505 -3.603072 -0.555769
 H -3.449887 3.120683 0.816737
 H -4.242374 3.104595 -0.760922
 H -1.891988 4.146707 -0.765616
 H -2.066227 2.786197 -1.893961
 H -0.048549 -0.462180 -1.517561
 H -0.800000 0.906552 -2.352456
 H 0.753323 1.119742 -1.519129
 H -0.108255 -0.468845 1.150167
 H -0.761490 0.979016 1.957537
 H 3.189180 0.920295 0.930345
 H 3.018293 -2.486979 -0.265241
 H 8.414430 -0.115549 -0.493939
 H 5.337036 -2.969126 0.437692
 H 4.286234 0.995129 -0.877815
 H 6.671637 1.567571 -1.054192
 H 7.735107 -2.394731 0.239711

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32169190**

Comp_29Z_c13

B3LYP/6-31G* Geometry

C -1.634382 0.615221 1.077040
 C -2.984769 1.680028 -1.177410
 C -2.290082 -0.248838 0.164805
 C -1.671102 1.967717 0.824575
 C -2.332412 2.494321 -0.280233
 C -2.961819 0.286180 -0.947086
 O -2.231772 3.866218 -0.274361
 C -1.346353 4.181526 0.807227
 O -1.132318 2.992237 1.572306
 C -3.692886 -0.623610 -1.911152
 C -3.144493 -2.039301 -1.815482
 O -3.156243 -2.470014 -0.462072
 C -2.278121 -1.763571 0.431562
 C -2.841813 -2.086956 1.821496
 C -0.862898 -2.401954 0.228904
 C 0.261592 -1.845049 1.078347
 N 1.390579 -1.372612 0.424816
 O 0.254991 -1.819401 2.303558
 N 1.480195 -1.240126 -0.923966
 C 2.544867 -0.744541 -1.453206
 C 3.805910 -0.281815 -0.834632
 C 6.235781 0.676681 0.216463
 C 4.426818 -0.931818 0.248582
 C 4.443936 0.838293 -1.397064
 C 5.640746 1.318883 -0.872214

C 5.630346 -0.453875 0.767044
 H -1.123561 0.235606 1.953436
 H -3.505123 2.092800 -2.036248
 H -0.387540 4.536185 0.402503
 H -1.806356 4.945438 1.441583
 H -3.602060 -0.247261 -2.938501
 H -4.765600 -0.641203 -1.671731
 H -2.131406 -2.085801 -2.243599
 H -3.770333 -2.754078 -2.358562
 H -2.177358 -1.739330 2.613659
 H -3.828038 -1.627484 1.936037
 H -2.951415 -3.172359 1.916687
 H -0.587568 -2.337724 -0.823458
 H -0.961158 -3.461549 0.492280
 H 2.093963 -0.968968 1.041801
 H 2.473576 -0.627476 -2.534160
 H 7.171003 1.048593 0.625494
 H 3.996022 -1.840072 0.659735
 H 3.986048 1.337269 -2.247750
 H 6.112406 2.191962 -1.314803
 H 6.098629 -0.972829 1.598797

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32258895**

Comp_29Z_c15

B3LYP/6-31G* Geometry

C 2.361429 -1.005412 0.062334
 C 4.814811 0.413806 0.003284
 C 2.372006 0.407066 0.155131
 C 3.568247 -1.652828 -0.072528
 C 4.774073 -0.957595 -0.106323
 C 3.589649 1.105673 0.134950
 O 5.818765 -1.846110 -0.215341
 C 5.210418 -3.123329 -0.439032
 O 3.811951 -3.005725 -0.158214
 C 3.599192 2.612325 0.281280
 C 2.328013 3.065548 0.987558
 O 1.196050 2.571150 0.289966
 C 1.031814 1.148339 0.295354
 C 0.315353 0.734703 1.596593
 C 0.165502 0.858564 -0.965875
 C -1.222710 1.476206 -0.933920
 N -2.287459 0.635434 -0.607463
 O -1.470421 2.637025 -1.209834
 N -2.134406 -0.653057 -0.213723
 C -3.162993 -1.363687 0.101187
 C -4.604137 -1.033857 0.088180
 C -7.373610 -0.525022 0.153548
 C -5.215477 -0.249395 -0.908436
 C -5.415636 -1.580402 1.098758
 C -6.783351 -1.322239 1.137371
 C -6.587216 0.000772 -0.872536
 H 1.435976 -1.570428 0.095360
 H 5.758602 0.950346 -0.003450

H 5.350912 -3.416498 -1.489466
H 5.655926 -3.860493 0.234924
H 3.646641 3.096662 -0.704060
H 4.487338 2.935124 0.840025
H 2.225900 4.154624 0.980768
H 2.331785 2.731374 2.037027
H 0.044342 -0.324302 1.588918
H 0.961069 0.915202 2.461850
H -0.597604 1.325271 1.718924
H 0.086827 -0.218489 -1.112745
H 0.684128 1.301917 -1.819759
H -3.191794 1.101073 -0.555089
H -2.906029 -2.359776 0.460179
H -8.440976 -0.324372 0.180871
H -4.630174 0.128871 -1.741377
H -4.960331 -2.205461 1.863199
H -7.390374 -1.746032 1.932726
H -7.042128 0.602611 -1.654406

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1184.32122103

Comp_29Z_c18

B3LYP/6-31G* Geometry

C -2.199555 0.725605 0.759408
C -4.252412 0.457255 -1.179928
C -2.441839 -0.528262 0.146421
C -2.978430 1.792139 0.372468
C -3.983840 1.666778 -0.580797
C -3.468001 -0.656964 -0.806345
O -4.586804 2.886215 -0.787085
C -4.034919 3.755743 0.209704
O -2.909237 3.101498 0.799406
C -3.776465 -2.006818 -1.416840
C -3.305008 -3.103812 -0.474130
O -1.926790 -2.922275 -0.195108
C -1.578686 -1.735972 0.555927
C -1.727858 -2.064138 2.052247
C -0.098097 -1.573733 0.122520
C 0.811723 -0.638826 0.897376
N 2.079579 -0.465550 0.360581
O 0.559205 -0.071220 1.953235
N 2.437840 -0.956788 -0.853961
C 3.622720 -0.742978 -1.312194
C 4.777909 -0.041877 -0.711998
C 7.038538 1.301788 0.293538
C 5.113109 -0.120732 0.653064
C 5.615632 0.699353 -1.564643
C 6.728444 1.372146 -1.066867
C 6.233781 0.546251 1.147628
H -1.417307 0.845552 1.498454
H -5.048325 0.356281 -1.911414
H -3.709379 4.687365 -0.262528
H -4.793284 3.953014 0.981466
H -3.263643 -2.126904 -2.381741

H -4.852634 -2.100199 -1.612442
H -3.386544 -4.096344 -0.928278
H -3.906113 -3.102179 0.448468
H -1.421192 -1.227813 2.681069
H -2.769542 -2.312710 2.280374
H -1.105544 -2.931854 2.297284
H -0.066311 -1.303972 -0.936924
H 0.353562 -2.573232 0.170765
H 2.670302 0.194380 0.863963
H 3.769188 -1.125501 -2.321893
H 7.908229 1.823607 0.682916
H 4.526398 -0.741246 1.323952
H 5.380070 0.751015 -2.624881
H 7.357120 1.948029 -1.740438
H 6.481536 0.467671 2.202555

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -1184.32126767

Comp_29Z_c19

B3LYP/6-31G* Geometry

C -2.212831 0.603171 0.978140
C -4.111192 0.484930 -1.123431
C -2.400032 -0.594862 0.250571
C -2.979863 1.693359 0.633576
C -3.913905 1.637047 -0.395584
C -3.342071 -0.650186 -0.787240
O -4.513780 2.867601 -0.545891
C -4.043504 3.658030 0.551044
O -2.957731 2.961714 1.171693
C -3.506631 -1.932881 -1.570614
C -2.193065 -2.704809 -1.558290
O -1.782983 -2.959799 -0.216227
C -1.618920 -1.844011 0.672029
C -2.183695 -2.358219 2.014381
C -0.102967 -1.586490 0.873399
C 0.644509 -0.938511 -0.278457
N 1.955681 -0.563463 -0.008782
O 0.197586 -0.709420 -1.391792
N 2.586273 -0.900748 1.145834
C 3.823065 -0.585840 1.323389
C 4.760992 0.162849 0.459796
C 6.658753 1.536197 -1.102364
C 4.386614 1.283179 -0.306082
C 6.110084 -0.234658 0.447941
C 7.047660 0.437869 -0.331471
C 5.329522 1.961055 -1.078626
H -1.493222 0.676024 1.786380
H -4.828844 0.449994 -1.937197
H -3.689755 4.623636 0.177540
H -4.856088 3.794815 1.279417
H -3.806650 -1.712424 -2.603071
H -4.297779 -2.559333 -1.133410
H -1.421434 -2.150352 -2.101275
H -2.309420 -3.695894 -2.008497

H -2.065026 -1.618465 2.812713
H -3.248449 -2.580994 1.901314
H -1.667221 -3.279480 2.305268
H 0.368430 -2.555688 1.075549
H 0.075241 -0.992947 1.775696
H 2.470372 -0.198969 -0.808928
H 4.235074 -0.966233 2.257700
H 7.389573 2.063911 -1.708753
H 3.367691 1.656412 -0.264248
H 6.416930 -1.085596 1.051325
H 8.083093 0.108507 -0.334588
H 5.023945 2.828450 -1.657190

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32065849

Comp_29Z_c20

B3LYP/6-31G* Geometry

C 2.973195 -0.015256 0.893962
C 2.637287 0.713265 -1.826214
C 1.814585 0.683183 0.478378
C 3.910062 -0.333797 -0.060770
C 3.746271 0.020499 -1.398286
C 1.654744 1.047100 -0.867043
O 4.837430 -0.394306 -2.123331
C 5.596063 -1.215084 -1.225698
O 5.112874 -0.980960 0.100588
C 0.419487 1.800199 -1.313685
C -0.227497 2.503025 -0.128480
O -0.440742 1.577182 0.934092
C 0.761032 1.048126 1.533025
C 1.316939 2.085168 2.530728
C 0.277132 -0.190582 2.329018
C -0.144026 -1.404194 1.498566
N -1.347875 -1.222593 0.829564
O 0.509802 -2.427318 1.453258
N -1.911170 -2.257094 0.157989
C -3.053450 -2.125705 -0.421580
C -3.981809 -0.981863 -0.546458
C -5.897309 1.071496 -0.814223
C -3.586730 0.366073 -0.634129
C -5.356384 -1.275511 -0.625268
C -6.303905 -0.263555 -0.748575
C -4.537235 1.378895 -0.765301
H 3.121607 -0.314501 1.925075
H 2.518189 0.996442 -2.867406
H 5.451886 -2.272718 -1.488153
H 6.651115 -0.935103 -1.282916
H -0.304931 1.108400 -1.766741
H 0.678416 2.534108 -2.087966
H -1.216212 2.900095 -0.378466
H 0.395553 3.343976 0.208263
H 2.204330 1.700082 3.042243
H 1.608526 3.007636 2.019401
H 0.555830 2.326893 3.280184

H -0.553055 0.142090 2.964930
H 1.076498 -0.542265 2.983772
H -1.813667 -0.324990 0.924905
H -3.410497 -3.055676 -0.864887
H -6.634056 1.863849 -0.913276
H -2.534491 0.629839 -0.642119
H -5.676575 -2.313680 -0.579457
H -7.359806 -0.515539 -0.798007
H -4.210952 2.413181 -0.836912

Number of Imaginary Frequencies= 0

SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32271497

Comp_29Z_c21

B3LYP/6-31G* Geometry

C -2.210926 0.716649 0.783408
C -4.272460 0.466642 -1.149125
C -2.453128 -0.530235 0.156412
C -2.990099 1.787370 0.408562
C -3.999813 1.670935 -0.541410
C -3.483619 -0.649999 -0.792866
O -4.636704 2.880677 -0.696746
C -3.861471 3.816480 0.063007
O -2.955986 3.080069 0.887806
C -3.788704 -1.992093 -1.421584
C -3.309594 -3.100161 -0.495833
O -1.930755 -2.917535 -0.220475
C -1.582991 -1.740019 0.544528
C -1.723000 -2.088778 2.037119
C -0.105195 -1.567265 0.105770
C 0.806563 -0.641836 0.889661
N 2.074105 -0.464856 0.353170
O 0.556001 -0.084705 1.951486
N 2.430749 -0.945582 -0.865991
C 3.616562 -0.732056 -1.322019
C 4.774703 -0.041956 -0.714873
C 7.041446 1.281412 0.303867
C 5.109124 -0.135210 0.649493
C 5.616278 0.703211 -1.560273
C 6.732142 1.365972 -1.055910
C 6.232808 0.521744 1.150597
H -1.429539 0.827890 1.524738
H -5.075778 0.371110 -1.873233
H -3.293825 4.461625 -0.623636
H -4.528311 4.411425 0.693882
H -3.278656 -2.096906 -2.389709
H -4.865222 -2.086650 -1.614894
H -3.389643 -4.086716 -0.963075
H -3.906719 -3.113071 0.429224
H -1.094851 -2.956278 2.267564
H -1.417891 -1.259274 2.675662
H -2.762197 -2.345939 2.266949
H -0.079583 -1.281642 -0.949740
H 0.348931 -2.566280 0.136530
H 2.667457 0.187196 0.863637

H 3.761575 -1.105197 -2.335435
H 7.913533 1.795330 0.698354
H 4.519381 -0.759312 1.314361
H 5.381413 0.765831 -2.620082
H 7.363847 1.945041 -1.723895
H 6.479883 0.431988 2.204789

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.32127104**

Comp_29Z_c22

B3LYP/6-31G* Geometry

C -1.345360 1.050661 1.142177
C -1.641711 1.648508 -1.614934
C -1.844415 0.073020 0.247933
C -1.007333 2.282002 0.627443
C -1.154766 2.579065 -0.725349
C -1.991726 0.374251 -1.115667
O -0.719608 3.860024 -0.968332
C -0.503236 4.433841 0.326116
O -0.458558 3.364919 1.278210
C -2.507199 -0.673815 -2.079079
C -3.296502 -1.742141 -1.335498
O -2.529401 -2.247844 -0.244304
C -2.251812 -1.297023 0.809298
C -3.504462 -1.167370 1.700978
C -1.126521 -1.959613 1.638315
C 0.282300 -2.060655 1.041076
N 0.313671 -2.337746 -0.313990
O 1.277460 -1.935769 1.735285
N 1.407248 -2.895405 -0.973168
C 2.557826 -2.318204 -0.944140
C 3.069367 -1.019909 -0.472602
C 4.240137 1.431003 0.262943
C 4.466080 -0.880495 -0.391374
C 2.268299 0.103366 -0.198969
C 2.851488 1.315696 0.158162
C 5.048280 0.327257 -0.014390
H -1.213053 0.844873 2.198634
H -1.750012 1.882185 -2.669444
H 0.450342 4.966453 0.332886
H -1.336238 5.108869 0.570971
H -1.664115 -1.146810 -2.602456
H -3.136627 -0.210961 -2.849789
H -3.510128 -2.606637 -1.970466
H -4.254860 -1.339510 -0.978727
H -3.316524 -0.495409 2.544012
H -4.349638 -0.758476 1.138972
H -3.787018 -2.150373 2.092080
H -1.463448 -2.976957 1.878377
H -1.002468 -1.437317 2.589435
H -0.562137 -2.705193 -0.673861
H 3.314721 -2.922814 -1.449721
H 4.689345 2.376511 0.555496
H 5.097906 -1.736081 -0.619153

H 1.191998 0.034302 -0.286971
H 2.214360 2.170054 0.370894
H 6.129615 0.408047 0.057434

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -1184.31889897**

Comp_29Z_c24

B3LYP/6-31G* Geometry

C 2.769809 -0.874420 0.725302
C 4.485319 0.581447 -0.998605
C 2.340641 0.350401 0.159351
C 4.025321 -1.332909 0.398811
C 4.868565 -0.621624 -0.451352
C 3.197631 1.072812 -0.686168
O 6.063265 -1.287346 -0.582915
C 5.879271 -2.542038 0.084989
O 4.660599 -2.472415 0.833543
C 2.757558 2.402871 -1.260412
C 1.670039 3.007155 -0.384873
O 0.614222 2.063890 -0.233383
C 0.934856 0.864814 0.504534
C 0.803695 1.153286 2.012275
C -0.126444 -0.165754 0.032505
C -1.572285 0.141076 0.437611
N -2.099116 1.269007 -0.180174
O -2.199590 -0.570157 1.204805
N -3.213668 1.945325 0.322469
C -4.344887 1.340779 0.421037
C -4.875486 0.040793 -0.026577
C -6.133058 -2.325828 -0.886738
C -6.107858 -0.362798 0.515830
C -4.291258 -0.758753 -1.025659
C -4.921520 -1.922975 -1.455192
C -6.725377 -1.541303 0.103710
H 2.137854 -1.445474 1.396684
H 5.152502 1.142338 -1.645691
H 5.806445 -3.345790 -0.660973
H 6.715886 -2.715991 0.767487
H 2.361538 2.273487 -2.277439
H 3.611625 3.088064 -1.335132
H 1.216234 3.890071 -0.843583
H 2.074924 3.300665 0.594300
H 0.954907 0.245161 2.603324
H 1.549569 1.887415 2.332609
H -0.192468 1.545392 2.238024
H 0.093191 -1.146009 0.457827
H -0.050211 -0.241691 -1.058472
H -1.377375 1.935547 -0.446367
H -5.097639 1.976720 0.893172
H -6.613253 -3.242784 -1.217926
H -6.579638 0.256562 1.275291
H -3.357594 -0.452142 -1.480973
H -4.461802 -2.524186 -2.235206
H -7.670368 -1.841646 0.548293

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.31905277

Comp_29Z_c25
B3LYP/6-31G* Geometry

C -2.240277 0.587228 1.002167
C -4.134451 0.475457 -1.103871
C -2.412499 -0.602783 0.257958
C -3.014998 1.674937 0.667140
C -3.946899 1.621680 -0.364369
C -3.352666 -0.655046 -0.781753
O -4.596333 2.832295 -0.465338
C -3.892498 3.712954 0.416357
O -3.045909 2.921019 1.255650
C -3.498225 -1.927431 -1.585500
C -2.174188 -2.681209 -1.583185
O -1.762951 -2.951936 -0.244629
C -1.615227 -1.847796 0.661284
C -2.175872 -2.389329 1.994483
C -0.103031 -1.575232 0.868664
C 0.639385 -0.906467 -0.274606
N 1.955448 -0.547278 -0.007010
O 0.184689 -0.646860 -1.378087
N 2.592572 -0.916561 1.134171
C 3.832949 -0.614578 1.309117
C 4.768904 0.148279 0.455780
C 6.662779 1.545828 -1.089657
C 4.395948 1.289387 -0.279526
C 6.114929 -0.258241 0.422254
C 7.050443 0.426430 -0.349073
C 5.336885 1.979239 -1.043814
H -1.527606 0.655355 1.816964
H -4.855579 0.441039 -1.914567
H -3.277138 4.407754 -0.174169
H -4.610830 4.257771 1.035405
H -3.800176 -1.695472 -2.614805
H -4.280954 -2.571461 -1.158794
H -1.409573 -2.107357 -2.115989
H -2.275774 -3.666421 -2.049569
H -2.067620 -1.660435 2.804184
H -3.237671 -2.623042 1.876075
H -1.648881 -3.308618 2.272501
H 0.379403 -2.540387 1.063157
H 0.066566 -0.987886 1.776946
H 2.466588 -0.167630 -0.802372
H 4.249869 -1.020340 2.230474
H 7.392053 2.082937 -1.689619
H 3.379992 1.668309 -0.219911
H 6.420968 -1.125691 1.002054
H 8.083401 0.089994 -0.369399
H 5.032513 2.862474 -1.598565

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.32072192

Comp_29Z_c26
B3LYP/6-31G* Geometry

C 2.325730 0.438771 -1.234236
C 3.141126 0.521573 1.480788
C 2.052008 -0.649219 -0.371296
C 2.982996 1.526940 -0.709773
C 3.382301 1.570915 0.624156
C 2.460559 -0.606429 0.970358
O 4.039669 2.751904 0.871573
C 3.860851 3.540635 -0.311731
O 3.377517 2.679785 -1.347940
C 2.177081 -1.776890 1.887396
C 2.003445 -3.045473 1.065400
O 0.999310 -2.845252 0.071153
C 1.308206 -1.863273 -0.944336
C 2.134058 -2.556775 -2.044934
C -0.077312 -1.464237 -1.521455
C -0.957797 -0.635120 -0.582599
N -1.394207 -1.355439 0.524556
O -1.259645 0.523909 -0.807017
N -1.797952 -0.738267 1.710637
C -2.804437 0.063022 1.712626
C -3.843619 0.433429 0.735781
C -5.992619 1.191848 -0.915559
C -4.163197 -0.313930 -0.412299
C -4.633472 1.554405 1.044495
C -5.687998 1.941762 0.221108
C -5.233350 0.058699 -1.220340
H 2.018817 0.435468 -2.274075
H 3.463276 0.555353 2.516804
H 3.122279 4.330831 -0.116127
H 4.822021 3.966531 -0.611861
H 1.262898 -1.594550 2.470042
H 2.994466 -1.904852 2.608668
H 1.650678 -3.884198 1.672406
H 2.954292 -3.338981 0.597759
H 2.353816 -1.871361 -2.869090
H 3.089776 -2.912104 -1.646923
H 1.580044 -3.414688 -2.439794
H -0.592499 -2.392532 -1.798072
H 0.054487 -0.867230 -2.425667
H -0.776672 -2.138102 0.730909
H -2.950579 0.518631 2.694950
H -6.818626 1.484456 -1.558371
H -3.587523 -1.198846 -0.653992
H -4.408953 2.129432 1.940031
H -6.275551 2.821108 0.470974
H -5.473502 -0.535090 -2.098370

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G**) = -1184.31941460

Comp_30E_c01
B3LYP/6-31G* Geometry

C 2.005960 -1.538002 0.001161
N 3.237151 0.965285 -0.000311
C 3.379567 -1.457855 -0.002520
C 1.200988 -0.380616 -0.000234
C 1.895119 0.881951 -0.003392
C 3.955569 -0.161400 -0.004832
N -0.161915 -0.595018 0.002027
N -0.934156 0.421479 0.000983
C -2.315732 0.110643 0.001050
C -5.090435 -0.291746 0.001119
C -3.193328 1.204660 0.004106
C -2.840513 -1.194052 -0.002254
C -4.217617 -1.386451 -0.002205
C -4.572469 1.004598 0.004278
N 5.318676 -0.002789 -0.051638
N 1.213693 2.044915 -0.003098
H 1.494750 -2.496200 0.003716
H 4.005722 -2.344186 -0.012965
H -6.165371 -0.451079 0.001023
H -2.773627 2.206762 0.006416
H -2.153427 -2.032497 -0.005004
H -4.618065 -2.397232 -0.005012
H -5.242317 1.860431 0.006733
H 5.656605 0.925904 0.161310
H 5.902629 -0.767582 0.253429
H 0.197781 2.001323 -0.007032
H 1.738528 2.906870 -0.016031

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -699.430066934

Comp_30E_c04

B3LYP/6-31G* Geometry

C 1.711670 -1.332563 0.005260
N 3.438980 0.871881 -0.000035
C 3.074937 -1.528908 -0.014167
C 1.180675 -0.029172 0.019949
C 2.109915 1.053283 0.026816
C 3.908242 -0.380448 -0.024145
N -0.168756 0.304692 0.010610
N -0.981778 -0.670508 0.033966
C -2.349650 -0.312049 0.010330
C -5.115405 0.148220 -0.029188
C -3.251314 -1.386964 0.031882
C -2.847809 1.002855 -0.030780
C -4.220127 1.224799 -0.050018
C -4.625705 -1.158579 0.011971
N 5.274018 -0.508172 -0.104152
N 1.667671 2.339786 0.097903
H 1.016995 -2.165752 0.002719
H 3.507457 -2.524556 -0.040024
H -6.186607 0.330481 -0.044735
H -2.844844 -2.393444 0.064203
H -2.147398 1.830170 -0.045994
H -4.599840 2.243103 -0.081355

H -5.314181 -1.999294 0.028713
H 5.800250 0.327442 0.113047
H 5.691075 -1.379601 0.189153
H 0.684725 2.498463 -0.068669
H 2.328860 3.066390 -0.132562

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -699.426390077

Comp_30E_c07

B3LYP/6-31G* Geometry

C 1.712093 -1.332686 -0.026137
N 3.438677 0.872151 0.014219
C 3.075439 -1.528825 -0.013669
C 1.180584 -0.029404 -0.026318
C 2.109648 1.053454 -0.021348
C 3.908387 -0.380272 0.012098
N -0.168693 0.304183 -0.011189
N -0.981815 -0.671102 -0.032773
C -2.349582 -0.312385 -0.009587
C -5.115279 0.148602 0.031793
C -2.847747 1.003073 0.007096
C -3.251313 -1.387488 -0.007501
C -4.625618 -1.158742 0.014012
C -4.219993 1.225358 0.027479
N 5.276037 -0.508447 -0.000819
N 1.667091 2.339859 -0.074634
H 1.017645 -2.166053 -0.032094
H 3.508800 -2.524395 -0.021935
H -6.186431 0.331130 0.047648
H -2.147333 1.830514 0.001600
H -2.844913 -2.394402 -0.022712
H -5.314100 -1.999623 0.016113
H -4.599659 2.244101 0.039232
H 5.792973 0.329643 0.228430
H 5.680287 -1.377623 0.315824
H 2.330090 3.066825 0.148508
H 0.683850 2.499253 0.088244

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-
31+G**) = -699.426368094

Comp_30Z_c01

B3LYP/6-31G* Geometry

C -0.615115 -0.656806 -0.572908
N -3.197411 0.072000 0.236498
C -1.622455 -1.599432 -0.538520
C -0.873027 0.677374 -0.198843
C -2.218022 0.985545 0.184610
C -2.909343 -1.186253 -0.115022
N -0.048700 1.807994 -0.324856
N 1.209395 1.830960 -0.385221
C 2.040207 0.699172 -0.114953
C 3.921361 -1.294575 0.469587
C 3.010183 0.344563 -1.062506

C 2.039502 0.075678 1.143585
C 2.980313 -0.911106 1.429641
C 3.930608 -0.663448 -0.776448
N -3.960153 -2.070219 -0.098066
N -2.536348 2.253487 0.571247
H 0.369669 -0.941057 -0.921261
H -1.446692 -2.623072 -0.854434
H 4.649833 -2.067882 0.696742
H 3.026961 0.863450 -2.016633
H 1.307845 0.374937 1.888142
H 2.978555 -1.384034 2.408474
H 4.667250 -0.945027 -1.524480
H -3.756712 -3.057557 -0.044815
H -4.780992 -1.759585 0.403730
H -3.519311 2.486359 0.567627
H -1.869154 2.969649 0.310352

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -699.403865147**

Comp_30Z_c03

B3LYP/6-31G* Geometry

C -0.616174 -0.659230 -0.569512
N -3.198759 0.075080 0.233753
C -1.623163 -1.602090 -0.526850
C -0.872167 0.675643 -0.197479
C -2.216320 0.985671 0.187899
C -2.909305 -1.186707 -0.103876
N -0.048309 1.805910 -0.331347
N 1.209739 1.828388 -0.393781
C 2.040788 0.697854 -0.118949
C 3.922262 -1.293484 0.472258
C 3.014161 0.343937 -1.063303
C 2.036840 0.075013 1.139927
C 2.977858 -0.910577 1.429263
C 3.934773 -0.662977 -0.774047
N -3.939314 -2.088521 0.003731
N -2.533065 2.254926 0.570069
H 0.367360 -0.944607 -0.920591
H -1.443054 -2.631528 -0.820808
H 4.650700 -2.066050 0.702026
H 3.033420 0.862715 -2.017459
H 1.302352 0.373152 1.882084
H 2.973230 -1.383320 2.408132
H 4.674100 -0.944066 -1.519625
H -4.861834 -1.684873 0.095180
H -3.882917 -2.948740 -0.521589
H -3.515968 2.487472 0.576458
H -1.866747 2.971038 0.307241

Number of Imaginary Frequencies= 0
SCF Energy (PCM/mPW1PW91/6-31+G) = -699.403888572**