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Supporting Information.

A Theoretical Study of the Gas Phase (Proton Affinity) and Aqueous (pK_a) Basicity of a Series of 150 Pyrazoles[†]

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Contents

Table S1. Complete data set.

Table S2 Torsion angles (°) between the phenyl substituent and the pyrazole ring

Table S3 Equations relating experimental and calculated pK_a s

B3LYP Energy (Hartree), number of imaginary frequencies (NIMAG) and Cartesian coordinates of the neutral and protonated pyrazoles in gas phase

Table S1. Complete data set.

No	Name	R ¹	R ³	R ⁴	R ⁵	ΔH Gas (kJ· mol ⁻¹)	ΔG Gas (kJ· mol ⁻¹)	ΔH Aqueous (kJ· mol ⁻¹)	ΔG Aqueous (kJ· mol ⁻¹)	Calc. pK _a	Calc. pK _a	PA NIST (kJ· mol ⁻¹)	PA (kJ· mol ⁻¹) ^k	PA NIST corr. (kJ· mol ⁻¹)	pK _a
1	Parent	H	H	H	H	891.03	890.67	1106.14	1105.37	-1.25	3.44	894.1		894.1	2.48
2a	3-Me	H	CH ₃	H	H	913.28	917.07	1116.87	1118.68	1.08	5.77	906.0	901.2	906.0	3.32
2b	5-Me	H	H	H	CH ₃	914.75	917.84	1116.84	1119.46	1.22	5.91	906.0	901.2	906.0	3.32
3a	3-Et	H	C ₂ H ₅	H	H	917.81	920.21	1117.16	1118.49	1.05	5.74				3.30
3b	5-Et	H	H	H	C ₂ H ₅	919.54	922.14	1116.25	1114.78	0.40	5.09				3.30
4a ^a	3- <i>t</i> -Bu	H	<i>t</i> -C ₄ H ₉	H	H	927.31	928.31	1114.83	1120.98	1.48	6.17	922.8		922.8	3.30
4b	5- <i>t</i> -Bu	H	H	H	<i>t</i> -C ₄ H ₉	928.93	931.39	1115.48	1115.01	0.44	5.13	922.8		922.8	3.30
5	4-Me	H	H	CH ₃	H	906.77	910.60	1112.78	1112.96	0.08	4.77	906.8	901.6	906.8	3.09
6 ^b	4-Adamantyl ^c	H	H	1-Ad	H	927.21	926.65	1120.72	1116.94	0.78	5.47	913.1		913.1	
7	3,5-diMe	H	CH ₃	H	CH ₃	934.66	942.65	1125.82	1126.47	2.45	7.14	933.5	927.5	933.5	4.12
8a	3,4-diMe	H	CH ₃	CH ₃	H	927.05	930.80	1123.23	1124.55	2.11	6.80	927.3	922.1	927.3	3.91
8b	4,5-diMe	H	H	CH ₃	CH ₃	930.39	931.49	1124.28	1125.95	2.36	7.04	927.3	922.1	927.3	3.91
9	3,4,5-triMe	H	CH ₃	CH ₃	CH ₃	947.04	952.09	1132.45	1139.18	4.67	9.36	949.3	938.0	949.3	4.63
10a	3,4-diMe,5-Et	H	CH ₃	CH ₃	C ₂ H ₅	949.81	954.54	1132.41	1134.56	3.87	8.55				4.60
10b	3-Et,4,5-diMe	H	C ₂ H ₅	CH ₃	CH ₃	951.41	953.25	1133.77	1136.93	4.28	8.97				4.60
11	3,5-diEt,4-Me	H	C ₂ H ₅	CH ₃	C ₂ H ₅	955.78	957.76	1133.91	1135.99	4.12	8.80	952.8		952.8	4.51
12a	3,4-triCH ₂	H	CH ₂	(CH ₂) ₂	H	927.61	929.95	1120.63	1122.05	1.67	6.36				3.61
12b	4,5-triCH ₂	H	H	(CH ₂) ₂	CH ₂	933.4	935.36	1125.15	1126.05	2.37	7.06				3.61
13a	3,4-tetraCH ₂	H	(CH ₂) ₂	(CH ₂) ₂	H	935.43	937.63	1124.74	1126.61	2.47	7.16				4.01
13b	4,5-tetraCH ₂	H	H	(CH ₂) ₂	(CH ₂) ₂	936.02	938.16	1124.70	1126.58	2.47	7.15				4.01
14a	3,4-pentaCH ₂	H	(CH ₂) ₂	(CH ₂) ₃	H	937.89	940.27	1124.68	1125.86	2.34	7.03				3.96
14b	4,5-pentaCH ₂	H	H	(CH ₂) ₃	(CH ₂) ₂	938.64	940.52	1124.22	1125.49	2.28	6.96				3.96
15a	2 <i>H</i> -campho ^d	H	H	--	--	943.29	945.15	1121.93	1123.64	1.95	6.64				3.35
15b	1 <i>H</i> -campho ^d	H	--	--	H	955.10	957.05	1132.16	1133.89	3.75	8.44				3.35
16a	3,4-triCH ₂ ,5-Me	H	CH ₂	(CH ₂) ₂	CH ₃	947.95	950.77	1130.68	1131.40	3.31	8.00				4.38
16b	3-Me,4,5-triCH ₂	H	CH ₃	(CH ₂) ₂	CH ₂	951.39	956.13	1134.42	1136.03	4.12	8.81				4.38
17a	3-Me,4,5-tetraCH ₂	H	CH ₃	(CH ₂) ₂	(CH ₂) ₂	953.61	957.93	1133.27	1134.81	3.91	8.60				4.65
17b	3,4-tetraCH ₂ ,5-Me	H	(CH ₂) ₂	(CH ₂) ₂	CH ₃	955.23	957.56	1134.16	1137.28	4.34	9.03				4.65
18a	3-Me,4,5-pentaCH ₂	H	CH ₃	(CH ₂) ₃	(CH ₂) ₂	955.77	959.44	1133.56	1136.50	4.21	8.89				4.57
18b	3,4-pentaCH ₂ ,5-Me	H	(CH ₂) ₂	(CH ₂) ₃	CH ₃	956.93	959.42	1134.01	1138.23	4.51	9.20				4.57
19	3,5-di <i>t</i> -Bu	H	<i>t</i> -C ₄ H ₉	H	<i>t</i> -C ₄ H ₉	957.62	961.57	1127.03	1127.05	2.55	7.24	952.7		952.7	3.99
20a	3- <i>t</i> -Bu,5-Me	H	<i>t</i> -C ₄ H ₉	H	CH ₃	946.87	949.53	1127.69	1130.13	3.09	7.78			946.2	
20b	3-Me,5- <i>t</i> -Bu	H	CH ₃	H	<i>t</i> -C ₄ H ₉	946.99	948.59	1126.06	1128.89	2.87	7.56	946.2		946.2	
21	3,5-di <i>t</i> -Bu,4-Me	H	<i>t</i> -C ₄ H ₉	CH ₃	<i>t</i> -C ₄ H ₉	967.90	970.29	1134.01	1135.85	4.09	8.78	967.5		967.5	4.25
22	3,5-diMe,4- <i>t</i> -Bu	H	CH ₃	<i>t</i> -C ₄ H ₉	CH ₃	950.11	951.87	1130.08	1134.20	3.80	8.49				4.28
23a	5-NO ₂	H	H	H	NO ₂	814.17	815.83	1054.64	1055.73	-9.95	-5.26	820.8		820.8	-4.66
23b	3-NO ₂	H	NO ₂	H	H	815.41	816.30	1040.79	1041.59	-12.42	-7.73	820.8		820.8	-4.66
24	4-NO ₂	H	H	NO ₂	H	814.25	816.12	1058.82	1060.76	-9.06	-4.38	822.2		822.2	-1.96
25	3,5-NO ₂	H	NO ₂	H	NO ₂	749.13	750.48	993.93	995.15	-20.56	-15.87	759.4		759.4	

26	4-F	H	H	F	H	860.65	862.01	1089.01	1090.15	-3.92	0.77	863.0		863.0	
27	4-Cl	H	H	Cl	H	865.73	865.29	1088.09	1087.38	-4.40	0.29	868.5		868.5	0.60
28	4-Br	H	H	Br	H	868.64	868.22	1088.36	1087.75	-4.34	0.35				0.64
29a	3-Cl	H	Cl	H	H	868.03	869.99	1079.56	1081.63	-5.41	-0.72				-0.48
29b	5-Cl	H	H	H	Cl	874.68	876.33	1091.96	1093.43	-3.34	1.35				-0.48
30a	3,4-diBr	H	Br	Br	H	857.91	859.85	1066.29	1067.21	-7.94	-3.25				-1.83
30b	4,5-diBr	H	H	Br	Br	860.73	862.33	1075.47	1076.06	-6.39	-1.70				-1.83
31a	4-NO ₂ ,5-Me	H	H	NO ₂	CH ₃	839.04	840.94	1068.05	1067.13	-7.95	-3.26				-1.25
31b	3-Me,4-NO ₂	H	CH ₃	NO ₂	H	840.60	843.17	1070.90	1072.40	-7.02	-2.34				-1.25
32a	3-Me,4-Cl	H	CH ₃	Cl	H	889.20	891.88	1098.97	1100.68	-2.07	2.62				1.42
32b	4-Cl,5-Me	H	H	Cl	CH ₃	890.50	890.15	1098.68	1100.31	-2.14	2.55				1.42
33a	3-Me,4-Br	H	CH ₃	Br	H	891.58	894.05	1098.81	1100.73	-2.06	2.63				1.46
33b	4-Br,5-Me	H	H	Br	CH ₃	892.85	893.15	1098.61	1101.94	-1.85	2.84				1.46
34a	3-Br,4-Me	H	Br	CH ₃	H	888.29	891.22	1087.06	1089.06	-4.11	0.58				0.24
34b	4-Me,5-Br	H	H	CH ₃	Br	893.73	893.87	1097.88	1100.61	-2.08	2.61				0.24
35a	4-Cl,5-Et	H	H	Cl	C ₂ H ₅	896.48	897.74	1099.92	1099.74	-2.24	2.45				1.50
35b	3-Et,4-Cl	H	C ₂ H ₅	Cl	H	897.05	897.83	1099.71	1099.57	-2.27	2.42				1.50
36a	4-Br,5-Et	H	H	Br	C ₂ H ₅	898.76	899.48	1099.17	1100.59	-2.09	2.60				1.53
36b	3-Et,4-Br	H	C ₂ H ₅	Br	H	899.29	899.98	1100.21	1100.08	-2.18	2.51				1.53
37a	3-Cl,5-Me	H	Cl	H	CH ₃	891.01	896.04	1089.59	1094.03	-3.24	1.45				0.30
37b	3-Me,5-Cl	H	CH ₃	H	Cl	896.36	901.97	1102.50	1106.37	-1.07	3.61				0.30
38a	3-Br,5-Me	H	Br	H	CH ₃	895.69	902.26	1091.35	1094.32	-3.19	1.50				0.45
38b	3-Me,5-Br	H	CH ₃	H	Br	899.16	906.58	1102.01	1104.13	-1.47	3.22				0.45
39	3,5-diMe,4-NO ₂	H	CH ₃	NO ₂	CH ₃	863.07	865.97	1078.16	1079.13	-5.85	-1.16				-0.46
40	3,5-diMe,4-Cl	H	CH ₃	Cl	CH ₃	911.71	914.99	1107.95	1107.30	-0.91	3.78				2.22
41	3,5-diMe,4-Br	H	CH ₃	Br	CH ₃	913.59	915.38	1107.78	1108.28	-0.74	3.95				2.30
42a	3,4-DiBr,5-Me	H	Br	Br	CH ₃	880.37	881.84	1075.49	1075.44	-6.49	-1.80				-0.96
42b	3-Me,4,5-diBr	H	CH ₃	Br	Br	882.30	885.46	1085.06	1085.26	-4.77	-0.08				-0.96
43a	3-Cyclopropyl	H	c-C ₃ H ₅	H	H	926.75	929.26	1118.70	1121.90	1.65	6.34				3.10
43b	5-Cyclopropyl	H	H	H	c-C ₃ H ₅	928.38	929.44	1121.35	1124.35	2.08	6.76				3.10
44a	3-Cycloprop.,4-Me,5-Et	H	c-C ₃ H ₅	CH ₃	C ₂ H ₅	955.10	956.00	1127.69	1123.72	1.97	6.65				4.30
44b	3-Et,4-Me,5-cycloprop.	H	C ₂ H ₅	CH ₃	c-C ₃ H ₅	952.76	954.31	1134.57	1134.58	3.87	8.56				4.30
45a	3-Ph	H	C ₆ H ₅	H	H	920.97	920.00	1105.55	1108.09	-0.77	3.92	914.2		914.2	2.13
45b	5-Ph	H	H	H	C ₆ H ₅	922.68	924.85	1108.83	1111.37	-0.20	4.49	914.2		914.2	2.13
46a	4-Cl,5-Ph	H	H	Cl	C ₆ H ₅	898.75	900.57	1090.28	1091.42	-3.69	1.00				0.26
46b	3-Ph,4-Cl	H	C ₆ H ₅	Cl	H	901.53	903.42	1089.99	1091.13	-3.74	0.94				0.26
47a	4-Br,5-Ph	H	H	Br	C ₆ H ₅	900.63	902.36	1090.75	1091.9	-3.61	1.08				0.30
47b	3-Ph,4-Br	H	C ₆ H ₅	Br	H	903.71	905.75	1090.72	1093.54	-3.32	1.37				0.30
48a	4-Me,5-Ph	H	H	CH ₃	C ₆ H ₅	933.66	935.02	1113.44	1114.24	0.31	4.99				2.68
48b	3-Ph,4-Me	H	C ₆ H ₅	CH ₃	H	934.84	937.12	1113.01	1113.97	0.26	4.95				2.68
49a	3-Ph,5-Me	H	C ₆ H ₅	H	CH ₃	940.18	939.05	1114.97	1120.28	1.36	6.05	932.1		932.1	2.92
49b	3-Me,5-Ph	H	CH ₃	H	C ₆ H ₅	940.76	943.56	1118.59	1125.29	2.24	6.93	932.1		932.1	2.92
50a	3-Ph,5-Et	H	C ₆ H ₅	H	C ₂ H ₅	943.85	943.65	1114.95	1118.23	1.00	5.69	935.6		935.6	
50b	3-Et,5-Ph	H	C ₂ H ₅	H	C ₆ H ₅	944.10	947.02	1118.31	1121.55	1.59	6.27	935.6		935.6	

51a	3,4-diMe,5-Ph	H	CH ₃	CH ₃	C ₆ H ₅	950.04	952.97	1122.18	1124.30	2.07	6.76				3.47
51b	3-Ph,4,5-diMe	H	C ₆ H ₅	CH ₃	CH ₃	953.76	956.42	1121.73	1123.74	1.97	6.66				3.47
52a	3-Me,4-Br,5-Ph	H	CH ₃	Br	C ₆ H ₅	919.70	921.99	1099.99	1102.23	-1.80	2.89				1.20
52b	3-Ph,4-Br,5-Me	H	C ₆ H ₅	Br	CH ₃	923.66	923.83	1099.68	1100.84	-2.04	2.65				1.20
53	4-Ph	H	H	C ₆ H ₅	H	906.42	908.08	1102.06	1102.86	-1.69	3.00	906.0		906	1.64
54	3,5-diPh	H	C ₆ H ₅	H	C ₆ H ₅	944.72	948.48	1106.36	1108.46	-0.71	3.98	946.3		946.3	1.43
55a	3-CF ₃ ,5-Me	H	CF ₃	H	CH ₃	863.85	867.90	1073.29	1081.59	-5.41	-0.73		869.0 ^l	866.8	-0.50
55b	3-Me,5-CF ₃	H	CH ₃	H	CF ₃	868.22	872.83	1086.94	1091.87	-3.61	1.07		869.0 ^l	866.8	-0.50
56	3,5-biB3LYP ₃	H	CF ₃	H	CF ₃	798.34	799.21	1031.09	1031.48	-14.20	-9.51		814.7 ^l	808.7	-8.23
57	4-CO ₂ Et	H	H	CO ₂ Et	H	878.61	880.81	1086.64	1088.02	-4.29	0.40	880.7		880.7	
58a	3-Me,5-CO ₂ Et	H	CH ₃	H	CO ₂ Et	905.86	909.68	1097.26	1102.78	-1.70	2.99	902.6		902.6	
58b	3-CO ₂ Et,5-Me	H	CO ₂ Et	H	CH ₃	912.53	916.99	1093.33	1095.06	-3.06	1.63	902.6		902.6	
59	3,5-diCO ₂ Et	H	CO ₂ Et	H	CO ₂ Et	884.44	887.67	1062.36	1066.22	-8.11	-3.42	881.6		881.6	
60a	3-Ph,5-CO ₂ Et	H	C ₆ H ₅	H	CO ₂ Et	908.81	910.00	1084.07	1083.51	-4.18	0.51	899.7		899.7	
60b	3-CO ₂ Et,5-Ph	H	CO ₂ Et	H	C ₆ H ₅	921.16	924.10	1086.32	1088.65	-5.08	-0.39	899.7		899.7	
61a	3-NH ₂	H	NH ₂	H	H	927.37	929.37	1125.48	1128.50	2.80	7.49	921.5		921.5	4.11
61b	5-NH ₂	H	H	H	NH ₂	938.35	939.26	1131.18	1133.44	3.67	8.36	921.5		921.5	4.11
62	4-NH ₂	H	H	NH ₂	H	913.88	914.35	1114.84	1116.47	0.70	5.38	907.6		907.6	5.57
62c	4-NH ₂	H	H	NH ₃ ⁺	H	864.08	864.80	1103.60	1103.14	-1.64	3.05				5.57
63	3,5-diPh,4-OH	H	C ₆ H ₅	OH	C ₆ H ₅	944.29	945.72	1103.56	1108.47	-0.71	3.98				2.01
64	1-Me	CH ₃	H	H	H	912.83	912.85	1113.05	1113.02	0.09	4.78	912.0	904.5	912.0	2.09
65	1,3-diMe	CH ₃	CH ₃	H	H	932.53	934.60	1123.06	1124.37	2.08	6.77	933.9	922.5	933.9	2.82
66	1,5-diMe	CH ₃	H	H	CH ₃	932.60	937.49	1121.94	1122.87	1.82	6.51	934.3	926.3	934.3	2.89
67	1,4-diMe	CH ₃	H	CH ₃	H	927.56	928.31	1119.61	1121.13	1.51	6.20	928.4	920.8	928.4	2.48
68	1,3,5-triMe	CH ₃	CH ₃	H	CH ₃	951.07	955.32	1131.47	1129.83	3.04	7.72	949.3	941.7	949.3	3.80
69	1,3,4-triMe	CH ₃	CH ₃	CH ₃	H	944.95	947.18	1127.90	1127.96	2.71	7.40		938.8 ^m	941.5	
70	1,4,5-triMe	CH ₃	H	CH ₃	CH ₃	945.83	946.97	1128.64	1130.28	3.12	7.80		938.8 ^m	941.5	
71	1-Me,3- <i>t</i> -Bu	CH ₃	<i>t</i> -C ₄ H ₉	H	H	944.82	943.05	1177.83	1183.88	2.87	7.56	944.4		944.4	
72	1-Me,5- <i>t</i> -Bu	CH ₃	H	H	<i>t</i> -C ₄ H ₉	942.28	943.95	1121.39	1123.46	1.92	6.61	939.2		939.2	
73	1-Me,3,5-di- <i>t</i> -Bu	CH ₃	<i>t</i> -C ₄ H ₉	H	<i>t</i> -C ₄ H ₉	969.17	971.47	1132.77	1137.85	4.44	9.13	970.8		970.8	
74	1,3,4,5-tetraMe	CH ₃	CH ₃	CO ₂ Et	CH ₃	960.86	964.96	1136.02	1138.02	4.47	9.16		958.05 ^m	962.1	4.27
75	1,4-diMe-3,5-di- <i>t</i> -Bu	CH ₃	<i>t</i> -C ₄ H ₉	CH ₃	<i>t</i> -C ₄ H ₉	976.75	978.91	1136.28	1137.19	4.33	9.01	979.6		979.6	
76	1-Me,3,5-diNO ₂	CH ₃	NO ₂	H	NO ₂	773.55	777.06	1000.15	999.75	-19.75	-15.07	788.8		788.8	
77	1-Me,4-Br	CH ₃	H	Br	H	890.16	890.48	1094.63	1095.68	-2.95	1.74				0.18
78	1,3-diMe,4-Br	CH ₃	CH ₃	Br	H	910.51	912.11	1104.72	1106.76	-1.00	3.68				0.87
79	1,5-diMe,4-Br	CH ₃	H	Br	CH ₃	908.61	909.70	1102.90	1104.78	-1.35	3.34				0.91
80	1,3,5-triMe,4-Br	CH ₃	CH ₃	Br	CH ₃	927.75	928.30	1112.34	1113.67	0.20	4.89				1.78
81	1,3-diMe,5-Br	CH ₃	CH ₃	H	Br	917.44	919.25	1108.19	1111.17	-0.23	4.46				1.20
82	1,3-diMe,4,5-diBr	CH ₃	CH ₃	Br	Br	899.37	901.02	1091.73	1093.86	-3.27	1.42				-0.60
83	1,5-diMe,3,4-diBr	CH ₃	Br	Br	CH ₃	895.35	896.49	1080.67	1082.22	-5.31	-0.62				-1.52
84	1,3-diMe,5-CO ₂ Et	CH ₃	CH ₃	H	CO ₂ Et	920.78	925.79	1100.44	1101.01	-2.01	2.67	924.9		924.9	
85	1,5-diMe,3-CO ₂ Et	CH ₃	CO ₂ Et	H	CH ₃	929.40	931.41	1098.25	1102.22	-1.80	2.89	933.4		933.4	
86	1-Me,3,5-diCO ₂ Et	CH ₃	CO ₂ Et	H	CO ₂ Et	902.42	907.71	1070.36	1073.83	-6.77	-2.09	913.4		913.4	
87	1-Me,3-NO ₂	CH ₃	NO ₂	H	H	839.78	836.58	1048.78	1051.41	-10.70	-6.01	850.3		850.3	-4.58

88	1-Me,5-NO ₂	CH ₃	H	H	NO ₂	836.78	840.05	1060.95	1062.41	-8.78	-4.09	847.6		847.6	-2.35
89	1-Me,4-NO ₂	CH ₃	H	NO ₂	H	837.46	838.63	1064.79	1065.80	-8.18	-3.49				-2.18
90	1,3,5-TriMe,4-NO ₂	CH ₃	CH ₃	NO ₂	CH ₃	879.52	882.04	1082.57	1084.18	-4.96	-0.27				-0.95
91	1-Me,3-Ph	CH ₃	C ₆ H ₅	H	H	937.51	933.71	1110.63	1113.49	0.17	4.86	932.6		932.6	
92	1-Me,5-Ph	CH ₃	H	H	C ₆ H ₅	939.67	941.36	1115.46	1117.76	0.92	5.61	932.4		932.4	
93	1,3-diMe,5-Ph	CH ₃	CH ₃	H	C ₆ H ₅	956.43	959.76	1124.49	1127.04	2.55	7.24	956.6		956.6	
94	1,5-diMe,3-Ph	CH ₃	C ₆ H ₅	H	CH ₃	954.29	953.77	1118.65	1122.14	1.69	6.38	954.3		954.3	
95	1-Me,3,5-diPh	CH ₃	C ₆ H ₅	H	C ₆ H ₅	958.71	959.82	1112.48	1116.11	0.63	5.32	958.9		958.9	1.26
96	1-Me,3-NH ₂	CH ₃	NH ₂	H	H	942.81	945.28	1129.19	1133.65	3.71	8.39	937.4		937.4	3.81
97	1-Me,5-NH ₂	CH ₃	H	H	NH ₂	951.47	954.26	1133.48	1134.52	3.86	8.55	949.5		949.5	4.23
98	1-Me,4-NH ₂	CH ₃	H	NH ₂	H	933.11	936.58	1120.05	1119.02	1.14	5.83				5.52
98c	1-Me,4-NH ₂	CH ₃	H	NH ₃ ⁺	H	877.75	881.81	1107.19	1107.61	-0.86	3.83				5.52
99	1-Me,3,5-diPh,4-OH	CH ₃	C ₆ H ₅	OH	C ₆ H ₅	958.30	961.65	1109.39	1111.89	-0.11	4.58				1.96
100	1,3-diMe,5-EtO	CH ₃	CH ₃	H	OC ₂ H ₅	965.61	969.83	1133.29	1135.96	4.11	8.80				3.51
101	1,5-diMe,3-EtO	CH ₃	OC ₂ H ₅	H	CH ₃	967.24	970.17	1125.99	1128.66	2.83	7.52				2.05
102	1-Et	C ₂ H ₅	H	H	H	919.72	921.26	1113.50	1115.45	0.52	5.21				2.00
103	1-Et,3-NO ₂	C ₂ H ₅	NO ₂	H	H	847.92	848.04	1048.43	1049.76	-10.99	-6.30				-4.71
104	1-Et,5-NO ₂	C ₂ H ₅	H	H	NO ₂	846.90	849.38	1062.04	1060.91	-9.04	-4.35				-2.32
105	1-Et,4-NO ₂	C ₂ H ₅	H	NO ₂	H	845.68	848.49	1064.03	1064.35	-8.44	-3.75				-2.13
106	1- <i>n</i> -Bu	<i>n</i> -C ₄ H ₉	H	H	H	926.30	926.72	1113.34	1113.66	0.20	4.89	928.8	923.8	928.8	
107	1- <i>t</i> -Bu	<i>t</i> -C ₄ H ₉	H	H	H	933.83	936.79	1115.61	1115.21	0.48	5.16				1.95
108	1-Adamantyl	1-Ad ^c	H	H	H	948.26	950.80	1118.93	1119.34	1.20	5.89	954.5	947.2	954.5	
109	1-Phenyl (Ph)	C ₆ H ₅	H	H	H	922.77	925.26	1099.19	1102.41	-1.77	2.92				0.44
110	1-Ph,3,5-diMe	C ₆ H ₅	CH ₃	H	CH ₃	964.57	974.98	1121.89	1124.14	2.04	6.73				2.65
111	1,5-diPhenyl,3-Me	C ₆ H ₅	CH ₃	H	C ₆ H ₅	966.07	971.92	1115.76	1119.17	1.17	5.86				1.51
112	1,3,5-triPhenyl	C ₆ H ₅	C ₆ H ₅	H	C ₆ H ₅	968.83	968.72	1105.78	1106.68	-1.02	3.67				0.39
113	1-Phenyl,4-Cl	C ₆ H ₅	H	Cl	H	899.68	902.24	1082.93	1085.87	-4.67	0.02				-1.40
114	1-Phenyl,4-Br	C ₆ H ₅	H	Br	H	901.93	904.10	1082.21	1085.31	-4.76	-0.08				-1.32
115	1-Phenyl-3-NH ₂	C ₆ H ₅	NH ₂	H	H	946.74	951.88	1115.69	1118.39	1.03	5.72				2.91
116	1-Phenyl-5-NH ₂	C ₆ H ₅	H	H	NH ₂	968.47	977.58	1128.33	1133.54	3.69	8.37				3.09
117	1-Phenyl-4-NH ₂	C ₆ H ₅	H	NH ₂	H	938.97	940.69	1104.66	1106.77	-1.00	3.68				4.73
117c	1-Phenyl-4-NH ₂	C ₆ H ₅	H	NH ₃ ⁺	H	873.39	876.80	1098.15	1099.75	-2.23	2.45				4.73
118	1-Phenyl,3-Me,5-NH ₂	C ₆ H ₅	CH ₃	H	NH ₂	982.53	990.91	1135.11	1135.54	4.04	8.73				4.76
119	1-Phenyl,3-Me,5-EtO	C ₆ H ₅	CH ₃	H	OC ₂ H ₅	971.99	980.31	1119.75	1123.13	1.86	6.55				2.34
120	1-Phenyl,3-MeO,5-Me	C ₆ H ₅	OCH ₃	H	CH ₃	946.64	955.65	1103.60	1111.86	-0.11	4.58				1.17
121	1Phenyl,3,4-diMe,5OEt	C ₆ H ₅	CH ₃	CH ₃	OC ₂ H ₅	979.55	986.23	1124.54	1127.44	2.62	7.31				2.55
122	1-pNP	pNP ^e	H	H	H	878.30	880.42	1081.42	1084.03	-4.99	-0.30				-0.65
123	1-pNP,3-Me	pNP ^e	CH ₃	H	H	895.22	899.97	1090.14	1089.56	-4.02	0.67				0.14
124	1-pNP,5-Me	pNP ^e	H	H	CH ₃	906.47	913.89	1097.65	1100.91	-2.03	2.66				0.62
125	1-pNP,4-Me	pNP ^e	H	CH ₃	H	889.85	893.83	1085.55	1087.28	-4.42	0.27				-0.16
126	1-pNP,3,4-diMe	pNP ^e	CH ₃	CH ₃	H	904.84	904.56	1093.33	1097.13	-2.69	1.99				0.51
127	1-pNP,4,5-diMe	pNP ^e	H	CH ₃	CH ₃	918.41	924.91	1102.42	1106.75	-1.01	3.68				1.08
128	1-pNP,3,5-diMe	pNP ^e	CH ₃	H	CH ₃	922.32	933.98	1105.40	1107.25	-0.92	3.77				1.50
129	1-pNP,3,4,5-triMe	pNP ^e	CH ₃	CH ₃	CH ₃	931.38	943.72	1110.00	1117.74	0.92	5.61				1.87

130	1-pNP,3-NH ₂	pNP ^e	NH ₂	H	H	902.81	907.02	1099.32	1108.37	-0.72	3.96				1.93
131	1-pNP,5-NH ₂	pNP ^e	H	H	NH ₂	925.14	933.04	1111.31	1112.81	0.05	4.74				2.11
132	1-pNP,4-NH ₂	pNP ^e	H	NH ₂	H	893.19	893.95	1084.64	1086.33	-4.58	0.10				4.05
132c	1-pNP,4-NH ₂	pNP ^e	H	NH ₃ ⁺	H	839.00	840.76	1087.11	1087.04	-4.46	0.23				4.05
133	1-DNP	DNP ^f	H	H	H	875.64	876.58	1078.16	1076.97	-6.22	-1.54				-1.40
134	1-DNP,3-Me	DNP ^f	CH ₃	H	H	893.82	896.01	1086.16	1087.35	-4.41	0.28				-0.28
135	1-DNP,3-Et	DNP ^f	C ₂ H ₅	H	H	898.03	899.65	1085.46	1089.17	-4.09	0.60				-0.42
136	1-DNP,3- <i>t</i> -Bu	DNP ^f	<i>t</i> -C ₄ H ₉	H	H	906.49	906.24	1086.41	1083.38	-5.10	-0.41				-0.60
137	1-DNP,5-Me	DNP ^f	H	H	CH ₃	893.45	899.27	1088.04	1099.03	-2.36	2.33				-0.13
138	1-DNP,4-Me	DNP ^f	H	CH ₃	H	886.73	888.95	1081.62	1081.76	-5.39	-0.70				-0.90
139	1-DNP,3,4-diMe	DNP ^f	CH ₃	CH ₃	H	903.41	905.99	1089.08	1089.02	-4.11	0.57				-0.10
140	1-DNP,4,5-diMe	DNP ^f	H	CH ₃	CH ₃	904.78	909.72	1089.56	1096.79	-2.75	1.94				0.20
141	1-DNP,3,5-diMe	DNP ^f	CH ₃	H	CH ₃	909.19	919.11	1095.55	1106.27	-1.09	3.60				0.55
142	1-DNP,3,4,5-triMe	DNP ^f	CH ₃	CH ₃	CH ₃	917.65	925.75	1100.55	1102.90	-1.68	3.01				0.70
143	1-DNP,2 <i>H</i> -campho ^d	DNP ^f	---	---	H	917.69	918.13	1089.43	1091.69	-3.65	1.04				-1.00
144	1-DNP,1 <i>H</i> -campho ^d	DNP ^f	H	---	---	933.05	938.00	1102.18	1106.08	-1.13	3.56				0.36
145	1-TNP	TNP ^g	H	H	H	857.16	862.63	1066.04	1067.45	-7.89	-3.20				-2.00
146	1-Acetyl	COCH ₃	H	H	H	865.79	867.77	1075.68	1077.59	-6.12	-1.43				2.94
147	1-NO ₂	NO ₂	H	H	H	834.43	837.72	1047.96	1049.75	-10.99	-6.30				-4.15
148	1-Amino	NH ₂	H	H	H	894.13	895.17	1100.76	1099.84	-2.22	2.47				<0.4
148c	1-NH ₂	NH ₂	H	H	H	799.31	801.83	1047.65	1048.75	-11.17	-6.48				<0.4
149	1-Chloro	Cl	H	H	H	866.32	867.80	1075.59	1077.60	-6.11	-1.43				
150	1-C(NH)NH ₂ ,3,5-diMe	^h	CH ₃	H	CH ₃	927.85	933.20	1103.20	1103.90	-1.51	3.18				
150c	1-C(NH)NH ₂ ,3,5-diMe	^h	CH ₃	H	CH ₃	994.31	997.37	1167.66	1169.23	9.94	14.63				

^a Tautomer **4a** with solvent effect has an imaginary frequency (*i* 17 cm⁻¹); ^b Compound **6** with solvent effect has an imaginary frequency (*i* 52 cm⁻¹); ^c 1-Ad; ^d (4*S*,7*R*)-7,8,8-trimethyl-4,5,6,7-tetrahydro-4,7-methano-2(1)*H*-indazole; ^e pNP; ^f DNP; ^g TNP. ^h 3,5-dimethyl-1*H*-pyrazole-1-carboximidamide; ⁱ p*K*_a = 0.1752*[Δ*G*_{aq} + Δ*G*_s(H⁺)]; where Δ*G*_s(H⁺) = -1112.5 kJ·mol⁻¹. ^j p*K*_a 0.1752*[Δ*G*_{aq} + Δ*G*_s(H⁺)]; where Δ*G*_s(H⁺) = -1085.7 kJ·mol⁻¹. ^k From references 12-22; ^l From reference 18; ^m From reference 15.

Table S2 Torsion angles (°) between the phenyl substituent and the pyrazole ring

	45a	46b	47b	48b	49a	50a	51b	52b	60a
	3-Ph	3-Ph,4-Cl	3-Ph,4-Br	3-Ph,4-Me	3-Ph,5-Me	3-Ph,5-Et	3-Ph,4,5-diMe	3-Ph,4-Br,5-Me	3-Ph,5-CO ₂ Et
θ	0.03	30.51	33.29	29.13	0.03	4.04	31.18	32.67	0.03

Table S3 Equations relating experimental and calculated p*K*_as

All compounds	n = 163	p <i>K</i> _a exp. = (-0.22±0.11) + (0.53±0.02) p <i>K</i> _a ^j calc.	R ² = 0.786
Removing 15b , 29b , 30b , 34b , 37b , 38b , 42b , 55b , 56 , 62 , 98 , 117 , 132 , 146 , 148c	n = 148	p <i>K</i> _a exp. = (-0.30±0.01) + (0.54±0.02) p <i>K</i> _a ^j calc.	R ² = 0.786

1, B3LYP Energy= -226.265996831 Hartree,
NIMAG= 0

N,-0.6609457355,0,-0.8270821445
N,0.6856061555,0,-0.8911103669
C,1.0748012316,0,0.3803745209
C,-0.0260746652,0,1.2670096763
C,-1.1342450268,0,0.4455047328
H,-1.1896245942,0,-1.6842072262
H,2.1286178565,0,0.6150192677
H,-0.0137651632,0,2.3443615678
H,-2.1905187386,0,0.6617899521

1H, B3LYP Energy= -226.618654088 Hartree,
NIMAG= 0

N,-0.675111914,0,-0.8594777245
N,0.675111914,0,-0.8594777245
C,1.110864006,0,0.4105448301
C,0,0,1.2464070086
C,-1.110864006,0,0.4105448301
H,-1.2046277626,0,-1.723043184
H,2.1669087426,0,0.6325431324
H,0,0,2.3233990733
H,-2.1669087426,0,0.6325431324
H,1.2046277626,0,-1.723043184

2a, B3LYP Energy= -265.596765023 Hartree,
NIMAG= 0

N,-0.8177211213,-0.0490223434,-0.8567887981
N,0.5312687027,-0.0687060666,-0.9247022115
C,0.9399475781,-0.0061227643,0.341115059
C,-0.1672979885,0.054066603,1.2277537642
C,-1.2805786512,0.0240341462,0.4162911978
H,-1.3506633488,-0.0884655972,-1.7097633331
C,2.3996803002,-0.0062698716,0.6738862858
H,-0.1501669289,0.1112752985,2.3042437269
H,-2.3351520757,0.0484999173,0.640913837
H,2.9886175611,-0.0618951589,-0.2423254395
H,2.6838886977,0.9023787997,1.2127895039
H,2.6623049946,-0.8597729628,1.3058572975

2b, B3LYP Energy= -265.596355339 Hartree,
NIMAG= 0

N,-0.5077216697,-0.0591384409,-0.858740564
N,0.8428547053,-0.0518249478,-0.9206157343
C,1.2239782694,0.0136445221,0.3494143432
C,0.1168613807,0.0484995936,1.2284276707
C,-0.9971378962,-0.0003266135,0.4106444392
H,-1.0321509899,-0.1051925303,-1.7177753683
H,2.2763650092,0.0335435554,0.5906090275
H,0.1245966387,0.1015263313,2.3051871583
C,-2.4602607153,0.0037460998,0.7157391344
H,-2.9524405444,-0.9033216652,0.3506830809
H,-2.6153953592,0.0553152929,1.7937872414
H,-2.9655040087,0.8635288031,0.264311731

2H, B3LYP Energy= -611.632422765 Hartree,
NIMAG= 0

N,-0.7825928024,0.0055064402,-0.893758424

N,0.5705977098,-0.0052765607,-0.8617543107
C,0.9972543983,-0.0093438072,0.4167695809
C,-0.1485150086,-0.0045874068,1.2221532495
C,-1.2400520959,0.004494336,0.3697073688
H,-1.2930002198,0.0012203966,-1.7674280362
C,2.4420299226,-0.0011323076,0.7765963142
H,-0.1733935638,-0.0080263032,2.2991040815
H,-2.2996632755,0.0086743812,0.5732401539
H,1.1159206663,-0.0059103844,-1.7147623239
H,3.0769810841,-0.2298725082,-0.0803986384
H,2.7260222247,0.9811813708,1.1643179697
H,2.6368858401,-0.7369276466,1.5586311346

3a, B3LYP Energy= -304.920577307 Hartree,
NIMAG= 0

N,-0.8189677017,0.063678836,-0.8416620572
N,0.5303900049,0.0824699177,-0.8916318235
C,0.9232446253,-0.0199248355,0.3772026475
C,-0.1960702916,-0.1064595543,1.2468931644
C,-1.2986623598,-0.0504487239,0.422297008
H,-1.3411330723,0.1202278827,-1.7004347139
C,2.3814752519,-0.0047928232,0.7318228629
H,-0.1943599602,-0.2006135096,2.3209169213
H,-2.3561180773,-0.0865428578,0.6313194657
H,2.9519324897,-0.204599015,-0.1786137507
H,2.5923707539,-0.8246745998,1.4270837211
C,2.8423969567,1.3237997374,1.3542450101
H,2.2967018595,1.5416908976,2.276527288
H,3.9087852932,1.2901480726,1.5946648625
H,2.6752456579,2.1536429752,0.6628895836

3b, B3LYP Energy= -304.920098401 Hartree,
NIMAG= 0

N,-0.4870206705,0.1746075495,-0.8937503003
N,0.8632236448,0.1419416432,-0.9344625901
C,1.2206082706,-0.0246723921,0.3339528075
C,0.0982761609,-0.0958085879,1.1900373859
C,-1.0011060952,0.0382274387,0.3603795745
H,-0.994424008,0.3064338774,-1.7541754167
H,2.2681260899,-0.0833293968,0.5897475484
H,0.0866692041,-0.2228456157,2.2606854111
C,-2.4735208771,0.0127413615,0.6380340112
H,-2.6237067306,0.2584716205,1.6923158664
H,-2.9684008674,0.8066757125,0.066619495
C,-3.1409376586,-1.3388770426,0.3248425738
H,-4.2082850109,-1.3048100128,0.5592862673
H,-3.0375791324,-1.6000914969,-0.731758257
H,-2.6872265196,-2.1413550284,0.911070953

3H, B3LYP Energy= -305.283505600 Hartree,
NIMAG= 0

N,-0.8729415929,0.0297364604,-0.8739522233
N,0.4810531085,0.0430588407,-0.8790898615
C,0.9455066301,-0.0082366906,0.3850040332
C,-0.1782712249,-0.0542413989,1.2216045769
C,-1.2935052525,-0.0306679589,0.4014009397
H,-1.4079655811,0.0523377558,-1.7323009236
C,2.4053557989,0.0146195677,0.7043723006
H,-0.1742322247,-0.1031260116,2.2975999456
H,-2.3467543754,-0.0546166134,0.634290644

H,1.0025225475,0.0779827895,-1.7461153832
H,2.9804451437,-0.1397688055,-0.212928832
H,2.6181070328,-0.8392151475,1.3541289114
C,2.8439099778,1.3206775406,1.3958720071
H,2.3162505795,1.468882732,2.3398389197
H,3.9120916202,1.2742017567,1.6117029176
H,2.6626977238,2.1893929753,0.7597294306

4a, B3LYP Energy= -383.567825889 Hartree,
NIMAG= 0

N,-0.8492929537,-0.0485493137,-0.8258406681
N,0.4967668791,-0.0686247455,-0.9265387823
C,0.9411031121,-0.0077333069,0.3270736008
C,-0.1476375487,0.0513924648,1.2412227542
C,-1.2799666473,0.0230718181,0.4585928303
H,-1.4030843614,-0.0863744731,-1.6655609605
C,2.4247836581,-0.0069286582,0.6516056417
H,-0.1121416979,0.1070143315,2.3168465726
H,-2.3285157053,0.0476478988,0.7101079261
C,2.77610724,1.2899516977,1.4149947111
H,2.2081906614,1.3748183859,2.3455740878
H,3.8405747959,1.3049953066,1.6689554785
H,2.5585175783,2.1717902206,0.80646837
C,3.2647985022,-0.0815265215,-0.6349580553
H,4.3290725691,-0.0799464311,-0.3811047641
H,3.0452231502,-0.9896397772,-1.2001401949
H,3.0639874191,0.7688651633,-1.2898036518
C,2.7491704946,-1.2266693529,1.5432679324
H,2.5119893509,-2.160960622,1.027379149
H,3.8133889239,-1.2386237465,1.7984364742
H,2.1806757393,-1.2042551686,2.4770976782

4b, B3LYP Energy= -383.567519284 Hartree,
NIMAG= 0

N,-0.5297040208,-0.0626592816,-0.8663652709
N,0.8187613658,-0.0584225083,-0.9525436132
C,1.2224335145,0.007943496,0.3101488951
C,0.1315321461,0.0460082983,1.2082023771
C,-1.00100121,-0.0009332055,0.4119245739
H,-1.0637113884,-0.1088421733,-1.7186145983
H,2.278853837,0.0260002448,0.5335778579
H,0.1691412475,0.1001703702,2.2832324425
C,-2.4810693265,0.0058575296,0.7382798611
C,-3.1574405041,1.2314075866,0.0815722385
H,-3.071377465,1.2086232911,-1.0086131373
H,-4.2232471181,1.2533351014,0.327328655
H,-2.7053005831,2.1621642046,0.4329580642
C,-2.6742225634,0.0840491202,2.2630348893
H,-3.7408897881,0.0890539188,2.5031081745
H,-2.220407664,-0.7734329941,2.7664070581
H,-2.2327783108,0.9955132786,2.6740468182
C,-3.1394978996,-1.2908192589,0.2132047084
H,-2.6747045248,-2.1734271501,0.6595300152
H,-4.2051482909,-1.3020155348,0.4603635228
H,-3.0523933932,-1.3805205837,-0.8734489121

4H, B3LYP Energy= -383.934409124 Hartree,
NIMAG= 0

N,-0.8964531626,-0.0492177181,-0.8514713835
N,0.456970297,-0.0656227761,-0.888889255

C,0.9562677599,-0.0062593947,0.3603274741
C,-0.1502142301,0.0504743158,1.2243866024
C,-1.2846459065,0.0216127372,0.4344296466
H,-1.4512830587,-0.0871205981,-1.6961340327
C,2.4393091498,-0.0068918867,0.6572130576
H,-0.1240321519,0.1059712361,2.2991371543
H,-2.3315053866,0.046292949,0.6941609021
H,0.9592730444,-0.1163206135,-1.7656445121
C,2.7797889172,1.2975276408,1.4176944142
H,2.2285569143,1.3735011003,2.357325842
H,3.8455492459,1.3064148351,1.6555284221
H,2.5596381178,2.1829224744,0.8164524932
C,3.2612422423,-0.0821431253,-0.643238712
H,4.3245972645,-0.0809216336,-0.3994720073
H,3.0684144013,-1.0039958927,-1.2018391057
H,3.087244672,0.781715248,-1.2932283481
C,2.7527272277,-1.2339883094,1.5470677898
H,2.5131367883,-2.1711505276,1.0389270157
H,3.818308951,-1.2412823621,1.7857612021
H,2.2009609438,-1.2020483808,2.4889081514

5, B3LYP Energy= -701.267354150 Hartree,
NIMAG= 0

N,-0.6651137935,0.0553479538,-0.9845602706
N,0.6643350334,-0.1432192079,-1.0480189053
C,1.050637295,-0.1823465455,0.2235036469
C,-0.0328993488,-0.0082713369,1.1220260532
C,-1.1267810448,0.1424759846,0.2921679513
H,-1.191773686,0.1216776451,-1.8399676213
H,2.0946064211,-0.3342168942,0.4579283024
C,-0.000486638,0.0085332247,2.6211181013
H,-2.1711749949,0.3007962521,0.5114205102
H,0.3817411724,-0.9338420242,3.0248934108
H,0.6412492366,0.8098246825,2.9996875066
H,-0.9995591227,0.1632402659,3.0344761546

5H, B3LYP Energy= -701.621541990 Hartree,
NIMAG= 0

N,-0.6735064956,-0.0036080699,-1.004185282
N,0.6738283009,-0.0036551749,-1.004539538
C,1.1059421131,0.0022619565,0.2686861646
C,0.00022538,0.0052883325,1.1200036341
C,-1.1067021145,0.0023731165,0.2675477819
H,-1.2041439161,-0.0026867947,-1.8665092012
H,2.1624727937,0.005818239,0.489015147
C,0.0003126259,-0.0001443908,2.6185689853
H,-2.1637972181,0.0058701607,0.4857453785
H,1.2041987181,-0.0026464567,-1.8668957056
H,-0.2630956042,-0.9881625142,3.0037720222
H,0.9845633186,0.2609059306,3.0075729922
H,-0.7202979019,0.7183856654,3.012355041

6, B3LYP Energy= -572.192084578 Hartree,
NIMAG= 0

N,0.007334679,-1.1120938741,-0.0532548855
N,1.1520142852,-0.4157092966,0.0599231808
C,0.7580496964,0.8554279936,0.08782866
C,-0.6513076285,0.9902156899,-0.008352046
C,-1.0948226162,-0.3198390199,-0.0985129537
H,0.0475434102,-2.1173761238,-0.0971917787

H,1.5015021271,1.632690451,0.1750925888
C,-1.4913112037,2.2483437988,-0.0057267522
H,-2.0843075098,-0.7390048949,-0.1893725064
C,-0.6016200629,3.5158468003,0.0340332556
C,-2.4268004224,2.2774496179,1.2358514271
C,-2.3768694295,2.3194931067,-1.2810438083
H,0.0310362009,3.4949257447,0.9287972093
H,0.0690978426,3.5220432659,-0.8328872352
C,-1.4647792939,4.7924978394,0.0372434281
H,-1.8201811983,2.2255175302,2.1469722035
H,-3.0684190795,1.3889626699,1.2329886137
C,-3.2924668308,3.5520397924,1.2397984394
H,-1.7350329809,2.2980190894,-2.1688561661
H,-3.0191363684,1.4328410034,-1.3332238635
C,-3.2435306297,3.5935385814,-1.2770568392
H,-0.8074790631,5.6684626645,0.0642246057
C,-2.3787196305,4.7922435229,1.2782644124
C,-2.3295130243,4.8335566537,-1.238040964
H,-3.94015208,3.5444343451,2.1234997992
C,-4.1573048729,3.5900297599,-0.0357900616
H,-3.855605662,3.6154337133,-2.1855459951
H,-2.9830826583,5.7065489798,1.3018236904
H,-1.773367678,4.7858752199,2.1922802969
H,-1.6887918832,4.8570675336,-2.1273336777
H,-2.932967318,5.748612838,-1.2551092365
H,-4.826720354,2.7218463279,-0.0630667882
H,-4.7937557626,4.4826122758,-0.033690753

6H, B3LYP Energy= -572.559367963 Hartree,
NIMAG= 0

N,-0.0407576011,-1.1429692731,-0.0285492732
N,1.0873551295,-0.4072260814,0.0171205064
C,0.751116527,0.8964228685,0.0335989792
C,-0.6404545349,1.0080368305,-0.0024966442
C,-1.0978471168,-0.3144404104,-0.041139838
H,-0.0134907507,-2.1544797217,-0.0479215101
H,1.5169539712,1.6541518945,0.0697251749
C,-1.480925279,2.2636949136,-0.000884868
H,-2.0988997982,-0.7142087552,-0.0764299731
H,2.0017242087,-0.8400541844,0.0331620689
C,-0.5889636928,3.5285703548,0.0493382175
C,-2.4217303951,2.2671897038,1.2382992578
C,-2.3509581924,2.3176814549,-1.289653518
H,0.0347471833,3.5123817712,0.9519247424
H,0.0842070967,3.5477612641,-0.8169259375
C,-1.465243352,4.7972348959,0.0501697311
H,-1.8235760148,2.2210649566,2.1553392034
H,-3.0625577063,1.3772682429,1.2259279554
C,-3.2946900357,3.5373120917,1.2332782759
H,-1.7023904906,2.3075452759,-2.1729051103
H,-2.9904206271,1.4286491968,-1.3486661743
C,-3.2242686342,3.5875479294,-1.2827567313
H,-0.8125863492,5.6742595177,0.0859282675
C,-2.3867852905,4.7815766031,1.285106558
C,-2.3162792011,4.8318900399,-1.2340291886
H,-3.9462177127,3.517881169,2.1118231393
C,-4.1479228709,3.5690527007,-0.0494925199
H,-3.8255919655,3.6039442631,-2.1964602165
H,-2.9972922018,5.6894858817,1.3065675243
H,-1.7911000906,4.7791311992,2.2049285128
H,-1.670067951,4.86549921,-2.1184455516
H,-2.9256518124,5.7406093253,-1.2533306162

H,-4.8129830537,2.6983730668,-0.0854581179
H,-4.7901737369,4.4550737912,-0.0497722904

7 B3LYP Energy= -701.262360231 Hartree,
NIMAG= 0

N,-0.6650095671,-0.1045802238,-0.8811676042
N,0.6884268961,-0.1116783113,-0.9466933197
C,1.0883832384,-0.0115870542,0.3172147998
C,-0.025449423,0.0601449132,1.1953435206
C,-1.1442438562,-0.0025875788,0.3878820181
H,-1.193079334,-0.170544098,-1.7361352004
C,2.5459429972,0.0130649658,0.6585485066
H,-0.0138627943,0.1455938148,2.2706793563
C,-2.6047682922,0.0251363164,0.7041917019
H,3.1408901331,-0.0605111281,-0.2526557792
H,2.8176120361,0.9387981804,1.1747671897
H,2.814554107,-0.8202049983,1.3148720435
H,-3.1088371573,-0.8874172112,0.3701472087
H,-2.7507506204,0.1105366562,1.7814231248
H,-3.1054871432,0.8758357569,0.2308655034

7H B3LYP Energy= -701.620524002 Hartree,
NIMAG= 0

N,-0.6779266758,1.104964029,0.0882986273
N,0.6786540127,1.1058936828,0.0659110547
C,1.1265727678,-0.1631962915,-0.0196996774
C,-0.0004258657,-0.9846176769,-0.0647956296
C,-1.1266474608,-0.1641358572,0.0014229721
H,-1.2041712579,1.9678032874,0.1294446745
C,2.5784159291,-0.495238361,-0.0340036716
H,-0.0008831887,-2.0597062986,-0.1375971381
C,-2.5787191858,-0.4935079777,-0.0339266473
H,1.2057649928,1.9655840463,0.144968064
H,3.1968307166,0.390125747,-0.1880056133
H,2.8674802118,-0.9570914273,0.9138729673
H,2.7919900791,-1.2089529954,-0.8314578657
H,-2.8845351478,-0.7364391407,-1.0554210164
H,-2.7805824408,-1.364617224,0.5908905886
H,-3.1923344866,0.3360344577,0.3204603109

8a total Energy= -304.924349329 Hartree,
NIMAG= 0

N,-0.8238747561,0.0492210078,-0.9919015689
N,0.5060753638,-0.1565659122,-1.0789662399
C,0.9313117304,-0.1793972322,0.1825247404
C,-0.143625669,0.0154807179,1.0971079303
C,-1.2551097852,0.158269394,0.2920088391
H,-1.3674973503,0.1050001531,-1.8368378428
C,2.3784867228,-0.3890731536,0.5004737782
C,-0.0740568717,0.0548410218,2.593711937
H,-2.293465683,0.3246966169,0.5340658008
H,0.3163432453,-0.8822043998,3.004158262
H,0.5811715608,0.8582401295,2.9460967656
H,-1.0615444718,0.2196738809,3.030405356
H,2.9479978503,-0.5067209427,-0.4220964265
H,2.7925500012,0.4588663358,1.0556002569
H,2.5274802025,-1.2833463772,1.1142139019

8b, B3LYP Energy= -304.923258173 Hartree,
NIMAG= 0

N,-0.5081976997,0.0847237925,-1.0069269782
N,0.833208556,-0.0470550573,-1.0488958976
C,1.1896017044,-0.0945054178,0.2300014068
C,0.0798622424,0.0102602277,1.1043891889
C,-1.013115798,0.1278699903,0.2584523217
H,-1.0184290686,0.1584871215,-1.8724559371
H,2.2337479869,-0.1959266001,0.4905268599
C,0.0864774072,-0.0192826227,2.6039162704
C,-2.4757972542,0.2511249597,0.5383586755
H,-0.1590602043,-1.0117122666,2.9974680892
H,1.0716756948,0.2498336237,2.9918584522
H,-0.6348785494,0.6859060787,3.0274103326
H,-2.9658055461,-0.7274669892,0.5852141443
H,-2.6409597902,0.7461104906,1.4974711752
H,-2.9829103412,0.8410444189,-0.2303957337

8H, B3LYP Energy= -305.290694968 Hartree,
NIMAG= 0

N,-0.8699761623,0.0557465845,-1.0094878921
N,0.4651213765,-0.1489180138,-1.0458933908
C,0.9539258024,-0.1815189973,0.209036811
C,-0.1287369624,0.0129306953,1.0880434729
C,-1.2482972487,0.1565571118,0.2782199137
H,-1.4220924449,0.1123627639,-1.8547660382
C,2.3982585412,-0.3921707695,0.498569478
C,-0.0705814868,0.0540578252,2.5838544153
H,-2.2834134519,0.3229749694,0.5341767785
H,0.9578700267,-0.2537500115,-1.923611344
H,0.3146161058,-0.8846814611,2.9896795846
H,0.5799455971,0.8605007269,2.9313775654
H,-1.061731027,0.2188621117,3.0064177406
H,2.985478656,-0.5121882692,-0.4126259606
H,2.7985824092,0.4578305907,1.0571905388
H,2.5327955077,-1.2844926388,1.1154002809

9, B3LYP Energy= -740.596020443 Hartree,
NIMAG= 0

N,-0.6717679792,-0.0094107347,-0.9760789441
N,0.6778407507,-0.041400599,-1.0421870137
C,1.0754060275,-0.0313541407,0.2260915099
C,-0.0341133858,0.0099184674,1.1195026027
C,-1.1500977581,0.0242469664,0.2992679467
H,-1.2022239182,-0.0007518942,-1.8317705969
C,2.5306269091,-0.0576368035,0.5738117596
C,0.0178775071,0.0264161076,2.6172910861
C,-2.6141718251,0.0397780587,0.6006958725
H,3.1288932833,-0.0753288041,-0.3379536238
H,2.8184856585,0.8225119819,1.1581751656
H,2.7843477824,-0.9402082101,1.1701377494
H,-3.0535481766,-0.9617040505,0.538412288
H,-2.7943177615,0.4154533481,1.6091191879
H,-3.1588767797,0.6863348534,-0.0937820119
H,0.6741642754,0.820627816,2.9875264995
H,-0.9707895874,0.190861953,3.0520469836
H,0.3975154177,-0.9183543052,3.0219914789

9H, B3LYP Energy= -740.953936983 Hartree,
NIMAG= 0

N,-0.712604309,0.0420129253,-1.0041607522
N,0.6408495195,0.0234609088,-1.0157729815
C,1.0968641117,-0.0055921141,0.2535015654
C,-0.0184300027,-0.0063721561,1.1018252823
C,-1.1475848057,0.0238401212,0.273058109
H,-1.2472844812,0.0708218026,-1.8617039063
C,2.5514534008,-0.032327934,0.5712159775
C,-0.0036277982,-0.0524215963,2.5993778704
C,-2.5975750441,0.0331397697,0.6132097051
H,1.1614077682,0.0427765959,-1.8822602264
H,3.1656353542,0.026542509,-0.3283693035
H,2.8126281687,0.8075587875,1.2195187787
H,2.80748249,-0.9526358995,1.1022124441
H,-2.8738428571,-0.8909918242,1.1271884038
H,-2.8239462166,0.8658246881,1.2832017773
H,-3.2226402413,0.1306102023,-0.2754956279
H,0.8531378304,0.490264657,3.0024484972
H,-0.9055197387,0.3976226244,3.016593447
H,0.0532438923,-1.0818127376,2.9652152722

10a, B3LYP Energy= -383.577865428 Hartree,
NIMAG= 0

N,-0.5912677045,-0.4792459816,-1.0733704352
N,0.7592781294,-0.4496147694,-1.0656341319
C,1.0808976297,-0.161555684,0.1922675553
C,-0.0795455756,-0.0083049535,1.0037772036
C,-1.1458992046,-0.2246664851,0.1453085005
H,-1.0690575181,-0.7026156682,-1.9311038186
C,2.5133580563,-0.0394683572,0.6079072687
C,-0.120402125,0.3193216141,2.4659642218
C,-2.6286206707,-0.1750926491,0.3556759954
H,3.1645170006,-0.2355245255,-0.2448161824
H,2.7366716424,0.9626193542,0.9886544285
H,2.7617047037,-0.7511431358,1.4021412973
H,-3.1098269582,-0.9310485624,-0.2756452451
H,-2.8456049789,-0.4644935501,1.3878038691
H,0.2087140123,1.3454212668,2.664615921
H,-1.1299095487,0.2181631262,2.8716383488
H,0.5318354568,-0.3437099161,3.0433101839
C,-3.2514867265,1.2038564855,0.0695624607
H,-3.0758006193,1.509756214,-0.9650923378
H,-4.3319026954,1.1835022266,0.237720917
H,-2.8197398758,1.9692077904,0.7189181794

10b, B3LYP Energy= -383.577135033 Hartree,
NIMAG= 0

N,-0.7271787625,-0.0457244987,-0.9838693864
N,0.6213608972,-0.0721125113,-1.0759152488
C,1.0449485375,-0.0355731484,0.1820035006
C,-0.0485468638,0.0150964667,1.0977333169
C,-1.1802783182,0.0067727412,0.300721684
H,-1.2738635189,-0.0658817954,-1.8289839983
C,2.5076581983,-0.0486032431,0.5287179563
C,0.0393993002,0.0656777485,2.5928341078
C,-2.6383049939,0.0432301124,0.6283302707
H,2.7339764139,0.8415263377,1.1299495967
H,2.7040067837,-0.9018591673,1.1908575839
H,-3.1591517888,-0.8458856797,0.257945879

H,-2.7841118627,0.0834615026,1.7081910787
H,-3.1288314861,0.921649344,0.1961799005
H,0.5886859595,0.9491097838,2.9357140114
H,-0.9500119854,0.0989846101,3.0545135688
H,0.5580841772,-0.8102844425,2.9970540101
C,3.4478791816,-0.1068943893,-0.6771846002
H,3.2996009389,0.7527872705,-1.3339930433
H,4.4900298787,-0.1132536069,-0.3467971225
H,3.2694088838,-1.0047217448,-1.2725773757

10H, B3LYP Energy= -383.952844829 Hartree,
NIMAG= 0

N,-0.6133017513,-0.5645290301,-1.1276085476
N,0.7369375719,-0.5120279953,-1.0449058972
C,1.0924173413,-0.1711503666,0.2103308777
C,-0.08556329,0.0006131552,0.9505610857
C,-1.1482989206,-0.2576836159,0.0738335913
H,-1.0786493506,-0.8258588816,-1.986154304
C,2.5169382084,-0.0321315636,0.6207781903
C,-0.1730628863,0.3916358575,2.3943720586
C,-2.627813325,-0.2023703991,0.2820542817
H,1.3235332419,-0.7273384769,-1.8396595192
H,3.2013236891,-0.2827424482,-0.1908473234
H,2.7223447824,0.9931140846,0.9391626801
H,2.7327011699,-0.6898437089,1.4663621683
H,-3.1216426036,-0.8337879247,-0.4623924387
H,-2.8497204337,-0.6449351155,1.256484262
H,0.0228282447,1.4588817443,2.5311885302
H,-1.1631936648,0.1825760634,2.8003095678
H,0.5535413802,-0.1582967631,2.9962699379
C,-3.1912945678,1.2314878167,0.2164327503
H,-3.0121568339,1.6862711047,-0.7602968996
H,-4.2688253092,1.2086772799,0.3859413031
H,-2.7430853786,1.871626123,0.9785262374

11, B3LYP Energy= -740.594001537 Hartree,
NIMAG= 0

N,-0.7012126391,0.0526133293,-1.022161095
N,0.6468539012,0.0203342638,-1.1004430054
C,1.056332411,-0.0197247687,0.1635156699
C,-0.0467812622,-0.0092529952,1.0668645765
C,-1.1700012599,0.0407870837,0.2578733005
H,-1.2379454922,0.1077162744,-1.8722877436
C,2.5153961158,-0.0638573815,0.5234127447
C,0.0131545145,-0.0482016208,2.5640671814
C,-2.6347694335,0.0410584889,0.5737772217
H,2.740437792,0.7853095497,1.1815755608
H,2.7010156175,-0.9584270562,1.131794088
H,-2.787033214,0.5534103948,1.5281445912
H,-3.1662755483,0.638772082,-0.1756874298
H,0.6720859596,0.7310273924,2.9608439124
H,-0.9738490456,0.1016386412,3.0080976409
H,0.3939627963,-1.0072706425,2.9326749616
C,3.4671839411,-0.0508889873,-0.6749867081
H,3.3296015132,0.8496195235,-1.2771188312
H,4.5060331018,-0.0842252851,-0.3358713402
H,3.2897871392,-0.9081047259,-1.3277216774
C,-3.2573102359,-1.3654972652,0.6435475371
H,-4.3240246873,-1.3060004648,0.8773076304
H,-3.1483896973,-1.8937609269,-0.3073526519
H,-2.7726646879,-1.9688784037,1.4148380255

11H, B3LYP Energy= -740.958244385 Hartree,
NIMAG= 0

N,-0.7311458132,0.0933111661,-1.090795222
N,0.6217025182,0.0461988603,-1.0910363178
C,1.0653307847,-0.0316744227,0.1789674641
C,-0.059837985,-0.0352655384,1.0179604905
C,-1.1808104745,0.046872829,0.1825968748
H,-1.2551343683,0.1796256791,-1.9507452526
C,2.5203583176,-0.1004627594,0.5212204048
C,-0.0479654577,-0.1206700072,2.513957503
C,-2.6422605177,0.0515108742,0.49871651
H,1.1535993146,0.0867265939,-1.9494276425
H,2.7265758315,0.6966371043,1.2437224057
H,2.6892538117,-1.0380265285,1.0625006177
H,-2.8005666606,0.7020147383,1.362811738
H,-3.1909570246,0.5047533063,-0.3320957071
H,0.7514922497,0.4906756212,2.9375847545
H,-0.9901547814,0.2303102688,2.9363314284
H,0.1056814871,-1.1486221355,2.8548306158
C,3.4799156189,0.0028485881,-0.668105297
H,3.374198,0.9542074566,-1.1974748385
H,4.5100703715,-0.0524891712,-0.3154060062
H,3.3438960304,-0.8190833878,-1.377397406
C,-3.1981753072,-1.3559955336,0.7938723727
H,-4.2617064301,-1.2880712798,1.0277029261
H,-3.0823679327,-2.018826014,-0.0664435156
H,-2.693319719,-1.8127739928,1.6470114339

12a, B3LYP Energy= -343.020660727 Hartree,
NIMAG= 0

N,-0.8757918026,0.3348727071,-1.1049825618
N,0.4179917977,0.0164897396,-1.3650655556
C,0.9091331081,-0.2431404759,-0.1627417815
C,-0.0425111877,-0.1015452604,0.8658488367
C,-1.2000268604,0.2763027606,0.2237425913
H,-1.4868384866,0.5513055843,-1.8753778034
C,2.2598470402,-0.6310540449,0.3632868165
C,0.5659414049,-0.3792255496,2.210685374
H,-2.1979135553,0.5006215472,0.5662131224
H,0.7553024746,0.5513345816,2.7587212619
H,-0.0453442072,-1.0127828109,2.8582676172
H,2.7437634534,-1.4229806109,-0.2123444034
H,2.9373040145,0.2306084125,0.3637926483
C,1.9101198871,-1.0800635506,1.817605316
H,2.7123165942,-0.8611997909,2.5252702453
H,1.7560511949,-2.1626187988,1.8248534062

12b, B3LYP Energy= -343.018698340 Hartree,
NIMAG= 0

N,-0.4741473358,-0.0753753125,-1.2310764536
N,0.8737832587,-0.247794482,-1.2029851577
C,1.2001621033,-0.2122992468,0.0906745506
C,0.0587651082,-0.0035229878,0.895967462
C,-0.9875958564,0.0810029041,0.0114217212
H,-0.9396389329,-0.0546635035,-2.1234277041
H,2.2360902676,-0.3317501049,0.3721120549
C,-0.4290755111,0.0995335605,2.3156787131
C,-2.3282333801,0.2485243311,0.6557215079
H,-0.4074620784,-0.8750539935,2.8173561353
H,0.1484246068,0.7895242819,2.9363951192

H,-2.9070934252,-0.6822102288,0.6181775837
H,-2.9472657138,1.0322473707,0.2102313929
C,-1.8993527222,0.6026065212,2.1193608212
H,-1.9196827259,1.6890834445,2.2354851854
H,-2.5850089027,0.1841447058,2.8588634781

12H, B3LYP Energy= -343.387306301 Hartree,
NIMAG= 0

N,-0.9199536884,0.3635390827,-1.1186359673
N,0.3816900803,0.0293767429,-1.3330215877
C,0.9365736859,-0.2578771313,-0.1485014673
C,-0.0259825682,-0.1069321021,0.8457896526
C,-1.190421023,0.2840974768,0.2055146752
H,-1.5397618674,0.5814823396,-1.887879453
C,2.2805384506,-0.6540615503,0.3641543305
C,0.562219344,-0.3928241639,2.2001576073
H,-2.1817586131,0.5102138955,0.5671568388
H,0.7736714427,0.0289565377,-2.2660466242
H,0.7145965931,0.5386407086,2.7530007448
H,-0.0645000023,-1.038224463,2.8164066419
H,2.7491151164,-1.4577055224,-0.2068159747
H,2.9579233006,0.2064193486,0.3371416131
C,1.9222529356,-1.074009507,1.8299852939
H,2.7158265769,-0.807178052,2.5263558344
H,1.8038217287,-2.1582273405,1.8670663884

13a, B3LYP Energy= -382.361113995 Hartree,
NIMAG= 0

N,-0.9932086174,0.213078687,-1.134307412
N,0.3329950796,-0.0129652866,-1.2473959755
C,0.7584539905,-0.1053103302,0.0100681052
C,-0.2986673666,0.0634724078,0.9401680108
C,-1.4175229614,0.2672456384,0.1568611323
H,-1.5435020496,0.3208240495,-1.9701956166
C,2.1799436795,-0.3806062378,0.4035062656
C,-0.1018883207,0.0336001045,2.4303892416
H,-2.4522967645,0.4427808638,0.4073864532
H,-0.1325976782,1.0544986228,2.8326181652
H,-0.9092176774,-0.5162068466,2.9248390379
H,2.8665046955,0.187819991,-0.2300194411
H,2.4062442551,-1.440785278,0.2343365891
C,1.2607895888,-0.6013330633,2.7719948582
H,1.4887062891,-0.4353689859,3.8292698111
H,1.2011906239,-1.6873056207,2.628895476
C,2.3906604357,-0.0401830226,1.8913490207
H,3.3567469492,-0.4301495208,2.2253057804
H,2.4325025989,1.0492352677,2.0135446478

13b, B3LYP Energy= -382.361074835 Hartree,
NIMAG= 0

N,-0.3089656515,0.1838904704,-1.05465181
N,1.039873322,0.2806704748,-1.0895038469
C,1.4053421543,0.2474514299,0.1885711261
C,0.2907043016,0.1270698539,1.0540442794
C,-0.8018741137,0.0907770377,0.2096717933
H,-0.8194508903,0.1885371437,-1.9227973646
H,2.4540863222,0.309490708,0.4420117547
C,0.1633322789,0.0545887206,2.5494409488
C,-2.2344280732,-0.044811217,0.6188229853
H,0.9292420986,-0.6014528815,2.9754272923

H,0.328265561,1.0454471751,2.9923383182
H,-2.5942686472,-1.059534126,0.403963855
H,-2.8757994213,0.6399899712,0.0531073201
C,-2.3513378133,0.2409961347,2.1309084656
H,-3.3341446999,-0.0794571996,2.4882653152
H,-2.2915871031,1.3230462215,2.2963703339
C,-1.2400481621,-0.454312687,2.9368026185
H,-1.2933513938,-1.5354818238,2.7598120718
H,-1.4080114993,-0.3026595165,4.0072074034

13H, B3LYP Energy= -382.730740102 Hartree,
NIMAG= 0

N,-1.0430595559,0.2165221159,-1.1536769931
N,0.2905909196,-0.0105467967,-1.2166375879
C,0.7814539809,-0.1089154301,0.0338580136
C,-0.283537039,0.0661709667,0.927353603
C,-1.4117590912,0.2679011695,0.1403351206
H,-1.6019705535,0.3240520316,-1.9895224569
C,2.201980136,-0.3738820326,0.4070003117
C,-0.0987332285,0.0325140362,2.4190649825
H,-2.4429432508,0.4430770613,0.4065153601
H,0.7682180319,-0.0861917231,-2.1054583921
H,-0.1476466104,1.055330301,2.8082642336
H,-0.9142977398,-0.5206012554,2.8909093306
H,2.8834366946,0.2072769591,-0.2211166393
H,2.421991339,-1.4318038777,0.219522048
C,1.2625148379,-0.6006275661,2.7711541832
H,1.4791514181,-0.4197672713,3.8255115763
H,1.2029864707,-1.6876842164,2.6467125117
C,2.402857065,-0.0452324287,1.9025467299
H,3.3598697892,-0.4580277327,2.2259211685
H,2.4694657077,1.0404975954,2.0281852377

14a, B3LYP Energy= -421.681054013 Hartree,
NIMAG= 0

N,-0.9527866341,-0.1779847661,-1.0316263108
N,0.365090975,-0.4404534664,-1.1361997455
C,0.8484372459,-0.2560322797,0.0917149684
C,-0.175122645,0.1425123475,0.9989105347
C,-1.3205984702,0.1729364047,0.2275248573
H,-1.5339920644,-0.25189566,-1.8500019494
C,2.3117770431,-0.4563875523,0.3767830721
C,-0.0438674424,0.4414924704,2.4694701777
H,-2.3428671008,0.4120172296,0.4776596348
H,0.1683259811,1.5071867923,2.6285995555
H,-1.0070059648,0.2525133278,2.9542266683
H,2.8564255845,-0.2975159221,-0.5574788367
H,2.5004433617,-1.4985298061,0.6660862283
C,1.0453524574,-0.4024897389,3.1563903037
H,0.8674004578,-0.4134893792,4.2367849066
H,0.9376085145,-1.440129682,2.8219611978
C,2.8404807855,0.4895545241,1.4684885523
H,3.9301398219,0.5589840926,1.3888075554
H,2.4599710668,1.4969789224,1.2666056288
C,2.490172718,0.0786804457,2.9128464919
H,2.6981917499,0.9325533127,3.5684189317
H,3.1702776287,-0.7194013869,3.2330382171

14b, B3LYP Energy= -421.680922028 Hartree,
NIMAG= 0

N,-0.3521691801,0.4690852463,-1.0039400981
N,0.9649970006,0.1879136042,-1.0844783317
C,1.2892067575,-0.1828428309,0.1496836548
C,0.1826635119,-0.1411453853,1.033463664
C,-0.8731443871,0.2847109794,0.2416016378
H,-0.836548347,0.779452608,-1.8309755075
H,2.3072945971,-0.4720285132,0.3698370486
C,0.1380681781,-0.5098725563,2.4924776323
C,-2.3114182192,0.5483722562,0.5778338366
H,0.935780632,-1.232610896,2.6915523552
H,0.3620625206,0.3615006813,3.1225608412
H,-2.9224823874,-0.3442463367,0.3886856407
H,-2.6959761707,1.3262399227,-0.0917199037
C,-2.4868926266,1.0040459877,2.0376178823
H,-3.468887401,1.4748089617,2.1493497398
H,-1.7492694028,1.7878290334,2.2388334303
C,-2.365068087,-0.1118249791,3.094692887
H,-2.269234535,0.3700893954,4.0745283103
H,-3.304397815,-0.676142135,3.1286772976
C,-1.2111529968,-1.1201138593,2.9141837783
H,-1.0866582446,-1.6616063188,3.8577670529
H,-1.4902635977,-1.8732672656,2.169082721

14H, B3LYP Energy= -422.051639857 Hartree,
NIMAG= 0

N,-1.002930751,-0.1799264714,-1.0484534538
N,0.3244399008,-0.4290718693,-1.1027502592
C,0.8709853996,-0.2529440733,0.1178437676
C,-0.1628936776,0.1396353009,0.9885646749
C,-1.3170685341,0.16584559,0.2132203878
H,-1.5924814162,-0.2573500471,-1.8662433508
C,2.3323804856,-0.448683039,0.3744661902
C,-0.0414568856,0.4394125783,2.4599541156
H,-2.3359239543,0.4046903977,0.4772226738
H,0.7722662525,-0.7065630409,-1.9665582675
H,0.1597619905,1.5073493991,2.6013975152
H,-1.010515793,0.2488849826,2.9279941365
H,2.8814741598,-0.2786050018,-0.5568743285
H,2.5090341322,-1.4951565954,0.6510424762
C,1.0459997635,-0.4035264771,3.1520927563
H,0.8563947548,-0.4005139591,4.2279591848
H,0.9318368031,-1.446876041,2.8370262298
C,2.8529999267,0.4938169243,1.4780091256
H,3.9404521977,0.5492692917,1.3914188251
H,2.4866728779,1.505076259,1.2729551044
C,2.4931082337,0.0722678069,2.9154711736
H,2.7048237926,0.9227829333,3.5705671104
H,3.1673652526,-0.7284610583,3.2349473339

15a, B3LYP Energy= -538.410172654 Hartree,
NIMAG= 0

N,-2.343452003,1.1744942762,-0.1016714108
N,-1.7801068374,2.4151341048,-0.0614622816
C,-0.4887336983,2.1482414652,0.0063304098
C,-0.20033951,0.7658539684,0.0145769423
C,-1.4253303497,0.1521212518,-0.0580500295
H,-3.3468962922,1.0965239692,-0.0979865439
C,0.8135234189,2.9130393213,0.0135939079

C,1.3017804837,0.6452582216,0.0220673186
H,-1.7410029093,-0.8792279907,-0.0760333736
C,1.6737582513,1.9050671623,0.9009771504
C,1.7585351379,1.1088099727,-1.3983363317
H,2.8275958508,0.9359079691,-1.5420022365
H,1.2317354997,0.5586309326,-2.1792997739
C,1.4182710461,2.633168614,-1.4083636071
H,2.3117605401,3.2423515154,-1.5666672198
H,0.7035657391,2.8983803091,-2.1895175134
H,1.728763617,-0.3029244626,0.351329117
C,1.1978212906,1.7974768397,2.3580611459
H,1.7405220975,0.9991325189,2.8745539543
H,1.399890485,2.7276929516,2.8976744648
H,0.1315563193,1.5860410147,2.4406152139
C,3.178524651,2.2163317465,0.9303341727
H,3.367596533,3.1295530878,1.5024047652
H,3.7169051002,1.4056234274,1.4318012605
H,3.6248860115,2.3472600394,-0.0547865121
C,0.7631072321,4.3758864923,0.4174695007
H,0.1339283638,4.943070667,-0.2741885677
H,0.3403784259,4.4989109621,1.4178715277
H,1.7609333053,4.8240698523,0.4066827498

15b, B3LYP Energy= -538.405856500 Hartree,
NIMAG= 0

N,-1.785533385,2.3112662263,-0.1460448589
N,-2.417447364,1.1068674004,-0.2159469792
C,-1.4399816482,0.1959586462,-0.1362775175
C,-0.1848033013,0.8166255007,0.0200787744
C,-0.4514729861,2.1662676894,0.0127587971
H,-2.3446925119,3.1484180098,-0.1601659605
H,-1.7003114548,-0.8514713454,-0.1785622586
C,1.3222639338,0.6887426007,0.0361371112
C,0.8392532624,2.9509521526,0.0173350344
C,1.7021479119,1.9475601781,0.9090665769
C,1.7881563826,1.1434804688,-1.3862925733
H,2.8576848029,0.9713594181,-1.5284420604
H,1.2618641517,0.5902280058,-2.165003248
C,1.4486344288,2.6668784259,-1.4050975026
H,2.3419585043,3.2771317242,-1.5612646104
H,0.7371910681,2.9294077332,-2.1905966331
H,1.7426213779,-0.2606261059,0.3698690203
C,1.2366810705,1.84912907,2.370497026
H,1.4325770065,2.7859696231,2.9015793313
H,0.1753159101,1.6205526076,2.4628852404
H,1.7951899088,1.0632755457,2.8886889677
C,3.2067995932,2.2635718093,0.929787221
H,3.399130962,3.1757048265,1.5027635812
H,3.7471989447,1.4525725094,1.4280361749
H,3.6488344129,2.3941002536,-0.0570179522
C,0.7889102564,4.4158243491,0.4183613666
H,0.1803262084,4.994868546,-0.2840887095
H,0.3616928568,4.545419095,1.416538749
H,1.7893460668,4.8570246356,0.4181025117

15H, B3LYP Energy= -538.782858306 Hartree,
NIMAG= 0

N,-2.3856022527,1.1305080719,-0.1500641304
N,-1.783163013,2.3550713635,-0.0651798007
C,-0.4654293015,2.1641523222,0.0159785352
C,-0.2070932648,0.7881022428,0.014549023

C,-1.4293528154,0.1612233745,-0.081354219
H,-3.3867678118,1.039222772,-0.0409720258
C,0.8222458122,2.9334758927,0.0214663054
C,1.2953880852,0.6517623996,0.0255513551
H,-1.7210004044,-0.8774594183,-0.1045513205
H,-2.3276773777,3.2057796391,-0.1235086822
C,1.6739123009,1.9057833226,0.9099989206
C,1.7438293211,1.1100620762,-1.3988204727
H,2.8107952421,0.9348056641,-1.5346132703
H,1.2245135697,0.5566984221,-2.1817792791
C,1.4058024508,2.6311606612,-1.4135245558
H,2.2948157188,3.2446980797,-1.5634824775
H,0.6974285631,2.9026075287,-2.1986147884
H,1.6957672047,-0.3055388064,0.3528129051
C,1.2000889409,1.8021309029,2.3681136135
H,1.7495212827,1.0102577033,2.8833260486
H,1.4009234999,2.732886481,2.9042658779
H,0.1357545905,1.5810545882,2.4713306929
C,3.1767630631,2.216487265,0.9289566425
H,3.3709670499,3.1185179448,1.5142652225
H,3.7127724918,1.398010116,1.4168277837
H,3.6193670487,2.3581591316,-0.0554630974
C,0.7801638986,4.3980171223,0.4205915464
H,0.191371035,4.9883502228,-0.2882889341
H,0.3553013317,4.5363954128,1.4178961081
H,1.7874515296,4.8184553402,0.4244260531

16a, B3LYP Energy= -382.350667305 Hartree,
NIMAG= 0

N,-0.7800168207,0.2187830394,-1.1666284248
N,0.519519674,-0.1088148483,-1.4089931327
C,1.0029836252,-0.3062452313,-0.1936814727
C,0.0432352955,-0.1190207699,0.8197446155
C,-1.1207274389,0.2232614937,0.1629759565
H,-1.390425174,0.3839142567,-1.9508246814
C,2.3505762004,-0.664306579,0.3607162711
C,0.6415222071,-0.3297865747,2.181419143
C,-2.4956021684,0.5703634837,0.6356178244
H,0.8258119629,0.6247418699,2.6893645685
H,0.0290849198,-0.9356158153,2.8550695774
H,2.8422861722,-1.4810295101,-0.1722810626
H,3.025722362,0.1986131216,0.3266425333
C,1.9903906711,-1.04513052,1.8319228512
H,2.786624999,-0.7917961071,2.5349549351
H,1.8380429535,-2.1265343818,1.8887988981
H,-3.2670648229,0.0765393496,0.0368065734
H,-2.626309239,0.254116189,1.671601867
H,-2.6799793689,1.6492663738,0.5929268797

16b, B3LYP Energy= -382.349503015 Hartree,
NIMAG= 0

N,-0.6106409927,-0.084155394,-1.2555388488
N,0.7404135635,-0.2587443123,-1.2499481847
C,1.1044513934,-0.2110323246,0.0349633455
C,-0.0306421149,0.0117463254,0.8556315203
C,-1.095394051,0.0884114634,-0.0047156781
H,-1.0926372683,-0.0691602907,-2.1387309611
C,2.5406027886,-0.3775695872,0.4217167675
C,-0.4843627154,0.1283588793,2.2855100435
C,-2.4213618897,0.2608895351,0.6677091868
H,-0.4473138314,-0.8395923789,2.8001319883

H,0.1041532315,0.827749583,2.8860438112
H,-3.0007814191,-0.6701469517,0.6492832268
H,-3.0504829615,1.0415389485,0.2307891595
C,-1.9606476835,0.6250456159,2.1193114996
H,-1.982483286,1.712071714,2.2300187625
H,-2.62811841,0.208497154,2.8763703976
H,3.1533946117,-0.5121423536,-0.4704969212
H,2.9095835255,0.4969866857,0.9666424896
H,2.6794453194,-1.2483388914,1.0704059552

16H, B3LYP Energy= -382.725006551 Hartree,
NIMAG= 0

N,-0.6622143811,-0.080275708,-1.2737560387
N,0.6884250482,-0.2644295419,-1.2178754682
C,1.1143767468,-0.217283382,0.0709497283
C,-0.0232860896,-0.004727116,0.848877677
C,-1.1030222213,0.0730763257,-0.0168756816
H,-1.156705618,-0.0959673377,-2.1555240662
C,2.5503693616,-0.3818336289,0.4301084299
C,-0.4746873429,0.1301635081,2.2775822948
C,-2.4173138127,0.2618296665,0.6636788457
H,1.2383916113,-0.3436763033,-2.0629411444
H,-0.437664616,-0.8375946274,2.7868762301
H,0.1298790776,0.8261936405,2.8611321286
H,-2.9853456301,-0.6745869316,0.6466566898
H,-3.0420497033,1.0317754098,0.2070994268
C,-1.9465622843,0.6377037649,2.1094675729
H,-1.9666841094,1.7236268099,2.215739869
H,-2.6110330042,0.2229027372,2.8660946155
H,3.186353928,-0.4686027085,-0.4518772327
H,2.8909722199,0.473007745,1.0187346821
H,2.6851550455,-1.2786198439,1.0402946731

17a, B3LYP Energy= -421.691948538 Hartree,
NIMAG= 0

N,-0.4313888038,0.1458231423,-1.0784423193
N,0.9197179478,0.245121967,-1.1348112281
C,1.3181927546,0.2296082918,0.1354712033
C,0.2072624537,0.1151282374,1.0163366462
C,-0.8999415572,0.0663583902,0.1945530493
H,-0.9551383062,0.1376969158,-1.9380999263
C,2.7706520357,0.3273781504,0.4828859806
C,0.1108969074,0.0624806861,2.5140985286
C,-2.3241692948,-0.0637051616,0.6335166322
H,0.8797330724,-0.5952109499,2.9340672005
H,0.2956716218,1.0566068599,2.9433532778
H,-2.686102848,-1.0832769962,0.4465209126
H,-2.9775795842,0.6080978862,0.0658618564
C,-2.4120563408,0.2528335065,2.141259103
H,-3.3885635656,-0.0576610595,2.5239577209
H,-2.3461431114,1.3378140298,2.2835977829
C,-1.287811095,-0.4299914377,2.9393965193
H,-1.3496388692,-1.5142852816,2.7858354213
H,-1.4341821739,-0.2555068535,4.0095404897
H,3.3682252221,0.3714772204,-0.4285013484
H,2.9806321246,1.22332121,1.0761696729
H,3.09991491,-0.5359665938,1.0702087346

17b, B3LYP Energy= -421.691251893 Hartree,
NIMAG= 0

N,-0.8911338395,0.1051689048,-1.1739388115
N,0.4402934725,-0.1222205253,-1.2680481582
C,0.8506689369,-0.1620511122,-0.0046805
C,-0.2183489872,0.0396463626,0.9045519034
C,-1.3390066545,0.210067994,0.109194865
H,-1.4345533922,0.1704309185,-2.0193358395
C,2.2670209002,-0.4203149623,0.41797979
C,-0.0414675242,0.069773304,2.3964852507
C,-2.7674151323,0.4893453677,0.4475649221
H,-0.0821241295,1.1045692148,2.7624988773
H,-0.8523827296,-0.464841096,2.9040057136
H,2.9620690757,0.1210766943,-0.2299168238
H,2.4953705756,-1.4867151171,0.2965034781
C,1.318825532,-0.5457135324,2.7817445089
H,1.5331950939,-0.3356424655,3.8340433409
H,1.2641034155,-1.6368357199,2.682427604
C,2.4583260249,-0.0181800688,1.8929533716
H,3.4208594982,-0.3912283428,2.2553752523
H,2.4957627953,1.0755233233,1.9706248113
H,-3.4501298675,0.0136491654,-0.2624774967
H,-3.0035442968,0.1058491677,1.4422322306
H,-2.9835447672,1.5633905254,0.44940971

17H, B3LYP Energy= -422.068346579 Hartree,
NIMAG= 0

N,-0.4821918685,0.1489673093,-1.097499961
N,0.8721819851,0.2427074723,-1.1019684694
C,1.3305741045,0.2272619363,0.1679945456
C,0.2153745856,0.1150258728,1.007066827
C,-0.9067797347,0.0686580195,0.1797271199
H,-1.011287983,0.143589876,-1.9588515192
C,2.7813097486,0.3227899076,0.4894342842
C,0.1178877438,0.0621031736,2.5057043391
C,-2.3238165926,-0.0606185869,0.6307229386
H,1.3914038648,0.3153321845,-1.9663385278
H,0.8923478689,-0.5909797558,2.9171202105
H,0.3041363022,1.061146065,2.9164400413
H,-2.6616733103,-1.0864798249,0.4406775149
H,-2.9770827711,0.5994874581,0.0525201585
C,-2.4049701926,0.2564715458,2.1396394919
H,-3.379293551,-0.0623296799,2.5139266894
H,-2.3511121972,1.3406381974,2.2840989474
C,-1.280568314,-0.4297874005,2.931702252
H,-1.3436157611,-1.514510358,2.7898185483
H,-1.4158547636,-0.2472607043,3.9993671265
H,3.3975980695,0.3677317877,-0.409491578
H,2.978064399,1.2169020538,1.0864985068
H,3.0953360509,-0.5426487633,1.0781481772

18a, B3LYP Energy= -461.011501991 Hartree,
NIMAG= 0

N,-0.4746502421,0.458346268,-1.0277133231
N,0.8471609411,0.1942738111,-1.127776282
C,1.2104108867,-0.1685676055,0.1000238335
C,0.1063003556,-0.1373352003,0.9988492117
C,-0.9687877702,0.2718482606,0.2264942612
H,-0.9758150062,0.7618823393,-1.8466734297
C,2.6299477917,-0.5429542009,0.393669631
C,0.0914144498,-0.5020047122,2.4593441136
C,-2.401747717,0.531147823,0.5894895509
H,0.8763682858,-1.2434143472,2.6416337824

H,0.3547177053,0.3638289807,3.0831804266
H,-3.0094364803,-0.3713426356,0.4407735801
H,-2.8083679382,1.285854633,-0.0932549153
C,-2.5456839287,1.0281956573,2.0394040577
H,-3.5274699199,1.4968976597,2.1621203219
H,-1.8077525202,1.820930212,2.1999686686
C,-2.390694455,-0.0578127324,3.1228389636
H,-2.2506045821,0.4492447155,4.0844967505
H,-3.3326054013,-0.612020973,3.2105886675
C,-1.2568146186,-1.0830203128,2.9231052421
H,-1.1152715752,-1.6152419258,3.8697451314
H,-1.5673746682,-1.840870855,2.1953766517
H,3.2191803158,-0.4992195571,-0.5231337694
H,3.0816456516,0.1342910519,1.1256090593
H,2.7020357799,-1.5569126841,0.8005761743

18b, B3LYP Energy= -461.010993916 Hartree,
NIMAG= 0

N,-0.8542241695,-0.2619530059,-1.0540332082
N,0.4675286208,-0.5271778142,-1.1375900958
C,0.9307143223,-0.3154111545,0.0917002712
C,-0.1076704467,0.1014000903,0.973999318
C,-1.2515038271,0.1195826585,0.1904471598
H,-1.4247323574,-0.3557414246,-1.8785964619
C,2.3910118092,-0.5030560691,0.4007361151
C,0.0031040102,0.4294603327,2.4394384878
C,-2.6663238809,0.485483202,0.5040369554
H,0.1824119771,1.5036643509,2.5864136726
H,-0.958237203,0.222920325,2.9225288133
H,2.9446081695,-0.379582046,-0.5335792562
H,2.5793494951,-1.5326289714,0.7325967126
C,1.1044041054,-0.3727764852,3.1564526637
H,0.9167252629,-0.3587202184,4.2353736311
H,1.0201938723,-1.4209081337,2.8492444512
C,2.9059902159,0.4865314372,1.4600325322
H,3.9962786415,0.5574003789,1.38922056
H,2.5238585884,1.4837546574,1.2154536133
C,2.5412237396,0.1290893408,2.9148571867
H,2.7216513091,1.012625637,3.5385715352
H,3.2315333437,-0.6414233652,3.2780163998
H,-3.3688533149,-0.048564863,-0.1419404318
H,-2.9098115668,0.2317281675,1.5380057126
H,-2.8474927867,1.5584886632,0.3785963121

18H, B3LYP Energy= -461.388772666 Hartree,
NIMAG= 0

N,-0.5209845196,0.4844840365,-1.0430286436
N,0.802447738,0.2014818831,-1.0925084498
C,1.2212333724,-0.1795427229,0.1320979789
C,0.113519212,-0.1372413646,0.9898868451
C,-0.9745053576,0.2831277469,0.2125196263
H,-1.0242766643,0.7958449515,-1.8625131618
C,2.6382335951,-0.5536828707,0.3986041322
C,0.0931049464,-0.4995726998,2.4516744936
C,-2.4022890356,0.5310358409,0.5892049303
H,1.3306437394,0.2949841025,-1.9493402183
H,0.8857894939,-1.2299579339,2.6358062738
H,0.3482362529,0.378873988,3.0564340233
H,-2.9772202999,-0.3921093,0.4485686961
H,-2.8266234816,1.266348997,-0.1015128466
C,-2.5340486259,1.0312742108,2.041511039

H,-3.5138358793,1.5014299275,2.1526215352
H,-1.8013939852,1.8290270613,2.2013720801
C,-2.3847013225,-0.0593288245,3.1192201299
H,-2.2413174479,0.4431568427,4.0807004986
H,-3.3263975365,-0.6103828592,3.2058264516
C,-1.2558850802,-1.0860889682,2.9083330545
H,-1.1017918219,-1.621014215,3.8485591832
H,-1.5660660196,-1.8478921713,2.1843763597
H,3.2384420612,-0.5465496344,-0.5123349623
H,3.0881940722,0.1415241142,1.1117669604
H,2.6904334587,-1.5542518853,0.8343711493

19, B3LYP Energy= -540.869052217 Hartree,
NIMAG= 0

N,0.6258218413,-1.4044970827,-0.0158991261
N,-0.7256160054,-1.4715670274,-0.014588126
C,-1.1312260423,-0.2061183261,0.0036168942
C,-0.0149029847,0.6755976258,0.0151673894
C,1.1080986645,-0.1304615203,0.0030663925
H,1.1488053169,-2.2642915281,-0.0218057401
C,-2.6047930828,0.1624586789,0.0000995845
H,-0.029946788,1.7525114148,0.0315189322
C,2.5911520827,0.1826954743,0.0038366641
C,-3.4827399744,-1.0984760705,0.0773201552
H,-3.2822256264,-1.6659427017,0.9886604858
H,-4.5393050361,-0.813808177,0.0720042458
H,-3.2983270938,-1.7623016031,-0.7695277189
C,-2.9081892659,1.0681437639,1.2145744313
H,-2.3191009294,1.9890437807,1.1875289481
H,-3.966285263,1.3480266734,1.2247720254
H,-2.6833795002,0.5523940143,2.1520922454
C,-2.9313592618,0.9309462076,-1.300691057
H,-2.7312817332,0.3114627673,-2.1790616443
H,-3.9875042511,1.2181405368,-1.3186690738
H,-2.3329524939,1.8419836623,-1.3875045384
C,2.7994740022,1.7059578862,0.0687792904
H,2.3632009238,2.1284660625,0.9775036596
H,3.8681529267,1.9375042245,0.0693690558
H,2.3486637075,2.2061230324,-0.7922054204
C,3.2654535722,-0.4707004677,1.2323529654
H,3.1696373121,-1.5603031102,1.2181324162
H,4.3335983807,-0.2348261826,1.2485980675
H,2.8198343392,-0.1080392954,2.1619861582
C,3.2410858174,-0.3601399061,-1.2901221139
H,2.7800347473,0.0855517157,-2.1750891205
H,4.3098185524,-0.126417471,-1.3051077331
H,3.1388821456,-1.4461040514,-1.3709645947

19H, B3LYP Energy= -541.247247454 Hartree,
NIMAG= 0

N,-0.6664937513,-1.2978529888,-0.6190493644
N,0.6889804483,-1.3046114584,-0.5776411824
C,1.1317778257,-0.1406932135,-0.0592378498
C,-0.0045635203,0.6176290666,0.2323332511
C,-1.1285011967,-0.1295962678,-0.1278720127
H,-1.1885286765,-2.0857465936,-0.9763333655
C,2.6026748073,0.1687295686,0.1241497806
H,-0.0126842225,1.6053403663,0.6598591711
C,-2.604636495,0.1952511109,-0.0362364685
H,1.2240438502,-2.0967997538,-0.9048928721
C,3.47784263,-0.9986895582,-0.369770652

H,3.3418922066,-1.1926451608,-1.438691146
H,4.5301232092,-0.7486132787,-0.226925663
H,3.2937224354,-1.9193229781,0.1935844457
C,2.9358577788,1.4462646954,-0.6824417342
H,2.3491432222,2.3023591947,-0.3426710328
H,3.9917500455,1.692200573,-0.5503600538
H,2.751741225,1.306138038,-1.750447867
C,2.8638539147,0.4142735832,1.6293793353
H,2.6297909625,-0.4703060026,2.2268235034
H,3.9187988535,0.6542995699,1.7788327169
H,2.2739370266,1.2509327262,2.0094857365
C,-2.8778270638,1.4600167535,-0.884692452
H,-2.6344655473,1.2972617014,-1.9375402984
H,-3.9369346057,1.7182828595,-0.8180399427
H,-2.3022071762,2.3167106776,-0.5279958068
C,-3.4603876319,-0.9740053923,-0.558982619
H,-3.3160275172,-1.8860593388,0.0292603499
H,-4.5168805288,-0.7133829211,-0.4806587469
H,-3.2660807112,-1.1874039682,-1.6151621204
C,-2.9512386453,0.471656365,1.4460818838
H,-2.3783390988,1.3117128769,1.8443941168
H,-4.0111753031,0.7216411427,1.5290528455
H,-2.7593517499,-0.4026329944,2.0729601138

20a, B3LYP Energy= -422.898158248 Hartree,
NIMAG= 0

N,-1.1209505596,-1.0131993131,0.1018055139
N,-2.4459732116,-0.7332280459,0.1091366243
C,-2.5112331172,0.5915384303,0.0254065163
C,-1.2112028688,1.1584293386,-0.0354228652
C,-0.3300861006,0.0929158373,0.0161440662
H,-0.8336413909,-1.9759250981,0.1599266719
C,-3.8339497086,1.292872897,0.0055352052
H,-0.9601954819,2.2040577335,-0.1071373375
C,1.1832627139,0.0159169389,-0.0105938725
C,1.6966016886,-0.6732385555,1.2748858325
H,1.3287889297,-1.6998377727,1.360861576
H,2.7899431538,-0.7136598012,1.27218352
H,1.3758659894,-0.1274071398,2.1656798841
C,1.7735367986,1.4348540995,-0.0886391205
H,2.8655736391,1.3835690266,-0.1073129073
H,1.4458972949,1.9529460552,-0.993547774
H,1.4795046457,2.0361804086,0.7754159648
C,1.6445733459,-0.7903081646,-1.2469794925
H,1.2893625148,-0.3260238225,-2.1703198834
H,2.7371215458,-0.8358315321,-1.2838812477
H,1.2710428312,-1.8180691482,-1.2240466664
H,-3.9638705142,1.8714225509,-0.9141190086
H,-4.6414454557,0.5623613686,0.0693140254
H,-3.9290866823,1.9867678087,0.8462570751

20H, B3LYP Energy= -423.272060263 Hartree,
NIMAG= 0

N,-1.0477066866,-0.7582191618,0.8834243465
N,-2.3655952808,-0.4519396653,0.7804991201
C,-2.5166292941,0.5805227974,-0.0771481821
C,-1.2416742602,0.9297151016,-0.5124050908
C,-0.3244304366,0.0721504487,0.1075746223
H,-0.7235438095,-1.4930103998,1.4972944297
C,-3.8561631027,1.1289933389,-0.4306318767
H,-1.009351926,1.7222577999,-1.2034918219

C,1.1834971333,-0.0001450307,0.0062996884
H,-3.0680388884,-0.973755457,1.2869258382
C,1.7443508084,-1.1219982026,0.9004674126
H,1.377591234,-2.1102596162,0.604101805
H,2.8309332055,-1.1505653398,0.8063551786
H,1.5257472926,-0.9550509531,1.9604198205
C,1.7652661136,1.3626788465,0.4520824272
H,2.8539953241,1.3326899317,0.3729057112
H,1.4073345249,2.1794334571,-0.1782075423
H,1.5071770546,1.5900822125,1.4892639875
C,1.5566741833,-0.2740226547,-1.4703981405
H,1.1941729316,0.5164683791,-2.1308653447
H,2.6437590481,-0.3160067453,-1.5653273207
H,1.1491882144,-1.226509902,-1.817948413
H,-4.2645206211,0.6043532121,-1.2994106017
H,-4.5644790577,1.0287115017,0.3938439358
H,-3.7716157827,2.1851460393,-0.6858558511

20b, B3LYP Energy= -422.898100239 Hartree,
NIMAG= 0

N,2.3293909676,0.7068479255,-0.0005229196
N,1.0378261981,1.1134137149,-0.0006507045
C,0.3248370234,-0.0084186139,-0.0002041805
C,1.1821265971,-1.1446593609,-0.0000777625
C,2.4689980311,-0.6463751923,-0.0001614271
H,3.0577691395,1.4023771448,-0.0007464247
C,-1.1938138288,0.0081830004,0.0000170344
H,0.9055120035,-2.1868972275,0.0001356718
C,3.8012011853,-1.3242706009,-0.0000520907
C,-1.7099931197,-0.7246421384,-1.2587058335
H,-1.3684039237,-1.763008893,-1.286260692
H,-2.8044027678,-0.730165441,-1.273522909
H,-1.3591729608,-0.2306874302,-2.1688244875
C,-1.7237946541,1.4524600659,-0.0014445335
H,-2.818084253,1.4448055348,-0.0012443018
H,-1.3818473127,2.0013435416,0.8784175486
H,-1.3821668346,1.9994502739,-0.8826170665
C,-1.709547549,-0.7219346503,1.2605056703
H,-1.3585382085,-0.2258914969,2.1694127421
H,-2.8039540916,-0.727603787,1.275651394
H,-1.3677561669,-1.760174039,1.290248379
H,4.3898205049,-1.0602510223,-0.8844841401
H,4.3898855822,-1.0598628139,0.8842208492
H,3.6687886384,-2.4066527944,0.0001879841

21, B3LYP Energy= -580.189055067 Hartree,
NIMAG= 0

N,-0.6709072425,0.5381030515,-0.8450869495
N,0.670703118,0.5082811966,-0.9241065298
C,1.0810325927,0.1047000498,0.2763470934
C,-0.0354389131,-0.127207127,1.1423432899
C,-1.1578434014,0.1632859131,0.3698086472
H,-1.1963547937,0.8111753852,-1.657992715
C,2.5758661675,-0.0280337638,0.5519824599
C,-0.0152493327,-0.6080556771,2.5684318325
C,-2.6531687885,0.1337754616,0.660749658
H,0.8417210445,-0.2117927619,3.1146588239
H,-0.9071961224,-0.2972995333,3.1134789518
H,0.0392244436,-1.7003816148,2.6331431248
C,-3.4659708652,0.4173052953,-0.6205647164
H,-3.2698465989,-0.3251148423,-1.3999194196

H,-4.5339682481,0.377248574,-0.3929223448
H,-3.2612470795,1.4141901475,-1.0233287946
C,-3.0657742779,-1.2593881744,1.1869977057
H,-4.1431938656,-1.2846363712,1.3778482639
H,-2.8318367624,-2.0363795575,0.4543209487
H,-2.5558627643,-1.5125510707,2.1172166419
C,-3.0095949247,1.2197344484,1.7028630085
H,-2.4862210791,1.0661641488,2.6481471294
H,-2.7445677415,2.2138788548,1.3334947754
H,-4.0844773467,1.2076476276,1.90966124
C,2.9027275189,-1.4324850107,1.1072733915
H,3.9820682327,-1.5319135769,1.259363333
H,2.4156406199,-1.6270854642,2.064233968
H,2.5891115711,-2.2092908885,0.4042415903
C,3.0211391759,1.0534473772,1.5642877838
H,2.5059292186,0.9627203842,2.5233110912
H,4.095867929,0.9720239897,1.7562798855
H,2.8215824234,2.053543117,1.1705106437
C,3.3767347532,0.1718104484,-0.7495281161
H,3.1069363424,-0.5743870291,-1.4998754049
H,3.1925879335,1.1552679706,-1.1846069216
H,4.4462063833,0.0786450618,-0.5370567796

21H, B3LYP Energy= -580.571067639 Hartree,
NIMAG= 0

N,-0.7208547003,0.5376397895,-0.8595963375
N,0.6266153061,0.4950112887,-0.8834018342
C,1.0920423737,0.093213293,0.3173642708
C,-0.0320182964,-0.1264727106,1.1385870287
C,-1.1682809096,0.1632329674,0.3567972585
H,-1.2560913345,0.8017123486,-1.6742770085
C,2.5891321008,-0.0284245356,0.5612512562
C,-0.0220031517,-0.6071019586,2.5630822932
C,-2.6607029448,0.1334062645,0.652392467
H,1.1485730352,0.7318888225,-1.7148831202
H,0.8740013269,-0.2800887212,3.0871011734
H,-0.8765897714,-0.2249042192,3.118032256
H,-0.0554954711,-1.6987451223,2.6131405167
C,-3.4732073811,0.4037790747,-0.6317315359
H,-3.2914163031,-0.3504127518,-1.4039206337
H,-4.5377589877,0.3650012361,-0.3966424063
H,-3.2839532727,1.4010210096,-1.0434181566
C,-3.053569306,-1.2590383761,1.1976590899
H,-4.129927087,-1.2807243449,1.3817680194
H,-2.8204596114,-2.0480501446,0.4782084057
H,-2.5542810867,-1.4939750579,2.1374754115
C,-2.9935968694,1.2368344013,1.6862809884
H,-2.4732943405,1.0917528662,2.6337724485
H,-2.7360481842,2.228365387,1.3057744373
H,-4.0660287354,1.2235876828,1.8935523021
C,2.9141882047,-1.4430748448,1.0938624981
H,3.9928449941,-1.5310203913,1.241120732
H,2.4337623479,-1.6481666577,2.0503605599
H,2.6086563824,-2.2153218513,0.3833966864
C,3.0246187247,1.0511416395,1.582105436
H,2.5293822237,0.9370982193,2.5471109667
H,4.1007241965,0.971802523,1.7522510365
H,2.8155060007,2.0571050408,1.2098674516
C,3.3719048819,0.1931281372,-0.7504136641
H,3.1172250943,-0.5472077088,-1.515358062
H,3.2305175461,1.2007724497,-1.1559877813
H,4.4395172456,0.0883882401,-0.5522633053

22, B3LYP Energy= -462.216890656 Hartree,
NIMAG= 0

N,-0.6234839869,0.0202113204,-0.9677008086
N,0.719079235,0.0107418562,-1.0086685009
C,1.0964662343,0.0228252031,0.2667513703
C,-0.034275186,0.0408298964,1.1513820403
C,-1.1347386746,0.0342268925,0.2934104662
H,-1.1424632337,0.0111426875,-1.8309363663
C,2.5710267026,0.0258034656,0.5511249288
C,0.0013851392,0.0144307822,2.6812305557
C,-2.6269208069,0.017305579,0.4595002517
H,3.1042677904,-0.1962624084,-0.3743462315
H,2.9152062786,0.9997807587,0.9106697431
H,2.8541250566,-0.7203799272,1.2969959227
H,-2.974683706,-0.8915644857,0.9563524622
H,-2.9903421197,0.8699789466,1.0346874092
H,-3.1088873437,0.0553972845,-0.521432995
C,0.4834842679,-1.3742882606,3.1644887685
H,1.4766959538,-1.6153764462,2.7800626846
H,0.5314939369,-1.4051855632,4.2581035864
H,-0.2012844863,-2.1592689217,2.8317915006
C,0.9532432916,1.1051984697,3.2251495309
H,0.9276804035,1.1106637498,4.3195141404
H,1.9874981752,0.9420698388,2.923048535
H,0.6506995429,2.0960004073,2.8746345756
C,-1.3832315313,0.2764553253,3.3068866029
H,-1.7836196186,1.2491234736,3.0092176099
H,-2.1090788122,-0.4943284906,3.0419801055
H,-1.2941622825,0.2773709865,4.397057292

22H, B3LYP Energy= -462.592113256 Hartree,
NIMAG= 0

N,-0.6690098916,0.0245885477,-0.9937222806
N,0.6775486547,0.0327144367,-0.9774584062
C,1.1098532886,0.0463826234,0.2990229482
C,-0.0239843926,0.0415347947,1.1412404432
C,-1.136771854,0.0181493156,0.2732148814
H,-1.1884817878,-0.0062912517,-1.8603230735
C,2.5819909524,0.0676399837,0.5536841343
C,0.0036015044,0.0128875706,2.6768038119
C,-2.6195853252,-0.0325098121,0.4655376276
H,1.2182489466,0.0546503325,-1.8314601727
H,3.1348984338,-0.2021664157,-0.3484130705
H,2.9069412381,1.0624542951,0.8659237404
H,2.8547946517,-0.6369785921,1.3381234402
H,-2.914799778,-0.9472541504,0.9816108036
H,-2.9731228489,0.8140419609,1.0525507926
H,-3.1306698179,-0.0124593219,-0.4991534271
C,0.4374539772,-1.3973357511,3.1416154607
H,1.4294885314,-1.6693059005,2.7734037091
H,0.4719728601,-1.4332312731,4.2331321068
H,-0.2677770052,-2.1610411696,2.8034944312
C,0.9888803325,1.0751253463,3.2180076896
H,0.9308667582,1.0954764266,4.3083750161
H,2.0269081984,0.8648749483,2.961593427
H,0.7367482803,2.0749211604,2.8541898838
C,-1.3761511999,0.3239064077,3.2912145515
H,-1.7482286368,1.3060891923,2.9887084091
H,-2.1249638042,-0.4320674933,3.0520895335
H,-1.2790987541,0.3382687333,4.3784382241

23a, B3LYP Energy= -430.823060887 Hartree,
NIMAG= 0

N,0.0089258702,-1.0824421103,0.0000001517
N,1.1547084247,-0.3973683254,0.0000001517
C,0.7542184259,0.8642713281,0.0000001517
C,-0.6476684948,1.0095410076,0.0000001517
C,-1.1006837028,-0.2901846256,0.0000001517
H,0.0492878942,-2.0904855733,0.0000001517
N,1.7289930329,1.9475088949,0.0000001517
H,-1.2168028853,1.9220724072,0.0000001517
H,-2.0966171842,-0.7026938805,0.0000001517
O,1.2632813909,3.0840561179,0.0000001517
O,2.9146386282,1.6652791593,0.0000001517

23b, B3LYP Energy= -430.823440621 Hartree,
NIMAG= 0

N,-0.0101056713,-1.1001704515,-0.0000095906
N,1.1189691458,-0.3895457524,0.000006085
C,0.7267516771,0.8893082092,0.0000080509
C,-0.6748160281,1.0093036352,-0.0000066935
C,-1.1057235763,-0.3018443393,-0.0000190091
H,-0.0002407253,-2.1102615513,-0.0000145733
H,1.4672156984,1.6739854562,0.000019853
H,-1.2875920551,1.8940831956,-0.0000092756
N,-2.4253253959,-0.865692345,-0.0000381913
O,-3.3719548277,-0.091770258,0.0000288857
O,-2.5004855415,-2.0945939986,0.0000333589

23H, B3LYP Energy= -431.146273256 Hartree,
NIMAG= 0

N,-0.0091855916,-1.1177909549,0.0000001517
N,1.1033780698,-0.364574394,0.0000001517
C,0.7234631227,0.9210384421,0.0000001517
C,-0.6579606533,1.0040484738,0.0000001517
C,-1.0912282456,-0.3201949829,0.0000001517
H,0.0426495007,-2.1317682011,0.0000001517
N,1.7563242373,1.9648847307,0.0000001517
H,-1.2546191098,1.9016267442,0.0000001517
H,-2.0872378221,-0.7372190867,0.0000001517
H,2.0518154758,-0.7347286313,0.0000001517
O,1.3576012096,3.1067483156,0.0000001517
O,2.9055545456,1.5534079656,0.0000001517

24, B3LYP Energy= -430.825927904 Hartree,
NIMAG= 0

N,-0.6661018939,0.,-0.8001845271
N,0.688714655,0.,-0.8713444146
C,1.0944834254,0.,0.3872059958
C,-0.0168707264,0.,1.2601129136
C,-1.1429983883,0.,0.4577999091
H,-1.1969333869,0.,-1.6576822877
H,2.1425268516,0.,0.6391412579
N,-0.0055108322,0.,2.695513954
H,-2.1911502503,0.,0.7050701868
O,1.0889483997,0.,3.2493222407
O,-1.0903756957,0.,3.2723568245

24H, B3LYP Energy= -431.148754330 Hartree,
NIMAG= 0

N,-0.7041206597,0.,-0.8267661907
N,0.6502390191,0.,-0.8398908256
C,1.1079367787,0.,0.4172504356
C,-0.0071677255,0.,1.2462957057
C,-1.137865831,0.,0.4388056139
H,-1.2410812478,0.,-1.688105088
H,2.1613336489,0.,0.6552335628
N,0.0073461135,0.,2.7075561981
H,-2.1865301776,0.,0.6969304561
H,1.1718328305,0.,-1.7106489588
O,1.107066732,0.,3.2281137341
O,-1.0816551147,0.,3.2501340247

25, B3LYP Energy= -635.373590749 Hartree,
NIMAG= 0

N,0.0010665364,-1.0964676525,-0.000018746
N,1.132665874,-0.4057432049,-0.0000110517
C,0.7351061593,0.8626338398,-0.0000187028
C,-0.6612586983,1.0178427464,-0.0000307728
C,-1.0930357128,-0.2888207571,-0.0000323231
H,0.003990048,-2.1086008507,-0.0000163499
N,1.7179076473,1.9446410565,-0.0000135367
H,-1.2457492932,1.9204933565,-0.0000385969
N,-2.4206262864,-0.8516414974,-0.0000443569
O,-3.3591296982,-0.0733179421,0.0000562054
O,-2.4893604943,-2.0783714732,0.0000736059
O,1.2521164564,3.0783383769,0.0000396709
O,2.8979025618,1.6493522017,0.0000549546

25H, B3LYP Energy= -635.670984621 Hartree,
NIMAG= 0

N,-0.0265343386,-1.1188090201,-0.0000392592
N,1.0799750999,-0.3668512105,-0.00003768
C,0.7100383024,0.9233043426,0.0000045798
C,-0.6736481238,1.0234560152,0.0000460823
C,-1.0898876148,-0.2999274356,0.0000161995
H,-0.027887461,-2.1394045532,-0.0000718249
N,1.7563355505,1.9604444117,0.0000107426
H,-1.2798639347,1.9159711953,0.0000927311
N,-2.4394423246,-0.8904767144,0.0000327724
H,2.029522764,-0.7409985637,-0.000069654
O,-3.3584761352,-0.1065771274,0.0000613599
O,-2.4620168206,-2.1098587289,-0.0000336619
O,1.3660118691,3.1036155747,0.00003929
O,2.8981150402,1.5320111425,-0.0000525387

26, B3LYP Energy= -325.523089300 Hartree,
NIMAG= 0

N,-0.0011373189,-1.084472429,0.
N,1.1394477789,-0.3727672453,0.
C,0.7516592666,0.9009352155,0.
C,-0.6513366784,0.9779130127,0.
C,-1.1230404498,-0.3141986588,0.
H,0.0520050455,-2.0899447529,0.
H,1.4736557549,1.7020855843,0.
F,-1.3941502295,2.0954429971,0.
H,-2.1216752694,-0.7166813236,0.

26H, B3LYP Energy= -325.863972815 Hartree,
NIMAG= 0

N,-0.0227114068,-1.1216216395,0.
N,1.0931539876,-0.3675540821,0.
C,0.7565571732,0.9328484361,0.
C,-0.6333396017,0.9841030867,0.
C,-1.1040539534,-0.3243323727,0.
H,0.0222447187,-2.1339700707,0.
H,1.4955437366,1.7189742154,0.
F,-1.3671724414,2.0710506743,0.
H,-2.1086944769,-0.7177773341,0.
H,2.0159958152,-0.7862105802,0.

27, B3LYP Energy= -685.883110320 Hartree,
NIMAG= 0

N,-0.6657085615,0.,-0.89754498
N,0.678717125,0.,-0.9631056594
C,1.0813385565,0.,0.3031237664
C,-0.0242843227,0.,1.1790802983
C,-1.142919986,0.,0.373170245
H,-1.1964873897,0.,-1.7535919562
H,2.1317401161,0.,0.5483277255
Cl,0.0052287698,0.,2.9129129409
H,-2.1937729875,0.,0.6092875995

27H, B3LYP Energy= -686.225782201 Hartree,
NIMAG= 0

N,-0.6740358355,0.,-0.9229798085
N,0.6740358355,0.,-0.9229798085
C,1.116390877,0.,0.3445011869
C,0.,0.,1.1803337737
C,-1.116390877,0.,0.3445011869
H,-1.2043009731,0.,-1.7863940092
H,2.1701101002,0.,0.5765164044
Cl,0.,0.,2.887318869
H,-2.1701101002,0.,0.5765164044
H,1.2043009731,0.,-1.7863940092

28, B3LYP Energy= -2799.80407414 Hartree,
NIMAG= 0

N,-0.6672116911,0.,-0.9140937064
N,0.6780654668,0.,-0.9807276537
C,1.0808757494,0.,0.2851801366
C,-0.0239495147,0.,1.1635140668
C,-1.1424606401,0.,0.3570824265
H,-1.1984480493,0.,-1.7700463752
H,2.1317312976,0.,0.5282111628
Br,0.0091088868,0.,3.0516067265
H,-2.1938601853,0.,0.5909331963

28H, B3LYP Energy= -2800.14782454 Hartree,
NIMAG= 0

N,-0.673993298,0.,-0.9393518919
N,0.673993298,0.,-0.9393518919
C,1.1144644047,0.,0.3288508033
C,0.,0.,1.1670421947
C,-1.1144644047,0.,0.3288508033
H,-1.2048017955,0.,-1.8025879054

H,2.1686998437,0.,0.5582103675
Br,0.,0.,3.0336552482
H,-2.1686998437,0.,0.5582103675
H,1.2048017955,0.,-1.8025879054

29a, B3LYP Energy= -685.885866267 Hartree,
NIMAG= 0

N,-0.7329980594,0.,-0.8447099643
N,0.6148728376,0.,-0.9161702577
C,0.9930041869,0.,0.3503045911
C,-0.0941127792,0.,1.2514885726
C,-1.2006778773,0.,0.428924406
H,-1.2617623126,0.,-1.7017921034
Cl,2.6745667132,0.,0.7644518415
H,-0.0633796783,0.,2.3273340624
H,-2.2556617107,0.,0.6518288317

29b, B3LYP Energy= -685.883353433 Hartree,
NIMAG= 0

N,-0.5929789342,0.,-0.8487947666
N,0.7558784658,0.,-0.9074282987
C,1.1429255123,0.,0.3641101338
C,0.0478491651,0.,1.2578513721
C,-1.0502098068,0.,0.4270066606
H,-1.1372557867,0.,-1.6969764183
H,2.196255147,0.,0.6006766635
H,0.0497319002,0.,2.3343201626
Cl,-2.7383443427,0.,0.780894471

29H, B3LYP Energy= -686.229415147 Hartree,
NIMAG= 0

N,-0.7343534936,0.,-0.8791305113
N,0.6190840183,0.,-0.8790755602
C,1.048747685,0.,0.3995578095
C,-0.0688448846,0.,1.2346014543
C,-1.1697674718,0.,0.3916919687
H,-1.2605457324,0.,-1.7445232793
Cl,2.696979724,0.,0.7774378194
H,-0.0669165683,0.,2.3114853068
H,-2.2258465639,0.,0.6143459814
H,1.1614632872,0.,-1.7354507995

30a, B3LYP Energy= -5373.34126080 Hartree,
NIMAG= 0

N,-0.7567814217,0.,-0.931330278
N,0.5889276137,0.,-1.0086063874
C,0.9897887431,0.,0.2517631665
C,-0.1050544366,0.,1.1500678082
C,-1.2225127476,0.,0.3412773439
H,-1.2903025055,0.,-1.7860318343
Br,2.8219536921,0.,0.6802526784
Br,-0.0798640581,0.,3.0306374177
H,-2.2723035593,0.,0.5836300649

30b, B3LYP Energy= -5373.34028674 Hartree,
NIMAG= 0

N,-0.5806723772,0.,-0.9385507532

N,0.7661504501,0.,-0.9969688085
C,1.1632658796,0.,0.2697374806
C,0.0628614432,0.,1.1549336005
C,-1.0491308161,0.,0.3343468027
H,-1.1221976581,0.,-1.7887646481
H,2.2136471254,0.,0.5157558151
Br,0.1022380052,0.,3.0334760879
Br,-2.8823107321,0.,0.7276944031

30H, B3LYP Energy= -5373.68069761 Hartree,
NIMAG= 0

N,-0.749960285,0.,-0.9598925279
N,0.6015450016,0.,-0.9611980752
C,1.0444426412,0.,0.3131937605
C,-0.0804780954,0.,1.1528954006
C,-1.1872201936,0.,0.3097655601
H,-1.2794406982,0.,-1.8234987266
Br,2.8473726588,0.,0.7208770812
Br,-0.0957155041,0.,3.0167653662
H,-2.2410477014,0.,0.5415540137
H,1.1405021761,0.,-1.8195216625

31a, B3LYP Energy= -470.159385347 Hartree,
NIMAG= 0

N,2.0015059775,-0.16244656,0.0969254755
N,1.7522938282,-1.4991983743,0.0952502105
C,0.4385971641,-1.5913846408,0.0173366035
C,-0.144741748,-0.3034017643,-0.0306373347
C,0.9015572626,0.6157731358,0.0228022151
H,2.9586609651,0.1519910811,0.150680217
H,-0.0582476412,-2.5478420722,-0.0027289659
N,-1.5393048302,-0.0007403944,-0.1172409368
C,0.950896979,2.104537344,0.010554312
H,0.4922653211,2.4964204944,-0.8991257712
H,0.386539451,2.5142881321,0.8501962088
H,1.9829692186,2.4571716199,0.0695593242
O,-2.3240401151,-0.9440156623,-0.1533646175
O,-1.8673148329,1.1867646611,-0.1501859405

31b, B3LYP Energy= -470.158675533 Hartree,
NIMAG= 0

N,-0.8035167068,-0.0527861175,-0.9175811809
N,0.5536293488,-0.0715095965,-0.9792787063
C,0.9716754956,-0.0101740287,0.2786614017
C,-0.1614257338,0.0493737058,1.1414148634
C,-1.2835869506,0.0198052178,0.3323176819
H,-1.3288269642,-0.0925190954,-1.7771090161
C,2.4274610992,-0.0102788144,0.6057153241
N,-0.1944179633,0.1260459009,2.5724389608
H,-2.3320141461,0.0453979563,0.5773922903
H,3.0019883269,-0.0658343445,-0.3188818772
H,2.7046182887,0.8930947424,1.1531229189
H,2.6838241095,-0.857455069,1.2453621237
O,0.8804897624,0.1449638994,3.1670317461
O,-1.2970338937,0.1683515344,3.1152961901

31H, B3LYP Energy= -470.491500968 Hartree,
NIMAG= 0

N,-0.8485865097,-0.0534752132,-0.946399514

N,0.508984403,-0.0701053197,-0.9519729516
C,0.9879381174,-0.0089343133,0.3035524489
C,-0.1521888013,0.0483382446,1.1237656612
C,-1.2788707034,0.0188793258,0.3163507226
H,-1.3828871582,-0.0927760256,-1.8069811074
C,2.4409242846,-0.0100783293,0.6088820506
N,-0.1822480584,0.1261004406,2.5781102903
H,-2.3262238789,0.0453209741,0.5768552027
H,1.0298859694,-0.1227916867,-1.8204541557
H,3.0382758455,-0.065553335,-0.3018350362
H,2.7041333403,0.8939327092,1.1625178702
H,2.6832206504,-0.8564363669,1.2554146516
O,0.8993682199,0.1430981517,3.14161283
O,-1.2857028076,0.1666067484,3.090615891

32a, B3LYP Energy= -725.215333900 Hartree,
NIMAG= 0

N,-0.812655172,-0.0523337642,-0.9203853889
N,0.5351249169,-0.0719446615,-0.9810938722
C,0.9489302713,-0.0096836925,0.2830038578
C,-0.1715196037,0.0496296896,1.1493280116
C,-1.2899386089,0.0203649138,0.3459994327
H,-1.3411799458,-0.0910531395,-1.7764482654
C,2.3993738442,-0.008196829,0.6372149929
Cl,-0.1434654232,0.1412196017,2.8826973644
H,-2.3407035151,0.0453949829,0.5823178592
H,2.9985665701,-0.063868049,-0.2717750667
H,2.6713676562,0.9001098259,1.1822815521
H,2.65022673,-0.8596388784,1.2761304126

32b, B3LYP Energy= -725.215005396 Hartree,
NIMAG= 0

N,1.7969025628,0.0279729841,0.030917926
N,1.6869121316,-1.3177569863,0.0341558998
C,0.3808772043,-1.5462824321,-0.0045772154
C,-0.3369759988,-0.3320362299,-0.0330454594
C,0.6033726373,0.6820993497,-0.0095555343
H,2.7160620241,0.4402716546,0.054464
H,-0.0043795231,-2.5539173082,-0.0129227803
Cl,-2.0619206984,-0.1376605458,-0.0874395316
C,0.4682867788,2.1670304634,-0.0036594786
H,1.1801228489,2.6359789401,-0.6886511311
H,-0.5374378041,2.44875791,-0.3166536281
H,0.6356078366,2.5823072005,0.9953929331

32H, B3LYP Energy= -725.566910041 Hartree,
NIMAG= 0

N,-0.8580314458,-0.0531536394,-0.944198793
N,0.4938570285,-0.0698772414,-0.9552947724
C,0.9687554872,-0.0088166959,0.3035296039
C,-0.1569300256,0.0491476793,1.142698511
C,-1.2812615568,0.0194422243,0.3290790318
H,-1.396954678,-0.0920049732,-1.7999937655
C,2.4162770058,-0.0085295998,0.6355503457
Cl,-0.127589512,0.1393424049,2.8504001881
H,-2.3311498331,0.0450583605,0.5756539545
H,1.0120025618,-0.1220847652,-1.8238401731
H,3.0381128744,-0.0635663913,-0.2583788828
H,2.671585613,0.9003749239,1.1864355916
H,2.6504481272,-0.8596951803,1.2800978988

33a, B3LYP Energy= -2839.13614457 Hartree,
NIMAG= 0

N,-0.810183228,-0.0531447884,-0.9350373419
N,0.5385008264,-0.0724353657,-0.9917331863
C,0.9492302031,-0.0101920301,0.273259559
C,-0.1736131284,0.0490873406,1.1382037909
C,-1.2891702299,0.0195699852,0.3304383493
H,-1.335859191,-0.0921983254,-1.7929439647
C,2.4000118404,-0.008798058,0.6262478425
Br,-0.1558419712,0.1489776729,3.0261505126
H,-2.3411032767,0.0443923777,0.5617803483
H,2.9985152221,-0.0643785716,-0.283179133
H,2.6723763292,0.8993781648,1.1712144536
H,2.651264324,-0.8602584021,1.2648696596

33b, B3LYP Energy= -2839.13583575 Hartree,
NIMAG= 0

N,-2.3428645781,-0.0224247062,0.036336599
N,-2.1910592357,-1.3640809257,0.0234903509
C,-0.8777825599,-1.550308767,-0.0096329015
C,-0.197247728,-0.3142978977,-0.0161701878
C,-1.1710565027,0.6687992434,0.0147698694
H,-3.2742541125,0.3614998723,0.0658913152
H,-0.4626651284,-2.5459388808,-0.0249724617
Br,1.6726246787,-0.0362457102,-0.0592003977
C,-1.089519863,2.1578111397,0.0016084461
H,-1.9815399262,2.6063686248,0.4455712861
H,-0.2209977106,2.4955018576,0.5694201306
H,-0.9880503335,2.5429681498,-1.0179240487

33H, B3LYP Energy= -2839.48860003 Hartree,
NIMAG= 0

N,-0.8544061283,-0.0539873113,-0.9597873367
N,0.497703931,-0.0705162134,-0.9666632248
C,0.9676115277,-0.0092722957,0.2945860404
C,-0.1595599374,0.0486243527,1.1322742811
C,-1.2797362217,0.0185813917,0.3128985721
H,-1.3905595698,-0.0930286516,-1.8173317525
C,2.4157646679,-0.0091132196,0.6242419293
Br,-0.138484692,0.1473591364,2.9993725025
H,-2.3310088354,0.0439129046,0.5536459189
H,1.018357909,-0.1226757884,-1.8336842591
H,3.0367388844,-0.0641133279,-0.2703683745
H,2.6719242614,0.8996167817,1.1748780111
H,2.6508203692,-0.8602191933,1.2684253394

34a, B3LYP Energy= -2839.13466626 Hartree,
NIMAG= 0

N,-0.7543822163,0.0685873087,-0.9933432819
N,0.5753776931,-0.1303857541,-1.0773032804
C,0.9629620363,-0.1699692977,0.1855227606
C,-0.098637242,0.0013744393,1.1108024668
C,-1.1984899725,0.1531059058,0.288672105
H,-1.289661242,0.1359719272,-1.8435197466
Br,2.7854820662,-0.4345620425,0.617455946
C,-0.037974134,0.0138727671,2.6050991893
H,-2.2394837263,0.3113201813,0.5237417694
H,0.3554445759,-0.9292439791,2.9947692492
H,0.6146216916,0.8121752802,2.969681425

H,-1.0304790003,0.1677532639,3.0330962377

34b, B3LYP Energy= -2839.13265811 Hartree,
NIMAG= 0

N,0.8075107592,-1.465694908,-0.0194877959
N,2.1480790841,-1.3913019711,0.0834897674
C,2.404969326,-0.0864578177,0.1040030189
C,1.2348578697,0.7073862124,0.0152487729
C,0.229763457,-0.237878798,-0.0622795909
H,0.3502175274,-2.3628856601,-0.0530119575
H,3.4269034199,0.2556885297,0.1832731262
C,1.11588435,2.199331306,0.0026771612
Br,-1.6357472335,-0.0237950445,-0.2030476756
H,2.0914901694,2.6602336193,0.1680148309
H,0.7320192365,2.5660221827,-0.9540463795
H,0.4403860345,2.5562223493,0.7850787219

34H, B3LYP Energy= -2839.48589512 Hartree,
NIMAG= 0

N,-0.7950247021,0.0744012078,-1.0099989352
N,0.5407807413,-0.1247629333,-1.044179513
C,1.000577628,-0.1748872851,0.222291014
C,-0.0781738893,-0.0017752136,1.1033186031
C,-1.1861210919,0.1510784387,0.2746559271
H,-1.3404490026,0.143275325,-1.85981932
Br,2.7995789591,-0.4371489321,0.5899483383
C,-0.0368757541,0.0136009556,2.5980421976
H,-2.2244710313,0.3091002446,0.5236181854
H,1.0532654702,-0.2135493755,-1.9133549344
H,0.3498673802,-0.9312513471,2.9865906958
H,0.6097332554,0.8155515253,2.9614386984
H,-1.0341990846,0.1678920814,3.009405471

35a, B3LYP Energy= -764.539035023 Hartree,
NIMAG= 0

N,-2.3260282706,-0.0299368829,0.0170269738
N,-2.1774128564,-1.3712053382,0.0164532381
C,-0.8637073933,-1.561485384,0.0103593429
C,-0.1821973218,-0.3271648043,0.0098686328
C,-1.1521458208,0.6600218801,0.0167203139
H,-3.256849426,0.3559366244,0.0354859072
H,-0.4493687042,-2.5575906816,0.0098455886
Cl,1.5367642004,-0.0765896018,0.0079100555
C,-1.0604186143,2.1521092747,-0.0171693269
H,-1.9282983425,2.577505639,0.4982155773
H,-0.1811734026,2.4537653029,0.5583432102
C,-0.9648676947,2.7287124099,-1.4417379539
H,-0.8926280729,3.818879401,-1.4086030396
H,-0.0824025235,2.3444921644,-1.9576353818
H,-1.8434692569,2.4645634362,-2.035875058

35b, B3LYP Energy= -764.538544103 Hartree,
NIMAG= 0

N,-0.8731134162,-0.0511805282,-0.909343522
N,0.472584529,-0.072231169,-1.0069239486
C,0.9225603773,-0.0114252445,0.2439756215
C,-0.1746001049,0.0493420738,1.1415894702
C,-1.3145972381,0.0221639026,0.3705043473
H,-1.4248729713,-0.0892854518,-1.7505474891

C,2.3843198186,-0.0110629171,0.5818309678
Cl,-0.0999822409,0.1402846411,2.8739367088
H,-2.358478755,0.0487234557,0.6353710422
H,2.6045857798,0.8903146659,1.1658223156
H,2.5836725755,-0.8505448783,1.2582720422
C,3.3106693659,-0.0867244488,-0.6334710582
H,4.3547407383,-0.0821368399,-0.3110637844
H,3.1332689061,-0.9966667464,-1.2103888935
H,3.1543691559,0.7609880247,-1.3037342798

35H, B3LYP Energy= -764.893109311 Hartree,
NIMAG= 0

N,-0.9196371168,-0.0515447825,-0.9284680114
N,0.4316861618,-0.0699563639,-0.9704664591
C,0.9367960853,-0.0099472757,0.2752506817
C,-0.1704900168,0.0492390052,1.141137182
C,-1.3128264917,0.0212673839,0.3554938691
H,-1.4779962172,-0.0895117948,-1.7713745261
C,2.3978429092,-0.0113937227,0.5780923381
Cl,-0.10111503,0.1389602396,2.8485862924
H,-2.356480332,0.0481677214,0.6266547606
H,0.9333879389,-0.1226065599,-1.8483409411
H,2.6082592578,0.8899452331,1.1645586523
H,2.5873706943,-0.8502988469,1.2570208098
C,3.3159139573,-0.0873945041,-0.6449852036
H,4.3563002066,-0.0825976242,-0.3195598658
H,3.1663380718,-1.0095135877,-1.2143539656
H,3.1877396583,0.7725344508,-1.3090272242

36a, B3LYP Energy= -2878.45978266 Hartree,
NIMAG= 0

N,-2.332753205,-0.0227187169,0.0039699278
N,-2.1942716647,-1.3655103501,0.0048453066
C,-0.882305703,-1.5651630678,0.0129031659
C,-0.1898944654,-0.3359633518,0.0194078302
C,-1.1540008509,0.6581249927,0.0152644914
H,-3.2610393498,0.3699263329,0.0090973292
H,-0.4771487735,-2.5650004105,0.0176309944
Br,1.6843597059,-0.0802560663,0.0389803499
C,-1.0597594885,2.1503387533,-0.0172097817
H,-1.920782597,2.5757931127,0.5097042276
H,-0.1732892668,2.4492469619,0.5480924819
C,-0.9815699699,2.7296702275,-1.4415998342
H,-0.9096102589,3.8197909263,-1.4069114066
H,-0.1051199655,2.3471711012,-1.9689202125
H,-1.8670176469,2.4665629945,-2.0260467898

36b, B3LYP Energy= -2878.45932380 Hartree,
NIMAG= 0

N,-0.8689792116,-0.051947723,-0.9236825283
N,0.4777606573,-0.0728196588,-1.0150892948
C,0.9227772538,-0.0117826356,0.2375423046
C,-0.1785905226,0.048861965,1.1318731653
C,-1.314398339,0.0212554592,0.3541187851
H,-1.41674819,-0.0901997612,-1.7676093548
C,2.3849551624,-0.0114364576,0.5747519491
Br,-0.1149840826,0.1481991874,3.0194224899
H,-2.3597690208,0.0475330371,0.6131923781
H,2.6053910128,0.8899022552,1.1585551018
H,2.5844887136,-0.850885508,1.2510211731
C,3.3108304374,-0.0871187281,-0.6408572169

H,4.3550792635,-0.0825473696,-0.318779826
H,3.1331062236,-0.9971098938,-1.2176320432
H,3.1542071621,0.7606543715,-1.3109975431

36H, B3LYP Energy= -2878.81472401 Hartree,
NIMAG= 0

N,-0.91421168,-0.0524371411,-0.9439644068
N,0.4373747696,-0.0705327343,-0.9795888715
C,0.9357746077,-0.0102539647,0.2693977358
C,-0.1743755152,0.0488171071,1.1320960739
C,-1.3115340566,0.0203689115,0.3387909358
H,-1.4685200758,-0.09062626,-1.7895596821
C,2.3974921546,-0.0117786502,0.5709728005
Br,-0.1136817358,0.1471294404,2.9991277758
H,-2.3570707181,0.0469078846,0.6026933104
H,0.9430612324,-0.1230853809,-1.8552087925
H,2.6084165819,0.8893937474,1.1574159038
H,2.5875317979,-0.8505489859,1.2498418769
C,3.3149831019,-0.0877677204,-0.6522784736
H,4.3556763713,-0.0830273368,-0.3277493719
H,3.1650494784,-1.00987405,-1.2216325015
H,3.1864522993,0.7721754705,-1.3162834474

37a, B3LYP Energy= -725.217062329 Hartree,
NIMAG= 0

N,-0.5675207373,-0.0598539236,-0.8755029478
N,0.7847747333,-0.0543966984,-0.9483938651
C,1.1570219259,0.0114127883,0.3153225141
C,0.066665129,0.04753618,1.2121388747
C,-1.0483699745,-0.0013774503,0.3964876922
H,-1.0936143751,-0.105873023,-1.7335237125
Cl,2.8385101147,0.0447358459,0.7367148702
H,0.0960394897,0.1008456477,2.2871524374
C,-2.5084627378,0.0031114082,0.7132466906
H,-3.0014052037,-0.904323398,0.3512113896
H,-2.6548853281,0.0549021302,1.7922597712
H,-3.0147082162,0.8632804936,0.2645584455

37b, B3LYP Energy= -725.214844782 Hartree,
NIMAG= 0

N,-0.7621120599,-0.0503018482,-0.8793741205
N,0.590066678,-0.0687756787,-0.9368647163
C,0.9920712137,-0.0075902248,0.3308254266
C,-0.1134199892,0.0515481201,1.2204684405
C,-1.2126681516,0.021632462,0.3948334625
H,-1.3071724722,-0.0864293993,-1.7256901408
C,2.4496184112,-0.0068710413,0.6693430111
H,-0.1115897617,0.1072916993,2.2960342285
Cl,-2.9008290179,0.0598171006,0.7549181896
H,3.0400404052,-0.0625434909,-0.2458822939
H,2.7304965968,0.9024660562,1.2084340423
H,2.7096258677,-0.860243755,1.3022253602

37H, B3LYP Energy= -725.569181709 Hartree,
NIMAG= 0

N,-0.2332737261,1.204292847,0.0420493558
N,1.1199389255,1.1072204549,0.0561636382
C,1.4862413957,-0.1886540541,-0.0067311602
C,0.3122690247,-0.9456026707,-0.0594198029

C,-0.7428892283,-0.0432008178,-0.0263006888
H,-0.7161436763,2.0929351395,0.0912047774
C,2.9129048183,-0.6133747676,-0.0176435632
H,0.2341789077,-2.0183671383,-0.1149205005
Cl,-2.4158705391,-0.3071753637,-0.0581299252
H,1.7023381238,1.9340539592,0.1007267142
H,3.5896288332,0.2342910264,0.0972182661
H,3.0996420971,-1.3188926336,0.7948525311
H,3.1459760437,-1.117901981,-0.9585526421

38a, B3LYP Energy= -2839.13683615 Hartree,
NIMAG= 0

N,-0.5820622762,-0.0604791237,-0.8787454341
N,0.7700785248,-0.0540998472,-0.9533029583
C,1.1454807548,0.0111052801,0.3097267432
C,0.0555023983,0.0469514995,1.2077838573
C,-1.0611868271,-0.0015133715,0.3941846754
H,-1.1100050954,-0.1066538588,-1.7358290783
Br,2.9806611548,0.0474082783,0.7646024564
H,0.0853139405,0.1000573806,2.2826980234
C,-2.521037055,0.0031478889,0.7126978989
H,-3.0144824869,-0.9042880697,0.3513409184
H,-2.6664692258,0.0549873198,1.7918771943
H,-3.027748987,0.8633766244,0.2646378636

38b, B3LYP Energy= -2839.13542403 Hartree,
NIMAG= 0

N,-0.7479117513,-0.0503853746,-0.8835934022
N,0.6033238844,-0.0689180741,-0.9393423493
C,1.004935811,-0.0077406886,0.328938676
C,-0.1019662551,0.0512680122,1.2161713709
C,-1.2019587194,0.0212357671,0.3898662373
H,-1.2905248333,-0.0875524003,-1.7314240572
C,2.4623795731,-0.0070714747,0.6686714384
H,-0.0999783432,0.1070279532,2.2917017954
Br,-3.0427654127,0.063122725,0.7846973985
H,3.053669304,-0.0624353159,-0.2460405229
H,2.7429167251,0.9020884589,1.2082052308
H,2.7220077376,-0.8606395882,1.3014190741

38H, B3LYP Energy= -2839.49078005 Hartree,
NIMAG= 0

N,0.4529373783,1.2639097685,-0.0448430817
N,1.8001576381,1.1006411665,-0.0590392609
C,2.1010562488,-0.2116175664,0.0094480701
C,0.8899560564,-0.90724858,0.068224079
C,-0.1210872623,0.0457145444,0.0320555015
H,0.0171757721,2.1764921898,-0.091604911
C,3.5047104732,-0.7079484577,0.0166216617
H,0.7608302636,-1.9746905227,0.1296937518
Br,-1.9653699507,-0.1528781517,0.0729674078
H,2.4230941073,1.8968710979,-0.1122267327
H,4.2238801248,0.1075416023,-0.0696376545
H,3.7053871022,-1.2502562646,0.943632557
H,3.6621240481,-1.3982938262,-0.8150803881

39, B3LYP Energy= -509.491827550 Hartree,
NIMAG= 0

N,-0.7376301512,1.6245965233,-0.085683237

N,0.614738908,1.7813116512,-0.0832297157
C,1.110674312,0.5559048098,-0.0201210275
C,0.0358356482,-0.3830505109,0.0174627133
C,-1.1526664019,0.3466973273,-0.0267134619
H,-1.3205584448,2.4464508596,-0.129270443
C,2.5848619479,0.3259875724,0.001903213
N,0.1250349648,-1.8060432673,0.0869278971
C,-2.5899156925,-0.0449078468,-0.0184831437
H,3.0960346987,1.2879865123,-0.0407542703
H,2.8844306325,-0.2063260592,0.9070872684
H,2.8974103113,-0.2908090227,-0.8432867763
H,-3.2300045258,0.839102497,-0.0653797654
H,-2.8166021618,-0.6944187067,-0.8659502612
H,-2.829357499,-0.6109382626,0.8835671205
O,1.245475097,-2.3115150877,0.1198842215
O,-0.9278891403,-2.4481620489,0.1100493125

39H, B3LYP Energy= -509.833054074 Hartree,
NIMAG= 0

N,-0.784056559,1.6584215774,-0.0875938084
N,0.572475471,1.7523051248,-0.0820222978
C,1.1223337192,0.5287961039,-0.0187218822
C,0.0368603521,-0.3601375399,0.0162653609
C,-1.1603221028,0.3707586328,-0.0280007702
H,-1.3684719629,2.484715595,-0.1316321957
C,2.5926075321,0.3189149828,0.0023010822
N,0.1364544262,-1.8071943387,0.0870486149
C,-2.5876950045,-0.0399863428,-0.0186884097
H,1.0388171987,2.6507284927,-0.1221832664
H,3.1271144232,1.2688016381,-0.0396005772
H,2.8786920197,-0.2207216072,0.9074356497
H,2.8916544004,-0.3051886103,-0.842325398
H,-3.2477615617,0.8271190312,-0.0650646704
H,-2.7909525097,-0.698652236,-0.865558786
H,-2.8036836993,-0.6148077532,0.8842242489
O,1.2623831072,-2.2769619169,0.1182530374
O,-0.9146559798,-2.4269341228,0.1090774394

40, B3LYP Energy= -764.547186859 Hartree,
NIMAG= 0

N,-0.7425269381,1.7149133612,0.0115777078
N,0.6026638997,1.8626986385,0.0174333778
C,1.0902642057,0.6261069042,0.004036524
C,0.0228841958,-0.3061806769,-0.0116349543
C,-1.1533084972,0.4191733759,-0.0072204681
H,-1.3221802828,2.5386070987,0.0138151354
C,2.5591231933,0.3585398217,0.0042457973
Cl,0.1596818881,-2.0396190085,-0.032448533
C,-2.5836357417,-0.0015273139,0.0025863216
H,3.10306555,1.3033815397,0.0116556593
H,2.8545459705,-0.2237373739,0.8818207519
H,2.8570212552,-0.2116014652,-0.8803629717
H,-3.1965958015,0.65647072,-0.619300508
H,-2.6762290864,-1.0168654826,-0.3847781504
H,-2.9986648106,0.0069408612,1.0157543105

40H, B3LYP Energy= -764.907181371 Hartree,
NIMAG= 0

N,-0.7488770532,-1.7178948464,-0.0894448218
N,0.6055883703,-1.7699906914,-0.0845691637

C,1.1092680823,-0.5227867598,0.0056446365
C,0.0078548579,0.3373288613,0.0582227264
C,-1.1559255036,-0.4356418254,-0.0030348119
H,-1.3085585927,-2.5583724973,-0.1513024702
C,2.5653429133,-0.2294533286,0.0360116063
Cl,0.0732296847,2.0460030417,0.1772068113
C,-2.5853685386,-0.0312037523,0.0150176417
H,1.0995189887,-2.6511185874,-0.1404332771
H,3.1635110703,-1.1387351563,-0.0312680449
H,2.8312220403,0.4278074858,-0.79564305
H,2.8221376668,0.2917708361,0.9616948343
H,-2.8064136975,0.5183726763,0.9334240249
H,-2.7955196594,0.6351694065,-0.8252993768
H,-3.2511436298,-0.8927168629,-0.046365265

41, B3LYP Energy= -2878.46784309 Hartree,
NIMAG= 0

N,2.2792663776,-0.5151281345,-0.0528411252
N,2.2683901064,0.8378461304,-0.0484243906
C,0.9830441442,1.1767786909,-0.0038444682
C,0.1820851732,0.0071479951,0.018304725
C,1.0423479525,-1.0750767394,-0.0148796786
H,3.1643262006,-0.994908223,-0.09009524
C,0.5506594229,2.605773778,0.0134480324
Br,-1.7077228053,-0.0806032568,0.0829420925
C,0.7997457487,-2.5463805114,0.0068628398
H,1.4271518508,3.2535604812,-0.0136868323
H,-0.0839409015,2.836892861,-0.8468984827
H,-0.0266215955,2.8329618231,0.9142629619
H,0.5636457381,-2.8960677771,1.016659016
H,-0.0434336034,-2.8056333539,-0.6363775129
H,1.6769931907,-3.0947937635,-0.3445989371

41H, B3LYP Energy= -2878.82851335 Hartree,
NIMAG= 0

N,2.3148810274,-0.5580575864,-0.0973372468
N,2.2478959334,0.7956056164,-0.088548511
C,0.960563607,1.1865268436,0.0010962133
C,0.1979511523,0.0147457065,0.051885454
C,1.0726356283,-1.0752502877,-0.0110865193
H,3.2016649613,-1.0416121278,-0.1548404647
C,0.5481738268,2.6136513433,0.0319011202
Br,-1.6676606922,-0.0783185296,0.1814635846
C,0.8035150479,-2.5364354017,0.0056940052
H,3.0817942952,1.3651503283,-0.1496933328
H,1.4054413398,3.2847209797,-0.0315874612
H,-0.1259435353,2.8259296393,-0.801632098
H,0.0046014197,2.8257464946,0.9559903432
H,0.2825200925,-2.8099762349,0.9266128021
H,0.1547461286,-2.8064742436,-0.8312458801
H,1.7230805536,-3.1187067385,-0.0623523145

42a, B3LYP Energy= -5412.67376554 Hartree,
NIMAG= 0

N,-0.7695710672,2.3721754325,-0.1200076451
N,0.5557307719,2.1079994711,-0.1169578962
C,0.6199847071,0.7938096622,-0.0006693044
C,-0.6670276278,0.2105698421,0.071248678
C,-1.5556471743,1.2698021965,-0.009554487
H,-1.0701744516,3.3309285462,-0.201228946

Br,2.2813939506,-0.0901235379,0.0525740384
Br,-1.1254562421,-1.6077002351,0.2406726723
C,-3.0458965444,1.3151020209,0.0095376389
H,-3.406421984,2.3424785052,-0.076410517
H,-3.4646482685,0.7364125081,-0.8176949133
H,-3.4373700697,0.8929165881,0.9385446814

42b, B3LYP Energy= -5412.67296965 Hartree,
NIMAG= 0

N,-0.7392983643,-0.0555620252,-0.9600802273
N,0.6114117661,-0.0740855618,-1.0035227263
C,1.0121558388,-0.0114818321,0.2637718691
C,-0.1098062106,0.0481402732,1.131603809
C,-1.2148775038,0.0175243309,0.3051886719
H,-1.2720118428,-0.0945872389,-1.8143346677
C,2.4609388292,-0.0097040928,0.623275408
Br,-0.0937855472,0.1479850928,3.0102825716
Br,-3.051348338,0.0595584021,0.6865883386
H,3.0611450476,-0.0651724713,-0.2850926457
H,2.7303357751,0.8987557805,1.1690162952
H,2.70926827,-0.8613706575,1.2625741933

42H, B3LYP Energy= -5413.02156392 Hartree,
NIMAG= 0

N,-0.7895280676,2.3865713491,-0.0940011335
N,0.5233478996,2.0507067827,-0.0803681446
C,0.6253813291,0.7090355091,0.0231012761
C,-0.6697770291,0.1888782682,0.0762215784
C,-1.5499867986,1.2784710076,-0.0000721505
H,-1.0820910594,3.3532706524,-0.1654223674
Br,2.2689965773,-0.1397918729,0.0729994256
Br,-1.1576851436,-1.6068062476,0.2208355273
C,-3.0348865496,1.3157053024,0.0115851275
H,1.2599556865,2.7425486476,-0.1417873378
H,-3.4136848872,2.3354995489,-0.0644538732
H,-3.4292111305,0.7306054718,-0.8230626243
H,-3.412011827,0.8680055807,0.9345226964

43a, B3LYP Energy= -342.998029175 Hartree,
NIMAG= 0

N,-0.7223162147,-0.2924169364,-1.1746347829
N,0.6169189454,-0.1140775521,-1.1933152032
C,0.9703137095,-0.0342716373,0.0893337953
C,-0.1641196169,-0.1642816208,0.9362233857
C,-1.2318033089,-0.3285700436,0.0812808769
H,-1.2156190212,-0.3807027403,-2.047504782
C,2.3901485638,0.164505324,0.4492384518
H,-0.2001724648,-0.1417232984,2.0132522555
H,-2.2852943622,-0.4644413057,0.2679834061
H,3.038344587,0.2291420574,-0.4165939136
C,2.7794062082,1.005790036,1.6487181663
H,3.6511621487,1.6424118362,1.5553253785
H,1.9768840298,1.4293829147,2.2412199685
C,2.9784790474,-0.4844870101,1.6864677674
H,2.311215297,-1.0737337717,2.3045880228
H,3.9873008117,-0.8739607821,1.6190419769

43b, B3LYP Energy= -342.997701064 Hartree,
NIMAG= 0

N,-0.1251607406,-0.1733528481,-0.8491529841
N,1.2172540324,-0.2762682493,-0.7543014532
C,1.4638472127,-0.1185812967,0.5416458797
C,0.2769182947,0.0881623404,1.280457749
C,-0.7435576554,0.0458800558,0.3460205498
H,-0.5619496657,-0.278120219,-1.7510609741
H,2.4820220347,-0.1553755275,0.8996194734
H,0.1758456486,0.2571199545,2.3399188289
C,-2.2109869392,0.2041308712,0.4554670818
H,-2.6151266754,1.0567196013,-0.0837065701
C,-2.9229226989,-0.1505767531,1.7367641846
H,-2.3279261789,-0.5555663183,2.545767603
H,-3.7361616034,0.4904374271,2.0537737892
C,-3.1205784019,-1.0133041496,0.5192628583
H,-4.0680813651,-0.9628750302,-0.0035917385
H,-2.6472378585,-1.9875624486,0.5114512622

43H, B3LYP Energy= -343.364295181 Hartree,
NIMAG= 0

N,-0.7689183435,-0.2993483341,-1.202618537
N,0.5758461082,-0.1189376344,-1.1692717992
C,0.9970968631,-0.0301671397,0.1109185317
C,-0.1502101005,-0.1629662828,0.9152226672
C,-1.2241849536,-0.3280533327,0.062116191
H,-1.2700836779,-0.3886119676,-2.0760406246
C,2.4033849581,0.166082474,0.4426465502
H,-0.1893984142,-0.1408785881,1.990896145
H,-2.274751008,-0.4631572524,0.2670798391
H,1.1203577439,-0.067768239,-2.0202094812
H,3.0663904934,0.2329530667,-0.4122851538
C,2.78713032,0.9984193763,1.6675527777
H,3.6497178938,1.6414748607,1.5487825502
H,1.9789227135,1.4309167195,2.2444640466
C,2.9838453831,-0.4744022899,1.7049048423
H,2.3135443387,-1.0744469447,2.307999175
H,3.985665019,-0.8737965115,1.6125705109

44a, B3LYP Energy= -460.979167013 Hartree,
NIMAG= 0

N,-1.0218114322,1.3921274924,-0.6751758696
N,0.305374981,1.617536856,-0.5723613301
C,0.8278222545,0.4249963258,-0.2947197315
C,-0.1810168841,-0.5784439222,-0.2163315315
C,-1.3685424421,0.0914809307,-0.4687624136
H,-1.6320679737,2.1627831205,-0.8932435023
C,2.2874323764,0.2354508891,-0.1287171262
C,0.006453853,-2.0380087827,0.0728557645
C,-2.7937032619,-0.3704667502,-0.4955439255
H,2.5609669595,-0.7152527777,0.314854956
C,3.2585632784,0.7810233305,-1.1649216964
H,4.1236159123,0.1781583886,-1.4165825827
H,2.8217833839,1.3293184837,-1.9905211345
C,3.1868034675,1.4067586498,0.1992530627
H,2.7045658412,2.3725126263,0.2821017069
H,4.0045001847,1.2360491835,0.8897540564
H,0.7496791125,-2.488005625,-0.5925940223
H,0.3438783694,-2.2123190807,1.1004345506
H,-0.9261454858,-2.5916882651,-0.0594037681

H,-3.3528919808,0.2260528648,-1.225474824
H,-2.8224343967,-1.3995597011,-0.8652490144
C,-3.4970071954,-0.2986933551,0.872398403
H,-3.5122231813,0.7250675181,1.2553835483
H,-4.5308186052,-0.6470234551,0.7953304153
H,-2.982099935,-0.9200053447,1.6090234092

44b, B3LYP Energy= -460.978329618 Hartree,
NIMAG= 0

N,-0.387584819,-0.3761197735,-0.8204700729
N,0.9545081239,-0.5013372246,-0.830168535
C,1.334642041,-0.1667078754,0.4004031059
C,0.2156422501,0.1767644408,1.212688744
C,-0.8854033482,0.0244543719,0.3846772464
H,-0.9096781354,-0.5801525389,-1.6568439329
C,2.7806819992,-0.1723777025,0.8120328467
C,0.2370116892,0.6157604019,2.6453258337
C,-2.3330874938,0.2564294804,0.602335733
H,-2.6504265691,1.2903008301,0.4925536958
C,-3.0981893535,-0.5426352544,1.6352497953
H,-2.5529792426,-1.3060500352,2.1762530463
H,-3.8544420326,-0.0274271416,2.214986002
C,-3.3546836085,-0.7780840008,0.1704425018
H,-4.2852151406,-0.4225083478,-0.254793321
H,-2.9884502391,-1.7041860057,-0.2565116901
H,0.7434269772,-0.1156213999,3.2843046242
H,0.7657152705,1.5673247923,2.7691933619
H,-0.7749080799,0.7499416701,3.0324838411
H,3.0624884597,0.8423259402,1.1220661743
H,2.8869736193,-0.7899770736,1.7129826517
C,3.7468732387,-0.6658488071,-0.2675572006
H,3.685788912,-0.0452331828,-1.1637472702
H,4.775582704,-0.6395128718,0.1016504007
H,3.5136170875,-1.6902786722,-0.5655625221

44H, B3LYP Energy= -461.354577948 Hartree,
NIMAG= 0

N,-0.4380886384,-0.7485195958,-1.4051442648
N,0.8881937999,-0.5212089827,-1.2489838285
C,1.1443905453,-0.1824348199,0.0355565095
C,-0.0945328597,-0.1632137776,0.7101316703
C,-1.0662806369,-0.5192293256,-0.2330497381
H,-0.8322244628,-0.9660816172,-2.3097621564
C,2.533895328,0.0641005427,0.4357694865
C,-0.3714169871,0.1900405329,2.1428913387
C,-2.5540951759,-0.6189959998,-0.1152726758
H,1.5458502686,-0.7194877528,-1.990226741
H,3.223020136,0.0776514943,-0.4019623697
C,2.9057064368,0.9783086295,1.5964335988
H,3.7688813362,1.6123899227,1.4397388172
H,2.1033370577,1.4445362244,2.1513604933
C,3.1096457108,-0.49169253,1.737837392
H,2.4455714606,-1.049769178,2.3847915533
H,4.1142802872,-0.8902551649,1.6780385462
H,0.3657650404,-0.2397913228,2.8210872418
H,-0.3779701262,1.2726334561,2.2952238719
H,-1.3480482555,-0.1872684222,2.4484150287
H,-2.932548958,-1.2821969221,-0.8986430355
H,-2.7898486999,-1.1032522624,0.8357366206
C,-3.259006761,0.749770739,-0.1962010722
H,-3.0648954429,1.2426585281,-1.1514215887

H,-4.3371946233,0.6130000917,-0.0999186919
H,-2.9304317848,1.4160265386,0.6034960985

45a, B3LYP Energy= -457.381101399 Hartree,
NIMAG= 0

N,-0.7836435445,-0.0494696441,-0.8533412922
N,0.5593067338,-0.0691817918,-0.9197677963
C,0.9702363457,-0.006467776,0.3504124038
C,-0.1443715317,0.0542283258,1.2335087664
C,-1.2522299431,0.0241268375,0.4183242011
H,-1.3141065327,-0.0888665326,-1.7083140928
C,2.4053563448,-0.0062605317,0.679436528
H,-0.1442758836,0.1116559872,2.308843162
H,-2.3073236878,0.0487362385,0.6396020863
C,2.841216592,0.0599166255,2.0101565393
C,3.3709545945,-0.0725953149,-0.3369446097
C,4.1994469024,0.0598831547,2.3175128614
H,2.1177410489,0.1119819117,2.8152418164
C,4.7269219559,-0.0725111465,-0.0281435093
H,3.0432235225,-0.1239486579,-1.3673859316
C,5.1492377762,-0.0063268289,1.2999707699
H,4.5153949154,0.1116778043,3.3534518423
H,5.4581549425,-0.1243253872,-0.8272587715
H,6.2066804888,-0.0063851836,1.5386836367

45b, B3LYP Energy= -457.380544540 Hartree,
NIMAG= 0

N,-0.5167972286,-0.4499196016,-0.7718338823
N,0.8272027974,-0.3792605125,-0.8366947891
C,1.1856475305,0.1269191639,0.3399075632
C,0.0704322859,0.3687293085,1.1679880718
C,-1.0308596833,-0.0186167325,0.4167657264
H,-1.0195590383,-0.8701750442,-1.5369453883
H,2.2300119182,0.3038668178,0.5492171507
H,0.0608625001,0.7969857128,2.1567125092
C,-2.4675919663,-0.0025455822,0.7080963206
C,-2.9236288795,-0.157931632,2.0259859672
C,-3.416095206,0.171947535,-0.3117069971
C,-4.2844860039,-0.1387059454,2.3132911344
H,-2.2052952471,-0.3108383728,2.8229546757
C,-4.7778819276,0.1793231041,-0.0229918028
H,-3.089813988,0.3339000403,-1.3333793054
C,-5.2181937623,0.0251773536,1.2902613897
H,-4.6177260254,-0.2623526993,3.3376015807
H,-5.4950395022,0.318927595,-0.8240501458
H,-6.2784453434,0.0356688115,1.5151538611

45H, B3LYP Energy= -457.744995831 Hartree,
NIMAG= 0

N,-3.0460427604,-0.6311701422,0.2158141552
N,-1.7362076707,-0.9742118631,0.2951171124
C,-0.963620742,0.0899711896,-0.0281917855
C,-1.8466301038,1.1381902556,-0.3456499851
C,-3.1295507033,0.6481499526,-0.1893689757
H,-3.7799289918,-1.3093344536,0.3707332432
C,0.4926835694,0.035829823,-0.0179859086
H,-1.5750080347,2.1239725358,-0.6819204756
H,-4.0891552349,1.1128372671,-0.3542018811
H,-1.4518186304,-1.8570438132,0.698241557
C,1.2246990491,1.2111035374,0.2143498098

C,1.1732732033,-1.1733719033,-0.2394042129
C,2.6133385491,1.1711736256,0.2360768211
H,0.711145821,2.1465414585,0.402188103
C,2.5616534636,-1.2042556753,-0.2171440386
H,0.6289129372,-2.0823991527,-0.473167669
C,3.2825288746,-0.0338679434,0.0230690934
H,3.1737229062,2.0787600353,0.4239846897
H,3.08231893,-2.1361967696,-0.4001269928
H,4.3655185686,-0.0606889642,0.0378353399

46a, B3LYP Energy= -916.997370322 Hartree,
NIMAG= 0

N,-0.5547451475,-0.5471177798,-0.7741854509
N,0.7849640863,-0.4945203111,-0.8867447271
C,1.1947833184,0.0725416231,0.2415355554
C,0.1026704453,0.3650340543,1.0819680672
C,-1.037280758,-0.0475316785,0.4019175092
H,-1.089388618,-1.0075313784,-1.4938309179
H,2.2425620077,0.2571095379,0.4201341907
Cl,0.1889817669,1.1518370606,2.6256623614
C,-2.4706719142,-0.003463879,0.7090744587
C,-2.9385545385,-0.2502143231,2.0079903309
C,-3.4030822395,0.2738810841,-0.303263174
C,-4.3024477374,-0.2232787192,2.2823750609
H,-2.2330507064,-0.4721896262,2.7983792392
C,-4.7667677546,0.2916078826,-0.0257781081
H,-3.0590693985,0.5059988892,-1.3053760024
C,-5.2213540786,0.0434800812,1.2681804644
H,-4.6486852992,-0.4184982343,3.2909695851
H,-5.4730127157,0.5118355571,-0.8182302125
H,-6.2831074885,0.0621194797,1.4855554097

46b, B3LYP Energy= -916.996144571 Hartree,
NIMAG= 0

N,-0.7512373213,0.2850387817,-0.890620383
N,0.5887687798,0.377222805,-0.8909884094
C,0.9762066767,0.0494217557,0.3462501365
C,-0.1721633264,-0.2513761598,1.1331962472
C,-1.2617801154,-0.0880234389,0.3070572415
H,-1.2562735911,0.5134435482,-1.731645739
C,2.4088988196,0.0219536878,0.6904665644
Cl,-0.2598978768,-0.7923640968,2.7810869249
H,-2.3159107855,-0.2171451359,0.4875523087
C,2.8637781074,0.3323564281,1.978913913
C,3.3505147375,-0.3005870808,-0.2983715108
C,4.2258683326,0.3157461299,2.2705066028
H,2.1564490515,0.6002156405,2.7528290795
C,4.7095452112,-0.3142799835,-0.003951564
H,3.0035705481,-0.5388370346,-1.2961180349
C,5.1532273583,-0.0088110361,1.2828465832
H,4.5615255162,0.5627889605,3.271504674
H,5.4240879265,-0.5681590678,-0.7791063021
H,6.2127429912,-0.0227366131,1.5125802777

46H, B3LYP Energy= -917.352449198 Hartree,
NIMAG= 0

N,-0.7973049423,0.3541283491,-0.8979783681
N,0.5529883927,0.4187871293,-0.8472366508
C,0.9977459958,0.0331737652,0.3726005456
C,-0.1596718964,-0.3070601126,1.1089178767

C,-1.2526374618,-0.1016092786,0.2806906639
H,-1.3076348387,0.5663419434,-1.7451488626
C,2.4202621564,0.00747518,0.6930090873
Cl,-0.2339086379,-0.9315889807,2.7019915321
H,-2.3035429465,-0.2713063363,0.4542780351
H,1.0876398414,0.8498471806,-1.590548974
C,2.8664797018,0.3729403619,1.9729359945
C,3.352485417,-0.3679372274,-0.2908479516
C,4.2276433617,0.3748000517,2.2538560458
H,2.1596446169,0.6738121703,2.7350522808
C,4.709793011,-0.3686685884,0.0031195191
H,3.0191952262,-0.7034274597,-1.2673279281
C,5.1484015518,0.0054602327,1.2737833046
H,4.570024108,0.6669835877,3.2389845905
H,5.4238911989,-0.6729726076,-0.7522440364
H,6.2076819565,0.0023485862,1.501357647

47a, B3LYP Energy= -3030.91772654 Hartree,
NIMAG= 0

N,-0.5632151111,-0.5747379824,-0.7688352945
N,0.7760027008,-0.524666263,-0.8924166461
C,1.1932002706,0.0655388614,0.2208749486
C,0.1074253423,0.3767911911,1.0645333444
C,-1.0367863421,-0.0507557873,0.3998963809
H,-1.1034863937,-1.0503215798,-1.4745120704
H,2.2426813026,0.2531282361,0.3858907646
Br,0.2221525115,1.279436738,2.7212817521
C,-2.4710909585,-0.0053479527,0.707948365
C,-2.9417434266,-0.2707242094,2.001893555
C,-3.4005101371,0.2891235728,-0.3020646438
C,-4.3060496238,-0.243305166,2.2744899579
H,-2.2380376802,-0.5077327117,2.7894908794
C,-4.7647515967,0.3077446917,-0.0266168925
H,-3.0530501429,0.5337000821,-1.2999943122
C,-5.2221220152,0.0421974716,1.2629127416
H,-4.654783775,-0.4530983658,3.279295767
H,-5.4689393509,0.5425803919,-0.8167006972
H,-6.2841523437,0.0615481013,1.47896574

47b, B3LYP Energy= -3030.91640284 Hartree,
NIMAG= 0

N,-0.7462872355,0.3189883607,-0.89520441
N,0.5937736731,0.4181844186,-0.886436119
C,0.9768815702,0.0566049309,0.3426082449
C,-0.1731419508,-0.2732631982,1.116923476
C,-1.2590608565,-0.0912984564,0.2886087594
H,-1.2485972796,0.5703808441,-1.7314341786
C,2.4100964126,0.0271279394,0.6871721434
Br,-0.2909725358,-0.9293656332,2.8883231692
H,-2.3137955192,-0.231360192,0.457671034
C,2.8667961684,0.3606681769,1.9688075225
C,3.3492405298,-0.3190142859,-0.2955310439
C,4.2286678501,0.3416333091,2.2609159508
H,2.1603753091,0.6488908809,2.7363424693
C,4.7085039738,-0.33530848,-0.0010494972
H,3.0007282514,-0.573312268,-1.288825127
C,5.1538539174,-0.0079324811,1.2796220112
H,4.566136388,0.6063414833,3.2567869472
H,5.4214761203,-0.6082006318,-0.7711501098
H,6.2132462531,-0.0239066273,1.5098373679

47H, B3LYP Energy= -3031.27348503 Hartree,
NIMAG= 0

N,-0.7892087697,0.3800776905,-0.9059334781
N,0.5604180414,0.4459257858,-0.8448841948
C,0.9963451581,0.0389042441,0.3715417432
C,-0.1637783625,-0.3171181583,1.0962464139
C,-1.2500246724,-0.0970205744,0.2622592409
H,-1.2943102973,0.6067733833,-1.752575184
C,2.4201473187,0.0123569287,0.6919153732
Br,-0.2684081672,-1.0424084086,2.8194635198
H,-2.3025121013,-0.2700379741,0.4228364409
H,1.1000113828,0.8903807597,-1.5768153582
C,2.8695982639,0.3923540052,1.9661105456
C,3.3494014971,-0.3770301839,-0.2889488489
C,4.2311673684,0.3922681229,2.2453774556
H,2.1644153671,0.7060323869,2.7245711177
C,4.7073942696,-0.3799051851,0.0032895469
H,3.0127763284,-0.7216934655,-1.261056826
C,5.1491862142,0.0071571801,1.268834318
H,4.5760795544,0.6958127097,3.2262131304
H,5.4191980438,-0.696070955,-0.7493873414
H,6.2087200715,0.0023853993,1.4952257556

48a, B3LYP Energy= -496.707212318 Hartree,
NIMAG= 0

N,-0.5794862703,-0.5900199979,-0.8196258932
N,0.7581380275,-0.5352838834,-0.9340223165
C,1.1576727567,0.0304618499,0.2008808613
C,0.0787882438,0.3310431235,1.065295145
C,-1.0486371833,-0.0920827885,0.3648274726
H,-1.1160777387,-1.0448500157,-1.5408311482
H,2.2097519566,0.2157613246,0.3650445352
C,0.1582520653,0.9955098002,2.4074269258
C,-2.4830844193,-0.042487611,0.67037095
C,-2.9519569275,-0.2744373834,1.972627111
C,-3.4223198126,0.2322636576,-0.3376891459
C,-4.3141552169,-0.2313619798,2.2560481498
H,-2.2471645802,-0.5101062054,2.7604250077
C,-4.7843661714,0.2642341317,-0.0535861295
H,-3.0822558233,0.450863779,-1.344202975
C,-5.2364419323,0.0344623551,1.2450201144
H,-4.6566928804,-0.4169695197,3.2679493173
H,-5.4925307504,0.4819842057,-0.845249198
H,-6.2969402212,0.0645468281,1.4672138241
H,0.2200900593,0.2688276741,3.224991036
H,1.047828329,1.6268672719,2.4698340846
H,-0.7125836903,1.6280934733,2.5955383613

48b, B3LYP Energy= -496.706675021 Hartree,
NIMAG= 0

N,-0.7070317569,-0.4017526228,-0.9588539957
N,0.6323393223,-0.4754794944,-0.9496357732
C,0.9893427558,-0.1622687922,0.3009086507
C,-0.1589124184,0.1192457049,1.1067036193
C,-1.2243307053,-0.0501300082,0.2462196901
H,-1.2032674665,-0.6172659303,-1.8079839687
C,2.4199177298,-0.1117394356,0.6567933697
C,-0.2407892918,0.5526033578,2.540777156
H,-2.2859210704,0.064073331,0.4018157919
C,2.8685389686,-0.4012912305,1.9529504848

C,3.3723183044,0.2203022712,-0.3198551374
C,4.2258780372,-0.3540215304,2.2654770782
H,2.1597632607,-0.6888428444,2.7189473845
C,4.7265579632,0.264008371,-0.0070212573
H,3.0342269395,0.4416293791,-1.3245462989
C,5.160566315,-0.0194026886,1.2885456706
H,4.5522971764,-0.5873563716,3.2730451643
H,5.4463516157,0.5247009045,-0.7752855359
H,6.2163857732,0.0181693303,1.5322544674
H,-0.0929354295,-0.2806847429,3.2353829027
H,0.514329338,1.3078936837,2.7727849158
H,-1.221203471,0.9840798482,2.7556527512

48H, B3LYP Energy= -497.075919332 Hartree,
NIMAG= 0

N,-0.7562508909,-0.5088782095,-0.9536388898
N,0.5936870614,-0.540865395,-0.895446947
C,1.008212774,-0.165200192,0.3378079663
C,-0.1498145096,0.1422729426,1.0892423784
C,-1.2212670675,-0.0801046825,0.2337669263
H,-1.2549253882,-0.705539635,-1.8106813598
C,2.4316111364,-0.1073093463,0.6679252639
C,-0.2275990509,0.6510391456,2.4964974059
H,-2.279902228,0.060677805,0.388928909
H,1.1444250623,-0.9405931246,-1.6437828984
C,2.8801052506,-0.5026026754,1.9375050024
C,3.3616080104,0.3329771624,-0.2895347128
C,4.2375648545,-0.4672942861,2.2363952402
H,2.1775840172,-0.8629022575,2.6782731173
C,4.7159624314,0.3691368484,0.0194064518
H,3.02691129,0.6881345526,-1.2585426147
C,5.1553965874,-0.0328364336,1.2808223843
H,4.5796089138,-0.7835915239,3.2142850858
H,5.4266917969,0.7221057398,-0.7178686954
H,6.2116220621,-0.0021014352,1.5201336988
H,-0.1753832103,-0.1656583875,3.2211179578
H,0.5912050907,1.3404426403,2.7080185428
H,-1.1675954087,1.1788659226,2.6615400458

49a, B3LYP Energy= -496.711642706 Hartree,
NIMAG= 0

N,-0.6928631023,-0.073753868,-0.8861415086
N,0.6535805982,-0.0948047278,-0.9460493205
C,1.0541892992,-0.0137939276,0.3243287783
C,-0.068144733,0.0593901614,1.1965103145
C,-1.1803624457,0.0182365119,0.3818491884
H,-1.2173107324,-0.1255959487,-1.7448582928
C,2.4870309778,-0.008669577,0.6658300139
H,-0.074252192,0.1323192436,2.271563853
C,-2.6425682208,0.0571748783,0.687463382
C,2.9113692238,0.0769277764,1.9988541601
C,3.4612546912,-0.0897456367,-0.3411278145
C,4.2670913306,0.0814733765,2.3179783076
H,2.1800887369,0.1406775273,2.7962994521
C,4.8142938138,-0.0851023042,-0.0209074205
H,3.1415022095,-0.1561409769,-1.3734661381
C,5.225558055,0.0005011238,1.3099714131
H,4.5737604654,0.1484259122,3.3560469314
H,5.5524991474,-0.1485474636,-0.8129881412
H,6.2811082765,0.0039807554,1.5575901271
H,-3.15245639,-0.8466035802,0.339132661

H,-2.7959914978,0.1317185038,1.7643800108
H,-3.1303722314,0.91842839,0.220103763

49b, B3LYP Energy= -496.711433134 Hartree,
NIMAG= 0

N,-0.613153281,-0.4452351871,-0.808435229
N,0.7337176493,-0.3821802021,-0.8780758774
C,1.1154865969,0.105233075,0.3014646891
C,-0.0041556189,0.3382512372,1.1366436391
C,-1.1131600134,-0.0310259909,0.3907887948
H,-1.1211588079,-0.8631904892,-1.5708346817
C,2.5634006943,0.3451207233,0.59662365
H,-0.0060527982,0.7535576347,2.131646213
C,-2.5469916495,-0.0118063252,0.6956064161
C,-2.9917835191,-0.1754711202,2.0163867652
C,-3.5044469537,0.17289633,-0.3140891386
C,-4.3498484385,-0.1544156893,2.3163323145
H,-2.2666016428,-0.3363659488,2.8055143778
C,-4.8635670761,0.1827016876,-0.0128453137
H,-3.1864083045,0.3407117168,-1.3374241847
C,-5.2924799183,0.0203839608,1.3032071827
H,-4.6742762918,-0.2846957896,3.3426839024
H,-5.5875786982,0.3301842436,-0.8063320047
H,-6.350644939,0.0320902425,1.5378056955
H,3.1712224607,0.0334625492,-0.2536188606
H,2.7591267133,1.404028138,0.7903472107
H,2.8870854267,-0.2161820062,1.4780128196

49H, B3LYP Energy= -497.082868000 Hartree,
NIMAG= 0

N,2.510940179,1.0134056281,0.3487936361
N,1.1692605827,1.2408723907,0.3517026543
C,0.5208948216,0.0920875301,0.0387049072
C,1.5103265939,-0.8654501347,-0.2212454139
C,2.7488107655,-0.2587764228,-0.0357008995
H,3.1673314009,1.774340506,0.4622447219
C,-0.9342230034,-0.00044126,0.0114071764
H,1.345674081,-1.8795347163,-0.5437584115
C,4.1294692369,-0.7788234121,-0.2415201447
H,0.7879348273,2.062186705,0.8016631503
C,-1.5532853321,-1.2348466516,0.2628494873
C,-1.7243001131,1.1277783233,-0.2655195282
C,-2.939214755,-1.3330814407,0.2474231864
H,-0.9549010434,-2.1080661313,0.4940144161
C,-3.1093824183,1.0209166553,-0.2800406307
H,-1.2637301247,2.0784453983,-0.5129462583
C,-3.717965404,-0.2076525552,-0.0215613158
H,-3.4125130407,-2.2860183381,0.4500359489
H,-3.7139957638,1.890864844,-0.5054639253
H,-4.7983172524,-0.2883838216,-0.0351581096
H,4.8451684833,-0.298307143,0.4280569254
H,4.1542521247,-1.8532329962,-0.0602645351
H,4.4517831541,-0.6042539571,-1.2723830376

50a, B3LYP Energy= -536.035400466 Hartree,
NIMAG= 0

N,0.5508817566,-0.9569389143,-0.1994587993
N,1.817965283,-0.794980555,0.2283503416
C,2.0385540328,0.5198009158,0.1544768711
C,0.8837222766,1.1916366543,-0.3338765332

C,-0.0593381626,0.2080381166,-0.5542169469
H,0.1701215534,-1.888758647,-0.2441286207
C,3.3384212934,1.0903006438,0.5478461
H,0.748376112,2.2473848523,-0.5026156992
C,-1.4803863181,0.2714599853,-1.0249781585
H,-1.609298442,1.1966831165,-1.5922606028
H,-1.6689826501,-0.5467727391,-1.7296471203
C,-2.5134403359,0.2171466468,0.1153804698
H,-3.5299424689,0.2756146986,-0.2828158811
H,-2.4287962983,-0.7114585787,0.68612858
H,-2.3697310108,1.0479447874,0.8100329202
C,3.6036866863,2.4577494901,0.3932066357
C,4.3427736016,0.2722055803,1.0879073877
C,4.8338715956,2.9935721954,0.766657691
H,2.8470841958,3.1111910168,-0.0254803024
C,5.5705745658,0.808566798,1.4597876111
H,4.1454368557,-0.7852534962,1.2112279969
C,5.823699809,2.1718531769,1.3018618948
H,5.0186447091,4.0543491256,0.6373708013
H,6.3343328986,0.1604387929,1.8756698256
H,6.7817335615,2.587984237,1.5925758376

50b B3LYP Energy= -536.035205069 Hartree,
NIMAG= 0

N,1.6689222207,-0.4703013915,0.7438510896
N,0.4767191817,-1.0073129647,0.4088016803
C,-0.0671540194,-0.1344917761,-0.438697415
C,0.7871144226,0.9789703288,-0.6309441993
C,1.9062847011,0.7344886212,0.150442829
H,2.2340292527,-0.9326543721,1.4373808804
C,-1.4195348752,-0.3890487275,-1.0375389715
H,0.6294958605,1.8243380648,-1.2813272352
C,3.1381103654,1.5010186003,0.3601220887
H,-1.674214256,-1.436454144,-0.8579791404
H,-1.364640472,-0.2561154285,-2.123652102
C,-2.5200406279,0.5211457841,-0.4674469008
H,-2.2954103,1.5765912082,-0.6448759941
H,-3.4849675504,0.3005934342,-0.9325223893
H,-2.6216721158,0.377841044,0.6113175247
C,3.1272143605,2.900238939,0.2532331886
C,4.3507873502,0.8640666744,0.6669155952
C,4.2911997032,3.6368700208,0.4462363411
H,2.1959472555,3.4094383882,0.0340368247
C,5.5120738247,1.6042914132,0.8705263894
H,4.3963025507,-0.2184840162,0.7174288857
C,5.4882560534,2.9933918666,0.7600255038
H,4.261992743,4.7174000553,0.3611567324
H,6.4396560462,1.0933475308,1.1031595731
H,6.3937032247,3.5688675468,0.9145681209

50H, B3LYP Energy= -536.408029803 Hartree,
NIMAG= 0

N,0.6135708852,-1.010258836,-0.583508433
N,1.875871292,-0.7969491693,-0.1222743948
C,2.0514948581,0.5307593309,0.0945304515
C,0.8277514767,1.1470725767,-0.1926438114
C,-0.0627330714,0.1572296302,-0.6032248012
H,0.2617880365,-1.9481046513,-0.7225923909
C,3.3246112114,1.0850606506,0.542021182
H,0.6023136362,2.194293852,-0.0824595855
C,-1.5147509576,0.2293357043,-0.9515209466

H,2.5905690378,-1.5036826588,-0.2321142102
H,-1.6669505669,1.117893211,-1.5690994994
H,-1.7817645237,-0.6316401789,-1.5711502734
C,-2.424930785,0.293023,0.2917976622
H,-3.4676857411,0.3536827972,-0.0231376051
H,-2.3115831299,-0.5953046685,0.9171230485
H,-2.2031127813,1.1711458066,0.9009947904
C,3.6629899866,2.4038335423,0.2009767223
C,4.2153406747,0.3177208598,1.3108545699
C,4.87703043,2.9388205285,0.6143907959
H,2.9914898101,2.9993621667,-0.4061225601
C,5.4268722863,0.860329251,1.7211026067
H,3.9495398992,-0.6854534869,1.6272820148
C,5.7599904232,2.1692851619,1.3717363304
H,5.1373224382,3.9541658654,0.3413862964
H,6.1051938502,0.268520651,2.3234606241
H,6.7047197593,2.5905060107,1.6940937423

51a, B3LYP Energy= -536.037958138 Hartree,
NIMAG= 0

N,-0.6437623642,-0.5947164356,-0.8043676266
N,0.6982110855,-0.5490658793,-0.9064698448
C,1.10601719,0.0210243151,0.2254618177
C,0.0098782581,0.329201944,1.0780657631
C,-1.1142234801,-0.0926894002,0.3759897478
H,-1.1749216864,-1.0681775417,-1.5170492721
C,2.5601442469,0.2752565292,0.4718163828
C,0.0786951701,1.0123999405,2.410801807
C,-2.5500896637,-0.0433989987,0.6779766342
C,-3.0265784822,-0.3217605365,1.9683018259
C,-3.4823711883,0.2746233306,-0.3235377704
C,-4.3897336713,-0.2785183519,2.2475044175
H,-2.3262285064,-0.5945477761,2.7483062421
C,-4.8455942675,0.3066488636,-0.0441826949
H,-3.134390033,0.5258121722,-1.319646407
C,-5.3051835355,0.0331484697,1.2432607544
H,-4.738609997,-0.4997779599,3.2500701946
H,-5.5486997776,0.5583856942,-0.8303021969
H,-6.3664500297,0.0631415785,1.4619744348
H,0.3267419281,0.3156231393,3.220003172
H,0.8490125218,1.7887337608,2.4116187166
H,-0.8701506805,1.4886599059,2.6661262366
H,3.1450934678,-0.0749784621,-0.3793812403
H,2.7622768805,1.3422713148,0.6115488335
H,2.9117327944,-0.2430260665,1.3694709124

51b, B3LYP Energy= -536.036613337 Hartree,
NIMAG= 0

N,-0.6499526206,-0.3884006418,-0.9303464431
N,0.6925591981,-0.4533279292,-0.937652998
C,1.0539687471,-0.1596090256,0.3142430017
C,-0.0896819963,0.1007738149,1.1323286092
C,-1.1726872116,-0.0609162458,0.2830974093
H,-1.1526838914,-0.5913282363,-1.7794765369
C,2.4858223453,-0.1076288402,0.6648611168
C,-0.1460222813,0.5146420876,2.5730907903
C,-2.6446781094,0.0548637294,0.5142148218
C,2.9454142952,-0.4604791317,1.9414618998
C,3.4284866312,0.2870361441,-0.2976226139
C,4.3038609049,-0.4127793969,2.2492476973
H,2.2436433512,-0.7988725934,2.6934481434

C,4.7840675569,0.3309388477,0.0100358313
H,3.0815018128,0.5565254441,-1.2874800667
C,5.2288045873,-0.0149255831,1.286646986
H,4.6392955095,-0.6957778284,3.2410616174
H,5.4963706299,0.6404754213,-0.7470362194
H,6.2854876763,0.0227215119,1.52674763
H,-3.0752605385,-0.8862250961,0.8724570012
H,-2.8599927663,0.8197788655,1.2630809266
H,-3.1700032932,0.3342819472,-0.4031626181
H,-0.0899088708,-0.3396534954,3.2569504529
H,0.6774396525,1.1870369238,2.8245873212
H,-1.0795786487,1.0393748863,2.79258686

51H, B3LYP Energy= -536.412969168 Hartree,
NIMAG= 0

N,-0.6954259701,-0.4768666791,-0.9408232442
N,0.6599420815,-0.4639396547,-0.9076627188
C,1.0716029052,-0.1465576205,0.3455587859
C,-0.0797283964,0.1061729479,1.1125796016
C,-1.1738547692,-0.1005405533,0.2625087305
H,-1.1961377031,-0.6024130809,-1.8101496663
C,2.4972472206,-0.0960608718,0.6734175624
C,-0.1514437433,0.5619269182,2.5381642314
C,-2.6323603263,0.0655904483,0.5144312644
H,1.2028502921,-0.897392504,-1.6424537456
C,2.9587488834,-0.5880357109,1.903712712
C,3.4151661398,0.4332347699,-0.2492665551
C,4.3172604512,-0.556239546,2.1991832567
H,2.2647327707,-1.0195289641,2.6143328951
C,4.7709488808,0.4647597801,0.0560341533
H,3.0680763648,0.8567171539,-1.1857103939
C,5.2233529638,-0.0305831472,1.2788037596
H,4.6694336769,-0.9464730371,3.146348279
H,5.4724212106,0.8859232744,-0.6538719545
H,6.2803360555,-0.0036375788,1.5153182859
H,-2.9523141432,-0.5853763661,1.3314542706
H,-2.8534480662,1.0956263969,0.8058445016
H,-3.2268156094,-0.1755435251,-0.3678870004
H,-0.2681052093,-0.2803811827,3.2262812984
H,0.752679929,1.1021313087,2.820162619
H,-1.001609492,1.2294613546,2.6904066855

52a, B3LYP Energy= -3070.24980640 Hartree,
NIMAG= 0

N,-0.6355612437,-0.5818214809,-0.7489150859
N,0.7074245484,-0.526961113,-0.8609145355
C,1.1288931313,0.0728025321,0.2493452595
C,0.0224239372,0.3781474054,1.0804872359
C,-1.116130744,-0.0570853501,0.4139410642
H,-1.1657711563,-1.0771507179,-1.4480371827
C,2.5770711845,0.3475570192,0.4872202143
Br,0.1133516188,1.2928694467,2.7344258522
C,-2.5520898597,-0.0174602095,0.7150795324
C,-3.0300630186,-0.2843192013,2.0060503318
C,-3.4769403158,0.2697930375,-0.3013877029
C,-4.3963871761,-0.2656149887,2.2693760515
H,-2.3302858132,-0.5159729215,2.7987376485
C,-4.8431075316,0.2804176964,-0.035117487
H,-3.1236413107,0.5138882505,-1.297363957
C,-5.307627262,0.0133658295,1.2515297431
H,-4.7505855592,-0.4764502959,3.2720928196

H,-5.5434379452,0.5093235233,-0.8303880652
H,-6.3712270848,0.0258949374,1.4604135369
H,3.1642615252,-0.0445832285,-0.3434210495
H,2.7663092596,1.4213308333,0.574217116
H,2.920852406,-0.119918214,1.4140370398

52b, B3LYP Energy= -3070.24827140 Hartree,
NIMAG= 0

N,-0.6622524433,0.4486528898,-0.8597243087
N,0.6831469178,0.5038679524,-0.8645536098
C,1.0603437341,0.1238330692,0.3590873886
C,-0.0959209807,-0.1676433766,1.1375738222
C,-1.1932035826,0.0522173555,0.3245706475
H,-1.1635730869,0.724221046,-1.6895290653
C,2.4938626203,0.0466258889,0.6944898695
Br,-0.2252870067,-0.8303979405,2.9078205229
C,-2.6569187279,-0.1001501612,0.5661563588
C,2.9698448015,0.3489837085,1.9769593812
C,3.4163126813,-0.3116230275,-0.2999404502
C,4.3329488226,0.288596072,2.2581062912
H,2.2776795329,0.6450506482,2.7544201625
C,4.7768122567,-0.3689451934,-0.0165843383
H,3.0530434539,-0.5419756352,-1.293774182
C,5.241018311,-0.0716756531,1.2648188108
H,4.6849608718,0.5298579578,3.2549341416
H,5.4761637593,-0.6500479747,-0.7962388946
H,6.3014071235,-0.1193317893,1.486063075
H,-2.9202894275,-1.1476573893,0.737296627
H,-2.9667129072,0.4643086287,1.4488379606
H,-3.2343814439,0.2597290738,-0.2884264905

52H, B3LYP Energy= -3070.61286923 Hartree,
NIMAG= 0

N,-0.7056735816,0.5505566141,-0.8618352367
N,0.6511413137,0.5366015116,-0.8273055381
C,1.0743432426,0.109350231,0.388912929
C,-0.0894120129,-0.2000370543,1.1146051022
C,-1.1929420981,0.072263713,0.2995865194
H,-1.2052472755,0.758987263,-1.7163774561
C,2.4993415195,0.0311736609,0.7003271306
Br,-0.2096504493,-0.9446492102,2.83110023
C,-2.6455687293,-0.1225259741,0.5450801655
H,1.1941272777,1.0358356071,-1.5198190342
C,2.973442276,0.3945374114,1.9700804237
C,3.4059994344,-0.3882243764,-0.2888905307
C,4.3368274429,0.3476442898,2.2371919975
H,2.2861129571,0.7312921464,2.7351238812
C,4.7660051538,-0.4378771013,-0.0091639143
H,3.0475102089,-0.7162363122,-1.2587778735
C,5.2325280845,-0.0676707482,1.2522956744
H,4.700815538,0.6381631054,3.2151172588
H,5.4597258196,-0.7758797925,-0.7692425248
H,6.2933834446,-0.1080748235,1.4688573456
H,-2.858108928,-1.180247661,0.7206676708
H,-2.9493553586,0.4256818918,1.4398742376
H,-3.2472942219,0.2212604746,-0.2970195424

53, B3LYP Energy= -457.378461814 Hartree,
NIMAG= 0

N,-0.628895241,-0.13478312,-0.8110093203
N,0.6465443186,0.2965746389,-0.8608645484
C,1.0085815725,0.3968439046,0.4120098325
C,-0.038951824,0.0323265789,1.3013416508
C,-1.0837451742,-0.3068802521,0.4550303416
H,-1.1237688097,-0.2998774026,-1.6724849054
H,2.0003166839,0.7465741408,0.6569309515
C,-0.0197228395,0.0156773996,2.7708196767
H,-2.0790412135,-0.6684803062,0.6576665035
C,-1.1899929346,0.2275919588,3.5162669238
C,1.1758669235,-0.2130080863,3.4691503295
C,-1.1675097319,0.2017028322,4.9076384956
H,-2.1217496625,0.4342319488,3.0011953043
C,1.2002491328,-0.2280229776,4.8609520492
H,2.0901630579,-0.3978075824,2.9166158986
C,0.0284446589,-0.0241492305,5.587885026
H,-2.0841988727,0.3698868184,5.4621776175
H,2.1359176054,-0.4085542342,5.378599603
H,0.0470986901,-0.0389081091,6.67161736

53H, B3LYP Energy= -457.736760179 Hartree,
NIMAG= 0

N,-0.6597702837,-0.1835608161,-0.8209843334
N,0.5901446262,0.3203162471,-0.8249551769
C,1.0004117334,0.474921621,0.4451570438
C,-0.0156915266,0.037670053,1.3034119197
C,-1.0471259781,-0.3748966387,0.4514151421
H,-1.1455086652,-0.4017835254,-1.6817907866
H,1.9702450785,0.8944730695,0.6616702352
C,-0.0021692919,0.0166760148,2.7739420097
H,-2.0130869645,-0.8007194107,0.6729801342
H,1.0606138804,0.5633857428,-1.6876001535
C,-1.17488986,0.2785568455,3.4953730102
C,1.1835562672,-0.2653306746,3.4659042405
C,-1.1595815861,0.2566520334,4.8861435406
H,-2.0942568924,0.5260279971,2.9756660052
C,1.1938777274,-0.2828953367,4.8567903951
H,2.0931211572,-0.497849408,2.9225782605
C,0.0235805823,-0.0229922884,5.5684202403
H,-2.0686219482,0.4665485298,5.436717048
H,2.1128453289,-0.5081454759,5.3843351907
H,0.0335757199,-0.038347791,6.6516497612

54, B3LYP Energy= -688.495818399 Hartree,
NIMAG= 0

N,-0.6158525403,1.5554992217,-0.3468364544
N,0.7269481754,1.6061444994,-0.3722468151
C,1.1254044857,0.3597462126,-0.0981208325
C,0.0053335874,-0.4918557354,0.0866811885
C,-1.1100557026,0.3109968746,-0.0836534407
H,-1.1382246046,2.3772123921,-0.605410356
C,2.5573085168,0.0260644033,-0.0133337423
H,0.0030823353,-1.5341987226,0.3579992641
C,-2.5449653621,0.021257209,-0.0052207281
C,2.9838239932,-1.3076701172,0.0453088737
C,3.5265652863,1.0403019041,0.0067168527
C,4.3386677838,-1.6203185067,0.1234414167
H,2.2553656454,-2.1099970474,0.0197418895
C,4.8792616834,0.7261595977,0.0819098574
H,3.2043283137,2.0731372415,-0.0367967976
C,5.2929987875,-0.6050867726,0.1417455272

H,4.6484043282,-2.6587143881,0.1660017549
H,5.6144585531,1.5233146657,0.0967470423
H,6.3479490089,-0.8478402382,0.2018541864
C,-3.0290916642,-1.2503815925,-0.3477759004
C,-3.4629815361,0.9970870739,0.412983932
C,-4.3882909745,-1.536106268,-0.2724641394
H,-2.3355556211,-2.0092772663,-0.6906675053
C,-4.8240086945,0.7117576135,0.4768582539
H,-3.1108676796,1.9758670686,0.7205416249
C,-5.2925020639,-0.5557668317,0.135777949
H,-4.744225318,-2.5238168244,-0.5431067114
H,-5.5175515241,1.4773518556,0.8059364351
H,-6.3518871986,-0.7785655223,0.1894393746

54H, B3LYP Energy= -688.868598490 Hartree,
NIMAG= 0

N,-0.6665919164,1.5578373124,-0.5217862469
N,0.692615204,1.5511713519,-0.5283383826
C,1.1393530071,0.3314896035,-0.1447149384
C,0.0062463314,-0.4472907903,0.1091787165
C,-1.1215544887,0.3425728502,-0.1337985664
H,-1.1882893657,2.3426539004,-0.8854050387
C,2.5613711403,0.0213244399,-0.0264006626
H,0.0032267556,-1.44958496,0.5008575658
C,-2.5453470962,0.0463820307,-0.0017628312
H,1.2184515116,2.3308599034,-0.896992796
C,2.9977290879,-1.2978290421,-0.2216902499
C,3.4977487644,1.0219216685,0.2798720383
C,4.3491935487,-1.6055935699,-0.1209521671
H,2.2862187166,-2.0747786582,-0.475136738
C,4.8476088399,0.7063907019,0.3791043467
H,3.175463133,2.0375613967,0.4843383419
C,5.2749256914,-0.6058980067,0.1770613955
H,4.6814307255,-2.624225043,-0.2799260113
H,5.5641558714,1.4800220776,0.6266784134
H,6.3275817281,-0.849652747,0.2567176511
C,-2.996505246,-1.2684113311,-0.1927909969
C,-3.4688516767,1.0561093352,0.3134883657
C,-4.3498890204,-1.5628962441,-0.078990393
H,-2.2951367484,-2.0522949946,-0.4530624508
C,-4.8207259313,0.753841398,0.4257685879
H,-3.1346508689,2.0685258766,0.5147844329
C,-5.2628391161,-0.554174763,0.2279160124
H,-4.6936358725,-2.5782059608,-0.2347104638
H,-5.5272144425,1.5344593962,0.680224096
H,-6.3170187315,-0.7875889515,0.3177454504

55a, B3LYP Energy= -602.745032286 Hartree,
NIMAG= 0

N,-1.7004619163,1.0861645839,0.2953252345
N,-0.3731967142,1.2858639719,0.3419925034
C,0.1359170659,0.109129841,0.0027298878
C,-0.8656908414,-0.8515958678,-0.2610711939
C,-2.0568330719,-0.1804066453,-0.0626370575
H,-2.3117167076,1.8595522625,0.5082435116
C,1.6176136049,-0.0946801868,-0.0118875438
H,-0.7361401905,-1.8783754139,-0.5591074253
C,-3.4795882231,-0.6184746208,-0.1864962157
H,-4.0176980491,-0.031668973,-0.93705219
H,-3.520763792,-1.6650491828,-0.4884766789
H,-4.0142004841,-0.5226020942,0.7633641387

F,2.1106283672,-0.3493604844,1.2256688992
F,1.9434723508,-1.160782306,-0.783181978
F,2.2859586013,0.9708741158,-0.4873668922

55b, B3LYP Energy= -602.743241296 Hartree,
NIMAG= 0

N,-0.4661185563,-1.211670949,0.3381588355
N,-1.8067083782,-1.1399763059,0.2938915894
C,-2.0837160064,0.1197002898,-0.0458682876
C,-0.8925218028,0.8690330236,-0.2150990566
C,0.1240002322,-0.0239423492,0.0461419447
H,-0.0175593761,-2.0729050627,0.6093236588
C,-3.499678634,0.5798102976,-0.1952438371
H,-0.7905584749,1.9074199567,-0.4849054045
C,1.6031015682,0.1273425469,-0.0181963961
H,-4.1803461414,-0.2478352835,0.0056997352
H,-3.7266942434,1.3919293511,0.5010777778
H,-3.691092657,0.947952339,-1.2070345875
F,2.0013131467,1.3432201363,0.4003903347
F,2.2195811721,-0.8026721422,0.7546573919
F,2.0890231513,-0.0336278485,-1.2727986986

55H, B3LYP Energy= -603.087022717 Hartree,
NIMAG= 0

N,-0.4204562028,-1.2123255537,0.4216587924
N,-1.7637462499,-1.0924505076,0.369010169
C,-2.1020411094,0.1397302814,-0.0614823292
C,-0.9032041593,0.8288217424,-0.289717186
C,0.1210789927,-0.0485196734,0.0234021986
H,0.043194176,-2.0621099662,0.7242545247
C,-3.516800318,0.5702413829,-0.2268445684
H,-0.8001011789,1.8428328846,-0.6401708108
C,1.625770083,0.1247116452,-0.024121527
H,-2.3677306385,-1.8630135717,0.6308621998
H,-4.2175522395,-0.2082324868,0.0769619574
H,-3.7078842513,1.4630905664,0.3728794548
H,-3.7102753548,0.822818114,-1.2723188141
F,2.0048979374,1.1207652871,0.7761522365
F,2.2148999581,-1.014876021,0.3879215688
F,2.0244111014,0.3911942998,-1.267799268

56, B3LYP Energy= -900.556591627 Hartree,
NIMAG= 0

N,-0.6203463735,1.2869517666,0.5268568593
N,0.7106422889,1.3506279301,0.536565946
C,1.1030162932,0.1766345272,0.0498829446
C,0.0146230902,-0.6594779476,-0.2722839645
C,-1.088117392,0.0998153055,0.0555278789
H,-1.1604171559,2.0666906922,0.8734899168
C,2.563705433,-0.1447021657,-0.0555205241
H,0.0334203808,-1.6556069965,-0.6799893473
C,-2.5480262726,-0.1701262067,-0.0933947538
F,3.2731523648,0.865412952,-0.5866467599
F,3.1067969475,-0.4241371566,1.1502707517
F,2.7479918694,-1.2341573682,-0.8354619906
F,-2.8454589094,-1.4511157054,0.1808663163
F,-2.9916178314,0.0838827848,-1.3441076709
F,-3.2642377329,0.6188465882,0.7443573975

56H, B3LYP Energy= -900.873650730 Hartree,
NIMAG= 0

N,-0.6609799163,1.3261090814,0.4572236719
N,0.6813320051,1.3330674793,0.4455274011
C,1.1184106203,0.1300976285,0.0371953937
C,0.0147363362,-0.6758472308,-0.2184661562
C,-1.0925745205,0.1174569074,0.060022201
H,-1.2082507366,2.1342338254,0.7417194121
C,2.6063024197,-0.1622637667,-0.0615507844
H,0.0170548924,-1.6987622448,-0.5600956025
C,-2.57911155,-0.1816562544,-0.0388250191
H,1.2249000362,2.1522382919,0.7043697634
F,3.2895138493,0.971010681,0.182509239
F,2.9527330814,-1.0802870401,0.8382207559
F,2.9064533323,-0.6033676825,-1.2793920826
F,-2.8756913054,-1.2676979695,0.6685195087
F,-2.923092431,-0.375464733,-1.3102434406
F,-3.2673014887,0.8677387423,0.4467795893

57, B3LYP Energy= -493.544322992 Hartree,
NIMAG= 0

N,0.0095321366,-1.0239139876,-0.0002311123
N,1.1500544178,-0.2913016123,0.0006479679
C,0.7334099299,0.9654724457,0.0008803114
C,-0.6837934103,1.0467629232,0.0000640497
C,-1.1091146914,-0.2719721636,-0.0006401695
H,0.077404614,-2.0293420105,-0.0005291071
H,1.4458005487,1.7753007007,0.0015812824
C,-1.5669320861,2.2180205594,-0.0000503519
H,-2.1019771634,-0.6913544276,-0.0013660079
O,-2.7779754733,2.1704942686,-0.000701491
O,-0.8633237767,3.3716497106,0.0006591516
C,-1.6352452102,4.5975224808,0.0006405697
H,-2.2780741188,4.6049094857,-0.8825290654
H,-2.2796544093,4.6039628371,0.882658372
C,-0.6564301298,5.7539292941,0.0021183153
H,-0.0180783983,5.7282157339,-0.8838347965
H,-1.2053220578,6.6994736446,0.0021058277
H,-0.0196854217,5.7273047173,0.8892005539

57H, B3LYP Energy= -493.891860234 Hartree,
NIMAG= 0

N,-0.0091251105,-1.0683857808,-0.0003538191
N,1.1029400297,-0.2964704622,0.000709428
C,0.738477974,0.9941711512,0.0009897733
C,-0.6538673483,1.0459347551,0.0001024179
C,-1.0898321673,-0.2780029306,-0.000737197
H,0.0494394413,-2.0800017591,-0.0007401802
H,1.4700545999,1.7871596618,0.0017992014
C,-1.5633047202,2.2314878243,0.0000027765
H,-2.0927753035,-0.6777814034,-0.0015636457
H,2.0299998553,-0.7056079316,0.0011647337
O,-2.7604554775,2.1072261403,-0.0008854981
O,-0.8684910013,3.3613713144,0.0008564131
C,-1.6409912347,4.6183524121,0.0007911774
H,-2.2763140464,4.6101041517,-0.8856581854
H,-2.2776628435,4.6093746958,0.886264153
C,-0.6535443064,5.761402848,0.0020091603
H,-0.0198118016,5.7403542346,-0.8867573485
H,-1.20417915,6.7050849483,0.0019685966

H,-0.0211738191,5.7396357275,0.8917281226

58a, B3LYP Energy= -532.875738596 Hartree,
NIMAG= 0

N,-0.7859178316,-1.0060147083,-0.0528644631
N,-2.0862034227,-1.3191893318,-0.0688359247
C,-2.7338346609,-0.1490843466,-0.0045639418
C,-1.8179073954,0.9253292031,0.0530538825
C,-0.5658965687,0.3335499414,0.0197131724
H,-0.0787919202,-1.7247258545,-0.0936354419
C,-4.2300034309,-0.1046700886,-0.0006911819
H,-2.0283518804,1.980365271,0.1110748892
C,0.8101493454,0.8437655914,0.0447895472
O,1.7878799461,0.126004251,0.0026644663
O,0.8534256806,2.1840220048,0.118995559
C,2.1742720774,2.7856804918,0.1486998722
H,2.7157813995,2.3890336457,1.010314715
H,2.7118380439,2.4849757421,-0.7532463889
C,1.9907725239,4.286442609,0.2308058068
H,1.4463270713,4.5665747365,1.1352519716
H,2.969311192,4.7732601343,0.2551603999
H,1.4424323919,4.6629712577,-0.6354901528
H,-4.6105082346,0.3665521725,0.9100771349
H,-4.6121140127,0.465723389,-0.8521290103
H,-4.6300359139,-1.1175458117,-0.0572829115

58b, B3LYP Energy= -532.871219240 Hartree,
NIMAG= 0

N,2.0777209657,-1.2592176152,0.0879171249
N,0.7393063755,-1.1819452125,0.0769714709
C,0.4922733074,0.1252507935,-0.0099902585
C,1.6900465263,0.8815295007,-0.0544564467
C,2.7062115176,-0.0467922908,0.0109588132
H,2.5080486996,-2.169327288,0.149403033
C,-0.8748527768,0.6895882869,-0.0530097149
H,1.777971884,1.9526904227,-0.1244308111
C,4.1935328265,0.0930964525,0.0083896308
H,4.4665284915,1.1463405254,-0.0596840711
H,4.6389332279,-0.3093935535,0.9235489472
H,4.6468818677,-0.4255491021,-0.8421307484
O,-1.0927761055,1.8795290926,-0.1318783433
O,-1.8333427222,-0.247998178,0.0040801538
C,-3.2000663016,0.2278953951,-0.0329491658
H,-3.3560469844,0.9110710835,0.8053314998
H,-3.3492467375,0.7933534787,-0.9558876652
C,-4.1047456212,-0.9850202228,0.0445492591
H,-3.9357982319,-1.5395559141,0.970102252
H,-5.1504177423,-0.6662530095,0.0189741012
H,-3.9286414663,-1.6578226449,-0.7974970609

58H, B3LYP Energy= -533.233705402 Hartree,
NIMAG= 0

N,-1.3734845915,1.321430189,0.0278092129
N,-2.6066638485,0.7796753074,0.0239191192
C,-2.5175699525,-0.5677325822,0.0019172184
C,-1.1526693009,-0.8789028054,-0.0060647303
C,-0.4669834589,0.3292228577,0.0107954837
H,-1.1894747468,2.3199465709,0.0485903931
C,-3.719690946,-1.4463713536,-0.0191472461
H,-0.7141366391,-1.8624741319,-0.0216703471

C,0.9783710655,0.7262105149,0.0156797506
H,-3.435434801,1.3616848492,0.0343177879
O,1.2823455838,1.8945317288,0.0349449205
O,1.7688126436,-0.324277122,-0.0028834051
C,3.2260706158,-0.0687859392,-0.000269596
H,3.4472071142,0.5401963017,-0.877661499
H,3.4490628229,0.5119885621,0.8955714321
C,3.923301477,-1.4074221812,-0.0223072645
H,3.6691869596,-1.9736761669,-0.9202525233
H,5.0032838981,-1.2416312121,-0.0208610321
H,3.671157586,-2.0019162864,0.8577656341
H,-3.7769195589,-1.9812902376,-0.9706027622
H,-3.6547905974,-2.1895129582,0.7780978718
H,-4.6414453248,-0.8781359053,0.1124595813

59, B3LYP Energy= -760.816869994 Hartree,
NIMAG= 0

N,0.0962502417,-1.0012050877,-0.0002173638
N,1.4038932318,-0.772452615,-0.0001705472
C,1.5135272582,0.5639523328,-0.0001152064
C,0.2482069875,1.1879302576,-0.0001349231
C,-0.6539766265,0.1426549799,-0.0001665596
H,-0.2543813233,-1.9476809366,-0.0002684664
C,2.815854404,1.2711367743,-0.0000577056
H,0.0306983454,2.2420861618,-0.0001092026
C,-2.1247711967,0.1467002812,-0.0001846314
O,2.9026080607,2.478977775,-0.0000039739
O,3.8633160049,0.4357222743,-0.0000774317
C,5.1756779584,1.0521365154,-0.0000218742
H,5.2602755364,1.6900464316,-0.8828210147
H,5.2602042525,1.6900433149,0.8827854367
C,6.201447294,-0.0620727087,0.0000152841
H,6.0955218346,-0.6917705941,-0.8859787022
H,7.2074552559,0.3662303751,0.0000530211
H,6.0954562189,-0.6917724935,0.8860001704
O,-2.8085559797,1.1403907452,-0.0001943338
O,-2.6090480667,-1.1172216301,-0.0001831655
C,-4.0559323508,-1.2548877104,-0.000196817
H,-4.4488179702,-0.7472264641,-0.8835007091
H,-4.4488354774,-0.7472298665,0.8831014185
C,-4.3776254927,-2.734245977,-0.000202844
H,-3.9726078582,-3.2258655798,0.8872164172
H,-5.4621349761,-2.8708739108,-0.0002145048
H,-3.9725889665,-3.2258627448,-0.8876150711

59H, B3LYP Energy= -761.166347626 Hartree,
NIMAG= 0

N,0.0838779839,-0.964409823,-0.000163482
N,1.3864149527,-0.6387612232,-0.0001904459
C,1.5042142885,0.704152837,-0.000175185
C,0.2228790967,1.2475851761,-0.0001244135
C,-0.6519946862,0.1651080771,-0.0001329766
H,-0.250267132,-1.9225074376,-0.0001678814
C,2.8357225965,1.3925460736,-0.0002072386
H,-0.0385349761,2.2930727067,-0.0000966949
C,-2.1508209999,0.1460882213,-0.0001023263
H,2.1320622696,-1.3269588371,-0.0002253744
O,2.9272241641,2.587480952,-0.0001061605
O,3.8149374713,0.4921721126,-0.0001399146
C,5.200909482,1.0123719001,-0.0000315063
H,5.3083778684,1.6378741444,-0.8867430192

H,5.3082387015,1.6378826691,0.8866906874
C,6.1367657434,-0.1720346539,0.0000476584
H,6.0006410136,-0.7894158405,-0.8902281785
H,7.1662713386,0.1938115391,0.000126134
H,6.000501849,-0.7894068347,0.8903084124
O,-2.7937211415,1.1574826676,-0.0001010104
O,-2.5913566381,-1.1090723793,-0.0001575386
C,-4.0590731185,-1.3021342321,-0.0001831128
H,-4.4481645526,-0.8006893206,-0.8868766676
H,-4.4481855638,-0.8007586213,0.886540434
C,-4.3277147577,-2.7875663019,-0.000244426
H,-3.9170879019,-3.2683088568,0.8900085675
H,-5.4082880821,-2.9490899284,-0.0002634754
H,-3.9170668544,-3.2682392438,-0.8905252851

60a, B3LYP Energy= -724.659883407 Hartree,
NIMAG= 0

N,-0.8869399721,-0.9962908402,-0.0001083423
N,0.4088415433,-1.3044414855,-0.0003008531
C,1.0577516936,-0.1279476876,0.0000757915
C,0.1321947153,0.9442857959,0.0004930369
C,-1.1144008255,0.3448020211,0.0004070878
H,-1.5916265569,-1.71920867,-0.0003244421
C,2.5297010218,-0.0791467772,0.0000116888
H,0.3248774297,2.003117729,0.0008737403
C,-2.4937410609,0.8480936647,0.0007242396
C,3.2104399418,1.1457825752,-0.0001495995
C,3.2811560332,-1.2638569592,0.0001053375
C,4.6022441888,1.1872645813,-0.0002023813
H,2.6538271098,2.075847918,-0.0002611769
C,4.6711005315,-1.2200657818,0.0000481517
H,2.7627817369,-2.2143672033,0.0002267769
C,5.3392971036,0.0046729648,-0.0001025992
H,5.1104103652,2.1451416887,-0.0003307508
H,5.2359029008,-2.1458020085,0.0001263217
H,6.4229524447,0.0364059563,-0.0001430319
O,-3.4655230204,0.1213802266,0.0002091441
O,-2.5439380263,2.1890469221,0.0007985747
C,-3.868249959,2.7861480347,0.0006514055
H,-4.4054513189,2.4341902913,-0.8826465519
H,-4.4056792714,2.4341075777,0.8837778489
C,-3.6908051136,4.2898282687,0.0007451762
H,-3.1458554962,4.6209688846,-0.8859310197
H,-4.6714617328,4.7728816907,0.0006362046
H,-3.1460941061,4.6208866219,0.8875988219

60b, B3LYP Energy= -724.655053484 Hartree,
NIMAG= 0

N,0.1087430215,-0.9504066516,-0.0500849344
N,1.4289233144,-0.738011732,-0.0583429954
C,1.5456911628,0.5917424041,-0.0230342302
C,0.2829338982,1.2265199802,-0.0029754275
O,-0.6404738388,0.1966783216,-0.0215465142
H,-0.2305148247,-1.8966890262,0.1289617142
C,2.8500595089,1.2917538361,-0.0048468411
H,0.0942067059,2.2850743939,0.0503723016
C,-2.1064325281,0.1922741952,-0.0052139942
O,2.9453296818,2.4999990373,0.0070531801
O,3.8969430329,0.4533883803,-0.0027693534
C,5.2092156904,1.0663489706,0.0109782938
H,5.3065815045,1.7026740827,-0.8719038752

H,5.2866984059,1.7060879467,0.8932256773
C,6.232722499,-0.050242732,0.0242613108
H,6.1336475774,-0.6823380957,-0.8608535797
H,7.2399816392,0.375207316,0.0332543138
H,6.1158805796,-0.677459039,0.910690249
C,-2.8199181435,1.2614600845,-0.5671969216
C,-2.8255156857,-0.8664155488,0.570217355
C,-4.2106669285,1.2697443146,-0.5534738785
H,-2.278855287,2.0789716586,-1.029119224
C,-4.217619239,-0.8603614787,0.572970293
H,-2.2983492882,-1.6859371741,1.0469908295
C,-4.9156499297,0.2075584133,0.0122873162
H,-4.7459200989,2.1032520027,-0.9939900597
H,-4.7566874503,-1.6848691039,1.0256099749
H,-5.99947708,0.2137558434,0.0183758484

60H, B3LYP Energy= -725.020598123 Hartree,
NIMAG= 0

N,-0.6405238748,-1.9058461857,0.2863474483
N,0.6983870988,-1.7451125966,0.2493936036
C,1.0023695908,-0.4328054481,0.0893637867
C,-0.2244579937,0.2496696958,0.0103581692
C,-1.2235559263,-0.7037764337,0.1310011914
H,-1.1023202734,-2.8063351814,0.3610182555
C,2.3754311699,0.0524263197,0.0215334697
H,-0.3686718453,1.3041333916,-0.149270126
C,-2.7200585981,-0.6698832766,0.0983008658
H,1.3232585786,-2.5157752826,0.4468838621
C,2.6647786716,1.3619417184,0.4359862342
C,3.4114631812,-0.7704737563,-0.4511965421
C,3.9711780649,1.8327853256,0.38826096
H,1.8769686699,2.0004575272,0.8177251661
C,4.7147008568,-0.2917677852,-0.4962982774
H,3.2022731809,-1.7674212685,-0.8251447533
C,4.9963055437,1.0081450258,-0.0747472535
H,4.190834388,2.8411915312,0.7168062206
H,5.5082370437,-0.9260554669,-0.8718762671
H,6.0134683861,1.3793035726,-0.1125696062
O,-3.3521104843,-1.6939687813,0.1986584203
O,-3.1748238148,0.557266761,-0.0436292011
C,-4.6417719589,0.7278996815,-0.0884136104
H,-5.0115932303,0.1302835095,-0.922539405
H,-5.0430741914,0.3195736228,0.8400048567
C,-4.9237597223,2.2021633339,-0.251939906
H,-4.4989589614,2.5874630369,-1.1807521174
H,-6.0054058345,2.3528046202,-0.2858857272
H,-4.5277107155,2.777733789,0.5867592829

61a, B3LYP Energy= -281.643152021 Hartree,
NIMAG= 0

N,-0.7387387425,0.0083534448,-0.8418441295
N,0.6194504779,0.0128097179,-0.9047040826
C,1.0083000424,-0.0087566478,0.3657008954
C,-0.1001102354,-0.0154435228,1.2544089756
C,-1.2041299106,-0.0005278873,0.4284684055
H,-1.2652696849,0.0197139783,-1.6984847889
N,2.3602920024,-0.0872438679,0.6993262323
H,-0.0889389515,-0.045500957,2.3315432349
H,-2.2594392141,-0.001562324,0.6512391468
H,2.9667288132,0.1197579637,-0.0832557866
H,2.6175301743,0.4449819679,1.5185028603

61b, B3LYP Energy= -281.638999820 Hartree,
NIMAG= 0

N,-0.5713948366,0.061912292,-0.8744815844
N,0.7878727887,0.0444783694,-0.9094766894
C,1.1399966214,-0.0163462204,0.3667329831
C,0.0208348954,-0.0501933704,1.2328445021
C,-1.0732630811,0.0026499784,0.3871761659
H,-1.0866844588,0.1877541948,-1.7306202858
H,2.1872175219,-0.0453832549,0.6295612693
H,0.0102107399,-0.1211646044,2.308310208
N,-2.4515847377,0.0656143076,0.6188343704
H,-2.9810124971,-0.6695655118,0.1650985054
H,-2.6768899069,0.0936619538,1.6035840782

61H, B3LYP Energy= -282.009329792 Hartree,
NIMAG= 0

N,-0.7976020579,-0.1032231534,-0.8846840456
N,0.5684356834,0.0749142597,-0.9180497572
C,1.0369812044,0.0843083391,0.357464488
C,-0.0832491884,0.0339009718,1.2188449195
C,-1.1881576764,-0.0520945434,0.4065824814
H,-1.3457263221,0.1687046014,-1.6913233921
N,2.3411268662,0.107308236,0.6548787948
H,-0.0664079766,0.0509320588,2.2954948637
H,-2.236993421,-0.0735151597,0.6604846691
H,1.0780407387,-0.1987575818,-1.7485327646
H,3.0554191729,0.2476032695,-0.0427517112
H,2.6326665856,0.1259232574,1.6195877787

62, B3LYP Energy= -281.633759737 Hartree,
NIMAG= 0

N,-0.6142479507,-1.3885515968,0.0253708051
N,0.7229613725,-1.4399670971,0.0330661861
C,1.1089103175,-0.1669541202,-0.0369037062
C,0.0019627545,0.7158473614,-0.0946490381
C,-1.1036911647,-0.1140204142,-0.0499125039
H,-1.1390857599,-2.2459751226,0.0696619602
H,2.1608892293,0.0785308216,-0.0413432034
N,0.0370295769,2.1206709019,-0.1037061552
H,-2.1609320539,0.0961031938,-0.0573745932
H,0.8791350942,2.4966079951,-0.5171248297
H,-0.7745694156,2.5490390769,-0.5270849217

62H, B3LYP Energy= -281.994677338 Hartree,
NIMAG= 0

N,-0.6539084627,-1.4069899344,0.0362379437
N,0.6853158528,-1.4159849113,0.0411324056
C,1.1381532516,-0.1502838049,-0.0590908926
C,0.0306198395,0.7088576142,-0.1335961419
C,-1.0890246933,-0.1359380076,-0.0696474896
H,-1.1922897744,-2.260990601,0.1026290103
H,2.1960724989,0.0577761763,-0.0668471778
N,0.0391428429,2.0749766338,-0.1820677229
H,-2.1438013515,0.0868613015,-0.0877406913
H,1.2115117595,-2.2770084871,0.1136073591
H,0.8898998195,2.5434467104,-0.451760031
H,-0.8042505126,2.5534843878,-0.4571756141

62c, B3LYP Energy= -281.977913886 Hartree,
NIMAG= 0

N,-0.6188220464,-1.3798684672,-0.0272687097
N,0.7172710877,-1.4402151983,0.089654131
C,1.1306921339,-0.1829758874,0.084341599
C,0.0189798905,0.6753408031,-0.0392215982
C,-1.1040820808,-0.1250244223,-0.109842749
H,-1.146159423,-2.2427984064,-0.044520761
H,2.1825596982,0.0486027366,0.1673258476
N,0.042618202,2.1441905187,-0.0850327254
H,-2.1563622864,0.093200727,-0.2074924437
H,0.4473539959,2.5484826324,0.768416526
H,0.587731963,2.4948007475,-0.8822566151
H,-0.9038625214,2.5271817363,-0.1779535323

63, B3LYP Energy= -763.733713347 Hartree,
NIMAG= 0

N,0.6049896077,-1.5231725512,-0.4413509263
N,-0.7317136249,-1.5515022783,-0.4667896838
C,-1.1324510958,-0.320757881,-0.1213556535
C,0.007198989,0.5033462138,0.0930068596
C,1.1209132273,-0.2927585247,-0.1323315277
H,1.1173541628,-2.3264595684,-0.7682789074
C,-2.5639536826,0.0000457711,-0.0062430495
O,-0.0229110815,1.8111860926,0.4875797199
C,2.5528362408,-0.0063863776,-0.0317238556
C,-3.0120409098,1.3176197675,0.1725388556
C,-3.5177196058,-1.0286820346,-0.0837367596
C,-4.3747145539,1.5940688086,0.2690030421
H,-2.2959603816,2.1254652401,0.2357856254
C,-4.8750368031,-0.7463973051,0.011687159
H,-3.1788623494,-2.0479310641,-0.2199181837
C,-5.3121317895,0.5673644176,0.1890654365
H,-4.7022497785,2.6188711887,0.4061485523
H,-5.5958538635,-1.554458946,-0.0504046549
H,-6.3715027558,0.7858271195,0.2648294641
C,3.0672646066,1.2226866306,-0.4785621778
C,3.443471456,-0.9470164619,0.5122294165
C,4.4274403483,1.5028643327,-0.3746822016
H,2.4054286668,1.942940515,-0.9470517254
C,4.8039438065,-0.6687363633,0.5990503406
H,3.0629793129,-1.8892178784,0.8912904311
C,5.3011946004,0.5587144872,0.1617959263
H,4.807079662,2.4543778471,-0.7296831584
H,5.4760681337,-1.4067850651,1.022184304
H,6.3603957741,0.7758892957,0.2364888233
H,0.8477593106,2.0677168818,0.813300879

63H, B3LYP Energy= -764.106261605 Hartree,
NIMAG= 0

N,0.663960117,-1.5333755268,-0.5831540798
N,-0.6906157896,-1.4812887833,-0.6656256681
C,-1.1464137368,-0.2945114955,-0.2017147536
C,0.0042817116,0.4704087308,0.0899217241
C,1.1262828624,-0.3170011379,-0.1767008178
H,1.1749548145,-2.1950140557,-1.153413171
C,-2.562997106,-0.0029529957,-0.0306342456
O,-0.0440164654,1.7193099046,0.5905289863
C,2.5513837038,-0.0230648361,-0.0313349236
H,-1.2280802,-2.2988986709,-0.9154168329

C,-3.0072847706,1.3299748335,-0.0198086054
C,-3.4990817007,-1.0434792563,0.1112495077
C,-4.3632564689,1.6074337809,0.1114560211
H,-2.2978785821,2.139734666,-0.1210497855
C,-4.8503609787,-0.7558322115,0.2442109149
H,-3.1793447131,-2.0794980839,0.1580587932
C,-5.285334365,0.5704651187,0.2406697418
H,-4.7000825861,2.6369208252,0.1127551521
H,-5.5633098674,-1.562629295,0.3625475848
H,-6.3404229372,0.7929331251,0.346609384
C,3.0494277524,1.229505096,-0.4275818785
C,3.4278590723,-0.9817569001,0.5021803508
C,4.4045740564,1.5128878454,-0.2902903214
H,2.3911719706,1.961377242,-0.8829631677
C,4.7808918013,-0.6896525671,0.632286222
H,3.0475467012,-1.9379334373,0.8443701252
C,5.2699124118,0.5562250367,0.2391410766
H,4.7864306703,2.4757954991,-0.6072978186
H,5.4522416878,-1.4294005084,1.051283789
H,6.3244477886,0.780937694,0.3452634459
H,0.8125599376,1.9781234037,0.9560129758

64, B3LYP Energy= -265.587659367 Hartree,
NIMAG= 0

N,-0.662769258,0,-0.8373054727
N,0.6840596262,-0.0000000002,-0.8872484
C,1.0752437579,-0.0000000002,0.3858520087
C,-0.0247159226,0.0000000001,1.2680924206
C,-1.1293874004,0.0000000002,0.4382741204
C,-1.4274486551,0,-2.0714682287
H,2.1291691904,-0.0000000003,0.6205355042
H,-0.0173054439,0.0000000002,2.3455710299
H,-2.1859382259,0.0000000005,0.6544338588
H,-1.190018927,0.8891892545,-2.658367394
H,-1.1900189274,-0.8891892547,-2.6583673938
H,-2.4897454647,0.0000000002,-1.8277352331

64H, B3LYP Energy= -265.948857995 Hartree,
NIMAG= 0

N,-0.6917494543,0,-0.8562553675
N,0.6613646536,-0.0000000002,-0.8454655104
C,1.1056504033,-0.0000000002,0.4251605844
C,-0.0010627517,0.0000000001,1.2594013781
C,-1.1116719034,0.0000000002,0.4183610995
C,-1.4568972746,0,-2.1077700657
H,2.1622960062,-0.0000000003,0.6429379671
H,-0.0028827141,0.0000000002,2.3362352698
H,-2.1657815379,0.0000000004,0.6475559288
H,1.1908625535,-0.0000000004,-1.7084056379
H,-1.2273649259,0.8982010651,-2.6822372169
H,-1.2273649262,-0.8982010653,-2.6822372167
H,-2.5126493456,0.0000000002,-1.8462215872

65, B3LYP Energy= -304.918240079 Hartree,
NIMAG= 0

N,-0.8203911911,-0.0494758852,-0.8671534684
N,0.5291458297,-0.0685859317,-0.9217411153
C,0.9399868798,-0.0062206458,0.3458665277
C,-0.1660350073,0.0539683918,1.2280992242
C,-1.2760907965,0.0238175732,0.4085285878
C,-1.5905193639,-0.106359445,-2.0948865762

C,2.4004105811,-0.0061730349,0.6766488019
H,-0.1537383606,0.1111210825,2.304715019
H,-2.3310885673,0.0484383711,0.6326998794
H,-1.3453323386,0.7455189834,-2.73240828
H,-1.3705923234,-1.0296927957,-2.6347136493
H,-2.651553666,-0.077587155,-1.8464303321
H,2.9885763239,-0.0617014555,-0.2402472876
H,2.686169747,0.9024246933,1.2150649331
H,2.6651241532,-0.8594626465,1.3082580359

65H, B3LYP Energy= -305.287018260 Hartree,
NIMAG= 0

N,-1.0889111601,-0.032265128,-0.017049354
N,0.0297747185,-0.7996336297,-0.0171540837
C,1.1367099014,-0.0235493841,0.0109210085
C,0.6910361686,1.2977710904,0.0369727447
C,-0.6976587334,1.2507643119,0.0189595235
C,-2.4309888895,-0.618575878,-0.0143943711
C,2.5124291867,-0.5944671088,-0.0169461793
H,1.3055371604,2.1819131578,0.0655065047
H,-1.4274915653,2.0450877332,0.0317870179
H,-0.0357621183,-1.8091681198,-0.0456921051
H,-2.5658715147,-1.2435579656,-0.8982134871
H,-2.5841087253,-1.1992833217,0.8963734975
H,-3.1464708048,0.2002257674,-0.0438582084
H,2.5560085903,-1.5702754035,0.4704995455
H,2.8557689616,-0.7103998388,-1.0493522157
H,3.203993824,0.0762677173,0.492589162

66, B3LYP Energy= -304.917233693 Hartree,
NIMAG= 0

N,-0.515025185,-0.0596526065,-0.8714874731
N,0.8381670987,-0.0516695052,-0.9180550429
C,1.2214388273,0.0137770259,0.3529681823
C,0.1164810033,0.0484217026,1.2276211022
C,-0.9956067618,-0.0005319101,0.4038666351
C,-1.2753010487,-0.1260492834,-2.1062019624
H,2.2742639939,0.0335262079,0.592240486
H,0.1198787979,0.1014013978,2.3045802056
C,-2.4555213709,0.0041024251,0.7220407479
H,-0.5580110345,-0.1610422205,-2.9233335306
H,-1.9119324773,0.7554107157,-2.221908063
H,-1.8988767,-1.0238355419,-2.1342530342
H,-2.9555610559,-0.9014091635,0.3624781351
H,-2.5979314482,0.0558216077,1.8019204991
H,-2.9687483389,0.8626796484,0.2762530129

66H, B3LYP Energy= -305.285954700 Hartree,
NIMAG= 0

N,-0.1802897739,0.6339389818,0.0292331161
N,1.146009081,0.9159935034,0.0853175187
C,1.8516074844,-0.2283878223,0.0701206471
C,0.9514703385,-1.2753485604,0.0023006222
C,-0.3299479287,-0.7082155758,-0.0226665798
C,-1.1762764868,1.7076965142,0.0319504054
H,2.92959421,-0.2158699254,0.1081389669
H,1.1837973402,-2.3265991829,-0.0261711714
C,-1.6599273515,-1.3774002237,-0.0923178193
H,1.4740107824,1.8718642059,0.1300204129
H,-1.0336063506,2.3491456742,-0.8389542046

H,-1.0966892947,2.2861378825,0.9535582145
H,-2.1620000822,1.2532451377,-0.0187291038
H,-2.2105641671,-1.0806812503,-0.9889028676
H,-1.520740787,-2.4568779518,-0.1251080398
H,-2.2722400141,-1.1424374071,0.7823118826

67, B3LYP Energy= -304.914835324 Hartree,
NIMAG= 0

N,-0.6654262236,0.0549320638,-0.9949951676
N,0.6640256541,-0.1433533538,-1.0461362998
C,1.0538620838,-0.1827657983,0.2269351202
C,-0.0278542008,-0.0090027963,1.1217599208
C,-1.1192089031,0.1410098617,0.2851282786
C,-1.4291194225,0.1517128995,-2.2250824839
H,2.0982962532,-0.3347088643,0.4598570201
C,-0.0026899239,0.0089358597,2.6211799365
H,-2.163658474,0.2994254065,0.505548683
H,-2.4789089132,0.3069115626,-1.9761921807
H,-1.3269322597,-0.7683282477,-2.803967904
H,-1.0716856323,0.9913386381,-2.8245910706
H,0.377154598,-0.9329350432,3.0287074371
H,0.636447885,0.8107036211,3.0034780083
H,-1.0040443209,0.1637511906,3.029395702

67H, B3LYP Energy= -305.281603653 Hartree,
NIMAG= 0

N,-1.0685555378,-0.1581295422,-0.0151547213
N,-0.6856290847,1.1317899064,0.0925802093
C,0.6609360281,1.2021773734,0.1074368494
C,1.1720694429,-0.0869456399,0.0053879065
C,0.0418265953,-0.9108286353,-0.069134809
C,-2.4812176746,-0.5474857568,-0.0542275069
H,1.1613990118,2.1546834601,0.1890171289
C,2.610837281,-0.5045463374,-0.022663192
H,-0.0335656239,-1.9837922069,-0.1565807145
H,-1.3675885398,1.8771495726,0.1500885357
H,-2.5209601023,-1.6306349743,-0.1437690851
H,-2.9670473091,-0.0959470107,-0.9201466398
H,-2.9759987574,-0.2434233315,0.8690775404
H,2.8639212412,-0.9739255535,-0.9759792176
H,3.2661283764,0.3560059715,0.1124561349
H,2.8269116529,-1.2206002953,0.7729435811

68, B3LYP Energy= -344.247648303 Hartree,
NIMAG= 0

N,-0.6727855094,-0.1048527817,-0.8929585866
N,0.6834151863,-0.1109845486,-0.9435590283
C,1.0855890936,-0.0112529512,0.3213051628
C,-0.0256535489,0.0598882034,1.1951715034
C,-1.1429626114,-0.0027878689,0.3817759702
C,-1.4374830875,-0.2003897485,-2.1218034816
C,2.5444305875,0.0131065424,0.6589654615
H,-0.0178020851,0.1451216248,2.27075867
C,-2.6004149547,0.0257678508,0.71037052
H,-0.7234537392,-0.2677255635,-2.9399343094
H,-2.0656016111,0.6836333123,-2.2645120882
H,-2.0709630294,-1.0920544659,-2.1230370341
H,3.1375579313,-0.0601965103,-0.2536266502
H,2.8185374715,0.9385465871,1.1745661754
H,2.8156507341,-0.8204555156,1.3139717937

H,-3.1118334787,-0.8850026135,0.3812139626
H,-2.7345851913,0.1110093635,1.7892254355
H,-3.1086198575,0.8756193834,0.2425117234

68H, B3LYP Energy= -344.623488934 Hartree,
NIMAG= 0

N,-0.6856162085,0.6269123725,0.0379347561
N,0.6271340497,0.9824246325,0.0006146175
C,1.410569066,-0.116451421,-0.041902088
C,0.5513910324,-1.2103276994,-0.0451887024
C,-0.757166612,-0.7218349748,0.0018038046
C,-1.7389934155,1.641396376,0.0252371141
C,2.898404262,-0.0356750871,-0.0451800318
H,0.8397161809,-2.2478982906,-0.0766723406
C,-2.0484694055,-1.4665147684,0.0088852785
H,0.8992767743,1.9559734376,0.0313279363
H,-1.5623563067,2.3658083778,0.8215902793
H,-2.6885582883,1.145633106,0.2096099786
H,-1.7741507972,2.1410039841,-0.9446653089
H,3.2536876509,0.850544161,-0.574592891
H,3.2813071637,0.0002659491,0.9790386586
H,3.3181897387,-0.9172216897,-0.5291331187
H,-2.6558479802,-1.2219975195,-0.8666068635
H,-1.8501180202,-2.5371096417,-0.0071419484
H,-2.6331938846,-1.2452743044,0.9057288698

69, B3LYP Energy= -344.245585282 Hartree,
NIMAG= 0

N,-0.8254255875,0.0487424067,-1.0021612159
N,0.5048876204,-0.1564091525,-1.0768022891
C,0.9333708565,-0.1791407461,0.1863261844
C,-0.1397510412,0.0149275444,1.0969296552
C,-1.2488889957,0.1566481652,0.2847170346
C,-1.6122680895,0.1303538492,-2.2170291693
C,2.38128695,-0.3893981786,0.5013650474
C,-0.0771173033,0.0553933531,2.5939058828
H,-2.2875087405,0.3230497296,0.5271722509
H,-2.6570097902,0.290233112,-1.9496374198
H,-1.5238506423,-0.797185811,-2.7867787626
H,-1.2672879852,0.9615371787,-2.8359886412
H,2.5321379239,-1.2839881751,1.1144859501
H,2.7978022899,0.4578613791,1.0560114086
H,2.9492598117,-0.507035686,-0.4223051707
H,0.3111765891,-0.8810831001,3.0080789186
H,0.5756432851,0.8594019579,2.9499639818
H,-1.0668987513,0.2202116736,3.0257541542

69H, B3LYP Energy= -344.619066765 Hartree,
NIMAG= 0

N,-0.8605251205,0.053356957,-1.0210523591
N,0.4773725539,-0.1506620933,-1.0385192125
C,0.9661982052,-0.1829244408,0.2202831625
C,-0.1172510878,0.0112052451,1.0898463304
C,-1.2322955054,0.1533881919,0.2675260784
C,-1.6505072217,0.1351045648,-2.2499104235
C,2.4110118278,-0.3934876619,0.5120644437
C,-0.0732368762,0.0544981003,2.5866319346
H,-2.2675182449,0.3196315729,0.5229423712
H,0.9754370098,-0.2560181276,-1.9128902717
H,-2.6874444385,0.2954434675,-1.9629836869

H,-1.5740606373,-0.799319073,-2.8079045844
H,-1.3129636848,0.9755946622,-2.8582146717
H,2.5468978034,-1.286094178,1.1280605597
H,2.8125062921,0.4562701691,1.0700718292
H,2.9990560254,-0.5134401045,-0.398803198
H,0.3083095165,-0.8832494906,2.9982057054
H,0.5734735185,0.8615207628,2.9399364659
H,-1.0683816344,0.2195403553,3.0000161531

70, B3LYP Energy= -344.243986878 Hartree,
NIMAG= 0

N,-0.5168375912,0.072176457,-1.0200333853
N,0.83022013,-0.0264755818,-1.0461702401
C,1.1903295087,-0.0485170901,0.2338845572
C,0.0807777596,0.0374872288,1.1034429641
C,-1.0135748249,0.1155109396,0.2515734175
C,-1.2582533324,0.137809832,-2.2647863447
H,2.2367556859,-0.1252186801,0.493632209
C,0.0875532878,0.0352793665,2.604004175
C,-2.4747156116,0.2251272661,0.5441236374
H,-0.5387363636,0.0304659775,-3.0733590913
H,-1.773918832,1.097015208,-2.3665966163
H,-1.992757866,-0.6696389571,-2.3253128599
H,-0.3698957907,-0.869473529,3.0183718487
H,1.1120112084,0.0814889496,2.980181026
H,-0.4496113473,0.8936783857,3.0196665648
H,-3.0360612327,-0.6331983008,0.1589961058
H,-2.6374123184,0.2674582982,1.6218434217
H,-2.9147653696,1.12771773,0.1066248104

70H, B3LYP Energy= -344.617702224 Hartree,
NIMAG= 0

N,-0.5495366726,0.0782633248,-1.0404405857
N,0.8038010446,0.0633153474,-1.0060287981
C,1.2175571787,0.0400641417,0.2750969369
C,0.1017213844,0.0510124394,1.0984069631
C,-1.0087684331,0.0805974415,0.2304866523
C,-1.2696730087,0.1720064951,-2.3114024234
H,2.2694322938,0.0114753087,0.5136770022
C,0.0797392388,0.0318521176,2.5966828556
C,-2.4625820461,0.1120017092,0.5581652512
H,1.3475458354,0.0453654297,-1.8581455213
H,-0.8432506402,-0.5356338488,-3.0231687121
H,-1.2151970531,1.1885285476,-2.7050898258
H,-2.3083686503,-0.0956498621,-2.1354250939
H,-0.4327406969,-0.8557277099,2.9753803825
H,1.0943146375,0.0246473271,2.9956836855
H,-0.4287037127,0.9117559463,2.9978778212
H,-2.9830011249,-0.7614988153,0.1555654159
H,-2.5954573913,0.1095591024,1.6387400448
H,-2.9439919523,1.0102454801,0.1623299578

71, B3LYP Energy= -422.889209147 Hartree,
NIMAG= 0

N,-2.028379125,0.0992755911,0.0049641259
N,-0.8464202621,0.7517407044,0.0157836193
C,0.0918361055,-0.1960355483,0.0071305115
C,-0.5050333541,-1.4834798527,-0.0078021896
C,-1.8634296403,-1.247456061,-0.0078328017
C,-3.2668918471,0.8532870092,0.027720509

C,1.5725566777,0.1425897611,0.0114174262
H,-0.0197408368,-2.4457445694,-0.0193352692
H,-2.7057686234,-1.9214887944,-0.016899364
H,-3.2992142801,1.5434885994,-0.8171071988
H,-3.3482240036,1.4232477392,0.9558047986
H,-4.1033390688,0.1581007252,-0.0424934778
C,1.7846885946,1.6660494808,0.0302310761
C,2.2317999904,-0.4788035826,1.2635235679
C,2.2320570768,-0.4477035083,-1.2555494075
H,1.3343254093,2.1181836253,0.9163109161
H,2.8556105802,1.8907126221,0.033257924
H,1.334726622,2.1398609146,-0.8446399896
H,2.1123702422,-1.5655308882,1.2818184774
H,3.3037185621,-0.2581365761,1.2783562
H,1.788038626,-0.0764651495,2.1781849902
H,1.7882081354,-0.0231739593,-2.1600797813
H,3.3039252712,-0.2264555845,-1.2649426132
H,2.1128791479,-1.533685698,-1.3004730494

71H, B3LYP Energy= -423.262778938 Hartree,
NIMAG= 0

N,0.6081247266,1.2578666905,0.0056210351
N,-0.7480862626,1.2836746814,0.0046449871
C,-1.2529845995,0.0314505501,-0.0078424354
C,-0.1500107862,-0.8303745742,-0.0149821377
C,0.9838204001,-0.0323655295,-0.0062802754
C,1.4073165528,2.4835320572,0.0178721525
C,-2.7378256393,-0.2614703772,-0.0115509684
H,-0.1716445526,-1.9065959588,-0.0252193183
H,2.0296162267,-0.2969742096,-0.0077746865
H,1.2510085044,2.1611619036,0.0118796037
H,1.1966019712,3.0597801693,0.9200364843
H,1.1993161507,3.0760302006,-0.8743461843
H,2.4553754846,2.1920057143,0.0168349719
C,-3.5577937251,1.0421425556,-0.0040455995
C,-3.0677744438,-1.0783992772,-1.2838439942
C,-3.0705401927,-1.0946662286,1.2495148072
H,-3.371517725,1.6531129732,-0.8935016309
H,-4.6219544135,0.8015132981,-0.0072629578
H,-3.3744623825,1.6410431992,0.8942187402
H,-2.514893143,-2.0196662854,-1.3133932289
H,-4.1332911571,-1.317315803,-1.2930595584
H,-2.8383089344,-0.5167610152,-2.1926977622
H,-2.843164631,-0.5446459079,2.1659773369
H,-4.1360600528,-1.3337304589,1.2532947441
H,-2.5175370672,-2.0361331676,1.2682171752

72, B3LYP Energy= -422.883376030 Hartree,
NIMAG= 0

N,-0.5280097736,-0.0471489355,-0.928990727
N,0.8276257454,-0.0244256167,-0.9547411691
C,1.1989443007,0.0276022439,0.3170078913
C,0.0856481418,0.046013147,1.1769177374
C,-1.0279976618,0.0016986533,0.3493118529
C,-1.2017669397,-0.0184444224,-2.2182761811
H,2.2491751285,0.0452659203,0.5683171014
H,0.0927602419,0.0807311605,2.2529210838
C,-2.5013967336,-0.0244145073,0.7343741124
H,-0.4868071433,-0.378413632,-2.9552130042
H,-1.5047124783,0.9973913421,-2.485426676
H,-2.0755639045,-0.6676049204,-2.2192606447

C,-3.2852418779,1.1238692724,0.0576564179
C,-3.1364567981,-1.3884012049,0.3722890779
C,-2.6220365613,0.1607847296,2.2612796399
H,-3.3259161173,1.0224090008,-1.0275514509
H,-4.316194296,1.1337309761,0.4235809835
H,-2.8347327188,2.0921791977,0.2914293465
H,-3.6764110162,0.1476310446,2.5497620229
H,-2.1176593656,-0.642014629,2.8041234296
H,-2.1962731835,1.1143212981,2.58319095
H,-2.6020807998,-2.2050903902,0.8638964447
H,-4.1794216498,-1.4152549944,0.7025914461
H,-3.1290729391,-1.5839624336,-0.7018883852

72H, B3LYP Energy= -423.255781300 Hartree,
NIMAG= 0

N,-0.5627662807,-0.0469210502,-0.9449972116
N,0.7946571128,0.008212206,-0.9057887954
C,1.2111478458,0.0714872059,0.3679285465
C,0.0887552778,0.0673384086,1.1717517669
C,-1.0335055788,-0.001969316,0.3283212185
C,-1.221356825,-0.0354289591,-2.2565012279
H,2.2619912817,0.1076677836,0.6087104646
H,0.0784613009,0.1078108823,2.2461081252
C,-2.5027671761,-0.0323443836,0.7271157608
H,1.3377054694,-0.0204681818,-1.7583517393
H,-0.6235893524,-0.6261330998,-2.9514116651
H,-1.3225842208,0.9878393441,-2.6207160515
H,-2.1979235788,-0.4969549394,-2.1684547271
C,-3.2739868333,1.1349793169,0.0653152567
C,-3.1275480076,-1.3983285818,0.3496361594
C,-2.5996006159,0.1335113094,2.258773059
H,-3.3341835371,1.0521798582,-1.020673618
H,-4.2982163628,1.1411119872,0.4433024436
H,-2.8231911797,2.0991038517,0.3134665095
H,-3.6508547194,0.118860847,2.550419683
H,-2.1024674786,-0.6811777639,2.790417526
H,-2.1784734606,1.0843930543,2.5940643012
H,-2.5884677164,-2.2228665267,0.8217205521
H,-4.1599992991,-1.4266526225,0.7041484332
H,-3.1531410359,-1.5821381322,-0.7262289391

73, B3LYP Energy= -580.184719330 Hartree,
NIMAG= 0

N,0.6214631776,-1.482516903,0.0412275652
N,-0.7362908311,-1.4985262829,0.0516443551
C,-1.1192478624,-0.2282941724,0.0040472721
C,0.0121907812,0.6219833414,-0.028036487
C,1.1227521396,-0.2059438481,0.0022531141
C,1.2855657227,-2.7673288292,0.1898661424
C,-2.5859674913,0.1674930796,-0.008100363
H,0.0195047257,1.6976401917,-0.0767833372
C,2.5973396127,0.1731766172,-0.0395949648
H,0.586060024,-3.5275670669,-0.1523922984
H,1.5400719801,-2.9665567838,1.234817727
H,2.1893065574,-2.8151678708,-0.4150169559
C,-3.4880489585,-1.0782110363,-0.0449749376
C,-2.9004592013,0.9851628512,1.2652297997
C,-2.8712690313,1.0373521048,-1.2528067888
H,-3.317971222,-1.7169009058,0.8240080836
H,-4.539096155,-0.7735724293,-0.0514390216
H,-3.2974554466,-1.679671449,-0.9364832753

H,-2.2848003447,1.8870055394,1.3228311041
H,-3.9509974005,1.2929469383,1.2713384951
H,-2.7134672915,0.3919623858,2.1644086754
H,-2.6549149971,0.4860501114,-2.1719395608
H,-3.9239094534,1.3367864332,-1.2746175151
H,-2.2643208088,1.9469148673,-1.255413112
C,2.7228976489,1.7095762548,0.0247849313
C,3.3680731388,-0.4127039437,1.1661660127
C,3.2432485066,-0.2990456086,-1.3641730871
H,2.2920912521,2.1074967144,0.9468015252
H,3.7785856916,1.9923153284,-0.0039817015
H,2.2258097941,2.1888103984,-0.8218453625
H,3.4024287821,-1.5028596103,1.1534288102
H,4.4014219512,-0.0531512751,1.1559310267
H,2.9108290384,-0.0991800118,2.108451323
H,2.7210541038,0.1309142218,-2.2224511681
H,4.2891118391,0.0203080606,-1.4055717331
H,3.2271767278,-1.3850921126,-1.4744515932

73H, B3LYP Energy= -580.567677903 Hartree,
NIMAG= 0

N,0.6647705652,-1.5078102568,-0.0011097448
N,-0.6957042518,-1.4588921785,0.0277892515
C,-1.1328392704,-0.1868598796,0.0069879072
C,0.012413648,0.6077349375,-0.019646273
C,1.1317699774,-0.2303444284,-0.0172882275
C,1.313572379,-2.815142949,0.1206065274
C,-2.6011530177,0.1839617728,0.0086763129
H,0.0329851866,1.6823204723,-0.0431148278
C,2.6020569014,0.1647870935,-0.0387649266
H,-1.2400668161,-2.3103173524,0.0237989089
H,0.7621294683,-3.5380238809,-0.4823996225
H,1.3372817718,-3.1362090082,1.1635914977
H,2.323516717,-2.750435139,-0.2669705475
C,-3.4885883229,-1.0750808281,0.016034094
C,-2.8876590483,1.02853208,1.2728506159
C,-2.8963241461,1.0201605048,-1.25876988
H,-3.3315562963,-1.6853579234,0.9114611895
H,-4.5388591338,-0.7793464711,0.018047508
H,-3.3369149879,-1.6926055831,-0.8754050301
H,-2.2883195071,1.9411629191,1.2905248222
H,-3.9404140286,1.3193492517,1.283866438
H,-2.6819115521,0.4650771589,2.186315791
H,-2.6908433916,0.4534315649,-2.1702843003
H,-3.9506048323,1.305447254,-1.2677822528
H,-2.3024667294,1.9362645153,-1.2838355576
C,2.7016972561,1.7045042136,0.0019931196
C,3.3362948327,-0.3972662459,1.2022943323
C,3.2684301345,-0.3249123655,-1.3479532483
H,2.2586184555,2.1173355172,0.9113506654
H,3.7542326219,1.9922825359,-0.0111838062
H,2.2247785986,2.1674649834,-0.8650450091
H,3.3840569367,-1.4869665621,1.2182451712
H,4.3648146013,-0.0303288708,1.2048732074
H,2.8612845133,-0.0617769258,2.127540591
H,2.7560337469,0.0774055298,-2.2249075033
H,4.3027992896,0.0242513453,-1.3746264364
H,3.293602842,-1.4122471868,-1.4412631791

74, B3LYP Energy= -383.574446427 Hartree,
NIMAG= 0

N,-0.681340944,-0.046318536,-0.9874248378
N,0.6714614487,-0.0629201651,-1.0386549489
C,1.0717326874,-0.0304180187,0.2295293624
C,-0.0352493691,0.0140241339,1.1189754999
C,-1.1505125657,0.0057797398,0.2937779934
C,-1.4453763913,-0.021941486,-2.218697072
C,2.528291659,-0.0477221335,0.5740265182
C,0.0179680147,0.0519024629,2.6165624396
C,-2.6114645139,0.0406417514,0.6071455648
H,-0.7561640372,-0.2407876967,-3.0315237263
H,-1.8989112405,0.9596965798,-2.3895980701
H,-2.2332198986,-0.7788527331,-2.2013142903
H,3.1248417709,-0.0762376201,-0.3387448413
H,2.8158764226,0.8408615808,1.1457773582
H,2.7869985015,-0.9213415571,1.1816248389
H,0.5063387898,-0.8385031866,3.0274004701
H,-0.9811979155,0.1048167225,3.0549459784
H,0.5783145994,0.9204164587,2.9789795325
H,-3.1296268732,-0.8532934581,0.2434217328
H,-2.7647760899,0.0924700096,1.6854749667
H,-3.1053132551,0.9106082517,0.1612382307

74H, B3LYP Energy= -383.954074752 Hartree,
NIMAG= 0

N,-0.7136702101,-0.0578583443,-1.0123958471
N,0.6407683959,0.0168859039,-1.0028962796
C,1.0984407294,0.0487815958,0.2672186277
C,-0.0165941614,0.0061765229,1.1080257783
C,-1.1417217443,-0.0550582243,0.2699626931
C,-1.460273016,-0.0300239352,-2.2687854125
C,2.5555930176,0.1077112301,0.5769487027
C,-0.0141553754,0.0176772682,2.6074589871
C,-2.5871933568,-0.1084073086,0.6313680993
H,1.1661872893,0.0095219173,-1.8664618384
H,-1.0363479553,-0.7569730119,-2.9629549113
H,-1.4380627412,0.9703334486,-2.7055553695
H,-2.4894815394,-0.3102540018,-2.0595674642
H,3.1583878594,0.1682399271,-0.3304672684
H,2.7801561176,0.9818052591,1.1922860218
H,2.8655537302,-0.7804966325,1.1328776225
H,-0.4641343116,-0.8913033874,3.0143695415
H,-0.569511362,0.8724618702,3.0012214173
H,1.0027693802,0.0812307848,2.9952258841
H,-3.0629724812,-1.0162041793,0.2502019099
H,-2.6954173004,-0.1059397539,1.7147606673
H,-3.1317197821,0.7541632612,0.2376834783

75, B3LYP Energy= -619.499227278 Hartree,
NIMAG= 0

N,0.5783979285,1.1348509691,0.0186140777
N,-0.7666680942,1.2253981997,0.0253577095
C,-1.2275291278,-0.018480197,-0.006739971
C,-0.146415111,-0.9508169777,-0.0423600728
C,1.0155400418,-0.169216466,-0.0343161866
C,1.2891055608,2.4047226617,-0.0227178384
C,-2.7391110172,-0.2458491818,0.0039346504
C,-0.2803447054,-2.453246227,-0.0514195994
C,2.5048117664,-0.5349801207,-0.0159123977
H,0.5948800948,3.1572290447,0.3456570911
H,1.5833694273,2.666667829,-1.0425070841
H,2.1713829651,2.3918842351,0.6143757481

C,-3.4759401019,1.1085373744,0.0509084443
C,-3.1853299629,-0.9794462685,-1.2826210777
C,-3.1584421531,-1.0534748524,1.2547123759
H,-3.2289691011,1.7272920276,-0.8136262173
H,-4.556334714,0.9338709558,0.0557292545
H,-3.2128590834,1.6752721126,0.9458829877
H,-2.7325416107,-1.9672551104,-1.3853084711
H,-4.2720928144,-1.1111466621,-1.2822260496
H,-2.9165514121,-0.3962836007,-2.167624157
H,-2.8675853702,-0.5247919877,2.166607481
H,-4.2454125742,-1.1821565135,1.2713695612
H,-2.7069927548,-2.0465382556,1.2874824782
C,2.7334516034,-2.0401758272,-0.2651233916
C,3.2866520216,0.206703983,-1.129048389
C,3.1108316963,-0.2055258186,1.3710571531
H,2.3413806423,-2.3551720324,-1.2340801724
H,3.809484396,-2.2348619118,-0.2640289041
H,2.2877586801,-2.6628998983,0.5099139826
H,3.3325366666,1.2841558876,-0.9803258669
H,4.3171334955,-0.15973024,-1.1558418661
H,2.8383421205,0.0179467999,-2.108385965
H,2.5993400663,-0.7681575851,2.156230864
H,4.1708158612,-0.4781325135,1.3927278184
H,3.0374058549,0.8536590882,1.6233741047
H,0.2084552415,-2.9151862342,-0.9113967594
H,0.135640743,-2.9148359768,0.848835633
H,-1.3272208653,-2.7428482099,-0.0936816781

75H, B3LYP Energy= -619.885064709 Hartree,
NIMAG= 0

N,0.6230519442,1.145750934,0.043500557
N,-0.7284672342,1.1785033289,0.0324817531
C,-1.2467206119,-0.0603737488,-0.0052757309
C,-0.1548935841,-0.9476150069,-0.0292487745
C,1.0216020545,-0.1575058564,-0.0101081025
C,1.3236069526,2.4339091627,0.0160662596
C,-2.7588866861,-0.2555151427,-0.0071653342
C,-0.2777355907,-2.4487511494,-0.0441706168
C,2.5098235407,-0.5315480148,-0.0125512561
H,-1.2206209274,2.0596206547,0.0658950841
H,0.7184399213,3.1608352831,0.5593708716
H,1.473821214,2.7706635586,-1.0106497966
H,2.2778141247,2.3479653395,0.5220097458
C,-3.4780568491,1.1111913471,0.025579973
C,-3.1853814729,-0.9916718508,-1.2998364734
C,-3.1834252889,-1.0525010517,1.2495438641
H,-3.2507567228,1.7229683469,-0.8537295911
H,-4.5566570968,0.9477219887,0.0203279573
H,-3.2534745156,1.6789927492,0.9346835999
H,-2.7434219907,-1.9842872955,-1.384695713
H,-4.2710792203,-1.1117393359,-1.3037434128
H,-2.9072636767,-0.4203451505,-2.1890401223
H,-2.900932984,-0.5261612404,2.1647932568
H,-4.2694826407,-1.1693654155,1.2511570445
H,-2.7442521473,-2.0493012945,1.2840859943
C,2.728769838,-2.0413039025,-0.2447736292
C,3.256070965,0.1974259048,-1.1595558415
C,3.1274946057,-0.183731737,1.3659572226
H,2.3329310365,-2.3724972891,-1.2059373489
H,3.8043155765,-2.2274647879,-0.2555347272
H,2.3046851452,-2.6556123638,0.5481303975
H,3.3127287048,1.2777623467,-1.0371459267

H,4.2834774244,-0.1699613259,-1.1989721266
H,2.793088664,-0.0151735981,-2.1266867854
H,2.6302817056,-0.7359803624,2.1668831245
H,4.1823493029,-0.4674342126,1.3686840367
H,3.077062093,0.8779134505,1.6133202083
H,0.2070163,-2.8915728718,-0.9133985726
H,0.1580541039,-2.899017268,0.8488701568
H,-1.3218395483,-2.7454468776,-0.0735511377

76, B3LYP Energy= -674.695280209 Hartree,
NIMAG= 0

N,0.8562445805,0.6341860999,0.0000302411
N,2.0827255316,0.1247754925,0.0000672504
C,1.9157475238,-1.1953183865,0.0000947764
C,0.5742536433,-1.5833409174,0.0000684797
C,-0.0802291735,-0.3687536721,0.0000307987
C,0.6983767002,2.0932719255,-0.0000024903
N,3.0730755932,-2.0837633254,0.0001458582
H,0.1464077931,-2.5698361288,0.0000794956
N,-1.5065188119,-0.1433292363,-0.0000051353
H,1.7062855691,2.5000559816,0.0000096729
H,0.1529290124,2.4105859685,0.8867974269
H,0.1529651004,2.4105496443,-0.8868375978
O,-1.9008710714,1.019289994,-0.0000774874
O,-2.2155068314,-1.1378629902,-0.0000429304
O,2.8195435539,-3.283136516,-0.000196557
O,4.1829303866,-1.5830068337,-0.0001845972

76H, B3LYP Energy= -675.002273274 Hartree,
NIMAG= 0

N,0.829319931,0.6475351045,0.0000076504
N,2.0402211291,0.0683269533,0.0000278538
C,1.9029849173,-1.2676771524,0.0000070926
C,0.5624310781,-1.5948519382,-0.0000074114
C,-0.0746673496,-0.35791082,-0.000011715
C,0.6890899169,2.1265689613,0.0000160158
N,3.1106588861,-2.1029773524,-0.0000032766
H,0.1072575999,-2.5725061403,-0.0000156599
N,-1.5284131653,-0.1190214028,-0.0000265937
H,2.9135867077,0.5938014608,0.0000338709
H,1.6937724565,2.5464032388,0.0000357936
H,0.1465318938,2.4316669763,0.8919744349
H,0.1465613087,2.4316797595,-0.8919555737
O,-1.8878311929,1.0452114301,0.0000168149
O,-2.2106095811,-1.1187026309,-0.0000085721
O,2.9319037864,-3.2983116341,-0.0000817615
O,4.1622260532,-1.482095772,0.0000400353

77, B3LYP Energy= -2839.12631795 Hartree,
NIMAG= 0

N,2.0704475757,-0.145449462,0.0035301166
N,1.8967801189,1.1892142814,-0.0513305502
C,0.579257228,1.3771907522,-0.0340974672
C,-0.0962871676,0.1440610056,0.0271230611
C,0.8928244831,-0.8194079002,0.0479197809
C,3.4122104,-0.6998535413,-0.0553028766
H,0.1647464364,2.372746302,-0.0607146957
Br,-1.9623226541,-0.1493287381,0.0852134559
H,0.8375503034,-1.8944031799,0.0930680581
H,3.8191650262,-0.6121057362,-1.0650841235

H,4.0532523023,-0.1570573284,0.63892747
H,3.3740099479,-1.750568455,0.2307477707

77H, B3LYP Energy= -2839.47848496 Hartree,
NIMAG= 0

N,2.0925332066,-0.1686368318,-0.0214300885
N,1.858926023,1.1592902895,-0.104071902
C,0.5339778602,1.3969238744,-0.0604329228
C,-0.1051426109,0.1688316651,0.0549698729
C,0.9084608038,-0.7927625973,0.0763295859
C,3.4525645822,-0.72079956,-0.0443196932
H,0.1387981366,2.3992117749,-0.1129088187
Br,-1.9453702322,-0.1399719619,0.1604676271
H,0.8483198965,-1.8667962908,0.154439203
H,2.6218283222,1.8204578762,-0.1850920869
H,3.9388830846,-0.4651912286,-0.9864493735
H,4.0206929291,-0.3377276653,0.8041695924
H,3.3682011091,-1.8020917443,0.0365538051

78, B3LYP Energy= -2878.45816439 Hartree,
NIMAG= 0

N,-2.0790191124,-0.411731365,-0.003726877
N,-1.8958932474,0.9251528742,0.0374389659
C,-0.5765096819,1.1205933911,0.0076324791
C,0.0845055917,-0.1282195635,-0.0487425618
C,-0.9061366269,-1.0888713996,-0.0527486498
C,-3.4234179749,-0.9553977461,0.0614379458
C,0.0111563975,2.4933053016,0.029217669
Br,1.949932838,-0.4368853634,-0.1183209149
H,-0.8533315703,-2.1645486083,-0.0889003707
H,-3.3815951941,-2.0249643077,-0.142717646
H,-4.0488624583,-0.4676502842,-0.686812648
H,-3.8546795558,-0.7915412385,1.0515157286
H,-0.7880432001,3.2333363936,0.0761852453
H,0.6664244149,2.6291093315,0.894295398
H,0.6106563799,2.6809265841,-0.8661407637

78H, B3LYP Energy= -2878.81811831 Hartree,
NIMAG= 0

N,-2.1078603223,-0.4401761816,0.0148644638
N,-1.867293303,0.8921625144,0.0607377416
C,-0.5404981633,1.1434792218,0.010574533
C,0.0850736179,-0.1056623142,-0.0715443408
C,-0.9226684056,-1.0657925206,-0.0662696537
C,-3.4674509675,-0.9856811105,0.0547921282
C,0.0284757189,2.5160490805,0.0424438454
Br,1.927998088,-0.4162121039,-0.1697457102
H,-0.8617238041,-2.1414719996,-0.1150379176
H,-2.6301907428,1.5546158897,0.1244386884
H,-3.3871975808,-2.069251783,0.0037757908
H,-4.0380805917,-0.6263142319,-0.8026697041
H,-3.9541705777,-0.7044351555,0.9896836901
H,-0.7502750258,3.2757701487,0.1181514315
H,0.7042589945,2.6214890069,0.8947395657
H,0.6109169461,2.7011342714,-0.8635901995

79, B3LYP Energy= -2878.45734559 Hartree,
NIMAG= 0

N,-2.3560214157,-0.0145770311,0.0053475991

N,-2.1883581111,-1.356675338,0.0114727864
C,-0.8741116598,-1.5463249178,0.0354096321
C,-0.1974377421,-0.3128083527,0.0466658533
C,-1.175943035,0.6687478344,0.0272857574
C,-3.6979403354,0.5401657073,-0.0078135586
H,-0.4611463926,-2.5427550525,0.0431621137
Br,1.6756230727,-0.0405157793,0.0789487046
C,-1.0842210413,2.1568354749,0.0271831056
H,-4.3886653372,-0.2976509315,-0.0702502044
H,-3.8400220488,1.1925793078,-0.8726419445
H,-3.8967009441,1.1058292207,0.9061708205
H,-1.5865591902,2.5936002832,0.8961435568
H,-0.0375941278,2.4592701898,0.0565823815
H,-1.5352685914,2.5902299847,-0.8712178036

79H, B3LYP Energy= -2878.81652227 Hartree,
NIMAG= 0

N,-2.3831020532,0.0142415973,0.0073225477
N,-2.1527784187,-1.3180979994,0.0907254212
C,-0.8286471385,-1.5507980914,0.1127972742
C,-0.1918443566,-0.3220830001,0.0516701569
C,-1.197071873,0.6614191931,-0.0098311318
C,-3.748802238,0.5458601119,0.0337892205
H,-0.4319703207,-2.5523313729,0.162948334
Br,1.6583747609,-0.033932097,0.04669615
C,-1.0784072902,2.1428954393,-0.0809190576
H,-2.9177944316,-1.9801409589,0.1050561831
H,-4.3767661445,-0.0404525853,-0.6376705442
H,-3.7209111127,1.572205252,-0.3229546195
H,-4.1449637574,0.5199509801,1.0502903012
H,-1.5744235253,2.6237834712,0.766094456
H,-0.026057024,2.4211106622,-0.0615899402
H,-1.514754129,2.5320962126,-1.0050266657

80, B3LYP Energy= -2917.78900395 Hartree,
NIMAG= 0

N,1.9844657869,-0.2148714638,0.0051594194
N,1.7189148561,-1.5445135401,0.002563715
C,0.3926125431,-1.6540825092,0.0007833789
C,-0.1862485704,-0.3644062969,-0.0003776056
C,0.8566170716,0.5473209783,0.0020612062
C,3.3623699944,0.2404887822,-0.0053382175
C,-0.2811988384,-2.9870450944,0.0007476397
Br,-2.0366661513,0.0455902261,-0.0013804159
C,0.8685503254,2.0381611736,0.0023167718
H,3.991152263,-0.64559389,0.0458864629
H,3.5684946806,0.8803415855,0.8563370781
H,3.5881291203,0.7904975545,-0.9229745327
H,1.3856977058,2.4386179867,-0.8755183242
H,-0.1544242676,2.4140964144,-0.0093614624
H,1.3649660017,2.4384513272,0.8922341245
H,-0.9174876052,-3.1094979177,0.8820294747
H,-0.9181075356,-3.1089655367,-0.8801417184
H,0.4706368196,-3.7768194797,0.0002788054

80H, B3LYP Energy= -2918.15554603 Hartree,
NIMAG= 0

N,-1.9858156744,-0.1336528484,-0.0347238542
N,-1.6823744708,-1.45741277,-0.0111710357
C,-0.3460581981,-1.6397657526,0.002858776

C,0.214727237,-0.3620160257,0.0026249443
C,-0.8319922105,0.5704593468,-0.0155946874
C,-3.3758595066,0.3203289083,0.0272109678
C,0.2894784011,-2.983709153,0.0056731957
Br,2.0511769674,0.0171496583,0.0155235282
C,-0.7874961697,2.0580136256,-0.0127357474
H,-2.4130340097,-2.1564475521,-0.0391369428
H,-3.9729830605,-0.2396549151,-0.6935519308
H,-3.4020849866,1.3726255111,-0.2439634797
H,-3.7742090953,0.1923102114,1.0353903812
H,-1.2822943475,2.4689724712,0.8712054771
H,0.2497930058,2.388546283,-0.0053760348
H,-1.2690679914,2.4718511781,-0.9027920658
H,0.9055847538,-3.1102322061,-0.8881165594
H,0.9449571733,-3.086132963,0.8737746333
H,-0.453239117,-3.781971708,0.0334353344

81, B3LYP Energy= -2878.45675140 Hartree,
NIMAG= 0

N,-0.7657219597,-0.0501636215,-0.8894112801
N,0.5892777118,-0.0682802642,-0.9331230372
C,0.9985037948,-0.007359377,0.3341464593
C,-0.1018047075,0.0514827038,1.2209061995
C,-1.2035588195,0.0214188495,0.3925738138
C,-1.5372379239,-0.1046050943,-2.1194575752
C,2.4588091377,-0.0073248762,0.6632440815
H,-0.1003609692,0.1071969548,2.296629514
Br,-3.037519894,0.0656365377,0.8333894168
H,-0.8207355223,-0.1555098958,-2.9361257713
H,-2.1557864982,0.7887435832,-2.2283077813
H,-2.1771332171,-0.9893478009,-2.1362042977
H,3.0436877132,-0.062629855,-0.2558032707
H,2.744793681,0.9015121742,1.2006253701
H,2.723913973,-0.8612013183,1.2934444586

81H, B3LYP Energy= -2878.81943291 Hartree,
NIMAG= 0

N,0.4454028375,1.0371151785,0.0314283654
N,1.7964151526,0.8773725092,-0.0053726569
C,2.1229441006,-0.4329957792,-0.0405064475
C,0.9263378047,-1.1432529328,-0.0416210926
C,-0.0979435197,-0.198591627,0.0001035066
C,-0.1635642751,2.3690164682,0.0043120796
C,3.5367597746,-0.90220494,-0.0384938304
H,0.8072205766,-2.2131362988,-0.066957673
Br,-1.9353515094,-0.4872325287,0.0078379088
H,2.4075203441,1.6834397511,0.0225479416
H,0.3033907501,2.9940221324,0.7661197322
H,-1.2193498774,2.2570287909,0.2366642388
H,-0.050887543,2.81419888,-0.9855952202
H,4.2033785204,-0.1751110451,-0.5058624219
H,3.878310547,-1.0732204807,0.9866550203
H,3.6184203165,-1.844045078,-0.581005451

82, B3LYP Energy= -5451.99486061 Hartree,
NIMAG= 0

N,1.476137396,1.2917018274,0.0000003072
N,0.8140909833,2.473655492,0.0000015277
C,-0.4861433804,2.1812172522,0.0000002965
C,-0.6651022941,0.7791625759,-0.000001297

C,0.6117976284,0.2469668165,-0.0000012723
C,2.9296272047,1.2710835283,0.0000014456
C,-1.5243985159,3.254261635,0.0000003183
Br,-2.2947763564,-0.1668623257,-0.0000033353
Br,1.1741280272,-1.5442048774,-0.0000026653
H,3.2550269319,2.308653904,0.0000023359
H,3.3087572277,0.7660119213,-0.8904685865
H,3.3087558434,0.7660108182,0.8904714439
H,-2.1680876064,3.1820479258,-0.8813365167
H,-2.1680990123,3.1820367502,0.8813277744
H,-1.0387049773,4.2306945562,0.0000093069

82H, B3LYP Energy= -5452.35033940 Hartree,
NIMAG= 0

N,1.5512229689,1.1812684941,-0.0395872153
N,0.8865494806,2.3658413995,-0.0163160644
C,-0.4487670791,2.1729348576,-0.000310229
C,-0.6469571595,0.7903908259,0.0038628623
C,0.6222804793,0.199719337,-0.0141340929
C,3.0142265725,1.1265770974,0.0345644735
C,-1.428486616,3.2906874945,-0.0017740326
Br,-2.2980328758,-0.0824740498,0.0187975593
Br,1.0662453273,-1.6013255976,-0.0028343749
H,1.3958802959,3.2399550847,-0.046232477
H,3.4298536019,1.8977201442,-0.6144026688
H,3.3337004364,0.1524887687,-0.3271585609
H,3.3465580089,1.267543451,1.0643782425
H,-2.0481734834,3.2457699119,-0.9010260342
H,-2.0933886272,3.2060367293,0.86103577
H,-0.9321959308,4.2613499514,0.0329962426

83, B3LYP Energy= -5451.99544375 Hartree,
NIMAG= 0

N,-1.7253418383,-1.4181294509,-0.0149486986
N,-0.4576267816,-1.8938644405,-0.0386766202
C,0.307911646,-0.8169209761,-0.0353764395
C,-0.4608269668,0.365833113,-0.0067061336
C,-1.7820829599,-0.0576178784,0.0076507468
C,-2.8364710586,-2.3545755547,0.0128082045
Br,2.1852325902,-0.9706981124,-0.0701344656
Br,0.1492205333,2.1491634618,0.0048284401
C,-3.0584081626,0.7122387659,0.0391790382
H,-2.4175188765,-3.3510246274,-0.1061526741
H,-3.5305400099,-2.152077276,-0.8056467991
H,-3.3717621421,-2.2979263061,0.9640841638
H,-3.6719305345,0.5109720683,-0.8446405788
H,-3.6547625218,0.4675357265,0.9236396518
H,-2.8427569169,1.780098487,0.0628311643

83H, B3LYP Energy= -5452.34940506 Hartree,
NIMAG= 0

N,-1.7185617471,-1.470581578,0.0339777212
N,-0.4197814827,-1.856321482,-0.0610138469
C,0.3754225563,-0.7670394877,-0.1061468971
C,-0.4507008056,0.3529513051,-0.0506642033
C,-1.7719107675,-0.1209156352,0.0324985373
C,-2.7950226868,-2.4646612217,0.0352693317
Br,2.2193627445,-0.9121651075,-0.2122829676
Br,0.0952344276,2.1398210932,-0.0766243531
C,-3.0479986189,0.6413384449,0.1075582563

H,-0.1526930661,-2.8325969796,-0.0567306732
H,-2.5716644224,-3.2399749517,0.7691183176
H,-2.9098097695,-2.8985145804,-0.9595605449
H,-3.7158537187,-1.9648267512,0.3241340866
H,-3.7038672105,0.401159858,-0.7332323954
H,-3.581982766,0.4278258916,1.037520083
H,-2.8344285111,1.7083852008,0.0780873982

84, B3LYP Energy= -572.191728382 Hartree,
NIMAG= 0

N,-1.0545693998,-0.0975112224,0.017221333
N,0.0343396317,-0.8839382449,0.0046411511
C,1.0926837179,-0.0696740129,-0.0897947646
C,0.6737583963,1.2704755931,-0.1394657828
C,-0.711436948,1.2268307952,-0.0685646137
C,-2.3634199508,-0.7328032645,0.1138515427
C,2.4816653036,-0.6270832239,-0.1303687905
H,1.2708376142,2.1643213792,-0.2159141737
C,-1.6108344623,2.3908967736,-0.0808270583
H,-2.1810410853,-1.8045962918,0.1356027134
H,-2.877816007,-0.4217891902,1.0232406412
H,-2.9812972678,-0.4744510843,-0.7459322349
H,2.4472539102,-1.7147345471,-0.057258839
H,2.9893659136,-0.3601078466,-1.0617166214
H,3.087078297,-0.2445678277,0.6963127177
O,-1.2171396916,3.5304213607,-0.184701478
O,-2.916228368,2.0524810918,0.0330663914
C,-3.8796553952,3.139990735,0.0346702798
H,-3.5449035624,3.902351001,-0.6692085759
H,-4.7962744371,2.680679176,-0.3364853382
C,-4.0691326716,3.7159002613,1.4278346889
H,-3.1491864053,4.1801032658,1.7866068358
H,-4.8500542992,4.4814816303,1.4026072309
H,-4.3754848328,2.9399458933,2.1334924452

84H, B3LYP Energy= -572.555715688 Hartree,
NIMAG= 0

N,-1.0992970396,-0.140703247,0.0103409868
N,0.0457315453,-0.8659183832,0.0122609632
C,1.132443714,-0.0650017549,-0.054264622
C,0.6491180496,1.2381157987,-0.0912740141
C,-0.7426100366,1.1637932339,-0.0471129378
C,-2.39202256,-0.8294388201,0.1288626259
C,2.5207085551,-0.6026037473,-0.1075252491
H,1.2199796213,2.1498550658,-0.1466921746
C,-1.6389600421,2.3718010155,-0.066846253
H,0.0077914961,-1.877100437,0.0486186779
H,-2.4390139481,-1.6234560499,-0.6174885534
H,-2.4982134768,-1.2388982414,1.1349059538
H,-3.173403018,-0.1019445388,-0.0573349326
H,2.6039110881,-1.5624759708,0.4054682707
H,2.8358352468,-0.7392330962,-1.1462164003
H,3.2094155649,0.100274838,0.3612589411
O,-1.1519203816,3.4670196565,-0.1498808084
O,-2.9311739694,2.0739385013,0.0087149331
C,-3.8879134629,3.2042083022,-0.0050320964
H,-3.5084397707,3.9467722956,-0.7054769516
H,-4.795828183,2.7532661008,-0.4012788677
C,-4.0853110771,3.7702378985,1.3858564449
H,-3.1682061058,4.2201154145,1.7689424381
H,-4.8480882211,4.5519128982,1.3401671629

H,-4.431672304,3.0027702987,2.0811901968

85, B3LYP Energy= -572.192084578 Hartree,
NIMAG= 0

N,-0.1279499171,0.6264501569,-0.0630004689
N,1.1646884738,0.9855752644,-0.0849644803
C,1.8381888151,-0.1573159145,0.0665242057
C,0.9629898006,-1.2604797718,0.1863476634
C,-0.3044553376,-0.7237103494,0.099067021
C,-1.1573212983,1.6417337311,-0.2101850315
C,3.3135256133,-0.2295161105,0.1009307224
H,1.2346780496,-2.2944254625,0.3186815108
C,-1.6531025522,-1.363345801,0.1538118915
H,-0.6529065397,2.6011758024,-0.2955076163
H,-1.8165231726,1.6534332047,0.6611210626
H,-1.7530032799,1.4631172312,-1.1088112337
H,-2.2163565663,-1.2082756914,-0.7722109173
H,-1.544616012,-2.4379679618,0.3018729888
H,-2.257510063,-0.9711355572,0.9781052314
O,3.9176158247,-1.2726982565,0.2354930934
O,3.9004795331,0.9736359546,-0.0261622126
C,5.3484089123,1.0049958385,-0.0085751661
H,5.586549928,2.0007050528,0.3669756799
H,5.7100882136,0.2549525852,0.6959478589
C,5.9265209971,0.7838751144,-1.3969048721
H,7.0146180472,0.8934201767,-1.3632056226
H,5.6963706513,-0.219269829,-1.7600774384
H,5.5300263789,1.5168520928,-2.10350977

85H, B3LYP Energy= -572.559367963 Hartree,
NIMAG= 0

N,-0.1469110757,0.6261416256,-0.0472839818
N,1.1811030976,0.8792534939,-0.0850376361
C,1.8647285631,-0.2678967203,0.0894647484
C,0.9398323421,-1.2893211855,0.2352346405
C,-0.3274886757,-0.7032334151,0.1422151714
C,-1.1245566873,1.6955534035,-0.2620089694
C,3.3590178147,-0.3181015857,0.1156136889
H,1.1648664478,-2.3309636793,0.3931390827
C,-1.6747144415,-1.3354882937,0.2218563298
H,1.5570350856,1.8120405879,-0.2063514758
H,-0.861928018,2.5559580864,0.3541979668
H,-2.1010591758,1.3297218137,0.0445958962
H,-1.152478528,1.9747269816,-1.3166426758
H,-2.2382004704,-1.194625061,-0.7042601492
H,-1.562553088,-2.4056265148,0.3892339743
H,-2.2613966176,-0.9248422997,1.0480521183
O,3.9562659379,-1.3460538355,0.2770391056
O,3.8608316364,0.9050680157,-0.0537315196
C,5.3328500093,1.0462538922,-0.0539636802
H,5.4846367538,2.0677233416,0.2896766845
H,5.7288672758,0.3468856592,0.6813183994
C,5.9030480021,0.8120678703,-1.4373623577
H,6.9806409646,0.9932311896,-1.4075762536
H,5.7463036809,-0.2164843806,-1.7663866861
H,5.4668758745,1.4969793595,-2.1675522016

86, B3LYP Energy= -800.134181577 Hartree,
NIMAG= 0

N,-0.1043634251,0.5931626198,-0.0050264691

N,1.1815840698,0.9353536368,0.0041809978
C,1.8676063589,-0.2169829488,0.0139061829
C,1.0016554048,-1.3217665293,0.0100811561
C,-0.2694803712,-0.7754551042,-0.0017140095
C,-1.1017168956,1.6606903582,-0.0190538642
C,3.3462111929,-0.2808372826,0.0238844848
H,1.2560382106,-2.3676453159,0.0153118466
C,-1.534744553,-1.5313025903,-0.0110973908
H,-0.5469521335,2.5955576108,-0.0298207868
H,-1.7323064937,1.6043505098,0.8674537524
H,-1.7296601398,1.5824860471,-0.9057823532
O,3.9545346995,-1.3283565811,0.0406514887
O,3.9187062529,0.9334605492,0.0157612936
C,5.3685363678,0.9778209156,0.0123306399
H,5.6033624161,1.9345910169,0.4792089158
H,5.7473933844,0.166349855,0.6346741128
C,5.9218505031,0.8979055199,-1.4009519942
H,7.009546614,1.0122509033,-1.3755480173
H,5.6915104787,-0.066960852,-1.8558209229
H,5.5081176303,1.6933541056,-2.025113281
O,-1.5780415993,-2.7388018516,-0.0352281379
O,-2.6251750171,-0.7334834366,0.0060092191
C,-3.9226657293,-1.3917360074,-0.0037619389
H,-4.5869538061,-0.6552509343,-0.4563989197
H,-3.8606845412,-2.2693391381,-0.6474611973
C,-4.3710988563,-1.7613955108,1.399588674
H,-5.3768027941,-2.1894649048,1.3583965344
H,-3.7040211151,-2.503544107,1.840874961
H,-4.4023898132,-0.8808656532,2.045751223

86H, B3LYP Energy= -800.490909321 Hartree,
NIMAG= 0

N,-0.110445733,0.5527775211,-0.0171146094
N,1.2121970911,0.8055354006,-0.0101784417
C,1.9110950102,-0.3474240357,0.0056217362
C,0.9952910317,-1.3874351816,0.0097964894
C,-0.2678428976,-0.7941570594,-0.0036885118
C,-1.0861306321,1.6570299192,-0.0367680091
C,3.406686286,-0.379236866,0.0165179367
H,1.2053311029,-2.4440783077,0.0210555528
C,-1.5685690433,-1.5439202935,-0.0071186859
H,1.5840116039,1.7488854689,-0.0177065361
H,-0.5321881734,2.594273489,-0.0605272243
H,-1.7035979232,1.6107019557,0.8572781458
H,-1.7105433776,1.5713258831,-0.9229765063
O,4.0180910419,-1.4104048914,0.0384689045
O,3.888166801,0.8637001242,0.0063221506
C,5.3590659601,1.0269807691,0.0115021793
H,5.499773117,1.9951674762,0.4882250029
H,5.7729028521,0.2412485548,0.642170338
C,5.9154100032,0.9895811066,-1.3965509133
H,6.990899831,1.1802963825,-1.3534843665
H,5.7677925713,0.0125500132,-1.8594854609
H,5.4618416268,1.7603931289,-2.0231014879
O,-1.5700234215,-2.7443902885,-0.0300300367
O,-2.6200797741,-0.7320788063,0.011900778
C,-3.9600506336,-1.3622300275,0.0095012465
H,-4.5911152592,-0.5983905095,-0.4409854647
H,-3.9114447449,-2.2331908149,-0.6426517593
C,-4.3995201891,-1.7181379916,1.4145597362
H,-5.415892161,-2.118213983,1.3720726509
H,-3.7576337359,-2.4833789037,1.8536207844

H,-4.4117895585,-0.8388098043,2.0620461545

87, B3LYP Energy= -470.146380423 Hartree,
NIMAG= 0

N,-0.7515883066,-0.0000000961,-0.8606584271
N,0.5811499398,-0.0000001751,-0.9332673991
C,0.9700105685,-0.00000016,0.3350839712
C,-0.1012113256,-0.000000067,1.2458536895
C,-1.2079985315,-0.0000000274,0.4254118537
C,-1.5369670709,0.0000000376,-2.087863034
N,2.3855772154,-0.0000002538,0.6725178316
H,-0.056321648,-0.0000000457,2.3204239544
H,-2.2622125729,0.0000000513,0.6515546856
H,-2.5937002878,-0.0000005758,-1.8241515622
H,-1.3042556219,-0.8900441247,-2.6732172724
H,-1.304256491,0.8900448789,-2.6732165987
O,3.2025246258,0.0000002038,-0.2330824041
O,2.6501431066,0.000000346,1.8726061117

87H, B3LYP Energy= -470.479128604 Hartree,
NIMAG= 0

N,-0.7864188094,-0.0000000656,-0.8716201023
N,0.5598590231,-0.0000000277,-0.8679490227
C,0.9827269972,0.0000000073,0.4076340817
C,-0.1053304192,-0.0000000078,1.2560734174
C,-1.2113206964,-0.0000000543,0.4036545104
C,-1.5569989078,-0.00000011,-2.1249547982
N,2.422075182,0.0000000527,0.6773754171
H,-0.09270084,0.0000000121,2.3335289395
H,-2.2663661719,-0.0000000798,0.6308100008
H,1.1324984616,-0.0000000269,-1.7085354219
H,-2.6114576125,-0.0000001348,-1.8583840159
H,-1.323572667,-0.8988290307,-2.6963973437
H,-1.3235727175,0.8988288031,-2.6963973763
O,3.1358621773,0.0000000547,-0.3148203271
O,2.7489088483,0.000000083,1.8427661623

88, B3LYP Energy= -470.143345285 Hartree,
NIMAG= 0

N,-0.6202630712,0.000001335,-0.8762691558
N,0.7159524773,-0.000002836,-0.9104452205
C,1.1263857693,-0.0000017351,0.3636369997
C,0.046616959,0.0000031584,1.2520277981
C,-1.0581288244,0.0000056223,0.418880866
C,-1.3618210009,0.0000012381,-2.1371522657
H,2.1828021986,-0.0000046035,0.5822852022
H,0.0391105024,0.0000051392,2.3281657368
N,-2.4432616518,0.0000110447,0.8017107364
H,-0.610006825,-0.0000036012,-2.9227900156
H,-1.9909280831,0.8861364497,-2.2084032596
H,-1.9909350946,-0.8861293245,-2.2083990285
O,-3.2906177759,-0.0000113693,-0.0900389114
O,-2.6840011795,-0.0000105171,2.002657718

88H, B3LYP Energy= -470.475070520 Hartree,
NIMAG= 0

N,-0.6476388589,0.0000009423,-0.8876678528
N,0.7006515778,0.0000027729,-0.8640345818
C,1.1594810429,-0.0000001106,0.4006458318

C,0.0623677984,-0.000002549,1.2472488984
C,-1.0401294792,-0.0000018215,0.4033175625
C,-1.3938874389,0.0000019421,-2.1672006617
H,2.2186571903,0.0000010662,0.6078321567
H,0.0458816748,-0.0000043948,2.324440669
N,-2.4547617642,-0.0000094374,0.798915509
H,1.2266933787,0.0000057423,-1.7311559822
H,-0.6604208715,-0.0000047658,-2.9724050558
H,-2.0148957445,0.8911313768,-2.221828301
H,-2.0149059307,-0.8911206015,-2.221823375
O,-3.2761229423,0.0000073581,-0.1030120959
O,-2.6564191004,-0.0000138169,1.9936227431

89, B3LYP Energy= -470.149484034 Hartree,
NIMAG= 0

N,-0.7465255642,1.6407461932,-0.0729653702
N,0.6020428452,1.7843616789,0.009425585
C,1.0868087292,0.5536503107,0.0623340756
C,0.0355732059,-0.384645128,0.012977399
C,-1.1339091534,0.3529831493,-0.074104536
C,-1.584139873,2.8284797584,-0.1474631424
H,2.1468137441,0.3702956904,0.1326471215
N,0.1296551861,-1.8136661897,0.0448188224
H,-2.1620174509,0.037933266,-0.1339529643
H,-1.431772789,3.440065182,0.7424129816
H,-1.3199921058,3.4075437759,-1.0329685266
H,-2.6268817649,2.520170851,-0.2075642376
O,1.2516515043,-2.3050981092,0.1261187763
O,-0.9185434138,-2.4547142288,-0.0113684842

89H, B3LYP Energy= -470.481380452 Hartree,
NIMAG= 0

N,-0.7735813628,1.6621317398,-0.075225785
N,0.5800734445,1.7404474604,0.0090106318
C,1.1147722389,0.5119150658,0.0650602585
C,0.0536207319,-0.3765523916,0.0139869277
C,-1.1186095634,0.3707926885,-0.0737002562
C,-1.614705929,2.8668366156,-0.1502670957
H,2.1780286656,0.3388300793,0.1354709479
N,0.1442273898,-1.8316516336,0.0460209599
H,-2.1458585085,0.0452326121,-0.1328199967
H,1.0506307694,2.6387824906,0.0225596492
H,-1.4742031128,3.467397779,0.7489756648
H,-1.3608235069,3.4347701417,-1.0458382421
H,-2.649842299,2.5380852316,-0.2096735621
O,1.266224236,-2.2972444655,0.1255819269
O,-0.9132702741,-2.4334227376,-0.0103072115

90, B3LYP Energy= -548.812935257 Hartree,
NIMAG= 0

N,-0.757830676,1.6378383816,-0.086104053
N,0.6020444922,1.7771716917,-0.0828242564
C,1.100660366,0.5529186,-0.019955261
C,0.0285821462,-0.3815019843,0.0172587567
C,-1.1605738339,0.352997783,-0.026990701
C,-1.5774683488,2.8397229505,-0.150121594
C,2.5760957528,0.3282025392,0.0017992662
N,0.1215562922,-1.8026744635,0.0865580417
C,-2.5893512284,-0.073771803,-0.0169213579
H,-0.8920092383,3.6828074151,-0.186078884

H,-2.2116359529,2.9262776599,0.7343272661
H,-2.1989764157,2.839977903,-1.0476908709
H,3.0843501837,1.2918768932,-0.0409294475
H,2.8778733358,-0.2034513974,0.9067072124
H,2.8908173299,-0.2878483287,-0.8431990432
H,-3.259345665,0.7850804041,-0.0626246827
H,-2.7975900155,-0.7324450187,-0.8624405234
H,-2.8100949238,-0.6492921209,0.8842651316
O,1.2442504587,-2.3056018358,0.1192250458
O,-0.9284958594,-2.4509535692,0.1099205545

90H, B3LYP Energy= -549.160856593 Hartree,
NIMAG= 0

N,1.6971760546,0.2166509053,0.0203774161
N,1.0792365982,1.4330823705,-0.0060544866
C,-0.2575524423,1.3019782183,-0.0123444967
C,-0.4814982709,-0.077843676,0.0011930326
C,0.7572701527,-0.7467435524,0.0137796738
C,3.1625922296,0.1373539012,-0.0341363394
C,-1.1708316621,2.4745017008,-0.0239359032
N,-1.7871601799,-0.7099777177,0.0063539751
C,1.0656520056,-2.2016988023,0.0146965558
H,1.6226691181,2.2873507714,0.0059734979
H,3.5790403368,0.9583849915,0.5496212701
H,3.5070934735,0.1915733471,-1.0678300145
H,3.4797217003,-0.797766,0.4187229781
H,-0.6095728927,3.4099696891,-0.0217198676
H,-1.8131396025,2.4381790284,-0.906005362
H,-1.8301490771,2.4440850131,0.8457188122
H,2.1316382938,-2.3945077053,-0.0884433021
H,0.7022821388,-2.6578125358,0.9387035026
H,0.5324156723,-2.6911942691,-0.8017308918
O,-2.7545970818,0.0339899509,-0.0396366031
O,-1.8103335647,-1.929873629,0.0566605527

91, B3LYP Energy= -496.702985895 Hartree,
NIMAG= 0

N,-3.0116123688,-0.7288616799,-0.000061086
N,-1.7190939904,-1.0972194756,0.0000015914
C,-1.0167473397,0.0428353679,0.0000717039
C,-1.8910290516,1.1608495838,0.0003520538
C,-3.1589279669,0.6209543472,0.0002230351
C,-4.0486049046,-1.7446004765,-0.0001964733
C,0.4556651031,0.0226186729,0.0000123585
H,-1.6405200154,2.2083720863,0.0005611849
H,-4.1324650123,1.0852300475,0.0002902086
C,1.1942047624,1.2140387547,-0.0002085721
C,1.1535309126,-1.1950190486,0.0002024544
C,2.5865691423,1.1911201597,-0.0002387539
H,0.6810536886,2.1687128307,-0.00037372
C,2.5439986368,-1.2161337169,0.0001670819
H,0.5905047345,-2.119835836,0.0003817664
C,3.2689729234,-0.0238810655,-0.0000524953
H,3.1384493826,2.1247103792,-0.0004151605
H,3.065177304,-2.1672999664,0.0003179418
H,4.3530136476,-0.0420278509,-0.0000755918
H,-3.958242063,-2.3714612393,-0.8893818504
H,-3.9587755931,-2.3711999231,0.8892321795
H,-5.0215821321,-1.2535410511,-0.0005605569

91H, B3LYP Energy= -497.073493883 Hartree,
NIMAG= 0

N,2.6984653056,-0.1572930254,-0.0480340946
N,1.4363914329,-0.6485014522,-0.1486993856
C,0.5252543777,0.3285186451,0.0874903356
C,1.2620305846,1.4891964532,0.361695831
C,2.6011422941,1.1442846145,0.2706810566
C,3.8746983594,-1.0058091007,-0.2344742891
C,-0.9134916387,0.0915569449,0.0425565539
H,0.8655095337,2.4539561902,0.6272518582
H,3.4893602338,1.7356720089,0.4286655912
H,1.2735972364,-1.5895178402,-0.4807642913
C,-1.7768831962,1.1511059121,-0.276432977
C,-1.448365327,-1.1777510809,0.3181962256
C,-3.1492356746,0.9390032703,-0.327203713
H,-1.3756844738,2.1309204381,-0.5067795352
C,-2.8215402396,-1.382115601,0.2648125114
H,-0.8042839199,-1.9984718227,0.6165574627
C,-3.6729515621,-0.3255030651,-0.0592851422
H,-3.8101288127,1.7588065292,-0.5808045886
H,-3.2292062394,-2.3602914766,0.4888378746
H,-4.7435790138,-0.4869818471,-0.0975385155
H,3.8892426806,-1.7974876227,0.5162596545
H,3.8754360796,-1.4299812126,-1.2399029708
H,4.7550459794,-0.3784698595,-0.1126464524

92, B3LYP Energy= -496.699168265 Hartree,
NIMAG= 0

N,1.817460385,-0.9747394184,0.4192030878
N,3.1275129154,-0.6871557396,0.2630734484
C,3.1554425973,0.5104519193,-0.3155556452
C,1.8595252301,1.0107483591,-0.5301277421
C,1.0066517232,0.0248711456,-0.0497082488
C,1.4558108944,-2.2168156503,1.0836109558
H,4.1048979548,0.9660068096,-0.5543541358
H,1.5698090021,1.9388482598,-0.9952669565
C,-0.4648193555,-0.0022607058,-0.0243576745
C,-1.1707982236,1.1367341873,0.3927847238
C,-1.1955651614,-1.1236214723,-0.4452292445
C,-2.5625166923,1.1520633985,0.3915792175
H,-0.6190711609,2.0065204029,0.7301029947
C,-2.5880643589,-1.1090777066,-0.4387242412
H,-0.6735204199,-2.0023434353,-0.8052377041
C,-3.277102058,0.0277801337,-0.0199974272
H,-3.0896454046,2.0406560725,0.7205410301
H,-3.1349249793,-1.98381798,-0.7726218473
H,-4.3610593825,0.0387134511,-0.0176017057
H,0.5056276516,-2.0953639221,1.6017834526
H,1.3758752727,-3.0402692151,0.368690677
H,2.2397042706,-2.4487474939,1.8024535849

92H, B3LYP Energy= -497.070393530 Hartree,
NIMAG= 0

N,1.7836434426,-1.0119682095,0.4088587341
N,3.0832370656,-0.6681797173,0.2156109234
C,3.1510587827,0.550466161,-0.3516857634
C,1.8607656273,1.0050888782,-0.5274654565
C,1.0027262597,-0.0010170771,-0.0466363948
C,1.4450419609,-2.245515196,1.1244957484
H,4.102806058,0.9931323948,-0.6002205558
H,1.5571801566,1.9332327822,-0.9807552226
C,-0.4629296068,-0.0174263068,-0.0185044252

H,3.830434095,-1.2996816808,0.4706664785
C,-1.1452962648,1.1300290831,0.4142110827
C,-1.1919147489,-1.1319469408,-0.4624713194
C,-2.5354742874,1.150583613,0.4217323609
H,-0.5900338626,1.9935300392,0.7617481851
C,-2.5822439069,-1.0997056196,-0.45902999
H,-0.6796510151,-2.0053891591,-0.8495013798
C,-3.2545854613,0.0374620779,-0.012607081
H,-3.0571952742,2.0347169137,0.7673503128
H,-3.1401963242,-1.9570607072,-0.8155098001
H,-4.3378150062,0.0587919379,-0.0105443657
H,0.4094322265,-2.1720837249,1.4459930996
H,1.5682903081,-3.1123609083,0.4735697121
H,2.0861566989,-2.3347628478,2.0024207643

93, B3LYP Energy= -536.029760469 Hartree,
NIMAG= 0

N,-0.6952519749,1.1482157284,-0.2297849523
N,-1.9697047577,0.6995385175,-0.1566303163
C,-1.8833637064,-0.5904824873,0.1657182842
C,-0.5331519547,-0.9812301562,0.2929992992
C,0.2131197744,0.1608676889,0.0384281321
C,-0.4693380386,2.5284874289,-0.6238505331
C,-3.1191110109,-1.4171085427,0.3449460669
H,-0.1453198359,-1.9499622306,0.565559667
C,1.6742786504,0.3392607413,0.0470748717
H,0.5071991355,2.6214373727,-1.0967596994
H,-0.5194153248,3.2005883369,0.2376726034
H,-1.2476399135,2.8070126033,-1.3327879283
H,-4.0033370624,-0.8086850425,0.1506735167
C,3.1296934291,-2.2705657425,-0.3394926438
H,-3.1896598177,-1.8114776025,1.3631630473
C,2.2881089705,1.4152227998,0.7062088261
C,2.4917755324,-0.6109752605,-0.5840408542
C,3.6748813961,1.5411678162,0.7244089194
H,1.6796175415,2.1421449101,1.2313299182
C,3.8779462702,-0.487421763,-0.558768133
H,2.0303915247,-1.4415172718,-1.1055830362
C,4.4752825658,0.5914290299,0.0917583414
H,4.1308090251,2.3766158605,1.2439633637
H,4.4921733538,-1.2307592014,-1.054672304
H,5.5547577861,0.6894844666,0.1084440429

93H, B3LYP Energy= -536.407471755 Hartree,
NIMAG= 0

N,-0.6645552282,1.2009999121,-0.1826378528
N,-1.9247784279,0.6922459132,-0.1027388941
C,-1.883907244,-0.6315729766,0.1691912413
C,-0.5422290539,-0.9744349472,0.2521328661
C,0.2107621632,0.1894569374,0.0348412681
C,-0.4541491285,2.5829106433,-0.6182905199
C,-3.1191596023,-1.4420455148,0.3658054055
H,-0.1441501765,-1.9482894602,0.4824814534
C,1.6686564986,0.3532408914,0.0343128149
H,-2.7294602377,1.2953503036,-0.2061900885
H,0.5944832619,2.6949745703,-0.8806634327
H,-0.70784466,3.2802775024,0.1818193676
H,-1.0652637243,2.7786326076,-1.5007853198
H,-3.8800428186,-1.2016607295,-0.3801198366
H,-2.8831088086,-2.5024170567,0.2856727526
H,-3.5439911871,-1.2642914944,1.3580651415

C,2.2884584032,1.3842203109,0.7573887116
C,2.4567158934,-0.5747251657,-0.6630109557
C,3.675419399,1.4888132092,0.7698823218
H,1.6951412799,2.0774521447,1.3429040348
C,3.8424051704,-0.4583309966,-0.6516132371
H,1.9850766654,-1.3713241767,-1.2266457719
C,4.452605083,0.5723441691,0.0624010956
H,4.1494695462,2.2779234872,1.3409520077
H,4.4455373495,-1.1714038102,-1.200427148
H,5.5326801022,0.6573007153,0.0735154165

94, B3LYP Energy= -536.032603713 Hartree,
NIMAG= 0

N,1.5897746831,-0.5991297919,-0.0145160391
N,0.3681902294,-1.1732580121,-0.0099159664
C,-0.5043450752,-0.1615978611,0.0022671955
C,0.1814117931,1.0802840607,0.0136973086
C,1.5257600244,0.7636782609,0.0067292117
C,2.7728484029,-1.4375935652,0.0375837752
C,-1.9547578875,-0.4156668788,-0.0025427553
H,-0.2338106821,2.0747603172,0.0184658076
C,2.7371333588,1.6383294495,0.0158939368
H,2.4777589833,-2.4404809245,-0.2633432511
H,3.1891313572,-1.4751240932,1.0489701606
H,3.5346541714,-1.0635423656,-0.6488909587
H,3.3575309928,1.4870335873,-0.8736267231
H,2.4344648532,2.6857171793,0.034868116
H,3.366827401,1.4565158082,0.8929136367
C,-2.8738564331,0.6420100592,0.0397246288
C,-2.4509911352,-1.7279011315,-0.048944593
H,-4.2450837649,0.3984146568,0.0353657075
H,-2.518823541,1.665382689,0.0780371785
C,-3.8203717888,-1.9695065604,-0.0529849947
H,-1.7485044278,-2.5511607157,-0.0821792837
C,-4.7259972762,-0.9085927652,-0.0110445987
H,-4.9381538812,1.231942581,0.0688995963
H,-4.1838739729,-2.9907946095,-0.0895605842
H,-5.7933401847,-1.0990786744,-0.0145522119

94H, B3LYP Energy= -536.409537887 Hartree,
NIMAG= 0

N,1.6401539951,-0.5902311916,0.1755736744
N,0.3841866302,-1.1174477293,0.2065088211
C,-0.5375795411,-0.1493486322,-0.0173419962
C,0.1816984482,1.0291842419,-0.2324816374
C,1.53737344,0.7262760806,-0.1156693317
C,2.8143352974,-1.4493128282,0.3082303966
C,-1.9727832183,-0.4159208218,-0.0112386771
H,-0.2298462599,1.9927777457,-0.4801730983
C,2.7249088683,1.6111290683,-0.2882980488
H,0.2309593804,-2.0537994272,0.5548114048
H,2.9314083551,-2.0764263664,-0.5777799442
H,2.7179602714,-2.0690738129,1.2010834686
H,3.689072815,-0.8138289565,0.420607851
H,3.3531792523,1.2793534901,-1.1192062656
H,2.3940423063,2.6266906664,-0.5003041217
H,3.3382239378,1.6378066595,0.616245887
C,-2.8650769195,0.6087293442,0.3398211938
C,-2.4745610505,-1.6817986856,-0.3550322597
C,-4.2332616585,0.3652873688,0.3549473975
H,-2.489073746,1.5847671398,0.6228854463

C,-3.8438808895,-1.917860471,-0.3371080277
H,-1.8059031751,-2.4727207092,-0.6784196322
C,-4.7242538511,-0.8962437585,0.019404792
H,-4.9166468475,1.1581647194,0.633564149
H,-4.2255385262,-2.8930935053,-0.6137954638
H,-5.7915877572,-1.0820211024,0.0304523767

95, B3LYP Energy= -727.814603706 Hartree,
NIMAG= 0

N,0.6120337338,-1.5755427643,-0.5347501296
N,-0.7339705684,-1.5923912004,-0.5301732524
C,-1.1157265961,-0.3714443925,-0.1400292725
C,0.0159518715,0.4428682244,0.0995791068
C,1.1162299403,-0.3594880773,-0.156501883
C,1.317995847,-2.7650048696,-0.9833791602
C,-2.5423441887,-0.0317004589,-0.008931019
H,0.0467512598,1.459890283,0.4536728198
C,2.5489598534,-0.0384043127,-0.0509416972
C,-2.9498787771,1.2880486265,0.2301411736
H,0.7273497801,-3.2295704014,-1.7714895724
H,1.4436610171,-3.4804985194,-0.1660809649
H,2.2955765056,-2.4860881592,-1.3730787069
C,-3.5275062398,-1.0246649113,-0.1223094352
C,-4.2998165857,1.607246654,0.3529626789
H,-2.2096594811,2.0755088144,0.3136817188
C,-4.8753268123,-0.7037977581,-0.0014887196
H,-3.2209135719,-2.0469523366,-0.3049878142
C,-5.2696286435,0.6131894726,0.2375093564
H,-4.5937169488,2.6349201821,0.5364124058
H,-5.6222035619,-1.4850596403,-0.0918602791
H,-6.3207997336,0.861126571,0.3327110916
C,3.0317448011,1.1631927449,-0.5913048637
C,3.4504995062,-0.8826946189,0.6145599156
C,4.3750406456,1.5078734522,-0.471777559
H,2.3477854441,1.8190463071,-1.1174248424
C,4.7953342736,-0.5393341493,0.7271274705
H,3.0933186273,-1.7987473349,1.0704273452
C,5.262930164,0.6562572903,0.184162556
H,4.7302841487,2.4391023517,-0.8986836039
H,5.4761005612,-1.2016006545,1.2501962911
H,6.3096344288,0.9234523856,0.2742403451

95H, B3LYP Energy= -728.193095508 Hartree,
NIMAG= 0

N,0.6617554026,-1.5707855391,-0.6459541994
N,-0.6991204746,-1.5389558161,-0.6130788837
C,-1.1349861092,-0.3405089725,-0.1535193654
C,0.0082318184,0.4083697963,0.1245884781
C,1.1210582255,-0.3820482367,-0.1815323335
C,1.3580378758,-2.710944132,-1.240065383
C,-2.5536354488,-0.0295370671,0.004102369
H,0.0394433996,1.3867166224,0.5723326781
C,2.5460597841,-0.0637003964,-0.0249400048
H,-1.2399028091,-2.2894189799,-1.0192947833
C,-2.9834439471,1.3022721731,-0.0958102757
H,0.9183374139,-2.9371604642,-2.2132626145
H,1.2968161526,-3.5821144808,-0.5854828566
H,2.3990292541,-2.4313479827,-1.3786297455
C,-3.4937446813,-1.0411291257,0.2575238958
C,-4.3307142185,1.6121991871,0.0473314271
H,-2.2696268866,2.089624093,-0.3071080989

C,-4.8397209741,-0.7240825059,0.3981091831
H,-3.1769936118,-2.0706272677,0.3882313791
C,-5.260142032,0.601536901,0.2916182691
H,-4.6567722541,2.6417084703,-0.0373259191
H,-5.558523053,-1.5079024144,0.6037751518
H,-6.3095079848,0.8465573571,0.4039855932
C,3.0259452758,1.1642622681,-0.5031783238
C,3.4210639136,-0.9402712601,0.6344603496
C,4.3660799611,1.4990744472,-0.3397450172
H,2.3563607556,1.8442663039,-1.0170034463
C,4.7583738088,-0.5947091137,0.8004404772
H,3.0530635039,-1.8707487522,1.0519331537
C,5.2329282946,0.6211761185,0.3099158843
H,4.7335357128,2.4444014993,-0.7203375734
H,5.4266789274,-1.2690779625,1.3221857669
H,6.2752559834,0.8868336488,0.4398986303

96, B3LYP Energy= -320.964725148 Hartree,
NIMAG= 0

N,-0.7417209693,0.0103689284,-0.8520578302
N,0.6173751483,0.0180367589,-0.9020119592
C,1.0081460565,-0.0077070254,0.3699929374
C,-0.0986328407,-0.0210874174,1.2547930102
C,-1.199618817,-0.0055439614,0.4205957524
C,-1.5006711693,0.025673124,-2.0844985191
N,2.3619803453,-0.0835848219,0.6994159329
H,-0.0924980483,-0.0557000003,2.3318742138
H,-2.2554009865,-0.0102220587,0.6425108569
H,-2.5634049099,0.0214215024,-1.8421893401
H,-1.2641721722,-0.8553249054,-2.6852592269
H,-1.2663877865,0.9222266779,-2.6628785169
H,2.96441771,0.1381094346,-0.0823082265
H,2.6175049395,0.4421328643,1.5234324151

96H, B3LYP Energy= -321.336853676 Hartree,
NIMAG= 0

N,-0.7816670798,-0.0780981089,-0.8871298894
N,0.5898000328,0.0203269867,-0.898173053
C,1.0524289062,0.0639220868,0.3797710356
C,-0.0725250609,0.064913124,1.2245482818
C,-1.1744446746,-0.0138518284,0.3950879869
C,-1.5543214028,0.0343248774,-2.1218071691
N,2.3617111875,0.0674672352,0.6814247248
H,-0.0712733091,0.1092942118,2.3002288806
H,-2.2245321242,-0.0163500695,0.6431142731
H,1.1020938826,-0.2036411114,-1.7404821062
H,-2.5979317821,-0.1463322594,-1.8718725979
H,-1.2297564228,-0.7262509725,-2.8336618223
H,-1.4481598982,1.0316031303,-2.5532727684
H,3.0750987893,0.2073658804,-0.0164484234
H,2.6455979331,0.1520128347,1.6445224873

97, B3LYP Energy= -320.960764309 Hartree,
NIMAG= 0

N,-0.5745483784,0.0958939715,-0.8846855086
N,0.7834450074,0.0075949739,-0.9100090234
C,1.1382801101,-0.0745321599,0.3663095919
C,0.0235832106,-0.0656834973,1.2313576292
C,-1.0672793811,0.0385694657,0.3825479745
C,-1.3249786486,0.2081670176,-2.1186618478

H,2.1848441369,-0.143545866,0.6241740308
H,0.0082795451,-0.1337821453,2.3070905858
N,-2.4403107528,0.164568572,0.6294335578
H,-0.6611770693,0.6252518144,-2.8734349435
H,-2.1753566606,0.8754723489,-1.9671059416
H,-1.6848584058,-0.766933326,-2.4637974145
H,-3.0106924302,-0.5431940093,0.1810053532
H,-2.6486921833,0.1938660398,1.6180589563
97H, B3LYP Energy= -321.336223093 Hartree,
NIMAG= 0

N,-0.6078516056,0.164231217,-0.8951690762
N,0.76060374,0.0096583855,-0.8797766078
C,1.1685100323,-0.094204164,0.4035226583
C,0.069240968,-0.1117718438,1.2243868492
C,-1.0554030842,0.0322820532,0.3767123896
C,-1.3634085068,0.1066726607,-2.1448271536
H,2.2194115603,-0.1478979778,0.6418658407
H,0.0557387096,-0.2279455291,2.2948080884
N,-2.3600480317,0.0040534817,0.6937266705
H,1.3011923264,0.340246457,-1.6680286185
H,-0.7391245424,0.4877902933,-2.9521421698
H,-2.2327540481,0.7594123321,-2.0657665891
H,-1.671461645,-0.9165096881,-2.3702930664
H,-3.0891940793,0.1677817878,0.018990476
H,-2.6348729932,-0.0528197095,1.6612607094

98, B3LYP Energy= -320.955235372 Hartree,
NIMAG= 0

N,-0.0032897285,0.5957545181,-0.071578336
N,1.1049509556,-0.1436896674,-0.2025225735
C,0.6928220539,-1.4109476788,-0.1335124999
C,-0.7054326947,-1.4930982683,0.0587192193
C,-1.1220079924,-0.1732285236,0.0979711913
C,0.0905098907,2.0404981004,0.0043680268
H,1.4047333484,-2.2168674772,-0.2368670886
N,-1.4949135052,-2.6559913875,0.0960269151
H,-2.1013337265,0.2632291608,0.212628234
H,0.1785550402,2.3790891583,1.0413059154
H,0.975380802,2.350477441,-0.5488454761
H,-0.7952958986,2.4900562519,-0.4473532813
H,-0.9865044659,-3.4711910233,0.4108478566
H,-2.345803179,-2.5556573043,0.6327327968

98H, B3LYP Energy= -321.323793269 Hartree,
NIMAG= 0

N,-1.0766156114,-0.1052887109,0.0200164803
N,-0.6729512936,1.1738109909,0.0403310845
C,0.678132144,1.232783064,0.0402416344
C,1.1661211373,-0.0776142071,0.0155001927
C,0.0184544636,-0.8894641817,0.0020784568
C,-2.4939193679,-0.4756342437,0.0029605196
H,1.1908273656,2.1809534634,0.0531886887
N,2.4721399164,-0.4869286213,-0.0606865818
H,-0.077203757,-1.9629688799,-0.0236462408
H,-1.3394002838,1.9342272474,0.0582811646
H,-2.991711131,-0.080543101,0.8894938945
H,-2.966435249,-0.0999325369,-0.9056661484
H,-2.5502663648,-1.5615633115,0.0150295783
H,3.1916390305,0.1747273401,0.1865918667
H,2.6875692595,-1.4378742514,0.1957918558

98c, B3LYP Energy= -321.304537431 Hartree,
NIMAG= 0

N,-0.0066390484,0.5917482598,-0.0106445169
N,1.1155775071,-0.1461825595,-0.0556255852
C,0.7268666826,-1.4137467644,-0.0451455491
C,-0.6755252393,-1.4679221064,0.0131216565
C,-1.1257988755,-0.1590205538,0.0318901635
C,0.0944967211,2.0522331433,0.0079403752
H,1.4545317024,-2.2117856263,-0.0766185003
N,-1.5097768847,-2.6788501049,0.0180440866
H,-2.1149721908,0.2695640469,0.073324303
H,-1.7374136537,-3.0099803275,-0.9280108676
H,0.6124693279,2.3664680375,0.913446442
H,0.6532572287,2.3803748943,-0.8673070394
H,-0.9085567772,2.4742128076,-0.0122416587
H,-1.0318559212,-3.446108866,0.5035818243
H,-2.3951119379,-2.5251204416,0.5122722563

99, B3LYP Energy= -803.053334997 Hartree,
NIMAG= 0

N,0.5988846939,-1.5718136632,-0.5395012908
N,-0.7383742332,-1.5668972572,-0.5295304865
C,-1.1208643686,-0.3444621328,-0.1293398681
C,0.0313248126,0.4464657815,0.1045736818
C,1.1286470399,-0.3615006538,-0.1630428921
C,1.2968892008,-2.7737787563,-0.9617159261
C,-2.5463245139,-0.0062184548,0.0011976432
O,0.0372934929,1.7427054429,0.538082677
C,2.5582208335,-0.0390997638,-0.0558069988
H,0.6473149834,-3.3058168944,-1.6544778355
H,1.5199221369,-3.4251719255,-0.1115787109
H,2.2267405802,-2.5052263853,-1.4625723152
C,-2.969382107,1.294763684,0.3150194038
C,-3.5219553768,-0.998668487,-0.1940373816
C,-4.3268811202,1.5900149178,0.4271346073
H,-2.2368841118,2.0748336625,0.4708244821
C,-4.8739652031,-0.6976359031,-0.0817233826
H,-3.2038595382,-2.0051513047,-0.4348599268
C,-5.2855559574,0.5993571972,0.2297745924
H,-4.633726322,2.6017129868,0.6696066375
H,-5.6110264163,-1.4782590284,-0.2365206231
H,-6.3408639597,0.8324764369,0.3178001671
C,3.0501808832,1.1408611595,-0.639971505
C,3.4542333328,-0.8564777754,0.6523361519
C,4.3925580279,1.4923859895,-0.5154356779
H,2.3811315956,1.7661020359,-1.2213740625
C,4.7975963376,-0.509782211,0.7626142033
H,3.0914170351,-1.7563830125,1.1350685321
C,5.2714144132,0.667238884,0.1833630948
H,4.7536601545,2.4043330307,-0.977524325
H,5.4739050443,-1.153523905,1.3138058907
H,6.3169971802,0.9376215361,0.2757184912
H,0.9382500496,1.9951449688,0.7731754522

99H, B3LYP Energy= -803.431530774 Hartree,
NIMAG= 0

N,0.6504900182,-1.5615564082,-0.6675559493
N,-0.7022638603,-1.5186243108,-0.6251423496
C,-1.1413146891,-0.3205164669,-0.1555060918
C,0.0193879474,0.4209669051,0.1134037051

C,1.1266764059,-0.3760127087,-0.2072731189
C,1.3463413564,-2.6992044281,-1.2643824578
C,-2.5552563594,-0.0146292675,0.0230911832
O,0.0160141195,1.6618409468,0.6372249618
C,2.5523931308,-0.055786058,-0.0420293805
H,-1.2511570385,-2.2486531042,-1.0560781703
H,0.97417766,-2.8699657187,-2.2765886079
H,1.2080194453,-3.5926827781,-0.6529628912
H,2.4040127066,-2.4533032017,-1.3117888389
C,-2.9866779205,1.3219226727,0.0416987488
C,-3.4999036925,-1.0459827885,0.1684585257
C,-4.338785312,1.6124650371,0.1853235552
H,-2.2692073474,2.124793225,-0.0604076976
C,-4.8481336373,-0.7455682091,0.3111267576
H,-3.1864258319,-2.0840298876,0.2106852174
C,-5.2706799282,0.5843496928,0.3164980392
H,-4.6650373864,2.6453937939,0.1947453132
H,-5.5679932983,-1.5460325842,0.4314708673
H,-6.3226761994,0.8168719693,0.4311505902
C,3.0750604821,1.0878193461,-0.666357072
C,3.3842479764,-0.8472586956,0.7648548461
C,4.4148929295,1.4247565942,-0.4923510129
H,2.4440116194,1.693379064,-1.3079004255
C,4.7218298069,-0.5031517792,0.932453994
H,2.9809242783,-1.7123339749,1.2794173859
C,5.2376436588,0.6307443415,0.3048437345
H,4.8160900049,2.3026259716,-0.9842688894
H,5.3588054925,-1.113914896,1.5608818967
H,6.2794858963,0.8959946776,0.4394869436
H,0.9085982796,1.924081492,0.8997966684

100, B3LYP Energy= -458.803343464 Hartree,
NIMAG= 0

N,0.6546575258,1.1019805437,0.0350565716
N,1.964192358,0.7176685162,0.0306778289
C,1.9427795488,-0.6095958461,0.0019022687
C,0.6143966374,-1.1094714174,-0.0219587623
C,-0.1726433397,0.0291040611,-0.0051906673
C,0.2980149625,2.5052476745,-0.0046250516
C,3.2193945244,-1.3913915346,0.0045580873
H,0.2923079556,-2.1368893631,-0.0413822312
O,-1.5040937756,0.2393796921,-0.0201455764
H,-0.7407908791,2.6146644568,0.3034692866
H,0.4202057568,2.9122421397,-1.012521745
H,0.9456476184,3.0509712188,0.6814753437
H,4.0694837703,-0.7077991847,0.0085381424
H,3.2905002215,-2.0359120574,0.8862200268
H,3.2952689153,-2.0329603003,-0.8786929315
C,-2.3255502346,-0.9400035752,-0.0263617202
H,-2.0823237142,-1.5368130938,-0.9126248946
H,-2.0968726247,-1.5365925743,0.8639296495
C,-3.7753432953,-0.5005738933,-0.0391413109
H,-3.9923930583,0.096766491,-0.9273435184
H,-4.427586413,-1.3777691545,-0.0461122336
H,-4.0090154601,0.0948862011,0.8461204377

100H, B3LYP Energy= -459.184505424 Hartree,
NIMAG= 0

N,-0.6283253575,1.1330344035,0.0595609348
N,-1.9220947628,0.6951592009,-0.0028067369
C,-1.9569700541,-0.6546810057,-0.0374562811

C,-0.6435524823,-1.1039679543,-0.0405005364
C,0.1690880437,0.0409288717,0.014404286
C,-0.2706764967,2.5480170782,0.0083660658
C,-3.2400427247,-1.4126357614,-0.03402633
H,-0.3200961153,-2.1293148183,-0.0795900975
O,1.4666630242,0.224407389,0.0175553126
H,-2.6863573125,1.3473289893,0.1043812094
H,0.807845559,2.610520126,0.1331645325
H,-0.7573015626,3.0832562214,0.8249998582
H,-0.5522213339,2.9767050509,-0.9550899311
H,-4.0246195857,-0.8749264147,-0.5699082726
H,-3.1025618948,-2.3839332615,-0.5086219366
H,-3.5800431808,-1.5839206097,0.991632962
C,2.3358800025,-0.9628694948,-0.0186337331
H,2.097562819,-1.5729980944,0.8558852902
H,2.0997288533,-1.516715144,-0.9304304453
C,3.7663800972,-0.4805537924,-0.0018068339
H,3.9805966693,0.0852971377,0.9063548431
H,4.4323737966,-1.3462112832,-0.0292435514
H,3.9820502653,0.1427265021,-0.8712095139

101, B3LYP Energy= -458.800954750 Hartree,
NIMAG= 0

N,-1.6387897364,-0.6173850802,0.0255015483
N,-0.4305105349,-1.2443466858,0.00102519
C,0.4527293059,-0.2577642499,0.0003235061
C,-0.1682495104,1.0150734554,0.0129502388
C,-1.5270328062,0.7360654685,0.0224404779
C,-2.8386693791,-1.4251897501,-0.0632232141
O,1.7666880215,-0.579066229,-0.0044395189
H,0.2852006364,1.991669965,0.0250755664
C,-2.6988717054,1.6650578385,0.0300872348
H,-2.687809383,-2.3326849864,0.5201594312
H,-3.0537737572,-1.7023329718,-1.0999605821
H,-3.6858817666,-0.8727730998,0.3430002148
H,-3.3323569505,1.5174732434,0.9106267044
H,-2.3476100028,2.6973413771,0.044725824
H,-3.3278166721,1.5395467512,-0.8570457558
C,2.6904316459,0.5115493999,-0.010716395
H,2.5163067212,1.1354577525,-0.896513464
H,2.5318260892,1.1325515348,0.8800643499
C,4.0921770205,-0.0665074164,-0.023683192
H,4.2474389285,-0.6819461635,-0.9123877837
H,4.8294590687,0.7409604119,-0.027311208
H,4.2616487667,-0.6868105654,0.8590318269

101H, B3LYP Energy= -459.182764937 Hartree,
NIMAG= 0

N,-1.6900855789,-0.6172017303,0.0286695744
N,-0.4393527196,-1.1679355795,-0.0391169233
C,0.4873314455,-0.1808987342,-0.0200808718
C,-0.1977666964,1.0370295652,0.0179347353
C,-1.5580411397,0.7265539824,0.0396215452
C,-2.8756304333,-1.4631542229,-0.0789071182
O,1.7495513541,-0.5237684385,-0.0311975292
H,0.2275660173,2.0249943786,0.0333474894
C,-2.7278364391,1.6510244121,0.0620140993
H,-0.285851781,-2.1641982496,0.0395207589
H,-2.8327542649,-2.2549692731,0.6706332317
H,-2.9505243721,-1.8918839552,-1.0803230991
H,-3.7496454161,-0.8472470418,0.1168470351

H,-3.3632557849,1.4692254765,0.9324909748
H,-2.378208506,2.6811893528,0.1088831366
H,-3.3385538675,1.5413824789,-0.8381381985
C,2.7599978629,0.5467488384,-0.0169142135
H,2.5923881246,1.1694397313,-0.899004794
H,2.6009365495,1.137740324,0.8883152788
C,4.1188341934,-0.11070961,-0.0352572529
H,4.2529359473,-0.7117337151,-0.9360491008
H,4.887800408,0.6653521299,-0.0244972736
H,4.2612143767,-0.7443725644,0.8416036442

102, B3LYP Energy= -304.915162222 Hartree,
NIMAG= 0

N,-0.1444955668,-0.0819636087,-0.2586593298
N,0.5443352847,-0.7217724099,0.7080865929
C,1.7577982821,-0.1736407252,0.687462862
C,1.857909099,0.8318758297,-0.2962623862
C,0.6078344188,0.8608163368,-0.8837415213
C,-1.548109641,-0.4091788612,-0.4869911523
H,2.5138504792,-0.5240588693,1.3741928527
H,2.7118233151,1.4397447489,-0.5463804354
H,0.2080551752,1.463045612,-1.6842102234
H,-1.8225249828,0.0226805985,-1.4518813211
H,-1.6207399646,-1.4954309264,-0.5744462496
C,-2.4639328457,0.1035591305,0.6233964198
H,-3.4989671716,-0.1800948216,0.4141004852
H,-2.1740930419,-0.3263637833,1.583438569
H,-2.4143068399,1.1924477491,0.7019318376

102H, B3LYP Energy= -305.278969711 Hartree,
NIMAG= 0

N,-0.165216038,-0.0692520948,-0.2711309716
N,0.5702502085,-0.6624212824,0.6969609128
C,1.8171591283,-0.1547053786,0.6992971765
C,1.8833111394,0.8044262953,-0.2985533078
C,0.6189427202,0.8297678498,-0.8848190852
C,-1.5914882377,-0.4016669202,-0.4921681077
H,2.5588351453,-0.5086240809,1.3981581821
H,2.7361103342,1.403941387,-0.5684655684
H,0.2343161107,1.4271242148,-1.6965238523
H,0.1756546636,-1.388438916,1.2810051485
H,-1.8464840613,0.0662308407,-1.4428318534
H,-1.6531679561,-1.4833617837,-0.633712471
C,-2.4970926704,0.0864209205,0.634615269
H,-3.5296060054,-0.1664904377,0.3862403119
H,-2.2640442825,-0.3908257305,1.5892496078
H,-2.4305765173,1.1687297848,0.757212539

103, B3LYP Energy= -509.474377715 Hartree,
NIMAG= 0

N,1.6240164695,-0.1237926818,-0.0124214882
N,0.4787963723,-0.8045227904,-0.0920252996
C,-0.457137836,0.1345417074,-0.0449713214
C,0.0652391902,1.4352780495,0.067492578
C,1.4265513528,1.2230618724,0.0871090236
C,2.8979959878,-0.848180156,-0.0010440549
N,-1.8652317433,-0.2239133112,-0.1133032794
H,-0.4753658707,2.363632773,0.1200748212
H,2.2534759097,1.9113885378,0.1579928299
H,3.6807161795,-0.1025759374,-0.1522021883

H,2.8978280573,-1.5168583409,-0.8637799799
O,-2.1651536619,-1.4028305364,-0.2063466035
O,-2.6597308434,0.7127923492,-0.0692398371
C,3.1150554854,-1.6276526699,1.2934317719
H,2.3199087853,-2.3609886251,1.4350363827
H,4.0701665089,-2.1566629613,1.2479338978
H,3.1322044564,-0.959514279,2.1577433471

103H, B3LYP Energy= -509.810223959 Hartree,
NIMAG= 0

N,1.657706882,-0.0987976692,-0.0002371406
N,0.467612688,-0.724633438,-0.0510411952
C,-0.5052119632,0.2026470068,-0.0405624695
C,0.0565398492,1.4611188367,0.0216233104
C,1.4332390403,1.2253008166,0.046012363
C,2.9415622638,-0.8488534976,0.0199125896
N,-1.9007570009,-0.2339479901,-0.0933564154
H,-0.4601487037,2.4063071609,0.0445611069
H,2.2578123731,1.919960332,0.0914079362
H,0.3563909706,-1.7337818914,-0.0977017672
H,3.7114268473,-0.0826523226,-0.0690403206
H,2.9697507977,-1.4568156671,-0.8872434188
O,-2.0651338913,-1.4445040851,-0.1436746717
O,-2.7382001573,0.6402554638,-0.0803769104
C,3.1151922481,-1.6820524258,1.2855003905
H,2.3632821934,-2.4699089196,1.3708002015
H,4.091675839,-2.1683204257,1.2450071802
H,3.0806138541,-1.0595749723,2.1811112513

104, B3LYP Energy= -509.470612293 Hartree,
NIMAG= 0

N,0.7497127342,0.6173298715,-0.0134789405
N,1.9667433359,0.0963240598,-0.2022280523
C,1.8190348561,-1.2337632729,-0.1859318898
C,0.4847489849,-1.5988013587,0.013634596
C,-0.1728422343,-0.3846995659,0.1157894891
C,0.6083484938,2.0838947555,-0.030630792
H,2.6827181944,-1.8674456082,-0.3145532218
H,0.0391468741,-2.5759447148,0.0819696759
N,-1.5804512424,-0.1825420862,0.3300293262
H,1.5936146019,2.4532273037,0.251720342
H,-0.1120828563,2.3627384732,0.7348207851
O,-2.0081504946,0.9706497584,0.3649571536
O,-2.2660646051,-1.1890651652,0.4638925723
C,0.192619955,2.6172258403,-1.3990534178
H,-0.8010079044,2.2615018757,-1.675612888
H,0.1634843909,3.7092413607,-1.3657631628
H,0.9092902159,2.315988173,-2.1661265753

104H, B3LYP Energy= -509.806152272 Hartree,
NIMAG= 0

N,0.7226092145,0.6321058281,-0.0040315492
N,1.9247296029,0.0575380003,-0.2112901044
C,1.8290409259,-1.2845192423,-0.2003300255
C,0.5000064159,-1.6083151924,0.0166951409
C,-0.152660875,-0.3865770053,0.1278958194
C,0.5831008542,2.123818783,-0.0361809473
H,2.6998886772,-1.9064858676,-0.3392531519
H,0.0502902248,-2.5842958608,0.0908503026
N,-1.5909888525,-0.1891977533,0.3593624165

H,2.7497759617,0.635355383,-0.3287168249
H,1.5479496589,2.5044595982,0.3058828416
H,-0.1659162772,2.373989604,0.7097855361
O,-2.0024728109,0.9589516497,0.3650222846
O,-2.2282756319,-1.2076836817,0.5207252853
C,0.2106804265,2.6452259718,-1.4191697471
H,-0.7723416542,2.286732685,-1.7247600676
H,0.1703368402,3.7354263465,-1.3703875426
H,0.9497197473,2.3683966406,-2.1740913326

105, B3LYP Energy= -509.477383449 Hartree,
NIMAG= 0

N,-1.6338986433,-0.2204982863,-0.0334584518
N,-1.4545188592,1.1006324879,-0.2979442921
C,-0.146077547,1.2970893528,-0.258701778
C,0.5174682089,0.0868196088,0.0298842483
C,-0.4742411925,-0.8707276815,0.1686764998
C,-2.9878127151,-0.7774092776,-0.0395295179
H,0.2812468388,2.2722752233,-0.4278554639
N,1.9262391517,-0.1329143001,0.1672197962
H,-0.4105949521,-1.9224582135,0.3918319638
H,-2.9299469418,-1.7524678715,0.4476497011
H,-3.6034568206,-0.1250361931,0.5822015159
O,2.6675669019,0.8339266726,0.0155202176
O,2.3019591873,-1.2750791496,0.4266802591
C,-3.5659366078,-0.8934829658,-1.4478743339
H,-4.580907223,-1.295297209,-1.3960850856
H,-3.6059908916,0.0859438888,-1.9270879413
H,-2.9628800947,-1.5614643865,-2.0676098374

105H, B3LYP Energy= -509.812383813 Hartree,
NIMAG= 0

N,-1.6479792062,-0.2404890772,-0.0360164914
N,-1.4015075553,1.0671571124,-0.3078035741
C,-0.083749144,1.3133312475,-0.266959846
C,0.5262279117,0.1079500402,0.0366693384
C,-0.4773991904,-0.8488364673,0.1753373169
C,-3.0245979251,-0.80205974,-0.0500999037
H,0.3351451328,2.2922697207,-0.4438840248
N,1.9577425413,-0.120335579,0.1890149629
H,-0.4054541876,-1.8998821946,0.4089202219
H,-2.1613065573,1.7128597102,-0.4899124967
H,-2.9303393887,-1.7834793189,0.4143675094
H,-3.6276254208,-0.179748612,0.6151451488
O,2.676447806,0.8497850998,0.0309945885
O,2.2912224099,-1.2606812042,0.4587853265
C,-3.6096557045,-0.8932501396,-1.4556129459
H,-4.6036992482,-1.3392559768,-1.3865519653
H,-3.7233789335,0.0876102138,-1.9227787096
H,-2.9974705485,-1.524258338,-2.1020191325

106, B3LYP Energy= -383.563133060 Hartree,
NIMAG= 0

N,-0.0862074083,0.5224400228,-0.1676052329
N,0.4442403145,-0.0860986582,0.9152251636
C,0.2872869565,-1.3892283604,0.691233937
C,-0.3512281821,-1.6314104173,-0.542736164
C,-0.576426814,-0.3723397994,-1.064643059
C,-0.1257163798,1.9802010013,-0.2470065548
H,0.6421410085,-2.1027230143,1.4198738988

H,-0.6020126624,-2.578894289,-0.9909455868
H,-1.0315621333,-0.0548080926,-1.9895776318
H,0.6100578217,2.3357110325,0.4755450242
H,0.2122226242,2.2747634719,-1.2446555539
C,-1.5082147529,2.5782072834,0.0429946501
H,-1.4388089496,3.6596782045,-0.128481834
H,-2.2281836732,2.1981363476,-0.692071239
C,-2.0260421868,2.3125162156,1.4598480006
H,-2.0709554252,1.233296686,1.6343240515
H,-1.3041052915,2.7050073186,2.1853102558
C,-3.4022355994,2.9349077085,1.7122604477
H,-3.3797368196,4.0213031861,1.5783109997
H,-4.1520525208,2.5323288075,1.0235939421
H,-3.7468284267,2.7337323449,2.7300499851

106H, B3LYP Energy= -383.929601469 Hartree,
NIMAG= 0

N,-0.1016101377,0.5230080304,-0.2293500599
N,0.2361502995,-0.1182523991,0.9122830897
C,0.2040908615,-1.4492498777,0.7168815769
C,-0.1724783831,-1.6722957673,-0.5983818242
C,-0.35648724,-0.409929736,-1.1593761812
C,-0.1994618528,2.0001106177,-0.3156794057
H,0.4532726765,-2.1332635329,1.5128124923
H,-0.2892797855,-2.6239588887,-1.0884698748
H,-0.6448579029,-0.1214308093,-2.1580042467
H,0.460816417,0.4023339607,1.7503836021
H,0.5791558105,2.4031389652,0.3369800736
H,0.076447933,2.249429251,-1.3407859457
C,-1.5826503681,2.5506458927,0.0420920047
H,-1.5409076217,3.6240181857,-0.1724987848
H,-2.3273802062,2.1312483273,-0.6426533785
C,-2.0149669031,2.3351326156,1.4976605153
H,-2.1067422189,1.2622235067,1.7073486313
H,-1.2397498032,2.7284934527,2.168510197
C,-3.3500026014,3.0158583665,1.8161451967
H,-3.2885552414,4.0960917017,1.661129349
H,-4.1520045803,2.6301935242,1.181019794
H,-3.6368588441,2.8444394335,2.8552711434

107, B3LYP Energy= -383.565481059 Hartree,
NIMAG= 0

N,-0.0150513527,0.5919114489,0.0005715387
N,1.1275392908,-0.1282699179,0.00214652
C,0.7425936913,-1.4018203105,0.0023921552
C,-0.6609815249,-1.5178508575,0.0010697853
C,-1.1129443552,-0.2120394986,0.0000945458
C,0.0747344127,2.0771072792,-0.0004192678
H,1.4867596009,-2.1845182542,0.0034934974
H,-1.2598431332,-2.413884784,0.0009654898
H,-2.1147890452,0.1805958956,-0.0009608048
C,-1.3365997162,2.6756730781,-0.0017135335
C,0.8332126781,2.5139907167,1.2639922633
C,0.8348290354,2.5123133656,-1.264447339
H,-1.2558007772,3.7645312408,-0.0023787593
H,-1.9010640448,2.38394875,-0.890920674
H,-1.9022193648,2.3851120019,0.8871509401
H,0.9398689306,3.6002652953,-1.2815821805
H,1.827790825,2.0624687688,-1.2841447639
H,0.2979112807,2.202571357,-2.1648383078
H,0.9382018446,3.6019690673,1.2798337316

H,0.2951394079,2.2054171367,2.1640868278
H,1.826161216,2.0641959209,1.2856083357

107H, B3LYP Energy= -383.934568158 Hartree,
NIMAG= 0

N,-0.0227975956,0.6015108104,0.0004943189
N,1.0811948919,-0.181781284,0.0019466604
C,0.7299702765,-1.4809532999,0.0024156656
C,-0.6528256679,-1.5399165589,0.0012377357
C,-1.0884484661,-0.2146322473,0.0000698093
C,0.0845115862,2.1178321426,-0.000429765
H,1.4786156708,-2.2575661873,0.0035540017
H,-1.2678891304,-2.4237172803,0.0012394496
H,-2.0893537335,0.1811011787,-0.0010343177
H,2.0062025811,0.2248101902,0.0025120774
C,-1.3379208159,2.6838195512,-0.0017360733
C,0.8344774848,2.5369202969,1.2731196228
C,0.8361649461,2.5352548517,-1.2735317664
H,-1.2680050888,3.7722922355,-0.0023575344
H,-1.8957847041,2.3926026239,-0.8943388269
H,-1.8969876244,2.3936844852,0.8904662941
H,0.8949327649,3.6243215583,-1.3085629464
H,1.8629134064,2.1600693832,-1.296848829
H,0.3186325337,2.1925630753,-2.1715489943
H,0.8931399351,3.6260337689,1.3068287181
H,0.3157927646,2.1953522027,2.1709001224
H,1.8612238526,2.1618407677,1.2982614901

108, B3LYP Energy= -615.885320493 Hartree,
NIMAG= 0

N,1.7168937646,-0.0716824539,-0.0020915635
N,2.3807356557,0.773260837,0.8172996165
C,3.6713701539,0.5315196407,0.6022684984
C,3.8557057936,-0.4768146975,-0.3634674553
C,2.5733954939,-0.840300575,-0.7282879043
C,0.237585351,-0.0520292822,-0.0019262795
H,4.4169576731,1.0905969138,1.1481535743
H,4.7799190522,-0.8827545218,-0.741175031
H,2.2284165423,-1.573704103,-1.4360832429
C,-0.2556536504,1.3566767104,-0.4046965409
C,-0.278356943,-0.3888527785,1.4159464684
C,-0.3205377538,-1.0853685465,-0.999547499
H,0.1667184424,2.0907017103,0.2851664233
H,0.1196052046,1.5968654755,-1.40579684
C,-1.7958044312,1.3978850369,-0.3813131363
H,0.1436269934,0.3261858571,2.1257982538
H,0.0808533125,-1.3835469423,1.702774062
C,-1.8184481926,-0.3445562311,1.4361225662
H,0.0413658419,-0.8669403793,-2.0101065591
H,0.0254350127,-2.090240366,-0.7339657707
C,-1.8637442691,-1.0440376155,-0.979134779
H,-2.1300391454,2.401094476,-0.6657494435
C,-2.2980054041,1.0653587861,1.0377483591
C,-2.3490850536,0.3627593437,-1.3801081252
H,-2.1686997808,-0.5822034051,2.4460206808
C,-2.3716629784,-1.3792543685,0.4368373459
H,-2.2426915696,-1.7832565263,-1.6925057591
H,-3.3924373414,1.1144013504,1.0711831213
H,-1.9227328946,1.8062007182,1.7526115011
H,-2.0145007071,0.6030273046,-2.3959739918
H,-3.4444945798,0.3915781264,-1.3891722078

H,-2.0533080172,-2.3881496531,0.7239195308
H,-3.467387576,-1.3734998417,0.451863127

108H, B3LYP Energy= -616.260014959 Hartree,
NIMAG= 0

N,-0.0167203128,0.578804724,-0.0348924121
N,0.6287434912,-0.1842367431,0.8778115079
C,0.3698218141,-1.4871377592,0.6620986293
C,-0.4746487884,-1.5696078626,-0.4312790169
C,-0.6942397072,-0.2534557021,-0.8406505304
C,0.1006366408,2.0847381173,-0.0238109168
H,0.7985740116,-2.2497358152,1.2929702106
H,-0.8798724325,-2.4625369956,-0.8759907429
H,-1.2896296223,0.1270270574,-1.6523777144
H,1.2050492444,0.242450666,1.5896657582
C,1.5814461579,2.4786150526,-0.2175517351
C,-0.4265337322,2.6237095694,1.324229196
C,-0.743861821,2.6553871409,-1.1773669751
H,2.2032264676,2.0633175716,0.5844293097
H,1.9523519556,2.071713702,-1.1635133273
C,1.6919164592,4.0194932693,-0.2048396591
H,0.1502636237,2.2117703696,2.1608757635
H,-1.4685049656,2.3188560259,1.4632080549
C,-0.3028309217,4.1636304365,1.326816818
H,-0.3884958244,2.2654313314,-2.1369285841
H,-1.7934607685,2.3668147631,-1.0583349588
C,-0.6244543948,4.1968952617,-1.1667663153
H,2.7426314144,4.2901278451,-0.3376564919
C,1.1751811414,4.5597305997,1.1429247015
C,0.8503560988,4.5980839754,-1.358344079
H,-0.6732496792,4.5369495592,2.2851210711
C,-1.1472659052,4.7424200935,0.17551476
H,-1.2276551271,4.5895058101,-1.9892973181
H,1.2747819928,5.6484930969,1.1701782619
H,1.7810103758,4.1694135284,1.9687506548
H,1.2237232555,4.23509991,-2.3219815722
H,0.9404512305,5.6879081111,-1.375141098
H,-2.2029505539,4.4827349863,0.3091202302
H,-1.0875476177,5.834424247,0.1821017089

109, B3LYP Energy= -457.371946539 Hartree,
NIMAG= 0

N,-1.0159968057,0.0403199652,0.0065044525
N,-1.7165764849,-1.0860484451,0.2901603002
C,-2.9915503588,-0.734468205,0.1895712069
C,-3.1343712077,0.626180692,-0.1647906295
C,-1.8436484697,1.0903331064,-0.2764716533
C,0.4048724917,0.0225082084,0.0087610574
H,-3.7618929875,-1.4671501807,0.3786462292
H,-4.0429132388,1.1827224734,-0.3260015209
H,-1.4616979237,2.0575690756,-0.5555359697
C,1.0779101402,-1.1880756944,-0.1717649268
C,1.1246996578,1.2054424597,0.1930185494
C,2.4689858948,-1.2049024212,-0.1776991891
H,0.5030245907,-2.0947283112,-0.3001653861
C,2.5168536752,1.1763319327,0.1716704806
H,0.608535054,2.1400192993,0.3732929741
C,3.1957266963,-0.0261085856,-0.0131926179
H,2.986975338,-2.1468246558,-0.3181950337
H,3.0694597516,2.0977825717,0.3153339343
H,4.2791761862,-0.0453632851,-0.0231292576

109H, B3LYP Energy= -457.736817827 Hartree,
NIMAG= 0

N,-0.997700061,0.0434105967,-0.0403286172
N,-1.742187064,-0.8531896698,0.654201418
C,-3.0491997109,-0.6001041072,0.4676618452
C,-3.151890599,0.4959620481,-0.3767008519
C,-1.8447054328,0.8710051686,-0.6774845546
C,0.4448363042,0.0153676098,-0.0201962971
H,-3.8052290504,-1.2064526431,0.9414658925
H,-4.0572852504,0.9550305234,-0.7361046797
H,-1.4616183349,1.6543115483,-1.3119352076
H,-1.2883549213,-1.5400759553,1.244014425
C,1.1062160778,-1.1153694774,-0.4983935241
C,1.1301848285,1.1242606708,0.4717918426
C,2.4980694491,-1.1318103157,-0.4712306096
H,0.5509298934,-1.9520479456,-0.9068677735
C,2.5222420522,1.0959008909,0.4767245419
H,0.5896617472,1.9826944263,0.8524480705
C,3.2025112672,-0.0290095154,0.0114543856
H,3.0297790553,-1.9993720107,-0.841982741
H,3.0724191654,1.9488838306,0.8543050122
H,4.2855814991,-0.0457936417,0.0229974401

110, B3LYP Energy= -536.030101953 Hartree,
NIMAG= 0

N,-0.5332446228,0.0770651409,-0.0600353987
N,-1.2968299999,-0.9755359499,-0.4773110481
C,-2.5539003682,-0.5639003655,-0.3819512169
C,-2.6130350184,0.7616939856,0.114973753
C,-1.3048586587,1.1492084022,0.3190486532
C,0.8783735697,-0.0819771441,-0.0032160131
C,-3.6833683585,-1.4622733748,-0.7795575882
H,-3.4924013224,1.3541421177,0.3150279458
C,-0.7742158251,2.4269949119,0.8876307455
H,-3.2939680895,-2.4283954417,-1.1029263306
H,-4.3712313076,-1.6272626227,0.0552766317
H,-4.2624772585,-1.0309168002,-1.6016234729
H,-0.4246024794,3.1150835634,0.1118106432
H,-1.5697929365,2.9310059735,1.4385069785
H,0.0578471413,2.2510410427,1.5732024691
C,1.4075103516,-1.2916573722,0.455779608
C,1.7334501118,0.9388978631,-0.4233593025
C,2.7863472971,-1.467182841,0.5054486705
H,0.7301535794,-2.0800144981,0.7557166053
C,3.1136939731,0.7585094065,-0.3551704724
H,1.3269502549,1.8576216013,-0.8249781389
C,3.6456755765,-0.4420464704,0.1090855192
H,3.1910422263,-2.408047498,0.8609721549
H,3.7717380805,1.5547705894,-0.6842368911
H,4.7195560836,-0.5815215195,0.1542361956

110H, B3LYP Energy= -536.410813581 Hartree,
NIMAG= 0

N,-0.5186332557,0.0652224826,-0.0113254063
N,-1.3165337673,-0.8358345988,-0.6558888978
C,-2.6138753294,-0.5064630307,-0.5022456565
C,-2.6386678029,0.648652827,0.2756335245
C,-1.3168392445,0.9890626895,0.5721722897
C,0.9173895784,-0.0793175451,-0.0054451683

C,-3.717017766,-1.2943842594,-1.1222737274
H,-3.5184986665,1.1815581961,0.5963965209
C,-0.7743709748,2.1295837382,1.3620366523
H,-0.8979828523,-1.6075591067,-1.1587647326
H,-3.443120146,-2.3434175692,-1.2480856763
H,-4.6094594602,-1.243181558,-0.4983827943
H,-3.9707319494,-0.8863638838,-2.1049950728
H,-0.3654214595,2.8990367976,0.7010936745
H,-1.5705737836,2.5795247361,1.9537441666
H,0.0242279117,1.8064107668,2.0321816195
C,1.5087537532,-0.9279632129,0.9300296591
C,1.6733730767,0.6298115346,-0.9376046925
C,2.8945034289,-1.0666612636,0.9262033102
H,0.8980789796,-1.4619307056,1.6489157476
C,3.058326724,0.4836729531,-0.9268169949
H,1.188128314,1.2803217899,-1.6557795597
C,3.6650849087,-0.3619971362,0.0015464969
H,3.3699507723,-1.7203886893,1.6470729733
H,3.6606257572,1.0282273731,-1.6435739732
H,4.7429191966,-0.4717844038,0.0050328276

111, B3LYP Energy= -727.812008467 Hartree,
NIMAG= 0

N,-0.6784523547,-0.5987877142,-0.8294127805
N,0.6829465007,-0.5490290863,-0.8523893265
C,1.0471868562,-0.0491320872,0.3224174109
C,-0.0857092559,0.2270930109,1.1227861525
C,-1.1846337778,-0.1250801307,0.3596314716
C,-1.3517144748,-1.1941138126,-1.9354468216
C,2.4936816398,0.1551641351,0.6498153172
H,-0.1099976776,0.6768159087,2.102744068
C,-2.6121147544,0.0523696079,0.6787485216
C,-3.0894946311,-0.3179014709,1.944319293
C,-3.5032863098,0.6431154497,-0.2293276639
C,-4.4214638925,-0.1063901488,2.291734165
H,-2.4121727258,-0.783118956,2.6514459263
C,-4.8346057425,0.8497254752,0.1188420988
H,-3.1491234129,0.951142031,-1.205673433
C,-5.2997095238,0.4755545461,1.3793084035
H,-4.7738085393,-0.4022016833,3.2736073353
H,-5.5090504474,1.3110403233,-0.5938764488
H,-6.3372734387,0.638388128,1.6480420834
H,3.1131442791,-0.1640847694,-0.1891149992
H,2.7081936056,1.2078261903,0.8574620447
H,2.7849275506,-0.4202120948,1.5335018785
C,-0.9407597846,-0.8706224706,-3.2301878354
C,-2.3808112164,-2.1149419203,-1.7333469133
C,-1.5723273639,-1.4612632689,-4.3205135748
H,-0.125053047,-0.1724942287,-3.365224686
C,-3.0153477206,-2.6899565374,-2.831945754
H,-2.676918143,-2.3840894389,-0.7278754757
C,-2.615593788,-2.3664996987,-4.1271838759
H,-1.2494270949,-1.2098104642,-5.3244495148
H,-3.8150048867,-3.4040103024,-2.6711267091
H,-3.1076558279,-2.8216515218,-4.9789907576

111H, B3LYP Energy= -728.193517844 Hartree,
NIMAG= 0

N,-0.79087179,0.7775525654,-0.009182834
N,-1.5166337059,1.9121334727,0.2241651103
C,-0.7240329932,3.0015748931,0.1587711361

C,0.5549641722,2.54254441,-0.1251035019
C,0.5000707118,1.1435968488,-0.2233098778
C,-1.4688669074,-0.4907819308,-0.1178057817
C,-1.2385777827,4.3776926826,0.4119366396
H,1.4434346332,3.1457004045,-0.2062395933
C,1.5977162258,0.2079979838,-0.485277123
H,-2.5171956907,1.8441994557,0.3550071964
C,2.5981039139,0.5860562357,-1.3947631715
C,1.6989762952,-1.0238306006,0.1791851202
C,3.672156063,-0.260604384,-1.6440532086
H,2.5249351423,1.5306492623,-1.9211444356
C,2.7811411147,-1.8605472945,-0.0688213983
H,0.9516366868,-1.3194276574,0.9044679153
C,3.765684202,-1.4840833977,-0.9819784252
H,4.4346277992,0.0338275447,-2.3549944075
H,2.8601194588,-2.8043597323,0.4570935269
H,4.6060709399,-2.140691903,-1.1734129671
H,-2.2206176387,4.5290753908,-0.0414448297
H,-1.3257335656,4.5647129527,1.4861793036
H,-0.5511539369,5.1134946875,-0.0037392212
C,-2.0707661786,-1.0333057346,1.0171601903
C,-1.530894123,-1.1255920821,-1.3565945249
C,-2.7544037865,-2.2414527712,0.9017670369
H,-1.9924111378,-0.5305906807,1.9745989917
C,-2.2054237285,-2.3396404565,-1.4529637181
H,-1.0590530326,-0.6806025336,-2.2239488528
C,-2.8176852887,-2.8939019547,-0.3289104405
H,-3.226738639,-2.6754772976,1.7745284964
H,-2.2592121573,-2.8468042204,-2.4084888243
H,-3.3456498758,-3.8362270588,-0.4123474268

112, B3LYP Energy= -919.596487627 Hartree,
NIMAG= 0

N,0.6579903035,-1.5719362105,-0.5719788134
N,-0.6967968081,-1.585038033,-0.5847037355
C,-1.0794152198,-0.3674569929,-0.1999450517
C,0.0512929244,0.4460154863,0.0617201947
C,1.1552958338,-0.3502379849,-0.175090418
C,1.3521052897,-2.7308991044,-1.0298769769
C,-2.5071344514,-0.022825614,-0.0932142735
H,0.0768943156,1.456994239,0.4330248568
C,2.5772121986,-0.0265641012,0.0351611995
C,-2.9117251424,1.2812135239,0.2236038055
C,-3.4950782091,-0.9960109442,-0.3086007648
C,-4.2625710341,1.6044256849,0.3242604343
H,-2.1690712274,2.0530395977,0.3893244038
C,-4.8433921344,-0.6710427322,-0.2090907934
H,-3.1905262929,-2.0051266584,-0.5560746414
C,-5.2351238524,0.6300875803,0.108697139
H,-4.5546695032,2.6194414998,0.5700087569
H,-5.5929073982,-1.4361791949,-0.3794360082
H,-6.2869408013,0.8812067501,0.1864818706
C,3.0843662073,1.1943264973,-0.4323035838
C,3.4307402426,-0.8817359954,0.7475381083
C,4.4102423647,1.5494867524,-0.1968346246
H,2.4359326221,1.8588833228,-0.9918464465
C,4.7561211312,-0.5259997469,0.9781315324
H,3.0521574724,-1.8215707104,1.1309583286
C,5.251563228,0.6893991547,0.5065956099
H,4.7868741719,2.4958918664,-0.5684275905
H,5.4015591303,-1.1966262073,1.5341757546
H,6.2842736831,0.9644265578,0.6884886852

C,0.9276745283,-3.9880012607,-0.5959009292
C,2.4158398767,-2.6151919935,-1.9253878875
C,1.5807631381,-5.1289800704,-1.0522875822
H,0.0874319157,-4.0562637416,0.0826556968
C,3.0703191074,-3.7629009166,-2.3662318026
H,2.7225522434,-1.6396258221,-2.2793610189
C,2.6573158775,-5.0212619212,-1.9324433239
H,1.2489644266,-6.1045139962,-0.7154899022
H,3.8964515136,-3.6707033961,-3.0619367127
H,3.1656875284,-5.9119763643,-2.2831272953

112H, B3LYP Energy= -919.978926713 Hartree,
NIMAG= 0

N,0.7062903474,-1.5912182119,-0.5560764074
N,-0.6603109253,-1.544551043,-0.58635679
C,-1.1003362435,-0.3310431229,-0.1779851644
C,0.0363198785,0.4090332842,0.1460270138
C,1.1567988203,-0.3968817596,-0.0881188652
C,1.3897808002,-2.7469799675,-1.0762390983
C,-2.5207798275,0.0042123864,-0.1070019876
H,0.0531186114,1.3908566774,0.5867589014
C,2.5681204971,-0.0816201698,0.1577105474
H,-1.1673571887,-2.2718874486,-1.0721142654
C,-2.9234648428,1.3409217665,-0.2461282775
C,-3.4898686846,-0.9905464935,0.0986278013
C,-4.2719690723,1.6723288312,-0.1874099625
H,-2.1859218558,2.115100051,-0.42181098
C,-4.8368656419,-0.6521416079,0.1550019014
H,-3.1960100309,-2.0230716184,0.2548226083
C,-5.229864075,0.678220207,0.0107262649
H,-4.5766073871,2.7055247652,-0.3018778483
H,-5.5787043851,-1.4232360221,0.3238452291
H,-6.280198518,0.939943663,0.0572360134
C,3.0288372065,1.2109508104,-0.136183646
C,3.4484132432,-1.0165792693,0.7225505185
C,4.3513165793,1.5563900284,0.1190902618
H,2.3585404561,1.9372054665,-0.5812685911
C,4.7670049943,-0.6606765558,0.9830125775
H,3.1023979448,-2.0095628178,0.9805029699
C,5.2217147209,0.6221170025,0.6788892571
H,4.7020728051,2.553175285,-0.119517873
H,5.4386026057,-1.383141444,1.4309586004
H,6.2507197186,0.8941148662,0.8819221809
C,1.1972081375,-3.9819891947,-0.4569462466
C,2.2016319259,-2.609744394,-2.200714064
C,1.8328330363,-5.1040849698,-0.9831304439
H,0.5768028767,-4.0610898043,0.4285933456
C,2.8424117002,-3.7377607709,-2.7055248443
H,2.3299474135,-1.6412887981,-2.6680279676
C,2.6562825713,-4.9811169293,-2.1015800574
H,1.692913924,-6.0692860319,-0.511936543
H,3.4788750864,-3.6454184833,-3.5770573094
H,3.1535285979,-5.8556500167,-2.5035581111

113, B3LYP Energy= -916.989325269 Hartree,
NIMAG= 0

N,0.1683705975,0.2625290922,0.0599153088
N,0.6643780628,1.4914730676,0.3378318966
C,1.9835058087,1.3651644719,0.2842867656
C,2.3442339039,0.0398559396,-0.0339943908
C,1.159937741,-0.6461815299,-0.1768804834

C,-1.2373196798,0.044232969,0.0262700813
H,2.6263412972,2.2100288762,0.4766500459
Cl,3.9444985718,-0.5982028959,-0.2243934432
H,0.9672222602,-1.6694080024,-0.4471520459
C,-2.0923073111,1.1195033806,-0.2226971096
C,-1.7550921829,-1.2339108387,0.2446812361
C,-3.4664245264,0.9053041964,-0.259669598
H,-1.6712814598,2.1032348543,-0.3783837331
C,-3.1318963044,-1.4363893837,0.1914434601
H,-1.0968699313,-2.0620225199,0.4762970898
C,-3.993008298,-0.3703978508,-0.0595984099
H,-4.1283147911,1.7417659108,-0.4528288622
H,-3.5295882254,-2.430161913,0.3620764117
H,-5.0640955326,-0.5310538244,-0.0938452198

113H, B3LYP Energy= -917.345142982 Hartree,
NIMAG= 0

N,0.1534329289,0.2519227475,0.0291235374
N,0.7136542322,1.2860907073,0.7000815796
C,2.0518425132,1.2487382465,0.5724623634
C,2.3595007379,0.1445744062,-0.2145103812
C,1.1425846668,-0.4572999155,-0.5417684415
C,-1.2745271343,0.042770064,0.003819571
H,2.6882661626,1.9861293869,1.0354534227
Cl,3.9178844055,-0.3665737561,-0.7008933086
H,0.9274759717,-1.3192403204,-1.1526126185
H,0.1321085937,1.9116448442,1.2449656516
C,-2.092265133,1.0327944864,-0.540094245
C,-1.7864690081,-1.1462065791,0.5191565135
C,-3.4682288283,0.8211318857,-0.5556983122
H,-1.6659479874,1.9340514414,-0.9657712621
C,-3.1637477016,-1.3461845036,0.4806217022
H,-1.1276868468,-1.890320411,0.9507845305
C,-4.0005151049,-0.3649008333,-0.0503407164
H,-4.120283032,1.5759188573,-0.9774979762
H,-3.5813237908,-2.263951802,0.87574971
H,-5.0715351745,-0.5257414776,-0.072263088

114, B3LYP Energy= -3030.91022268 Hartree,
NIMAG= 0

N,-0.5454882553,0.3541843492,0.0725771624
N,-0.1195559085,1.6102465928,0.3482008786
C,1.2046509433,1.5563330552,0.3020776068
C,1.6412545189,0.2516607871,-0.0087724311
C,0.496279456,-0.4982878928,-0.1546706211
C,-1.9368998775,0.0587016969,0.0311289831
H,1.7969556428,2.4371844521,0.494754758
Br,3.4201939377,-0.3504338605,-0.2039521383
H,0.3596368311,-1.5313440143,-0.4218095832
C,-2.847869774,1.0828213444,-0.2341064208
C,-2.3847062353,-1.2442398983,0.2572713947
C,-4.207699949,0.792447149,-0.2803070124
H,-2.480689382,2.0870037636,-0.3954481521
C,-3.7476273776,-1.5232575941,0.1945721454
H,-1.6833581717,-2.0322711013,0.5016735774
C,-4.6642432025,-0.5088539221,-0.0732566952
H,-4.9132234708,1.5892092477,-0.4861826499
H,-4.0912286414,-2.5359511601,0.3711309812
H,-5.7244280843,-0.7290499944,-0.1148807835

114H, B3LYP Energy= -3031.26687054 Hartree,
NIMAG= 0

N,-0.5594850953,0.3405779497,0.0431138937
N,-0.0639089586,1.4116490151,0.7077467313
C,1.2757098285,1.4452892383,0.5922327046
C,1.6541184128,0.3522765579,-0.1793577599
C,0.4744416729,-0.3176366206,-0.5101268489
C,-1.9733504286,0.0533426138,0.0067098482
H,1.8636617942,2.222450666,1.0542946335
Br,3.3910450333,-0.1173506426,-0.689573351
H,0.3107675333,-1.1965256607,-1.11272708
H,-0.6846940972,2.010353236,1.2393612967
C,-2.839276074,0.9934476641,-0.5510014076
C,-2.4247292817,-1.1578078966,0.5270585847
C,-4.2016772929,0.7077575234,-0.5751657815
H,-2.4590842846,1.9133328641,-0.9805180338
C,-3.7888634896,-1.4323528259,0.4796156364
H,-1.7302250367,-1.8619215959,0.9696156077
C,-4.6732798237,-0.501501854,-0.0646165019
H,-4.8901240431,1.4232282626,-1.0075446689
H,-4.1592598234,-2.368569536,0.8785056956
H,-5.733886929,-0.7199886412,-0.093140976

115, B3LYP Energy= -512.750381010 Hartree,
NIMAG= 0

N,-0.7440782763,-0.0099162637,-0.8857363047
N,0.6109719345,0.1825475025,-0.9152609148
C,1.0048168784,0.0631246238,0.3446706116
C,-0.088438102,-0.2041463705,1.2134649921
C,-1.1827874306,-0.2425466493,0.3832442264
C,-1.496947795,0.0277230519,-2.0825700684
N,2.3516312167,0.1362932447,0.6834660561
H,-0.0694898623,-0.370318781,2.2781727874
H,-2.2177473843,-0.4445706347,0.6019004277
H,2.9244355398,0.5325520181,-0.0495792217
H,2.5373702327,0.5623915421,1.5799480265
C,-0.8498739297,-0.1351547432,-3.3115268679
C,-2.8808248975,0.2296283958,-2.0451225114
C,-1.5908686265,-0.1081854192,-4.4886226584
H,0.2214588388,-0.2787008893,-3.32422756
C,-3.6108305669,0.2418285667,-3.2302600723
H,-3.3872092892,0.3953658652,-1.1025353043
C,-2.9730334447,0.0735781135,-4.4578682927
H,-1.0814134515,-0.2360466758,-5.4371584432
H,-4.6828969924,0.3983015373,-3.190477025
H,-3.544823892,0.0901648653,-5.378206883

115H, B3LYP Energy= -513.123871891 Hartree,
NIMAG= 0

N,-0.7537368026,-0.086613925,-0.9208680462
N,0.5220790447,0.4256567133,-0.8383250221
C,1.0118901655,0.2236306479,0.4121832558
C,0.0306395472,-0.4833825659,1.1306966586
C,-1.034033005,-0.6527627959,0.2654779475
C,-1.5139543559,-0.0166042538,-2.1364879356
N,2.2167369239,0.6752570301,0.8052254505
H,0.1040809597,-0.8347328304,2.1457640554
H,-1.9697137521,-1.1694981519,0.4093669977
H,0.8373910919,1.0719805504,-1.5493280839
H,2.888743021,1.0479985471,0.1537082105
H,2.5567589568,0.4372690856,1.7231292369

C,-0.9635211405,-0.5116886534,-3.3193866418
C,-2.7905853283,0.5422220924,-2.0989378876
C,-1.7126472573,-0.4339292418,-4.4901536469
H,0.0182526325,-0.9711309475,-3.32133378
C,-3.5355570105,0.590728032,-3.2744634124
H,-3.1878543826,0.9415900324,-1.1733779947
C,-2.9965001588,0.1105763869,-4.4671045918
H,-1.2994821179,-0.8161850868,-5.4155085158
H,-4.530563976,1.0182045199,-3.2588025837
H,-3.5776139556,0.1594250924,-5.3799553338

116, B3LYP Energy= -512.744423857 Hartree,
NIMAG= 0

N,-0.6384744892,0.2939802266,-0.858430946
N,0.704774072,0.5874424781,-0.8505412508
C,1.083752356,0.3810630649,0.3983893003
C,0.0247266283,-0.0628432606,1.2204842164
C,-1.0695379888,-0.1187105636,0.3763755161
C,-1.3648424343,0.3774932842,-2.0760145145
H,2.1123347571,0.5598409888,0.6764093876
H,0.049676904,-0.3164367118,2.2678194954
N,-2.3912750174,-0.4673084644,0.6414682261
H,-2.8694260397,-0.9287999245,-0.122483555
H,-2.4873646277,-0.9925380285,1.4992901069
C,-0.742548408,-0.0114915908,-3.2660190255
C,-2.67380634,0.868208833,-2.0962007618
C,-1.437348493,0.0796565948,-4.4673021105
H,0.2795444251,-0.3641325648,-3.2319093364
C,-3.3643108514,0.9392394839,-3.3051445421
H,-3.1365396863,1.2138781512,-1.180722706
C,-2.7522668104,0.545758399,-4.492754827
H,-0.9496391192,-0.219965274,-5.3880396761
H,-4.378233639,1.3229775682,-3.3161318314
H,-3.2907092982,0.6096738104,-5.431187266

116H, B3LYP Energy= -513.126140634 Hartree,
NIMAG= 0

N,-0.6732668491,0.3498865436,-0.8481784117
N,0.5281520934,0.995464192,-0.6545440614
C,0.9792450776,0.7177966836,0.5812653899
C,0.1006447651,-0.1448774651,1.1958433332
C,-0.9424723274,-0.3722473144,0.2688781453
C,-1.3928087114,0.4193955307,-2.0932915485
H,1.8991351418,1.1502894731,0.9427017447
H,0.1903295496,-0.5707404459,2.1806168412
N,-2.0347108786,-1.1448841254,0.3746421148
H,0.8398286861,1.6830929121,-1.3256035059
H,-2.6896219733,-1.2385004649,-0.3858913369
H,-2.1848784608,-1.6969846034,1.2026448431
C,-1.0078466187,-0.4073437306,-3.1502880469
C,-2.4598357829,1.3116294377,-2.2094627245
C,-1.7095424246,-0.3314595481,-4.3504676596
H,-0.178520106,-1.0950600249,-3.0322268803
C,-3.1561027498,1.3714170578,-3.4143322307
H,-2.7351692627,1.9457330876,-1.3746807114
C,-2.7799698663,0.5539780176,-4.479997812
H,-1.4220062252,-0.9643422255,-5.1810555449
H,-3.9862601347,2.058867826,-3.5207011529
H,-3.3229535613,0.6073568315,-5.4160633172

117, B3LYP Energy= -512.740770639 Hartree,
NIMAG= 0

N,-0.1943566097,-0.6212397804,-0.8619066877
N,-0.1466141996,0.7254333107,-0.8628081804
C,0.0107216576,1.0754864389,0.4076007747
C,0.0784361841,-0.0561382089,1.259844035
C,-0.0564745676,-1.1331426857,0.4088770342
C,-0.3562682086,-1.3365288947,-2.0741045737
H,0.0652868659,2.1205539561,0.6762105468
N,0.1798957471,-0.0530362921,2.6580181678
H,-0.0406543396,-2.1912550918,0.6043800426
C,-0.0902310985,-0.7019958023,-3.291586215
C,-0.7817616031,-2.6682095001,-2.0598733549
C,-0.2447556801,-1.4048330285,-4.4814863333
H,0.229321568,0.3307676357,-3.2858275274
C,-0.9211013403,-3.3631095421,-3.258795082
H,-1.0240814119,-3.1581622045,-1.1255160843
C,-0.6546107763,-2.738259966,-4.4748156442
H,-0.0368646905,-0.9058251992,-5.4213251712
H,-1.252401685,-4.395162406,-3.237614774
H,-0.7689463024,-3.2812890712,-5.4055785934
H,0.5291213195,-0.9162711821,3.0507733724
H,0.699339171,0.7326038144,3.0250703481

117H, B3LYP Energy= -513.111507393 Hartree,
NIMAG= 0

N,-0.2108554343,-0.6519780774,-0.8628691969
N,-0.5613676182,0.6402916975,-0.7338769475
C,-0.3375544123,1.0552488196,0.5319628296
C,0.1932419808,-0.0212976535,1.2512641048
C,0.2584148832,-1.0784351132,0.3285937455
C,-0.3574988279,-1.3632302604,-2.1055019397
H,-0.5683717021,2.0641385014,0.8334738343
N,0.5188752029,-0.0602107281,2.5839353551
H,0.6284593703,-2.0847842934,0.4371486454
H,-1.0191278046,1.121752891,-1.4968975184
C,0.2465015516,-0.8533987881,-3.2546089002
C,-1.0977302753,-2.5439182376,-2.1209938768
C,0.0900202311,-1.5454494732,-4.4526197073
H,0.8491125782,0.0466721004,-3.2113832966
C,-1.2282374318,-3.2321038913,-3.3241176458
H,-1.5738673971,-2.9070972389,-1.2181358236
C,-0.6413451902,-2.7322564315,-4.4862385063
H,0.5547363907,-1.1653217636,-5.3539748753
H,-1.8003297952,-4.1511917327,-3.3540387458
H,-0.7526212149,-3.2698400098,-5.4200428874
H,1.1327205939,-0.7963038056,2.8972635483
H,0.6654681846,0.8173823207,3.0584764192

117c, B3LYP Energy= -513.088249467 Hartree,
NIMAG= 0

N,-0.1799893159,-0.6241537278,-0.8515532879
N,-0.3487027344,0.714143784,-0.8111456303
C,-0.1040162246,1.0825906907,0.4375292189
C,0.2203721881,-0.0511740947,1.2016594837
C,0.1743733936,-1.137738339,0.3489209277
C,-0.363764487,-1.3457285497,-2.0809997877
H,-0.1806856746,2.1205331869,0.7273021459
N,0.5831289868,-0.0815085298,2.6266612019
H,0.3837225706,-2.1853818866,0.493794563

H,1.535030802,0.2655704472,2.7981642361
C,0.0321942518,-0.7514277884,-3.2767777011
C,-0.9336448804,-2.617029852,-2.0525850988
C,-0.1394600073,-1.4560642511,-4.4644690381
H,0.460902235,0.2419074909,-3.2714178736
C,-1.0871403634,-3.3146679096,-3.2479711646
H,-1.2833325829,-3.0489848205,-1.1222224178
C,-0.6911624731,-2.7366361749,-4.4525582274
H,0.1646974724,-1.0034564509,-5.4004055084
H,-1.533488959,-4.3015436658,-3.2370494614
H,-0.8193371036,-3.279942284,-5.3808899625
H,0.5346882314,-1.0346699003,3.0007861596
H,-0.059308573,0.4896206233,3.1877854743

118, B3LYP Energy= -552.075754828 Hartree,
NIMAG= 0

N,-0.6248771744,0.1714286142,-0.8727887631
N,0.7378147205,0.3758219491,-0.8691924593
C,1.1262432673,0.1117956965,0.3679578061
C,0.0369868067,-0.2880455151,1.1841171356
C,-1.0665570225,-0.2494553946,0.3547108061
C,-1.3529068054,0.3346146508,-2.0789352646
C,2.5639597689,0.2543149257,0.7584166056
H,0.0541968472,-0.5752923972,2.223562601
N,-2.4045852894,-0.5229601976,0.6270092719
H,-2.9184626418,-0.9304110443,-0.1444358317
H,-2.5231379346,-1.068176582,1.4694435693
H,2.9636908028,-0.6869410806,1.1479015937
H,3.1562067815,0.5507177748,-0.1081261956
H,2.6884449243,1.0118149399,1.5382249941
C,-0.7594373104,-0.041186216,-3.2884272003
C,-2.6363384461,0.8906877253,-2.0724295471
C,-1.4566140357,0.1275387896,-4.4797866007
H,0.2438957039,-0.4450861248,-3.2757620571
C,-3.330315967,1.0390216432,-3.2723215246
H,-3.0756306028,1.2277766086,-1.1423517332
C,-2.7469268585,0.6588221538,-4.4784730501
H,-0.9903968673,-0.1629157332,-5.4145600081
H,-4.3238141996,1.4730242646,-3.2610017343
H,-3.2874328676,0.7831398494,-5.4096284136

118H, B3LYP Energy= -552.462992783 Hartree,
NIMAG= 0

N,-0.6345539519,0.1663136116,-0.8898809416
N,0.6854256857,0.5605063515,-0.7625841848
C,1.1552379607,0.1675695528,0.4467468427
C,0.164617016,-0.5670118251,1.0683279418
C,-0.9527431154,-0.5664364899,0.2051552587
C,-1.3734497258,0.356995935,-2.1091828265
C,2.5212087526,0.5371345619,0.9153691808
H,0.233791038,-1.0610388916,2.0229273638
N,-2.1472519173,-1.1631830406,0.3450074406
H,1.0159667763,1.3213417357,-1.3410494848
H,-2.8399602556,-1.1296798653,-0.3866640189
H,-2.3249548804,-1.7545915559,1.139698398
H,2.7807078885,-0.040295525,1.8016190327
H,3.269444772,0.3427982581,0.1437677887
H,2.5677576215,1.5983609265,1.1770642554
C,-1.0645243948,-0.4183177554,-3.2285852363
C,-2.3865399787,1.3163697785,-2.1405611078

C,-1.7859783025,-0.220053903,-4.4025937932
H,-0.2772912166,-1.1614372616,-3.1777394167
C,-3.1085065822,1.494664257,-3.3187627389
H,-2.5993179326,1.9131133009,-1.2611369417
C,-2.8060624255,0.7310067798,-4.4455463134
H,-1.5554079511,-0.8114719608,-5.2802404964
H,-3.8981803002,2.2349734124,-3.3574426317
H,-3.3662538543,0.8777819291,-5.3612449399

119, B3LYP Energy= -650.585866784 Hartree,
NIMAG= 0

N,0.0864694187,-0.6559945647,0.1054586087
N,0.3596404067,-2.0027489079,0.1416105898
C,1.6778232632,-2.103930461,0.1212026215
C,2.3005027398,-0.8289926782,0.0650962532
C,1.2496532292,0.0652772785,0.0530186362
C,-1.2643404283,-0.2169825102,0.0632406962
C,2.3380227157,-3.4459293354,0.1677009057
H,3.3537483808,-0.6072775351,0.0354664886
O,1.2037235891,1.4065928424,-0.0184564336
H,1.5802808284,-4.2296820481,0.200623389
H,2.9680128103,-3.6079755001,-0.7122302029
H,2.9758080095,-3.5432830486,1.0514693078
C,-2.2324129046,-1.0795713906,-0.4621436404
C,-1.6398889876,1.0358051037,0.55766658
C,-3.5649587544,-0.683079998,-0.4963133937
H,-1.9270929057,-2.0510595649,-0.8248233124
C,-2.9771172369,1.4230476061,0.5060070233
H,-0.8976887339,1.6982518825,0.9774843433
C,-3.9456475882,0.5705532273,-0.0186044745
H,-4.3087076474,-1.3585439279,-0.9040721428
H,3.2603846368,2.3964494112,0.8906940643
H,-4.9848853177,0.8767286091,-0.0510385061
C,2.4688265556,2.0713595902,-0.1906077396
H,3.1138057282,1.8323752051,0.6622005429
H,2.9448107594,1.6922932398,-1.1015086461
C,2.2047643595,3.5601532719,-0.2821532177
H,1.7336752643,3.9298215001,0.631171453
H,3.1486557944,4.0935075112,-0.4216335877
H,1.5518622889,3.7874161915,-1.1273752061

119H, B3LYP Energy= -650.969375260 Hartree,
NIMAG= 0

N,0.0856358535,-0.6502467685,0.1831280112
N,0.4134570056,-1.970828467,0.3617473179
C,1.7490055359,-2.1341798479,0.2999168074
C,2.3100236891,-0.8877622036,0.0467629062
C,1.2444528925,0.0238645628,-0.0246753842
C,-1.2812599099,-0.1974804085,0.1418106157
C,2.396349744,-3.4596596238,0.5156716096
H,3.3573671257,-0.6737820891,-0.0756000578
O,1.1783673199,1.3112381312,-0.2534307779
H,-0.3113658511,-2.6337804217,0.600345279
H,1.7378586274,-4.2798822382,0.2242383613
H,3.3136650395,-3.5292666106,-0.0691058989
H,2.658826101,-3.5883882561,1.5697507789
C,-2.0491945131,-0.4637987615,-0.9913652615
C,-1.8004546575,0.4901282047,1.2368041493
C,-3.3738148226,-0.0360078932,-1.0190305779
H,-1.6160112673,-0.9855525659,-1.8368576706
C,-3.1236040177,0.9212314416,1.1907499688

H,-1.1803837033,0.6854809067,2.1033037168
C,-3.9073304919,0.6557021324,0.0682328027
H,-3.9840371418,-0.2352466998,-1.891401617
H,-3.5417589167,1.4595227897,2.0324508391
H,-4.9372864829,0.9907295352,0.0396411244
C,2.4330770955,2.0326628801,-0.5027687131
H,3.0717342723,1.9042168054,0.3748369747
H,2.9110329896,1.5776469306,-1.373995611
C,2.0845954753,3.4825989894,-0.741326951
H,1.5923125947,3.9168423093,0.1303400056
H,3.0035891515,4.0425905938,-0.9299165014
H,1.4326402865,3.5920082452,-1.6094337372

120, B3LYP Energy= -611.258903496 Hartree,
NIMAG= 0

N,-0.690122006,0.1909792958,-0.651023887
N,0.6062614719,0.6418570361,-0.5851464621
C,0.9147400002,0.5724094359,0.6962799207
C,-0.14666891,0.0676422526,1.48325808
C,-1.164507532,-0.1757710435,0.5860034738
C,-1.307282176,0.0859873305,-1.9243694366
O,2.109649988,0.9481582736,1.1887754266
H,-0.1537015912,-0.1051970355,2.5465092006
C,-2.5111278709,-0.7737985431,0.8428468013
H,-2.7950314695,-1.4835529184,0.0626946501
H,-2.4895905976,-1.3039019768,1.7961094753
H,-3.2975961562,-0.0157019188,0.9055331162
C,3.0598595922,1.4397079643,0.2381672828
H,2.6712859526,2.3211067296,-0.2778714689
H,3.9455499095,1.6977730387,0.8160143279
H,3.3004088927,0.6725444372,-0.5022976385
C,-0.5455942755,-0.338504369,-3.0180296997
C,-2.6505140893,0.4268157871,-2.1029663485
C,-1.1342288394,-0.4362194885,-4.2741518392
H,0.4989429204,-0.5763719532,-2.8685663712
C,-3.2344709332,0.3093610145,-3.3627580218
H,-3.230065581,0.8064844757,-1.2723396516
C,-2.4819378227,-0.1224298765,-4.4523338624
H,-0.5376062723,-0.7658875911,-5.1172877487
H,-4.2772141469,0.5762448017,-3.4925388326
H,-2.9376009576,-0.2052910585,-5.4321880864

120H, B3LYP Energy= -611.632422765 Hartree,
NIMAG= 0

N,-0.6743815782,0.1025660615,-0.6885627493
N,0.5494284201,0.7160652773,-0.5451082412
C,0.9436853317,0.6159176636,0.7467628288
C,-0.0405942182,-0.0930801673,1.4379345272
C,-1.0354175584,-0.4013212457,0.5173496847
C,-1.3244283492,0.0472001492,-1.9730771668
O,2.0593403178,1.1010401587,1.2396737451
H,-0.0158229756,-0.3492316016,2.4832293359
C,-2.3105879104,-1.1461462936,0.7139627103
H,0.9600890593,1.2040989158,-1.3282021474
H,-2.46548934,-1.882316642,-0.0771147031
H,-2.2926468251,-1.6594196622,1.6743482896
H,-3.1644745133,-0.4632571094,0.7074518043
C,2.9695204121,1.8155125872,0.3737474383
H,2.4879638131,2.7114435372,-0.0264977263
H,3.8025803454,2.1028131993,1.0082640601
H,3.3253755997,1.1606993179,-0.4256810679

C,-0.9121374664,-0.9073200055,-2.9036173247
C,-2.3471711298,0.9520239585,-2.2554865374
C,-1.5418839397,-0.9506738777,-4.144823702
H,-0.1227734497,-1.6076779409,-2.6558723191
C,-2.9732294158,0.8921914291,-3.4981280129
H,-2.645728442,1.6869306407,-1.5171110058
C,-2.5698106236,-0.054897874,-4.4389911007
H,-1.2347651826,-1.6873895415,-4.8770189137
H,-3.771497109,1.5862591905,-3.7308077494
H,-3.0590073461,-0.0961358829,-5.4048236141

121, B3LYP Energy= -689.908102184 Hartree,
NIMAG= 0

N,-0.8581787615,0.1980386415,-1.2646244121
N,0.4885097827,-0.0206539455,-1.2668210916
C,0.864388253,0.0179220874,0.0046389051
C,-0.2370818405,0.2392678318,0.8752408958
C,-1.3180328786,0.348568033,0.0236429333
C,-1.5777823374,0.1174329231,-2.4875408469
C,2.3019291173,-0.1676759912,0.3754943871
C,-0.2395934222,0.288224953,2.3726655021
O,-2.6369616846,0.4798412234,0.2950173819
H,0.4745425267,-0.4288256501,2.7866764237
H,0.035318922,1.2757969304,2.7613041232
H,-1.2244479962,0.0349433526,2.7728077868
H,2.8922150495,-0.3588097516,-0.5215060288
H,2.7056441019,0.7204659954,0.8720594418
H,2.4315449719,-1.0114516769,1.061019112
C,-3.0474960548,1.7503416639,0.8530773571
H,-2.8319290768,2.5430326683,0.1264994701
H,-2.4658181013,1.9549544299,1.7563763332
C,-4.5283867381,1.6670466395,1.1598826055
H,-4.875034629,2.6159553459,1.5777614479
H,-5.1029069918,1.4568531422,0.2551531635
H,-4.7285715969,0.8755088626,1.8852657482
C,-1.0815969917,-0.703781149,-3.5051453339
C,-2.744731881,0.8567633,-2.6982503391
C,-1.7553809942,-0.7853843227,-4.7191640485
H,-0.1694554029,-1.25775074,-3.3317130537
C,-3.4174835313,0.7557650445,-3.9136466521
H,-3.123891094,1.510248501,-1.9268655489
C,-2.9291780356,-0.0626783272,-4.9294983346
H,-1.3619367244,-1.4234847739,-5.5024990695
H,-4.3229085628,1.332110686,-4.0675237017
H,-3.4541015972,-0.1328734275,-5.875133557

121H, B3LYP Energy= -690.294863083 Hartree,
NIMAG= 0

N,-0.8430417925,0.2379319396,-1.3371438832
N,0.5223981282,0.257187135,-1.3019482337
C,0.9478036623,0.3671737833,-0.0268333549
C,-0.1689676941,0.4633633707,0.8039215545
C,-1.2846492759,0.380191447,-0.0600533163
C,-1.5709807288,0.1867512382,-2.5772469975
C,2.400970021,0.3580562079,0.3103797059
C,-0.1290425749,0.5784949225,2.3019767081
O,-2.5894776855,0.4009194246,0.1060376535
H,1.0434748423,0.0079987855,-2.1314599869
H,0.9050314849,0.587593398,2.6474781941
H,-0.5967919952,1.4963853488,2.6621055177
H,-0.6225560353,-0.2674418661,2.7856147257

H,3.0168605556,0.2856866545,-0.5872758494
H,2.6790692026,1.273209514,0.8380793511
H,2.6414795504,-0.4883496313,0.9580792405
C,-3.188944835,0.9478713068,1.3297558442
H,-2.7731949968,1.9445719763,1.4913831915
H,-2.9230318319,0.2972758483,2.1634970548
C,-4.6832263047,0.990942653,1.1101246386
H,-5.1638130334,1.3899166101,2.0066848601
H,-4.9383779886,1.6354665081,0.2674651684
H,-5.0806555946,-0.008636947,0.9259088214
C,-2.3683271939,-0.921949116,-2.8529828692
C,-1.4495894836,1.2456739926,-3.4770095379
C,-3.0623669227,-0.9646142367,-4.0591133409
H,-2.4443952602,-1.7317641314,-2.1380571722
C,-2.1372450961,1.1816073795,-4.6861052141
H,-0.8391871529,2.1070652695,-3.2314423103
C,-2.9436650216,0.0810854653,-4.9740983962
H,-3.6886760585,-1.8185933154,-4.2863011892
H,-2.0513400531,1.9956220104,-5.3954631684
H,-3.4817262107,0.0388155342,-5.9134961846

122, B3LYP Energy= -661.935466907 Hartree,
NIMAG= 0

N,-2.1480807516,0.0429192013,-0.0130544576
N,-2.8352277196,-1.1185729779,0.1585800738
C,-4.1113517995,-0.7774519748,0.0928197503
C,-4.2750635971,0.6121143396,-0.127611627
C,-2.996105426,1.1055876041,-0.1918204875
C,-0.736486238,0.0373863137,-0.0028543076
H,-4.871667104,-1.5355350604,0.2073022012
H,-5.1926089681,1.1671837142,-0.2319305173
H,-2.6368457932,2.104881801,-0.3667501883
C,-0.0537928571,-1.1833384244,-0.0821287187
C,-0.0203465168,1.2378480352,0.0899262419
C,1.3322454923,-1.201044802,-0.0794817158
H,-0.6222555651,-2.0999205802,-0.1437307426
C,1.3665890817,1.221100507,0.0849843085
H,-0.5344145659,2.1849603896,0.1811045013
C,2.029860496,0.0013292639,-0.000447737
H,1.8781162737,-2.1321762302,-0.1427214895
H,1.9369544025,2.1366351162,0.1569006069
N,3.5023983266,-0.016443124,-0.0023400301
O,4.0854259293,1.0597714734,0.0708659247
O,4.0590168998,-1.1056615852,-0.0776035896

122H, B3LYP Energy= -662.283156016 Hartree,
NIMAG= 0

N,-2.1351664534,0.0392671786,-0.0531128884
N,-2.8758374883,-0.8734422584,0.6258628533
C,-4.1831143604,-0.6273836699,0.4345803362
C,-4.290422105,0.4762399701,-0.4002626582
C,-2.9863475148,0.8668663121,-0.6885388734
C,-0.6944902773,0.0225752129,-0.0314991066
H,-4.9370676384,-1.243376257,0.8997044758
H,-5.1977529815,0.9303405888,-0.7614932333
H,-2.6080562413,1.6589138172,-1.3153511889
H,-2.424153818,-1.5565210255,1.2222219918
C,-0.0245586699,-1.1238416142,-0.459482196
C,-0.0191143866,1.1589469887,0.4104301907
C,1.365818322,-1.1353787011,-0.4335617525
H,-0.5701926554,-1.982533117,-0.8326605499

C,1.3717795717,1.149929102,0.4178084347
H,-0.5641917148,2.0289258567,0.7555313135
C,2.0342937427,0.0022205541,0.0014701641
H,1.9304016034,-1.9990436109,-0.758321901
H,1.9404869641,2.0074642583,0.7515665241
N,3.527920695,-0.0093998188,0.0207373839
O,4.0814038963,1.0131779334,0.3855392669
O,4.0745322438,-1.0410392114,-0.3292977762

123, B3LYP Energy= -701.267354150 Hartree,
NIMAG= 0

N,-1.7203043138,0.2883905409,-0.1824119758
N,-2.5144150727,-0.6670312633,0.3809829018
C,-3.7599238871,-0.2990264378,0.122156482
C,-3.7855031559,0.9131089016,-0.6251020449
C,-2.4708865348,1.254971603,-0.8004819459
C,-0.3187707458,0.1887692114,-0.0875823755
C,-4.9172588418,-1.1174563481,0.5986623171
H,-4.6482072892,1.4500996528,-0.9852930864
H,-2.0260028328,2.0870640048,-1.3184666739
C,0.2550217103,-0.9809970322,0.4302168768
C,0.503353271,1.2464029064,-0.5020029428
C,1.6330694309,-1.0936093569,0.5233332733
H,-0.3919832047,-1.7839904557,0.7515364269
C,1.8822456545,1.1315000494,-0.4136775915
H,0.0776277972,2.1642094608,-0.8837940423
C,2.4357645599,-0.0382070542,0.0978310539
H,2.0933958974,-1.9888772229,0.9178222349
H,2.5309244702,1.9371996787,-0.7280080086
N,3.8986066206,-0.1584433498,0.1936480808
O,4.5756508798,0.790754764,-0.1876282918
O,4.3571003267,-1.2005360535,0.6486032861
H,-5.5290891677,-1.4588847474,-0.2413238321
H,-4.5589023785,-1.9906777152,1.1442174453
H,-5.5639234937,-0.5348898366,1.2611056324

123H, B3LYP Energy= -701.621541990 Hartree,
NIMAG= 0

N,-1.6839283853,0.3160438935,-0.1924459067
N,-2.5249779809,-0.6219777955,0.3227676232
C,-3.8101371822,-0.2712455907,0.1101091378
C,-3.7813951233,0.9410946749,-0.5849772266
C,-2.4460023952,1.2736636702,-0.7562360217
C,-0.2542179594,0.1879104856,-0.1130003844
C,-4.9536762468,-1.0922221072,0.5973053998
H,-4.6338148096,1.5012807036,-0.9316269712
H,-1.9848164223,2.1087821977,-1.2594546531
H,-2.1524953218,-1.3993345662,0.854299468
C,0.35379511,-0.9678302362,-0.6048756469
C,0.4817455164,1.2306340809,0.4480640081
C,1.7366839253,-1.0870127589,-0.5217725979
H,-0.2327894505,-1.7504072684,-1.0715191535
C,1.8665028048,1.1174419654,0.5109694831
H,-0.0148016174,2.1086041997,0.8425019933
C,2.4646619323,-0.0407208403,0.0310094858
H,2.2521361906,-1.962705235,-0.8925802659
H,2.4784199021,1.9011156805,0.9369962658
N,3.9498927791,-0.166441081,0.111202051
O,4.558563278,0.7793247465,0.5811658474
O,4.4379052004,-1.2056972545,-0.2989692239
H,-5.728985305,-1.1457266412,-0.1684344704

H,-4.6462250581,-2.108026907,0.8498063923
H,-5.3944783812,-0.6341510163,1.4872353666

124, B3LYP Energy= -701.262360231 Hartree,
NIMAG= 0

N,-1.9472977486,-0.2734032185,-0.1581933454
N,-2.4836456723,-1.4953378032,-0.4506258719
C,-3.7913577908,-1.3183951171,-0.3887005527
C,-4.1252167245,0.0093463379,-0.0408609631
C,-2.9231382096,0.6670509244,0.1080647395
C,-0.538190741,-0.1579802974,-0.1081218823
H,-4.4511054946,-2.1475389758,-0.5978776892
H,-5.1067359403,0.4322449958,0.1014047346
C,-2.6743551055,2.0784645766,0.5358284474
C,0.2127274566,-1.2556029841,0.3337941743
C,0.1088250532,1.0131193406,-0.5186809304
C,1.5954508553,-1.1753201298,0.3841722559
H,-0.3017788765,-2.1604868655,0.6246345986
C,1.4934486719,1.1009091672,-0.4585878634
H,-0.4581119064,1.8436571034,-0.9132405877
C,2.2209210189,0.0070295007,-0.0038173881
H,2.1928730805,-2.0088813845,0.7265134423
H,2.0124925332,1.994494283,-0.7762300396
N,3.6911586094,0.098361123,0.0573392927
O,4.2110506788,1.1550480825,-0.2830437
O,4.3070289689,-0.8867946009,0.446465612
H,-1.8532228181,2.1509463163,1.2525144485
H,-2.4433275238,2.7364778601,-0.3072853065
H,-3.5748943748,2.4660687652,1.0138303745

124H, B3LYP Energy= -701.620524002 Hartree,
NIMAG= 0

N,-1.947990594,-0.2403606544,-0.2388885907
N,-2.549503117,-1.2802787826,-0.8814291353
C,-3.8822432804,-1.1517731084,-0.7893724032
C,-4.1483115253,-0.0029765478,-0.0641071598
C,-2.9125126311,0.559591282,0.2771753698
C,-0.5097483789,-0.1403055833,-0.1667196589
H,-4.5418073386,-1.877349773,-1.2396436597
H,-5.1191062821,0.3843267406,0.1964998664
C,-2.6044523882,1.7939681394,1.0513406304
H,-1.991870188,-1.9798923313,-1.3547666945
C,0.1775605914,-0.9519973408,0.7358619379
C,0.1472958627,0.7616114777,-1.002384562
C,1.5641139255,-0.8594929839,0.8022958482
H,-0.3585225959,-1.6353243199,1.3837301158
C,1.5332183679,0.8586373333,-0.9295076892
H,-0.4100423152,1.3736205739,-1.7010656859
C,2.2111919448,0.0450998247,-0.0302743934
H,2.1405176602,-1.4667336441,1.4872234782
H,2.0868837779,1.544244011,-1.5568188274
N,3.6999709475,0.1484118439,0.0459586073
O,4.2332479576,0.9652610597,-0.684703822
O,4.2636782378,-0.5922776325,0.832860597
H,-1.7631362983,1.6419316527,1.7296562054
H,-2.3519558255,2.6198137303,0.3799232433
H,-3.4767252268,2.0889537451,1.6333736583

125, B3LYP Energy= -701.263976832 Hartree,
NIMAG= 0

N,1.7047843614,0.1829079316,0.0347158138
N,2.3113140972,1.3835553743,0.2282387951
C,3.6065151841,1.1254837083,0.1856121956
C,3.877774578,-0.2525278256,-0.0409494619
C,2.6299144131,-0.8197649514,-0.1329728508
C,0.2987202149,0.0948202122,0.0195351376
H,4.3135595914,1.931949242,0.3195722066
C,5.2116531241,-0.9238001298,-0.1594925144
H,2.3441032141,-1.8414116735,-0.3164710923
C,-0.4650812684,1.2704991186,0.0229351327
C,-0.3389275639,-1.1535154631,0.00503487
C,-1.848594992,1.1969040061,0.002762011
H,0.0411677409,2.2245742755,0.0411255212
C,-1.7235175336,-1.2270516901,-0.0204839319
H,0.2344181886,-2.0701139087,0.0239582555
C,-2.4666900368,-0.050962937,-0.0218823802
H,-2.4541516667,2.0926275918,0.002445166
H,-2.2319641683,-2.1810423758,-0.0313781985
N,-3.9354989241,-0.1296377843,-0.0469304171
O,-4.4472283305,-1.2442878996,-0.0655042048
O,-4.563457038,0.923277726,-0.0481785007
H,5.8013894561,-0.8015167034,0.7537548165
H,5.0997820607,-1.9944822278,-0.341278993
H,5.7962612979,-0.5055776161,-0.9840903759

125H, B3LYP Energy= -701.616096414 Hartree,
NIMAG= 0

N,-1.6785700926,0.1144759171,-0.1132563571
N,-2.3394838728,1.0967423178,-0.7710373327
C,-3.6657764597,0.8924748438,-0.6650933624
C,-3.8807440678,-0.2532370065,0.0971592118
C,-2.5996525906,-0.7088296968,0.4245254398
C,-0.2417619038,0.066243734,-0.0553216899
H,-4.36553201,1.566298359,-1.1352655389
C,-5.1942298554,-0.8519777724,0.4989843841
H,-2.2865591855,-1.5494826002,1.0240396396
H,-1.8296233442,1.7805562245,-1.3165989281
C,0.4555815618,1.1766985944,0.4214734782
C,0.4069498767,-1.0951667948,-0.4720324693
C,1.844363079,1.1259368703,0.4713970949
H,-0.0702894931,2.0555543416,0.7754826059
C,1.7949049508,-1.1494703234,-0.4028552605
H,-0.1560782984,-1.9358066738,-0.8583487486
C,2.4847898339,-0.0368030371,0.0615982195
H,2.4278856097,1.9604959425,0.836204559
H,2.3419589502,-2.0288412209,-0.7151848476
N,3.9754412715,-0.0927139117,0.1243080512
O,4.502446115,-1.1367610984,-0.21903751
O,4.5483378339,0.9104601206,0.5135875343
H,-6.0195849411,-0.3483440301,-0.0044372824
H,-5.2374627575,-1.9117297458,0.2403007674
H,-5.3520772101,-0.7619343536,1.576300342

126, B3LYP Energy= -740.596020443 Hartree,
NIMAG= 0

N,1.3658307249,-0.0928029609,0.0021246464
N,2.068061146,1.0740086111,0.0461286052
C,3.3443216688,0.7250319031,0.0381262192
C,3.4964915491,-0.6967368746,-0.012757441
C,2.211468579,-1.1749160493,-0.0345603168
C,-0.0396542468,-0.0722499783,-0.0020064938

C,4.4240562402,1.7578639551,0.0801104249
C,4.774462071,-1.475967819,-0.0375866077
H,1.850071451,-2.1883819856,-0.0750035417
C,-0.7121439554,1.1591921641,0.0103616347
C,-0.7751105308,-1.2670783607,-0.0174933772
C,-2.0969382807,1.193149128,0.0053389724
H,-0.133549752,2.0711117474,0.0234333355
C,-2.1608434913,-1.2323892102,-0.0232237689
H,-0.2766823192,-2.2265675349,-0.0231587134
C,-2.8117090257,-0.002361344,-0.0119433274
H,-2.6307020502,2.1334281504,0.0141071667
H,-2.7416513568,-2.1441768644,-0.0349121733
N,-4.280642738,0.0331849346,-0.0177842418
O,-4.8784287027,-1.0384133016,-0.0314940463
O,-4.8259860312,1.1317002837,-0.0087263251
H,5.3815262958,-1.2776116812,0.8514106424
H,4.5817622841,-2.5499202578,-0.0746713763
H,5.3844295279,-1.2173484761,-0.90896528
H,5.0609302782,1.6287750281,0.9608570218
H,5.0702275832,1.6909674634,-0.8007897383
H,3.9863510817,2.7557383297,0.1130911001

126H, B3LYP Energy= -740.953936983 Hartree,
NIMAG= 0

N,1.3478840767,-0.0888880073,-0.0287657874
N,2.0979290612,0.9714728342,0.3679298958
C,3.4110524371,0.6827836228,0.2634232949
C,3.5118102376,-0.6251238975,-0.2407487612
C,2.2026244217,-1.0629323977,-0.4082082741
C,-0.0867890023,-0.0565991533,-0.0236628791
C,4.474541412,1.65244842,0.6441842022
C,4.7721674402,-1.3756297967,-0.5437250679
H,1.8217621747,-1.9942919331,-0.7973232096
H,1.6526955168,1.7857952102,0.7723552061
C,-0.7478411579,0.9999774131,-0.6520171817
C,-0.779520209,-1.0907401016,0.605048449
C,-2.1378934194,1.0281426169,-0.6388816573
H,-0.1937785746,1.7736944807,-1.1703395329
C,-2.1698844456,-1.071839221,0.5973680933
H,-0.2457774801,-1.8884707682,1.1066065042
C,-2.820908875,-0.0102331578,-0.0181988615
H,-2.6916965969,1.8259711478,-1.1150726416
H,-2.7476834931,-1.8532085599,1.0724015947
N,-4.3124877662,0.0161448342,-0.0134006593
O,-4.8793597926,-0.9229156631,0.5188010947
O,-4.8491312354,0.9752887631,-0.5416810387
H,5.3878995203,-1.4907310728,0.3519029813
H,4.5489504608,-2.371966281,-0.9255767799
H,5.3713176367,-0.8554411613,-1.2952341608
H,5.1226562542,1.2209176394,1.4110392918
H,5.0998852952,1.8873758078,-0.2212827411
H,4.0591321378,2.5845322242,1.0293877019

127, B3LYP Energy= -740.589987799 Hartree,
NIMAG= 0

N,-1.5349993465,-0.3688588866,-0.1758479653
N,-2.0326413703,-1.604181429,-0.4661867673
C,-3.3449063496,-1.4583830448,-0.4259890533
C,-3.7331533602,-0.137072475,-0.0945123766
C,-2.5424228663,0.5473118736,0.067632738
C,-0.1320356332,-0.211532338,-0.1151894999

H,-3.982174572,-2.3057084034,-0.6373684525
C,-5.1280999047,0.3918322926,0.0559011823
C,-2.3328949265,1.9630433427,0.4996175832
C,0.6490986826,-1.2865930403,0.3313062387
C,0.4837972538,0.978332385,-0.5217217511
C,2.0282506765,-1.1655881301,0.3905396211
H,0.1594768561,-2.2061958606,0.618975677
C,1.8646382597,1.1068528422,-0.4524368516
H,-0.1047710464,1.791665755,-0.9206358489
C,2.6216301638,0.0349926868,0.0071376041
H,2.6476979625,-1.9812511893,0.7368466072
H,2.3590690501,2.0154005427,-0.7669507482
N,4.087208189,0.1696746567,0.0784218134
O,4.578500222,1.2417912291,-0.2572033274
O,4.7298469085,-0.7972553029,0.470797616
H,-5.2401694234,0.9961913899,0.9610008443
H,-5.4237086304,1.0172253511,-0.7928629856
H,-5.844589394,-0.42957869,0.1216521978
H,-1.4872895848,2.0630318151,1.18327614
H,-2.1642634447,2.6399674076,-0.3444772199
H,-3.2268213717,2.3140452198,1.0181409846

127H, B3LYP Energy= -740.952684621 Hartree,
NIMAG= 0

N,-1.5318483861,-0.3366113129,-0.2725209359
N,-2.0859881493,-1.4301148675,-0.8603650017
C,-3.4262996221,-1.3280273864,-0.8113933481
C,-3.7576725955,-0.1455957782,-0.1660454326
C,-2.532256921,0.4632891757,0.1687264232
C,-0.0995605598,-0.195740006,-0.1753550997
H,-4.0528163367,-2.0974783211,-1.2358614763
C,-5.1284946618,0.3801614826,0.1302724883
C,-2.2902727323,1.7449609025,0.8862168764
H,-1.4992942909,-2.1284125816,-1.2978230986
C,0.5962076204,-0.9938133113,0.7329540453
C,0.5470971552,0.72735738,-0.9960376015
C,1.9788273782,-0.8666825201,0.8199726758
H,0.0685175239,-1.6924536292,1.3712650053
C,1.9285318512,0.8611648723,-0.9009738111
H,-0.0156387152,1.3274769893,-1.7005636714
C,2.614677516,0.0598216523,0.0030362251
H,2.5604112983,-1.4625548509,1.5104226227
H,2.4728881664,1.56507906,-1.5160007222
N,4.0983444388,0.201355886,0.1022640961
O,4.6207948242,1.0405563292,-0.6109734854
O,4.6706625535,-0.5332697982,0.8889160509
H,-5.2849972052,0.4931546848,1.2062196802
H,-5.2869878954,1.3567497648,-0.3336657382
H,-5.8937004155,-0.2979304317,-0.2480074855
H,-1.2617753037,1.8314722594,1.2348676447
H,-2.504847245,2.5951736866,0.2315054784
H,-2.9593594444,1.819259906,1.7458074423

128, B3LYP Energy= -740.594001537 Hartree,
NIMAG= 0

N,-1.6031478823,0.0782619665,-0.0621592373
N,-2.2791538348,-1.1034351078,-0.2132016455
C,-3.5629978482,-0.7914213908,-0.1518389961
C,-3.7337117122,0.6021782423,0.0596020884
C,-2.4688017088,1.1395370617,0.1184143352
C,-0.1922476137,0.0406815154,-0.0408982442

C,-4.6156200876,-1.8435259873,-0.3033053356
H,-4.6603669314,1.1430504136,0.1723193107
C,-2.0676928251,2.5543228182,0.3919743846
C,0.4458969762,-1.1042657016,0.4586496589
C,0.5730975645,1.1055820347,-0.5330833592
C,1.8293671197,-1.1732919536,0.4865750386
H,-0.1579003919,-1.9274231673,0.8129177764
C,1.9595108085,1.0437880479,-0.4957311945
H,0.0945996836,1.9680622068,-0.9727242362
C,2.5736058025,-0.0929641446,0.0178752506
H,2.3383368048,-2.0450483809,0.8738790288
H,2.5661379961,1.8541307331,-0.8754188342
N,4.0443210505,-0.1588522524,0.0558173653
O,4.6697088282,0.812897462,-0.3546756399
O,4.5582757046,-1.1801602921,0.4976204388
H,-5.2442831517,-1.648379316,-1.1770454969
H,-4.1512337845,-2.8227080182,-0.4237113144
H,-5.2704308392,-1.8734432619,0.5724633524
H,-1.2379538024,2.6158752422,1.0999445482
H,-1.774205155,3.0894065013,-0.5162996709
H,-2.9184777705,3.0846307289,0.8216556277

128H, B3LYP Energy= -740.958244385 Hartree,
NIMAG= 0

N,-1.5964499316,0.0634887461,-0.0232279023
N,-2.3306966211,-1.0088548324,-0.4436035197
C,-3.6466973301,-0.7560097641,-0.3053915584
C,-3.7494628064,0.5236861931,0.2368536063
C,-2.4561945118,1.0189656879,0.4076656242
C,-0.1555404383,0.0299371522,-0.0316202919
C,-4.6947315233,-1.7315207797,-0.7186747071
H,-4.6629121042,1.0373312798,0.4877445931
C,-1.9946274037,2.3260293691,0.9530618833
H,-1.8662365278,-1.8204830823,-0.8303799895
C,0.5092005382,-0.7093980899,0.9474381662
C,0.5323964811,0.7335787587,-1.0194642259
C,1.8996863631,-0.7483824427,0.9355925937
H,-0.047607448,-1.2363370711,1.7131511078
C,1.9232396582,0.701664447,-1.0259105702
H,-0.0072916082,1.2925294839,-1.7741187764
C,2.5764265115,-0.0403085916,-0.0498102695
H,2.4576863503,-1.3064136666,1.6753621613
H,2.498816571,1.2326559926,-1.7720964396
N,4.0695959908,-0.0780327634,-0.059370906
O,4.6318848051,0.5653843997,-0.9287909722
O,4.6097897588,-0.7495352482,0.8028962673
H,-5.0633988237,-1.4897548036,-1.7197565983
H,-4.314213875,-2.7541773346,-0.7314420442
H,-5.5403333844,-1.6856125984,-0.0317121634
H,-1.150108233,2.1996778175,1.6331813765
H,-1.6809202245,2.9958765416,0.1474603338
H,-2.8098285344,2.8068171858,1.4922836002

129, B3LYP Energy= -779.921500834 Hartree,
NIMAG= 0

N,-0.7566983999,-0.0864667232,-0.8462548985
N,0.5988495653,-0.2461477631,-0.9142038832
C,1.022443964,-0.2172262237,0.3370041715
C,-0.0562387963,-0.0181766888,1.2487536296
C,-1.1859921955,0.0677768538,0.4608702536
C,-1.4833383212,-0.0485210994,-2.0538909946

C,2.4726631977,-0.3862130537,0.6602531538
C,0.0498340102,0.0817095458,2.7397167673
C,-2.5968413906,0.3566775975,0.8653111029
C,-0.8629022505,0.4704257915,-3.2006158156
C,-2.7906912092,-0.5463037971,-2.1361492539
C,-1.5472562425,0.5120986193,-4.4041691055
H,0.1539385063,0.8289160168,-3.1281481458
C,-3.4827983335,-0.4952579119,-3.3382926416
H,-3.2586372421,-1.0017169334,-1.2759483185
C,-2.8562717508,0.0377713678,-4.45950039
H,-1.0869224989,0.9144323451,-5.2959238376
H,-4.4899288131,-0.8796511315,-3.4206871782
N,-3.589347073,0.0898085609,-5.7346372119
O,-4.7435201358,-0.3253209245,-5.7473446724
O,-3.0051219755,0.5471463191,-6.7106833741
H,2.6380327698,-1.2626070613,1.2947639377
H,3.047950598,-0.5109244861,-0.2575154336
H,2.8626418812,0.4831309139,1.1991998111
H,-3.0887650432,1.0377906232,0.1677080778
H,-3.2087808757,-0.5482176029,0.9383290106
H,-2.6010860405,0.8285458184,1.8487508069
H,-0.9059297839,0.3413493923,3.1988310753
H,0.3757663943,-0.865553746,3.1826383326
H,0.7769943849,0.8431330811,3.0388499243

129H, B3LYP Energy= -780.289250518 Hartree,
NIMAG= 0

N,-0.751908233,-0.088408161,-0.8584063927
N,0.5611909355,-0.4510650995,-0.8416812203
C,1.042477646,-0.3939237943,0.4172284345
C,-0.0010743495,0.0369782958,1.2413976614
C,-1.1153953291,0.2237281285,0.4097413714
C,-1.4933788415,-0.0512392729,-2.0928760111
C,2.4542974817,-0.7516584054,0.7366794714
C,0.0491379625,0.2684615286,2.7211270808
C,-2.4842742845,0.6884392395,0.7669564904
H,1.0100201033,-0.7714838095,-1.6895281833
C,-1.2360489114,0.9723836123,-3.0055883819
C,-2.4407807074,-1.0427833785,-2.3457786996
C,-1.9414354291,1.0022461035,-4.2041800462
H,-0.5068751661,1.7411648969,-2.7793426937
C,-3.153871521,-1.0070679218,-3.5396864642
H,-2.6155096455,-1.8323089129,-1.6252155239
C,-2.8867890831,0.0128810568,-4.4444203303
H,-1.7763648435,1.7777088524,-4.939970655
H,-3.8988067321,-1.7544441363,-3.7773501336
N,-3.6484801451,0.0482061434,-5.7282340741
O,-4.484561216,-0.8227398842,-5.8981267324
O,-3.3753318192,0.9452315069,-6.507549172
H,2.4867344057,-1.5626218494,1.467874588
H,3.0000779047,-1.0720851279,-0.1519239265
H,2.977599298,0.105988798,1.1662816419
H,-3.0570080996,0.9859240174,-0.1108213111
H,-3.0342828484,-0.103496659,1.2843483864
H,-2.4214878662,1.5396382202,1.4478958166
H,-0.1837154242,1.3075403273,2.9691406794
H,-0.6678098828,-0.3664198745,3.247964163
H,1.0397746766,0.0493058575,3.1198105913

130, B3LYP Energy= -717.315654675 Hartree,
NIMAG= 0

N,-0.695617464,-0.0044646241,-0.8475015322
N,0.6705523733,-0.1342465617,-0.8797225574
C,1.0528087073,-0.0747953259,0.3855555199
C,-0.0592262033,0.0897924824,1.2647954198
C,-1.1487598545,0.1289922755,0.4373915006
C,-1.4319414021,-0.0118919024,-2.0410502916
N,2.3912932176,-0.105803642,0.7327437284
H,-0.0507017739,0.1855611409,2.3382178219
H,-2.191983135,0.2581495638,0.6694086259
C,-0.7551000362,0.0260902851,-3.2698799348
C,-2.8349954901,-0.0611577999,-2.0195918263
C,-1.4709152581,0.0259683394,-4.4558582962
H,0.3244767171,0.0575032491,-3.2714029813
C,-3.5499054183,-0.0558520041,-3.2061881288
H,-3.3745016777,-0.114357255,-1.0837847229
C,-2.8628475079,-0.0115079015,-4.4166628673
H,-0.9652550567,0.0582721918,-5.4110247519
H,-4.6303262146,-0.0939673351,-3.2066782934
N,-3.6219350827,-0.0091737361,-5.6735285002
O,-4.8468737799,-0.0435891872,-5.6021267356
O,-2.9895300196,0.0277333597,-6.7241679914
H,2.5990518758,-0.5198849202,1.6290397308
H,3.0025918836,-0.4314595926,-0.002984636

130H, B3LYP Energy= -717.672227670 Hartree,
NIMAG= 0

N,-0.7017910459,0.0452744334,-0.8746169617
N,0.5962641357,-0.4157720243,-0.8047203783
C,1.0702582336,-0.2298619502,0.4570421939
C,0.0636953892,0.4319389061,1.1865731479
C,-1.0022909763,0.582651293,0.3239519911
C,-1.4417951961,0.0212182966,-2.0984510705
N,2.2833092378,-0.6496132829,0.8465130925
H,0.123217073,0.7672335977,2.2081190978
H,-1.9501470665,1.0748571858,0.4751434665
H,0.9101278878,-1.0880643603,-1.4928857309
C,-0.8260321464,0.4228092499,-3.2857660873
C,-2.7713517848,-0.4010840387,-2.0671609982
C,-1.5559717621,0.392345658,-4.4684453553
H,0.1957331114,0.7827670746,-3.2880322323
C,-3.5063934501,-0.4058095708,-3.2470848075
H,-3.2223039919,-0.7384665455,-1.1420922109
C,-2.8832012197,-0.0161330014,-4.4259718921
H,-1.1189027702,0.6981295997,-5.4094369536
H,-4.5399287255,-0.7242938131,-3.2663100373
N,-3.6672142179,-0.038388831,-5.6932941385
O,-4.8350643371,-0.3806248943,-5.6147583892
O,-3.080582491,0.2872353899,-6.7119882762
H,2.5990570223,-0.4571438691,1.7839092531
H,2.9638829593,-1.0156679265,0.1996695412

131, B3LYP Energy= -717.308086181 Hartree,
NIMAG= 0

N,-0.7542355252,-0.0543565092,-0.861048168
N,0.5819055372,-0.3836516192,-0.9182865079
C,0.9827450497,-0.3729438053,0.3381365053
C,-0.0498185463,-0.0165663467,1.235463442
C,-1.1534270339,0.1941964342,0.4341616168
C,-1.4899667246,0.0205866077,-2.0632710299
H,2.0086926672,-0.6204065572,0.5688354127
H,0.0028117639,0.0934814242,2.3063325716

N,-2.4563403584,0.5456229635,0.7737147841
C,-0.8219588416,0.3828875879,-3.2416535736
C,-2.8556494308,-0.2939511654,-2.0976834502
C,-1.517103698,0.4520656298,-4.4383288826
H,0.2370120622,0.5946988561,-3.1998650883
C,-3.5543216725,-0.2146932849,-3.29525585
H,-3.3601547322,-0.6273412882,-1.2014745377
C,-2.879795432,0.1628182799,-4.451084022
H,-1.0220596344,0.7336581417,-5.3574022874
H,-4.6062112001,-0.4596746977,-3.345625777
N,-3.6224896891,0.2474257665,-5.720624844
O,-4.8233340376,0.000729188,-5.696430421
O,-2.9973075896,0.5615338734,-6.726866951
H,-2.5348099458,0.8379922102,1.7380612042
H,-2.8902346882,1.2233354105,0.1585584539

131H, B3LYP Energy= -717.673064284 Hartree,
NIMAG= 0

N,-0.7959043786,-0.1724324163,-0.8448342156
N,0.4307493026,-0.8025386735,-0.7729640718
C,0.9035038031,-0.6768844632,0.4839968363
C,0.0404658084,0.100496304,1.2171535958
C,-1.0315785231,0.4252530753,0.3526957886
C,-1.5166589389,-0.0540863135,-2.0831787772
H,1.8302427233,-1.149557219,0.7707785499
H,0.1594468064,0.4188943855,2.2389725457
N,-2.1089084665,1.1899677019,0.5780677752
H,0.6585998437,-1.5075476189,-1.4617009925
C,-0.9944584913,0.741171369,-3.1053829787
C,-2.7235082439,-0.7407284076,-2.2271026644
H,-1.6954104186,0.8486199689,-4.3017357503
H,-0.059729315,1.2710722976,-2.9669506682
C,-3.4320672032,-0.6197747023,-3.4188499895
H,-3.0982976891,-1.3670938616,-1.4263455392
C,-2.9012493721,0.1697703783,-4.4309759702
H,-1.3279629764,1.4511830165,-5.1215480087
H,-4.3715600838,-1.1328539034,-3.5744604623
N,-3.6586797189,0.2943935535,-5.7126211253
O,-4.7265847845,-0.2895396871,-5.7804453444
O,-3.1500555553,0.9709831458,-6.5896977002
H,-2.2158375946,1.659791126,1.4625080743
H,-2.7819032376,1.3887496622,-0.145760332

132, B3LYP Energy= -717.305740292 Hartree,
NIMAG= 0

N,-0.6946285966,-0.0148805371,-0.8657851756
N,0.6571071355,0.0259631123,-0.9047090459
C,1.0483474869,0.0060929872,0.3574812296
C,-0.0556126771,-0.0570718369,1.2536935449
C,-1.1610939256,-0.0683946534,0.433797685
C,-1.4361802199,-0.0056266721,-2.0596109226
H,2.101551308,0.0393224467,0.5964153462
N,0.000338403,-0.0252228818,2.6475874465
H,-2.2085951923,-0.1079774321,0.6738251408
C,-0.76393066,-0.0151339526,-3.2915818732
C,-2.8386503878,0.0133760528,-2.031111172
C,-1.4842894398,-0.008455693,-4.4740559821
H,0.3161019734,-0.0274872215,-3.2992400863
C,-3.5591946156,0.018221336,-3.2157476531
H,-3.3757086981,0.0296794621,-1.0929732511
C,-2.8771009788,0.0068009802,-4.4282179455

H,-0.9822058555,-0.016301786,-5.4316110247
H,-4.6401950774,0.0335331815,-3.2109826883
N,-3.6416669101,0.0121280642,-5.6828274314
O,-4.8664011822,0.0270855655,-5.606457521
O,-3.0122865911,0.0011159822,-6.735493679
H,-0.8198323303,-0.3823053305,3.1165555326
H,0.8418298316,-0.4231038736,3.0401081261

132H, B3LYP Energy= -717.658782540 Hartree,
NIMAG= 0

N,-0.7186959107,0.0340460846,-0.8636604208
N,0.4966010952,0.60507726,-0.7666205486
C,0.957785754,0.491759226,0.4969085581
C,0.0012766231,-0.2036077087,1.2480399634
C,-1.0404686474,-0.4750701774,0.346656947
C,-1.4591181972,0.0158997512,-2.0942681964
H,1.9126133365,0.9071400668,0.7767345686
N,0.0434012817,-0.500839511,2.5838774443
H,-1.9619488995,-1.0178170484,0.4807708661
H,0.8745516129,1.1391602814,-1.5387296908
C,-0.8421966263,-0.4612527657,-3.2514647954
C,-2.7767796509,0.4721480198,-2.0911202782
C,-1.5612939275,-0.4685632454,-4.4415985175
H,0.1689740789,-0.8497849097,-3.2243460261
C,-3.4992950853,0.4446802075,-3.2787749451
H,-3.2260758686,0.8594645794,-1.185056125
C,-2.8757132092,-0.0191466779,-4.4303911201
H,-1.1259768922,-0.8319422101,-5.3627390863
H,-4.5233244221,0.7901860962,-3.3246648658
N,-3.6488384001,-0.0368793939,-5.7067533316
O,-4.8061441425,0.3427053386,-5.6557149983
O,-3.0623419926,-0.4291480882,-6.7010901049
H,-0.5844235256,-1.2061193759,2.937103867
H,0.9361124537,-0.4739147903,3.0516045643

132c, B3LYP Energy= -717.639982636 Hartree,
NIMAG= 0

N,-1.6723223401,0.185651116,-0.0968259354
N,-2.276699618,1.3451360434,-0.4346647697
C,-3.5782314193,1.1231312734,-0.3494640037
C,-3.799839498,-0.2057587877,0.0548426967
C,-2.5592575333,-0.7898788854,0.2154692863
C,-0.2410868485,0.0987772859,-0.0722231932
H,-4.2836947382,1.9080745856,-0.5810630969
N,-5.1014574446,-0.8587063594,0.2586583127
H,-2.256217995,-1.771025192,0.543858271
H,-5.7689215928,-0.2191991152,0.7050914954
C,0.495429712,1.2311597568,0.2723935306
C,0.3807477133,-1.1069472464,-0.3959096868
C,1.8820514834,1.1503549665,0.3060747593
H,-0.0109478552,2.1574033087,0.5067869289
C,1.7671345604,-1.1906779039,-0.3491220857
H,-0.1962449045,-1.9673723705,-0.7114559838
C,2.4934474118,-0.0602160919,0.0028473012
H,2.4882293714,2.0060900939,0.5702755557
H,2.2861734882,-2.1064270253,-0.5966729558
N,3.9774873528,-0.1487626898,0.0486440899
O,4.4787513049,-1.2298999821,-0.2182018622
O,4.5864164825,0.8644359093,0.3517145657
H,-5.018666332,-1.6748450313,0.8742271749
H,-5.5248487613,-1.1799186584,-0.621363395

133, B3LYP Energy= -866.479177001 Hartree,
NIMAG= 0

N,-1.9731926068,-0.6036085505,-0.0125633051
N,-2.556663692,-1.7193066815,0.5182140919
C,-3.8442658982,-1.5827069307,0.2602552878
C,-4.1192835626,-0.3907416231,-0.4580290527
C,-2.899433879,0.2104717457,-0.6172292024
C,-0.5740173093,-0.4870662245,0.025765783
H,-4.5369666622,-2.3388983057,0.5984270466
H,-5.0711637325,-0.030493395,-0.8112748848
H,-2.6265740343,1.120987533,-1.1228721152
C,0.1067670294,0.7425462909,0.0462038358
C,0.1941016066,-1.6603685428,0.0001230196
C,1.4904475496,0.8126528461,-0.0275312284
C,1.5773900122,-1.6094439632,-0.026114097
H,-0.3276961876,-2.6067810227,-0.0062537162
C,2.2108893068,-0.3699248253,-0.0562375815
H,1.9942956312,1.7689414736,-0.0353641844
H,2.1699105092,-2.5136913519,-0.0460072102
N,3.6854898372,-0.3060940581,-0.1118535492
O,4.2927941005,-1.3681629399,-0.1331075262
O,4.2029431026,0.8022572089,-0.1346589254
N,-0.5926292372,2.0351258275,0.2267069997
O,-0.2510183799,2.9582647716,-0.4994302832
O,-1.4339835036,2.0977547177,1.1092897978

133H, B3LYP Energy= -866.825694249 Hartree,
NIMAG= 0

N,-1.9744391514,-0.562242134,-0.1423420875
N,-2.7956470123,-0.5982351501,0.9442069892
C,-4.0381426631,-0.8952008083,0.5500099866
C,-4.0217594036,-1.1169101138,-0.8248123603
C,-2.7130441151,-0.9037215307,-1.2257839048
C,-0.5408721419,-0.4649086521,-0.0673995623
H,-4.8502028718,-0.9145113249,1.2609076002
H,-4.8570380727,-1.3827347228,-1.4506783477
H,-2.2557389546,-0.969010973,-2.2002540055
H,-2.4707658838,-0.1394695078,1.7959306214
C,0.1447519404,0.654007843,0.4396750785
C,0.1926458265,-1.5147802423,-0.6200165003
C,1.5279864856,0.7275865958,0.3787665799
C,1.5824149761,-1.4598371832,-0.6730734048
H,-0.3266777183,-2.3846112653,-1.0025809926
C,2.2229427914,-0.3379958714,-0.1720325835
H,2.0547227771,1.5963598258,0.7524935488
H,2.1634805602,-2.2721115461,-1.0898273699
N,3.7153693075,-0.2668587176,-0.2224528962
O,4.2873069283,-1.2131264896,-0.7318852574
O,4.2306575206,0.7303261195,0.248625588
N,-0.5452815468,1.8009977064,1.0708957312
O,-0.1146056142,2.9065616922,0.8444127437
O,-1.4963047202,1.54174068,1.8132637947

134, B3LYP Energy= -905.811514636 Hartree,
NIMAG= 0

N,-1.6128842631,-0.7958207405,0.1655422777
N,-2.3687183266,-0.0934108471,-0.736618436
C,-3.6262534623,-0.354675966,-0.4233620953
C,-3.7022221099,-1.2181362469,0.7100009797

C,-2.4062670044,-1.475629253,1.0572958947
C,-0.2201966429,-0.6495456727,0.1419998399
C,-4.7518631411,0.222656448,-1.2198266613
H,-4.5880590135,-1.5893984977,1.1994234419
H,-2.0006179205,-2.0574306363,1.8674245773
C,0.6783144209,-1.6259589987,0.6100535533
C,0.3186647162,0.5559073395,-0.3359526329
C,2.0443776579,-1.3924848883,0.6737375654
C,1.6830236706,0.786080691,-0.3231100886
H,-0.3678155599,1.3038513628,-0.7060331764
C,2.5326955707,-0.1864326901,0.1991062974
H,2.7142997678,-2.1475919289,1.0601960448
H,2.0959731343,1.7155255145,-0.6901519706
N,3.986483318,0.0615274064,0.2416414282
O,4.3867537879,1.1342016969,-0.1915170825
O,4.6977004571,-0.8186966981,0.7077473521
N,0.2452168838,-2.990368097,0.9868563494
O,-0.5152316262,-3.5674258611,0.2250117372
O,0.7099830262,-3.4577006977,2.0174980817
H,-5.4233090504,0.8052047361,-0.5826637576
H,-4.3630636315,0.8724901498,-2.0039850329
H,-5.3454325591,-0.5685229249,-1.6866706867

134H, B3LYP Energy= -906.165039288 Hartree,
NIMAG= 0

N,-1.5994354869,-0.4955665837,0.3659254821
N,-2.413355666,-0.7859172019,-0.6939856272
C,-3.6909172525,-0.520503193,-0.3816263336
C,-3.6932833211,0.0304274703,0.909390113
C,-2.3819829726,0.0347165506,1.3389784505
C,-0.166528424,-0.4498728127,0.288903035
C,-4.8158027409,-0.8345051711,-1.3046485304
H,-4.5546665804,0.3642349245,1.463801862
H,-1.9455903746,0.3745482593,2.2648639377
H,-2.0415787533,-1.4107337576,-1.4087513086
C,0.6415349384,-1.575394232,0.0430625949
C,0.4478629835,0.7711400453,0.5697336762
C,2.0244423855,-1.4851127553,0.0921292568
C,1.8347428202,0.878824899,0.6090057426
H,-0.1648178557,1.6456192486,0.7497852894
C,2.5967901668,-0.2532207641,0.3678549116
H,2.6440596192,-2.3559240905,-0.0792063273
H,2.3216095719,1.8227666565,0.8161440046
N,4.0868799036,-0.1505874705,0.4043608708
O,4.5504584467,0.9428772497,0.6731204888
O,4.7113329263,-1.1676475566,0.1632637543
N,0.0842916284,-2.9065012323,-0.283113406
O,-0.8883727047,-2.9371457316,-1.0415739835
O,0.6343668565,-3.873944298,0.1881542225
H,-5.4865152839,0.0233311935,-1.3817358872
H,-4.461028498,-1.0914430128,-2.3031349988
H,-5.3949819284,-1.6761453461,-0.9143553281

135, B3LYP Energy= -945.135410974 Hartree,
NIMAG= 0

N,1.281792625,-0.7250724115,-0.2533081276
N,1.7976016044,-1.9745809453,-0.4791187612
C,3.1110066398,-1.8315773973,-0.4218116935
C,3.4649683913,-0.4793000707,-0.1328201704
C,2.2797634377,0.1923274371,-0.0299371602
C,-0.107344261,-0.5726051981,-0.1592248528

C,4.0231496634,-2.9952632994,-0.6683317435
H,4.4527815799,-0.0658482716,-0.0089638243
H,2.0766166971,1.222797468,0.2069654352
C,-0.7850095598,0.6298755621,-0.4329955635
C,-0.8727624657,-1.6674871103,0.2733969925
C,-2.1487125893,0.7664966917,-0.2171602367
C,-2.2411663686,-1.5610726029,0.449012171
H,-0.356969178,-2.595393471,0.4746745672
C,-2.8641144367,-0.3368551369,0.2175295591
H,-2.6449074795,1.7069903121,-0.4110793499
H,-2.8285324362,-2.4048845059,0.7838926889
N,-4.3186673504,-0.2073826079,0.4273879419
O,-4.922577286,-1.202300153,0.8068458952
O,-4.8273960813,0.8844444245,0.2105729987
N,-0.1147483902,1.799421106,-1.0446605873
O,0.6101550489,1.5908427782,-2.0052723672
O,-0.3642817549,2.8976790901,-0.5669684334
H,4.7441054164,-3.0613689343,0.1538703146
H,3.4232753639,-3.9079262324,-0.6428573114
C,4.7780217989,-2.8989892956,-2.0049738712
H,5.4323204012,-3.7642791748,-2.1375555953
H,4.0795064626,-2.8678635982,-2.8445268354
H,5.3976693069,-1.9995352525,-2.0504601795

135H, B3LYP Energy= -945.490634369 Hartree,
NIMAG= 0

N,1.2176537756,-0.9804805309,0.0451721733
N,1.8210957616,-1.7701924971,-0.8949814628
C,3.0797175614,-2.0520303821,-0.5258001412
C,3.2740181212,-1.4757797537,0.7405594576
C,2.1007253546,-0.8267718798,1.0644307942
C,-0.1884865649,-0.695019587,0.0718544249
C,4.0228685453,-2.7959365533,-1.4143549047
H,4.1717345007,-1.51745286,1.3347237509
H,1.8251066342,-0.2662920926,1.9436656829
H,1.401997158,-1.7932068016,-1.8236917448
C,-0.8543681987,0.0573368464,-0.9134959287
C,-0.9035868043,-1.1152433755,1.1942124032
C,-2.1926193755,0.3923756125,-0.7727046188
C,-2.2501596816,-0.7973321744,1.3420798378
H,-0.4034106502,-1.703825919,1.9530582091
C,-2.8695216268,-0.0495940839,0.3531641011
H,-2.6981053478,0.9866878527,-1.5228981607
H,-2.8160329542,-1.1264334119,2.203695543
N,-4.3155044147,0.2963977371,0.4984170979
O,-4.8676960171,-0.0880091198,1.513438318
O,-4.8196211772,0.9334718024,-0.4085925408
N,-0.1877197109,0.532301471,-2.1457850428
O,0.5913753235,-0.2479084383,-2.6991929394
O,-0.4716287314,1.6374633269,-2.5447263815
H,4.521235362,-3.5583407096,-0.8093238487
H,3.454109502,-3.3246304177,-2.1836875278
C,5.0736214868,-1.8728256075,-2.0652584485
H,5.7362262755,-2.468492145,-2.6945835555
H,4.6027622603,-1.1126051322,-2.6918806833
H,5.6839766444,-1.3703888615,-1.3125078612

136, B3LYP Energy= -1023.78282292 Hartree,
NIMAG= 0

N,-0.3572680737,0.8624193462,2.1100306768
N,0.9175354537,0.3705837002,2.0072106412

C,1.4921212069,0.6162355334,3.1717313154
C,0.574852937,1.2576615966,4.0623567748
C,-0.5848140101,1.3951539326,3.3559065225
C,-1.2450974696,0.6706617563,1.0447465249
C,2.9393814116,0.2539042358,3.4455029762
H,0.7427985877,1.5687310987,5.080170092
H,-1.5384575143,1.8003549122,3.6485802384
C,-2.3508334603,1.5020242253,0.7860756128
C,-1.0538948659,-0.4378394212,0.2036868803
C,-3.2697754735,1.2091317702,-0.2111061781
C,-1.9355919213,-0.7176432119,-0.825179026
H,-0.2000792502,-1.0726526684,0.3918380103
C,-3.047018629,0.1012260267,-1.0119474388
H,-4.1254830502,1.8486705317,-0.3757974194
H,-1.7876099926,-1.5727855621,-1.4701153763
N,-4.0059300004,-0.2054331934,-2.089864464
O,-3.7784771518,-1.1895857497,-2.781590127
O,-4.9666785394,0.5410531947,-2.2230591663
N,-2.5662382668,2.7830337242,1.4956120914
O,-1.6050231488,3.5275887587,1.6121988356
O,-3.7020266432,3.0220247268,1.8823157998
C,3.5519050628,-0.498036884,2.2518694555
H,4.5959630476,-0.7411893251,2.4680739571
H,3.0179253061,-1.4298840706,2.0523434448
H,3.5198208292,0.105136272,1.3425789387
C,3.7368732437,1.554492644,3.6966432723
H,3.3370408932,2.114827023,4.5459851158
H,4.7827029921,1.3174313157,3.9127504024
H,3.7091373522,2.2059173538,2.819418415
C,3.0061898131,-0.6400423846,4.7042318933
H,2.5978801344,-0.1343201269,5.5833020039
H,2.4468661109,-1.5679009008,4.5576063057
H,4.0455764789,-0.9007682801,4.923005899

136H, B3LYP Energy= -1024.14135641 Hartree,
NIMAG= 0

N,-0.5123858647,0.5023127625,2.2258015251
N,0.848875369,0.575432028,2.1066011895
C,1.4333481767,0.4290073452,3.3041442558
C,0.4012503407,0.1794432737,4.2294923938
C,-0.783156496,0.2267205272,3.5282653355
C,-1.4106387608,0.3800657908,1.1145899122
C,2.9253746871,0.5588727042,3.5118907688
H,0.5105464738,0.0078136335,5.2867780499
H,-1.8017209073,0.089617635,3.8550962485
H,1.2243015745,0.9959879965,1.2590520563
C,-1.6040426698,1.3842022553,0.1478151675
C,-2.2015592953,-0.7686450188,1.055842147
C,-2.5687575096,1.2497480045,-0.8394391694
C,-3.1647866619,-0.9224553051,0.0636290932
H,-2.0548338593,-1.5519285648,1.788867135
C,-3.3283210991,0.090898992,-0.8675978034
H,-2.7273705402,2.0319132802,-1.5705026451
H,-3.7763493986,-1.8131411437,0.0043441121
N,-4.3560566317,-0.0633027987,-1.9400583616
O,-5.0241749884,-1.0812461641,-1.9119522472
O,-4.4405859263,0.8405064813,-2.751826229
N,-0.8075043086,2.6300905428,0.1169386028
O,0.3993667805,2.5311044255,0.350657424
O,-1.3839632564,3.6553540027,-0.1637077209
C,3.6486216125,0.8187106057,2.1775840892
H,4.7217091719,0.8950789853,2.3586677089

H,3.5007312163,0.0031692678,1.4634439779
H,3.3392600634,1.76206519,1.7162054322
C,3.1739750335,1.7399958909,4.482168141
H,2.6952562268,1.5766200016,5.450024696
H,4.247703751,1.8413754513,4.6535515498
H,2.8068700554,2.6826676215,4.069390533
C,3.4400756646,-0.7575742345,4.1419207873
H,2.9603136552,-0.9643235187,5.1012280336
H,3.2731236049,-1.6116164391,3.4810450514
H,4.5141208757,-0.672914595,4.3198595519

137, B3LYP Energy= -905.807704167 Hartree,
NIMAG= 0

N,-0.7808707066,0.3369015065,-0.8276988617
N,0.4323977378,0.9654353863,-0.8384517487
C,0.8607803684,0.8819258905,0.4075735212
C,-0.0552226822,0.1903711331,1.2354039139
C,-1.1081251856,-0.1555024394,0.4182245463
C,-1.4942959644,0.2468031743,-2.0371399313
H,1.8105748661,1.3215759786,0.6735935055
H,0.0448850581,-0.0431295565,2.2830688737
C,-2.3411598351,-0.9467473528,0.7138412778
C,-0.8700760371,-0.1784156531,-3.2194191
C,-2.8289631311,0.6570778474,-2.1044946413
C,-1.5276028451,-0.1624310551,-4.4381537475
C,-3.522751885,0.6362666254,-3.3067252776
H,-3.3090974119,1.0311012766,-1.2103565739
C,-2.8574225055,0.2347415018,-4.4593051814
H,-1.0250624695,-0.4702960228,-5.344400422
H,-4.5540887176,0.954965759,-3.367526451
N,-3.5824025042,0.2323811445,-5.7491288141
O,-4.7553320915,0.580774985,-5.7343238348
O,-2.9638430629,-0.1186331363,-6.7434771655
N,0.4995955102,-0.7456231983,-3.2131650808
O,0.7428989136,-1.5869168658,-2.3636088465
O,1.2551946618,-0.3759661549,-4.0960630536
H,-3.2303125215,-0.3162369083,0.8091477167
H,-2.538808468,-1.6913007341,-0.0613243492
H,-2.2104497913,-1.4732135315,1.6597213257

137H, B3LYP Energy= -906.160853235 Hartree,
NIMAG= 0

N,-0.837396926,0.4805810582,-0.8021361073
N,0.2178875463,1.3274930765,-0.6333406465
C,0.7325683625,1.1530383987,0.5924288295
C,0.0044768324,0.1589204587,1.2237825021
C,-0.975277864,-0.265238939,0.3224191613
C,-1.5271431361,0.3923111846,-2.0593305522
H,1.5672536491,1.74716767,0.9312211349
H,0.1661043097,-0.2267486076,2.2164373867
C,-1.9771763471,-1.3571679578,0.4444001806
H,0.4652905161,1.9972246992,-1.3504448081
C,-1.0116055663,-0.3315281762,-3.1476751696
C,-2.7314283638,1.078526946,-2.1940790214
C,-1.6902850674,-0.3666647399,-4.3562897889
C,-3.4346830161,1.0326517452,-3.3959752713
H,-3.1141215523,1.6510565582,-1.3578144147
C,-2.8974700395,0.3109336554,-4.4508128936
H,-1.2905022667,-0.9112545638,-5.2017955777
H,-4.3762279452,1.5509346352,-3.5217569201
N,-3.642781533,0.2595189343,-5.7475698472

O,-4.6965551828,0.8679105292,-5.7934540807
O,-3.1333596306,-0.3848501498,-6.6456905986
N,0.263964058,-1.0939202843,-3.0591003264
O,0.599393859,-1.4915025493,-1.9498823368
O,0.8693820516,-1.2708038544,-4.0958770601
H,-2.966593972,-1.0457710606,0.1045475449
H,-1.6621247628,-2.2162577772,-0.1559150267
H,-2.0503071113,-1.6753100845,1.4833240887

138, B3LYP Energy= -905.808186779 Hartree,
NIMAG= 0

N,0.9651254822,-0.257814204,-1.6944441371
N,2.0970474689,0.3984676269,-1.3032359498
C,2.9871351646,0.1195603712,-2.2354733154
C,2.4698288858,-0.7413443121,-3.2468054344
C,1.1731682981,-0.9604341549,-2.8599746564
C,-0.1588879913,-0.2279368371,-0.8579237523
H,3.9792276659,0.5427947867,-2.1645038166
C,3.1813767106,-1.2819367235,-4.4484265277
H,0.4096055443,-1.572220378,-3.3098290285
C,-1.4795651352,-0.3894330273,-1.3147180647
C,0.0388423778,-0.0721388306,0.5232716362
C,-2.5520233354,-0.4696480088,-0.4380185564
C,-1.0253073907,-0.101563668,1.4072386673
H,1.0513006561,0.0621495509,0.8764391053
C,-2.3112561786,-0.3180981822,0.9173674606
H,-3.5562047122,-0.6196968246,-0.8087924738
H,-0.8714200211,0.0173565455,2.4708674151
N,-3.4481980318,-0.3801025745,1.8558323783
O,-3.202307151,-0.2384428438,3.0465396964
O,-4.561622522,-0.5704866098,1.3848927309
N,-1.8270122632,-0.4013396704,-2.7532691605
O,-1.3286326493,0.4636612373,-3.4567486279
O,-2.6182792612,-1.255608573,-3.128822792
H,4.0813181514,-1.8339713292,-4.1629540625
H,2.539259353,-1.9583091568,-5.0152692145
H,3.4902235845,-0.4757766098,-5.1203140192

138H, B3LYP Energy= -906.158948669 Hartree,
NIMAG= 0

N,-0.5632181682,0.164597325,-0.8852250957
N,0.4390924575,1.0297626245,-0.5748049508
C,0.7633138597,0.8837906502,0.7139114207
C,-0.0869416456,-0.0640100671,1.2969234035
C,-0.9072471197,-0.4842036482,0.2569641198
C,-1.294862353,0.1874296494,-2.1214770723
H,1.5845830455,1.4442812604,1.1351920229
C,-0.0983380195,-0.5300651685,2.7205785219
H,-1.7091354017,-1.205590498,0.2504713997
H,0.9805273479,1.4211716046,-1.3459656239
C,-0.7215029792,-0.0731118197,-3.3798064194
C,-2.6728480818,0.3905253821,-2.037883891
C,-1.5078139036,-0.1442925443,-4.519815177
C,-3.4711524853,0.3364927693,-3.1762941613
H,-3.1216014268,0.6021243445,-1.0754962591
C,-2.8716113988,0.0701539055,-4.39695197
H,-1.0679232718,-0.3625890819,-5.4844329323
H,-4.5392061396,0.5024371842,-3.1244820409
N,-3.7172991735,0.0100453657,-5.6274382014
O,-4.9144216703,0.1703198808,-5.4729339895
O,-3.1387397652,-0.1950780127,-6.6788494244

N,0.7308721024,-0.2780789282,-3.5752455016
O,1.4919148029,0.4573899153,-2.9407972361
O,1.0744572599,-1.1263301229,-4.3642331008
H,-0.3897718412,0.2795081044,3.3938273531
H,-0.8027999976,-1.3508853011,2.8555350462
H,0.8899769252,-0.8802188812,3.0251566799

139, B3LYP Energy= -945.140677407 Hartree,
NIMAG= 0

N,1.3676527972,-0.6037557189,0.037883442
N,2.0252396715,0.2560482607,0.8766976918
C,3.3107181741,0.0454737125,0.658746728
C,3.5177403242,-0.9482998027,-0.3541912043
C,2.2565460615,-1.3309651925,-0.7207331038
C,-0.0277230091,-0.5541612401,-0.0239214643
C,4.3523377064,0.7943989749,1.4247393188
C,4.8253292787,-1.4449045153,-0.8868479225
H,1.9369092299,-2.0364372882,-1.4690097837
C,-0.8351945738,-1.6322663044,-0.4344839469
C,-0.6715506573,0.6530318567,0.298021772
C,-2.2067090358,-1.5000344933,-0.5969345952
C,-2.04357801,0.7863655493,0.1866759518
H,-0.0573924689,1.4798803862,0.624548385
C,-2.7982300072,-0.2889719977,-0.2784558534
H,-2.802803921,-2.3348049989,-0.9376890703
H,-2.5355883342,1.7174262104,0.4319961581
N,-4.2577006675,-0.1460000097,-0.4274163264
O,-4.7506208594,0.935161983,-0.1314303627
O,-4.883457414,-1.1145706718,-0.8385951516
N,-0.2981989538,-2.9957875263,-0.6376636368
O,0.4478152479,-3.438798404,0.2224166864
O,-0.6694857674,-3.5995018199,-1.6352613938
H,5.4246309812,-1.9100811243,-0.0979028165
H,4.674658473,-2.1891856477,-1.6707017755
H,5.421342342,-0.6296845302,-1.3086899901
H,3.8807563488,1.4905420365,2.1184148342
H,4.9873777016,0.1105731258,1.9962180128
H,5.0054511414,1.3596385898,0.752615417

139H, B3LYP Energy= -945.497850284 Hartree,
NIMAG= 0

N,1.371140771,-0.6675899442,-0.1202593222
N,2.0962081236,-0.5981657547,1.034450062
C,3.4017972792,-0.4848668871,0.7509158653
C,3.5337273917,-0.4060742397,-0.6524129713
C,2.2470112215,-0.5154316493,-1.1490658768
C,-0.0566718428,-0.5533950401,-0.1782135968
C,4.4455187612,-0.4828867709,1.8111544433
C,4.8065911422,-0.2627719554,-1.4274370463
H,1.8899286117,-0.5017845699,-2.1668923025
H,1.6482126248,-0.933760475,1.8865961588
C,-0.9429666631,-1.4907676183,0.3850675286
C,-0.5835893532,0.503290049,-0.9228755778
C,-2.3128838517,-1.3813411695,0.1984607029
C,-1.95640894,0.6324656375,-1.1074289729
H,0.0879252138,1.2357899667,-1.3526913028
C,-2.7961666993,-0.313149395,-0.5402741821
H,-2.9900531054,-2.1138843726,0.6181999588
H,-2.3744636027,1.4537759615,-1.6744867698
N,-4.2721043626,-0.1842312714,-0.7273634415
O,-4.6552242925,0.747103688,-1.4123844465

O,-4.9685030593,-1.020496948,-0.180889026
N,-0.4867263975,-2.6371000581,1.201103562
O,0.4278386552,-2.4293430032,2.0028178794
O,-1.0584371871,-3.6918316274,1.0522461485
H,5.4755814074,-1.1081075766,-1.2471869881
H,4.6077300491,-0.2174254679,-2.4983255617
H,5.3392242149,0.6489888266,-1.1457222719
H,4.0105870748,-0.5175379341,2.8103496329
H,5.1070106735,-1.3452486464,1.6901494676
H,5.0604168646,0.417078806,1.7316849432

140, B3LYP Energy= -945.135615815 Hartree,
NIMAG= 0

N,-0.7980092777,0.3457052383,-0.82182396
N,0.4221116335,0.9546953818,-0.8337549118
C,0.8323887458,0.895383736,0.4187931946
C,-0.0982304738,0.2384977369,1.2665125792
C,-1.1456326916,-0.1094447693,0.4359312411
C,-1.5012737948,0.2439814384,-2.0334501252
H,1.7871787119,1.3253793521,0.6868046362
C,0.040728398,-0.0209092976,2.7361511598
C,-2.3920715518,-0.8789039506,0.7309473327
C,-0.8633193805,-0.1746217538,-3.2116256086
C,-2.8414583658,0.6370655507,-2.1124840435
C,-1.5104982652,-0.163226142,-4.4357954336
C,-3.5239568384,0.6106968169,-3.3204524544
H,-3.3348409656,1.002856961,-1.22221428
C,-2.8442339291,0.2200965822,-4.4688722881
H,-0.9971129954,-0.4658464214,-5.337695348
H,-4.5582563338,0.9178720086,-3.3894196566
N,-3.5569569383,0.2133883977,-5.7642184824
O,-4.7344947333,0.5474312419,-5.759498122
O,-2.9254617986,-0.1265663673,-6.7546355673
N,0.5092138886,-0.7346783817,-3.1955357514
O,0.7474852134,-1.583425895,-2.3518292694
O,1.2723495122,-0.3545175213,-4.0675190072
H,-3.2525883605,-0.2280680949,0.9183543973
H,-2.6539096396,-1.5556197218,-0.0855236884
H,-2.2430310982,-1.4814096378,1.6283602728
H,-0.445492607,0.7557324378,3.335920558
H,-0.4015108888,-0.9789114391,3.0218477495
H,1.0933930243,-0.046723787,3.0257413766

140H, B3LYP Energy= -945.493127320 Hartree,
NIMAG= 0

N,-1.4508172335,-0.5494994144,-0.6897344464
N,-2.0363922384,0.0331213048,-1.7713912414
C,-3.3709939758,-0.0695093449,-1.654312021
C,-3.6670840275,-0.7102293589,-0.4597685629
C,-2.4270697548,-0.9933855903,0.1394390266
C,-0.0277769509,-0.4980622968,-0.5031307673
H,-4.0205459147,0.3119039544,-2.4273587578
C,-5.022487138,-1.0182972695,0.0984738533
C,-2.1488807991,-1.6027224352,1.4663999703
H,-1.47802115,0.3806894229,-2.53962646
C,0.625277407,0.6511076967,-0.0261858123
C,0.717752105,-1.6247552159,-0.8413095765
C,2.005274419,0.674091465,0.1082483704
C,2.1026761755,-1.6226754138,-0.6897610658
H,0.2104706737,-2.5014257293,-1.2253943011
C,2.7158438814,-0.4718941099,-0.2185910519

H,2.5131885538,1.5616987352,0.4621438775
H,2.7014243087,-2.4889999841,-0.9385114797
N,4.203122503,-0.4572825626,-0.0569608831
O,4.7935769881,-1.4783675201,-0.3600246219
O,4.6977682314,0.5726991057,0.3626784471
N,-0.1168762347,1.882673828,0.3610324294
O,-1.2811025784,1.7451967448,0.715441251
O,0.4939720332,2.9301428694,0.3038137445
H,-2.8312157913,-2.4351227697,1.6466596209
H,-1.1251211961,-1.9659451654,1.5508387136
H,-2.3148140479,-0.8595935641,2.2530280901
H,-5.1444493716,-2.0897805531,0.2750734918
H,-5.1829527809,-0.5012850275,1.0477369639
H,-5.80556662,-0.7023032014,-0.5906786014

141, B3LYP Energy= -945.139933651 Hartree,
NIMAG= 0

N,-1.5090253262,0.6292416239,0.0506536682
N,-2.2182028874,-0.5317518652,0.2132130615
C,-3.4864317503,-0.1619703944,0.2576290414
C,-3.6090388096,1.2478228276,0.1087914667
C,-2.3310879296,1.7346857906,-0.0245051121
C,-0.1125953254,0.5441514419,-0.0587436259
C,-4.5727334516,-1.1725655005,0.4434177475
H,-4.5177362138,1.8285159653,0.0824664014
C,-1.8526362297,3.1293648078,-0.269634668
C,0.4957637719,-0.4209830798,-0.8775649917
C,0.7140587031,1.3702342055,0.7106529676
C,1.8688690232,-0.5968995972,-0.9034739556
C,2.0951634887,1.2440495094,0.6634431352
H,0.2616045393,2.0875797845,1.3816440135
C,2.6537412552,0.2533362118,-0.1364912891
H,2.3189462349,-1.3611370075,-1.5214903189
H,2.7384898168,1.8761365025,1.2596875363
N,4.1228345236,0.094616797,-0.1714691677
O,4.787819718,0.8667032922,0.5068166651
O,4.5786889916,-0.7953669307,-0.8755735035
N,-0.2927798256,-1.2445359971,-1.8247956443
O,-1.0998507092,-0.656201156,-2.5258528442
O,-0.0280117685,-2.433919815,-1.8781753213
H,-4.1447335357,-2.1725655601,0.5162449797
H,-5.1477972161,-0.9713054994,1.3518284356
H,-5.2693998489,-1.1537425394,-0.3995886269
H,-1.4484468634,3.5978827137,0.6328758558
H,-1.0786764973,3.1624631098,-1.040471257
H,-2.690139178,3.740170459,-0.6080054496

141H, B3LYP Energy= -945.499132370 Hartree,
NIMAG= 0

N,-1.4986780593,0.5969776783,0.1562679852
N,-2.2741289067,-0.4693754023,0.5187008489
C,-3.5768011019,-0.1498506213,0.4141164844
C,-3.6298536461,1.1623658477,-0.055583331
C,-2.3224876613,1.606228683,-0.2282422905
C,-0.073231495,0.4797805339,0.0524519355
C,-4.6628051309,-1.1105339081,0.7546833244
H,-4.5226353641,1.729565626,-0.2613180058
C,-1.8127285089,2.8901292552,-0.7796618789
H,-1.8510554727,-1.3088744056,0.8927925728
C,0.5481332788,-0.1953450806,-1.0118806044
C,0.7075618343,1.0337661538,1.0641623438

C,1.9280753352,-0.3215635229,-1.0615769362
C,2.0964699451,0.9382423848,1.0135084487
H,0.2235900232,1.5339820966,1.8941589777
C,2.6760723511,0.2605955493,-0.048306373
H,2.4085729039,-0.8542457757,-1.8717882912
H,2.7224745707,1.3685679206,1.7840654469
N,4.1662337953,0.1450215763,-0.1075351996
O,4.7894753894,0.6678294707,0.798810999
O,4.631021822,-0.4616520852,-1.0551071738
N,-0.2306228966,-0.7923872574,-2.130483555
O,-1.3075253526,-0.2746685054,-2.3996345128
O,0.267331074,-1.7433968649,-2.6982317299
H,-4.2885684914,-1.9654663627,1.319697589
H,-5.4342341265,-0.6138151773,1.345028542
H,-5.12966552,-1.4827237967,-0.1615589621
H,-1.03619866,3.3274376525,-0.1491464866
H,-1.3936734471,2.7278601365,-1.7773190443
H,-2.6308833721,3.6036406823,-0.8658921794

142, B3LYP Energy= -984.467850300 Hartree,
NIMAG= 0

N,-0.7348015158,0.1641108604,-0.8364122764
N,0.5789669563,0.5408454886,-0.872871361
C,0.9996963163,0.450063246,0.3751021467
C,-0.0385342812,-0.004780004,1.2467902151
C,-1.1412146783,-0.1820673023,0.4396037786
C,-1.451767666,0.1449611623,-2.0397679468
C,2.4062034519,0.8020140093,0.7378242036
C,0.0830299527,-0.2444114423,2.7201488811
C,-2.5031999368,-0.706720944,0.7625705568
C,-0.8929649972,-0.3916717498,-3.2119307568
C,-2.7182634687,0.7355654769,-2.1269210144
C,-1.5368847921,-0.3068288218,-4.4345961769
C,-3.4025127172,0.788120406,-3.3324035517
H,-3.145070301,1.1938776928,-1.2453631106
C,-2.7968104969,0.274932964,-4.4745367797
H,-1.0808373384,-0.7043283904,-5.3304764173
H,-4.3778042701,1.2489725041,-3.4056880087
N,-3.5076204435,0.3509789461,-5.7668595916
O,-4.6205116192,0.8615927433,-5.7679051834
O,-2.9409950248,-0.101690934,-6.7519705714
N,0.3743295633,-1.160069077,-3.1874539899
O,0.4778731441,-2.0248325635,-2.3326130534
O,1.1869489205,-0.9174798693,-4.0642127287
H,2.9543556242,1.1143233103,-0.1511485732
H,2.4359709472,1.6143066374,1.4706781725
H,2.9231183047,-0.0555907626,1.1796800234
H,-3.2393168404,0.0912214335,0.9050240785
H,-2.8752067233,-1.3703016108,-0.0214184223
H,-2.463618689,-1.2800742567,1.6894600846
H,0.9056222726,-0.9301218556,2.9455548048
H,0.2814640281,0.6862611388,3.262308511
H,-0.8293744822,-0.6752688356,3.1366629574

142H, B3LYP Energy= -984.830339002 Hartree,
NIMAG= 0

N,-1.2364303789,-0.5078288494,-0.2378160528
N,-1.9267550694,0.046597593,-1.2765266412
C,-3.2490327142,-0.003682077,-1.0254162196
C,-3.4152817982,-0.5747674552,0.2417168055
C,-2.1326076318,-0.8655073562,0.7188936525

C,0.1949576277,-0.4450304738,-0.1857658646
C,-4.2563216689,0.4908472991,-2.0050893055
C,-4.7117766869,-0.7923011593,0.9607332584
C,-1.7131630627,-1.393738974,2.0441095638
H,-1.4518210957,0.2910304584,-2.1355943235
C,0.8801675692,0.7411825914,0.1254221122
C,0.9185416621,-1.5957027592,-0.4898682979
C,2.2660585635,0.7818848256,0.1259362358
C,2.3113599252,-1.5782123594,-0.4655121182
H,0.3867293863,-2.5028103333,-0.7499563212
C,2.9546239782,-0.3884994238,-0.1593528447
H,2.7958591278,1.6987436471,0.3488518548
H,2.8932478699,-2.4625690986,-0.6893193437
N,4.4495693916,-0.3575158273,-0.1384966434
O,5.0202899283,-1.4007084569,-0.4022495673
O,4.9716335008,0.7065891929,0.1398483878
N,0.1622339646,1.9958777369,0.4748536684
O,-0.9240730273,1.8819355131,1.028634892
O,0.7158833475,3.0399138768,0.1936801884
H,-3.7912188832,0.8156179935,-2.9368782012
H,-4.9802247649,-0.2937451079,-2.2367958802
H,-4.8054921545,1.3373823377,-1.5849932991
H,-0.7916792618,-1.9737066867,1.9854605292
H,-1.5501860115,-0.561981787,2.7372306762
H,-2.496238899,-2.0274969026,2.4601495935
H,-4.9036284632,0.0072979228,1.6818743263
H,-5.549102381,-0.8164140654,0.2621967345
H,-4.7103838899,-1.7382278353,1.5053784449

143, B3LYP Energy= -1178.62783542 Hartree,
NIMAG= 0

N,-0.2081841623,-0.3716287375,-0.2171242952
N,0.5573357287,0.7806619784,-0.3299362698
C,1.785324873,0.3391302707,-0.2260080071
C,1.8717096284,-1.0662137155,-0.0232558657
C,0.5848528496,-1.5034196555,-0.0222671793
C,-1.5960180067,-0.2503625042,-0.1722913721
C,3.1823930177,0.898764369,-0.3022522259
C,3.3383043011,-1.3966812558,0.0342561355
H,0.1516126839,-2.477167225,0.1275860299
C,3.8852346072,-0.0903466493,0.7352107619
C,3.8486287441,-1.2074788856,-1.4304055816
H,4.8814340308,-1.5481000688,-1.5262819338
H,3.2482490088,-1.7836595213,-2.1352446963
C,3.7284014892,0.331782966,-1.6608936282
H,4.697463955,0.7818137246,-1.8879234147
H,3.0563653936,0.5813067534,-2.4837908104
H,3.6208023317,-2.3409881856,0.4992268424
C,3.3959298876,0.0786749942,2.1823108166
H,3.820020573,-0.7048480925,2.8177398239
H,3.7251430173,1.0392500374,2.5889646365
H,2.3101570842,0.0305676309,2.2754079599
C,5.4183012788,0.0070481544,0.7517138392
H,5.7338661296,0.9579822749,1.1904311352
H,5.8344634697,-0.7892522761,1.3765621085
H,5.8799592148,-0.0716263808,-0.2317967841
C,3.3505342193,2.3949015092,-0.1089605213
H,2.8191395033,2.9466521231,-0.8892222137
H,2.9511172678,2.7216349558,0.8545361299
H,4.4050599767,2.679162739,-0.1579912824
C,-2.4894626036,-1.2863433271,-0.5140894706
C,-2.1542575309,0.9603607421,0.2783826279

C,-3.8600832171,-1.1610086093,-0.3378549745
C,-3.5210229651,1.1161712338,0.4129365899
H,-1.4769705578,1.7637940356,0.5291268445
C,-4.3638784284,0.044393472,0.1211872882
H,-4.521755523,-1.9797780482,-0.5829923743
H,-3.9441699792,2.0474664496,0.7634375366
N,-5.8187956239,0.1930745181,0.2902268789
O,-6.2321704977,1.2751600272,0.6890024402
O,-6.5238643789,-0.7722947332,0.0239734159
N,-2.0454646649,-2.5372149907,-1.1660809215
O,-2.5272045117,-3.5845766493,-0.7549800373
O,-1.2589483138,-2.4375620482,-2.0962934817

143H, B3LYP Energy= -1178.99056493 Hartree,
NIMAG= 0

N,-0.2421004347,-0.5350802314,-0.1459906876
N,0.6037222956,0.4266253315,-0.6708683718
C,1.8449862547,0.1369697524,-0.3043521384
C,1.8327288089,-0.9916424431,0.5325852745
C,0.523912543,-1.3902730016,0.6186565316
C,-1.6565374265,-0.3496272116,-0.0377049239
C,3.2574267562,0.5544333107,-0.5842814416
C,3.2800910999,-1.3117275132,0.8121984766
H,0.0432061898,-2.2034196991,1.1392180382
H,0.236093747,0.994178626,-1.4331365646
C,3.8812590524,0.1487151691,0.835074939
C,3.8261226196,-1.8684660927,-0.5413657761
H,4.8415427773,-2.2431082884,-0.4135924773
H,3.221143911,-2.697255263,-0.9102829939
C,3.78597623,-0.6297841771,-1.48531808
H,4.7779489771,-0.3663998385,-1.8541530425
H,3.1514531004,-0.7799767619,-2.3606775913
H,3.4840130336,-1.9300114644,1.6840706468
C,3.3756970758,1.0064442364,2.0059407679
H,3.7494179736,0.6047364697,2.9512815578
H,3.7488208528,2.0299562067,1.9220237963
H,2.2870349109,1.0552056992,2.0783937483
C,5.4154126184,0.1858112675,0.8594197495
H,5.769619177,1.2188218032,0.8249730516
H,5.777225963,-0.2453500351,1.7966571881
H,5.8914845032,-0.3550118961,0.0432164223
C,3.4976029862,1.9515679893,-1.1280537072
H,3.0421574499,2.078972168,-2.1145746809
H,3.0951665316,2.7211687756,-0.4649957999
H,4.5676571372,2.1332465387,-1.2440666592
C,-2.5201156108,-0.2653577836,-1.1471028646
C,-2.2176593397,-0.354210137,1.2417226166
C,-3.8957972561,-0.1979754115,-0.9837785217
C,-3.5945405287,-0.2765502046,1.4218518386
H,-1.5657679233,-0.4099392762,2.1042612539
C,-4.4092762507,-0.1959560196,0.3031069742
H,-4.5546926831,-0.1513333659,-1.8409549953
H,-4.0343995651,-0.2698889826,2.4104060543
N,-5.8878199107,-0.1064115078,0.4818198252
O,-6.3026414726,-0.1431584669,1.6268323158
O,-6.5580688178,-0.0045446915,-0.530277229
N,-2.0304160916,-0.249952075,-2.5419647662
O,-2.664355622,-0.8714339485,-3.3637656001
O,-1.0229739086,0.4208791233,-2.7808225347

144, B3LYP Energy= -1178.61780481 Hartree,
NIMAG= 0

N,0.2285848365,1.0801473339,0.4025685042
N,0.4445819043,2.4314109213,0.5672556799
C,1.7670819929,2.5773535353,0.5829942325
C,2.4169720807,1.3427741165,0.3882701372
C,1.4165366656,0.4105017643,0.2725889471
C,-1.105926928,0.6506611723,0.2817096166
H,2.1785447825,3.5664800206,0.7225301633
C,3.7239238183,0.6023949857,0.2440515378
C,2.0295722976,-0.9615345017,0.030512488
C,3.2999323793,-0.4811336997,-0.8177297156
C,3.8640313058,-0.2602980612,1.5394455412
H,4.8455979029,-0.7363521968,1.5901860723
H,3.7516547352,0.3533701738,2.4339284153
C,2.7223794179,-1.3138811682,1.397294259
H,3.1163772622,-2.3320289454,1.3570962337
H,2.013264125,-1.2737882849,2.2233223652
H,4.6027753707,1.1964722812,-0.0079657607
C,2.9517721016,0.1029562894,-2.1962553404
H,3.8500238626,0.5190993549,-2.6625760144
H,2.5763180637,-0.6789097504,-2.8634436297
H,2.2054096631,0.8961914314,-2.1494898416
C,4.3553625683,-1.5761592047,-1.0428638101
H,3.9876227279,-2.3288102216,-1.7461094864
H,5.2508651605,-1.1329012552,-1.4894890262
H,4.6636614571,-2.0926668145,-0.1353225864
C,1.1811306018,-2.0659065408,-0.5805949403
H,0.4044632564,-2.4188873285,0.1010353602
H,0.6988718341,-1.7390956302,-1.5058963277
H,1.8058900293,-2.9309615427,-0.8177079335
C,-1.9433214273,1.3397235838,-0.6056437835
C,-1.6494705719,-0.4316479424,0.9928413401
C,-3.2562201628,0.9458717433,-0.8058289631
H,-1.5307280374,2.1872684735,-1.1356028391
C,-2.9497928423,-0.8684075341,0.7753812158
C,-3.7367835543,-0.1694838136,-0.1244770079
H,-3.9033074372,1.4737742063,-1.4926730461
H,-3.3443562499,-1.7151456435,1.3185514517
N,-5.1289127516,-0.6141947561,-0.3488358264
O,-5.515221575,-1.5970108211,0.2683475516
O,-5.8031417891,0.0305607386,-1.1407063173
N,-0.9162271637,-1.1061575213,2.0869666138
O,-1.0961869518,-2.3097713581,2.2197338446
O,-0.2150559614,-0.4132454898,2.8068980249

144H, B3LYP Energy= -1178.98630938 Hartree,
NIMAG= 0

N,0.2826496602,0.9535322814,0.6123520447
N,0.5747990657,2.2361211163,1.0341147247
C,1.9286068985,2.3866367412,1.0762880308
C,2.4993517326,1.2391077842,0.5799498856
C,1.4450605195,0.3623110285,0.2932155868
C,-1.0713756935,0.5321343961,0.379053692
H,2.3478529856,3.3089792859,1.4491242973
C,3.7694087008,0.4894246797,0.271344591
C,1.9991532459,-0.9489434882,-0.2003343005
H,-0.0919629068,2.6786377438,1.6575572486
C,3.2852997631,-0.3700856402,-0.960786012
C,3.8732656309,-0.5850307914,1.3991894267
H,4.8241647761,-1.1137203316,1.3351723787
H,3.820651233,-0.1350815431,2.3908108188
C,2.6705810822,-1.5310853663,1.1059631923
H,2.9958567472,-2.5518934206,0.9017450368

H,1.9602038552,-1.5841992485,1.9328465144
H,4.6641923975,1.089242169,0.1172764253
C,2.9461706702,0.4685341053,-2.2026670689
H,3.8558444343,0.9143747622,-2.6125714848
H,2.515994767,-0.1593222272,-2.9872497161
H,2.2478362375,1.2847527933,-2.0031595902
C,4.2840915576,-1.454089365,-1.3881480655
H,3.8843939675,-2.0340879687,-2.2234794944
H,5.2056111144,-0.9822300421,-1.7396609458
H,4.5540461701,-2.1529325206,-0.5981218738
C,1.0912626534,-1.9121563284,-0.9447778675
H,0.2610254261,-2.2511468512,-0.3193793391
H,0.6768815728,-1.4668715266,-1.8522182859
H,1.6530810226,-2.8006540324,-1.2388696335
C,-1.5587062298,0.5410947824,-0.9253935563
C,-1.89053764,0.0603394784,1.4154874472
C,-2.8464445639,0.08647365,-1.197675362
H,-0.9263298937,0.903588908,-1.7259412015
C,-3.1649324888,-0.4208461483,1.1602828581
C,-3.6211781873,-0.3876007923,-0.1493573521
H,-3.2480532282,0.0932356502,-2.202312459
H,-3.7887075476,-0.804358751,1.9571848944
N,-5.0016299376,-0.8846321587,-0.4342251374
O,-5.6547809571,-1.2655529089,0.5203916878
O,-5.3581890357,-0.8686427612,-1.5988308171
N,-1.4343922532,0.070450751,2.8234537455
O,-1.750175223,-0.8710911556,3.5192270952
O,-0.7831784022,1.0482201151,3.183055929

145, B3LYP Energy= -1071.01911829 Hartree,
NIMAG= 0

N,-0.6776511223,0.0381693434,-0.8261110095
N,0.6238152792,0.4485424639,-0.8662507834
C,1.0476430779,0.3276788142,0.3773976105
C,0.0366583728,-0.1735191609,1.2395827715
C,-1.0576647319,-0.3476309775,0.4363394675
C,-1.4199060782,0.0244100766,-2.0103009807
H,2.0615276439,0.6066988144,0.6221005158
H,0.1073922498,-0.3832592505,2.2938679415
H,-2.0448595344,-0.7268436459,0.645534659
C,-0.8786875268,-0.4875703981,-3.200829176
C,-2.7266840909,0.5296977011,-2.0891928164
C,-1.5645890701,-0.4613607938,-4.4025759594
C,-3.4720473749,0.5007015058,-3.2570146473
C,-2.8658037083,0.0211496375,-4.4072057865
H,-1.110894604,-0.8380980116,-5.3090585514
H,-4.4862350014,0.8750867819,-3.2800330824
N,-3.630761085,0.0208033561,-5.6761478701
O,-4.7740342449,0.4496300586,-5.6376628638
O,-3.0636064181,-0.408502907,-6.6688306725
N,0.4350896089,-1.1823137196,-3.2136123925
O,1.2174777418,-0.8544419383,-4.087228385
O,0.5910983098,-2.0696913436,-2.3936886495
N,-3.3651546668,1.1945580279,-0.9245378281
O,-4.492308,0.8207303033,-0.6360671526
O,-2.7356175262,2.0783552621,-0.3722816586

145H, B3LYP Energy= -1071.35856230 Hartree,
NIMAG= 0

N,-0.6868836901,0.0161410136,-0.8347269687
N,0.2629495571,0.9466183345,-0.5403241269

C,0.8144907535,0.6493016157,0.6440018165
C,0.2457645637,-0.5315691625,1.1067490887
C,-0.6873898046,-0.9052893809,0.152265518
C,-1.4165690325,0.0227159866,-2.0693182642
H,1.5639525186,1.293057377,1.0788314921
H,0.4858409639,-1.0557000806,2.0164887012
H,-1.3256368632,-1.7722453787,0.0917891585
H,0.2776491279,1.829819954,-1.037775304
C,-0.9625899272,-0.6738053371,-3.1978476411
C,-2.6309256156,0.7143711302,-2.1743730241
C,-1.6832874518,-0.6814728493,-4.3845714787
C,-3.396933023,0.6825862038,-3.3298389326
C,-2.8969259974,-0.0145417177,-4.4182499098
H,-1.3111154815,-1.2006037782,-5.2590078773
H,-4.3489419308,1.195791078,-3.3863350053
N,-3.6973753663,-0.0399927757,-5.6852681499
O,-4.7420000595,0.5825292315,-5.67587789
O,-3.2297951207,-0.6807498656,-6.6067706919
N,0.3197388838,-1.4344846539,-3.1842578155
O,0.9750614353,-1.3936971962,-4.2039499591
O,0.5953588737,-2.0410230751,-2.1599568698
N,-3.1312059502,1.5404356949,-1.044105064
O,-4.32218348,1.5100754221,-0.8281682634
O,-2.2920626886,2.2005807565,-0.4424622449

146, B3LYP Energy= -378.964816385 Hartree,
NIMAG= 0

N,0.0774198688,-0.0876368702,0.000203727
N,0.921364307,-1.1612432253,0.0002543921
C,2.1305384453,-0.6340542723,0.0000210845
C,2.0928775221,0.7889651138,-0.0001275962
C,0.7613021018,1.1041377577,-0.0000041425
C,-1.3360685375,-0.239033913,0.0003767125
H,2.9954120226,-1.2814770312,-0.000122288
H,2.9255704993,1.4730452176,-0.000305005
H,0.2312823409,2.0413496365,-0.0000503448
O,-2.034538954,0.7457064036,0.0004114745
C,-1.8380535154,-1.6565605358,0.0006911849
H,-1.4680972071,-2.1928192404,-0.8752649822
H,-1.467806779,-2.1925366234,0.8766987775
H,-2.9257332148,-1.6313204176,0.0008697467

146H, B3LYP Energy= -379.307318962 Hartree,
NIMAG= 0

N,0.0795782287,-0.1051925632,0.0003160016
N,0.9878618326,-1.1179440353,0.0002814006
C,2.2266909788,-0.6061549969,-0.0000159666
C,2.1200092595,0.7826129677,-0.000193898
C,0.7629863993,1.0622228649,0.0000098739
C,-1.408769734,-0.2528369893,0.0006180143
H,3.092686702,-1.2510049933,-0.0000817892
H,2.9295933587,1.4932424683,-0.0004430199
H,0.222440302,1.9960870896,-0.0000260714
H,0.6988529912,-2.0875129605,0.0004703819
O,-2.0255382109,0.7594480934,0.0003800591
C,-1.913007474,-1.6605970347,0.0006945254
H,-1.5787884425,-2.1989378942,-0.8918989218
H,-1.5788070682,-2.1988065381,0.8933732561
H,-3.0008048207,-1.6276399605,0.0006802119

147, B3LYP Energy= -430.790394781 Hartree,
NIMAG= 0

N,-0.6271007146,-0.0000001483,-0.8342931765
N,0.7176109364,0.0000001486,-0.8915423798
C,1.0804509731,0.0000002222,0.3783662212
C,-0.0401266379,-0.0000000294,1.2594288068
C,-1.1381354494,-0.0000002674,0.442792279
N,-1.4061383658,-0.000000314,-2.0401224747
H,2.1309476017,0.0000004526,0.6284767869
H,-0.0354647389,-0.0000000337,2.3371100585
H,-2.1981014103,-0.0000005021,0.6252084896
O,-0.7983940538,-0.0000001748,-3.0768252439
O,-2.6085949406,-0.0000005802,-1.8594707672

147H, B3LYP Energy= -431.120976512 Hartree,
NIMAG= 0

N,-0.678995078,-0.0000001598,-0.8225906062
N,0.6693353543,0.0000001377,-0.845597744
C,1.1108853349,0.0000002287,0.4208444039
C,0.0020863055,-0.0000000201,1.2689264835
C,-1.1200059455,-0.0000002635,0.4513134377
N,-1.4782990512,-0.0000003295,-2.1398097258
H,2.1690882319,0.000000461,0.6364863193
H,0.0118847214,-0.0000000234,2.346630658
H,-2.1765969957,-0.0000004976,0.6727393441
H,1.1670567299,0.0000002519,-1.7321181207
O,-0.7702996227,-0.0000001685,-3.0977010869
O,-2.6488648039,-0.0000005885,-1.968046302

148, B3LYP Energy= -281.607262725 Hartree,
NIMAG= 0

N,-0.7357363551,-0.1329657207,-0.7794792329
N,0.5971191838,-0.3160259414,-0.8760376936
C,1.0409416427,-0.1698341251,0.3708761527
C,-0.0097051187,0.108822993,1.2724125276
C,-1.1456821379,0.1244605558,0.4882392708
N,-1.5799180955,-0.2063752256,-1.8875010878
H,2.0963822246,-0.2691968903,0.576256714
H,0.0517120369,0.2729589952,2.3355653454
H,-2.1866852563,0.2912757541,0.7084268933
H,-1.2699708601,0.4831832034,-2.5674529318
H,-1.4712680645,-1.1263464983,-2.3066798576

148H, B3LYP Energy= -281.960572688 Hartree,
NIMAG= 0

N,-0.7489391727,-0.1372376243,-0.8170469517
N,0.6089391567,-0.3102315531,-0.8314981035
C,1.081838893,-0.1674274138,0.4167517571
C,0.0089435973,0.1037138555,1.2572331062
C,-1.1224799632,0.1153251442,0.4500901291
N,-1.5648264778,-0.2130907777,-1.9177326619
H,2.1363277681,-0.2662994658,0.6251662003
H,0.0473054188,0.2712029157,2.3203921433
H,-2.1644781963,0.2825606559,0.672938812
H,1.0986122756,-0.5118929582,-1.6951334134
H,-1.386194131,0.5248092671,-2.5908243558
H,-1.5960949133,-1.1439166898,-2.3202805473

148c, B3LYP Energy= -281.925371876 Hartree,
NIMAG= 0

N,0.5518430836,0.0825915181,0.203907186
N,-0.0787852496,-1.1196450257,0.140776219
C,-1.3506679445,-0.7944966033,0.0104606662
C,-1.5330454592,0.6160172056,-0.0985881934
C,-0.2818295686,1.1620804813,-0.0292888968
N,1.9411695107,0.0061918954,-0.0738595597
H,-2.1024836283,-1.5694994696,0.0045806331
H,-2.4638123283,1.1517237541,-0.1926886521
H,0.0706840713,2.181897808,-0.0430970037
H,2.2338397149,-0.9313083164,0.2455679281
H,2.1554467444,0.0879111767,-1.0802423256
H,2.4627520536,0.7186285758,0.4527009989

149, B3LYP Energy= -685.837136485 Hartree,
NIMAG= 0

N,0.0140599831,-1.0719845757,0.
N,1.1544437723,-0.3726225575,0.
C,0.7452797751,0.8956711985,0.
C,-0.6626407245,0.996956048,0.
C,-1.1131752689,-0.3072251364,0.
Cl,0.0561505902,-2.7795815713,0.
H,1.4812367949,1.6851898013,0.
H,-1.2671474449,1.8889980483,0.
H,-2.0966514773,-0.7454697553,0.

149H, B3LYP Energy= -686.180478417 Hartree,
NIMAG= 0

N,0.,0.6730642322,-0.871125183
N,0.,-0.6811461669,-0.8735605152
C,0.,-1.1134448041,0.3998015204
C,0.,-0.0017057624,1.2318181279
C,0.,1.1142004666,0.4008177602
Cl,0.,1.558786444,-2.3162022285
H,0.,-2.1696348947,0.6222469234
H,0.,0.0017012488,2.3092694277
H,0.,2.1709741417,0.6173382767
H,0.,-1.1988977053,-1.7457255095

150, B3LYP Energy= -453.783671521 Hartree,
NIMAG= 0

N,0.0551863791,-1.1688505513,-0.2124868168
N,1.2158970782,-0.4468693207,-0.2261574839
C,0.8503750503,0.8213463478,-0.2927851004
C,-0.5649050935,0.9367595512,-0.3051949692
C,-1.0567819406,-0.3465866663,-0.2455727245
C,0.1774853092,-2.5847792902,-0.041236631
C,1.872606417,1.9123459981,-0.3499767815
H,-1.1528443494,1.8410416951,-0.3376843846
C,-2.4852883478,-0.7876667746,-0.1775215385
N,1.1741222697,-3.1535903102,0.4962397199
H,1.8420823967,-2.4623046199,0.8301072316
N,-0.9231109859,-3.2998535833,-0.4892804011
H,-1.3068184715,-3.0092415962,-1.3777665649
H,-0.7553666581,-4.2957275762,-0.4372150289
H,1.7379500038,2.6211744658,0.4722253648
H,2.8749604076,1.4883258642,-0.2829279949
H,1.7962941283,2.4753452129,-1.2849523469

H,-2.8348851663,-1.2194792528,-1.1204481198
H,-2.6471191108,-1.5328175516,0.6023169145
H,-3.1082529163,0.0827479582,0.0330949564

150H, B3LYP Energy= -454.149699691 Hartree,
NIMAG= 0

N,0.0212095812,-1.1791210454,-0.2001492952
N,1.1605022151,-0.4285219206,-0.210363811
C,0.8586728437,0.8763183155,-0.3394848135
C,-0.5340688205,0.9610573583,-0.3657407279
C,-1.0439217026,-0.3319480903,-0.2688605232
C,0.1159216204,-2.611882443,0.1235666166
C,1.9044695365,1.9300889377,-0.4566707958
H,-1.1154722946,1.8660155634,-0.4336964453
C,-2.4623419285,-0.7843078085,-0.2051326157
H,2.0645173911,-0.8845613936,-0.2393581288
N,0.8089212796,-3.0635866217,1.0766533425
H,1.1744492507,-2.3632451902,1.7152701905
N,-0.6582965631,-3.3607900828,-0.7067076004
H,-0.7631368786,-3.0883623188,-1.6730072583
H,-0.6419068004,-4.3560434305,-0.5259854712
H,2.8721786696,1.5845375586,-0.0901184276
H,2.0192158507,2.2324674104,-1.5015672497
H,1.611708433,2.812186117,0.1144868532
H,-2.7910964967,-1.1847347155,-1.1677890473
H,-2.6044191832,-1.563206374,0.5452154418
H,-3.0985770035,0.0650494739,0.0412618664

150c, B3LYP Energy= -454.174958817 Hartree,
NIMAG= 0

N,0.0276855491,-1.2031083554,-0.1979707694
N,1.2132650786,-0.4824744231,-0.1320389343
C,0.8624803814,0.7792727407,-0.2083156444
C,-0.563623099,0.9083680286,-0.3259110474
C,-1.0862449527,-0.3462763425,-0.3188773655
C,0.1497114952,-2.5617903211,-0.1354217296
C,1.8729954558,1.8736649394,-0.1706885272
H,-1.1243104094,1.8264173098,-0.405584551
C,-2.5137397697,-0.7749902191,-0.4154561537
N,1.3738944922,-3.0530065848,-0.0198308182
H,2.1383790845,-2.3862760416,0.0146017542
H,1.5543375559,-4.0433975294,0.0330897342
N,-0.9167072954,-3.3592978567,-0.1884644702
H,-1.849984324,-2.9932962364,-0.2760945753
H,-0.8117040955,-4.361452925,-0.1412742949
H,1.6794981984,2.5420903477,0.6725935843
H,2.8787619658,1.4666036679,-0.0752695174
H,1.8185405296,2.4740155063,-1.0828271079
H,-2.7079645943,-1.3821567146,-1.3063697904
H,-2.8495030325,-1.312994702,0.4778227742
H,-3.1395155138,0.1128531115,-0.4994629499