Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Study of Heavy Atom Influence on Poly-halogenated Compounds using DP4/MM-DP4+/DP4+: Insights and Trends

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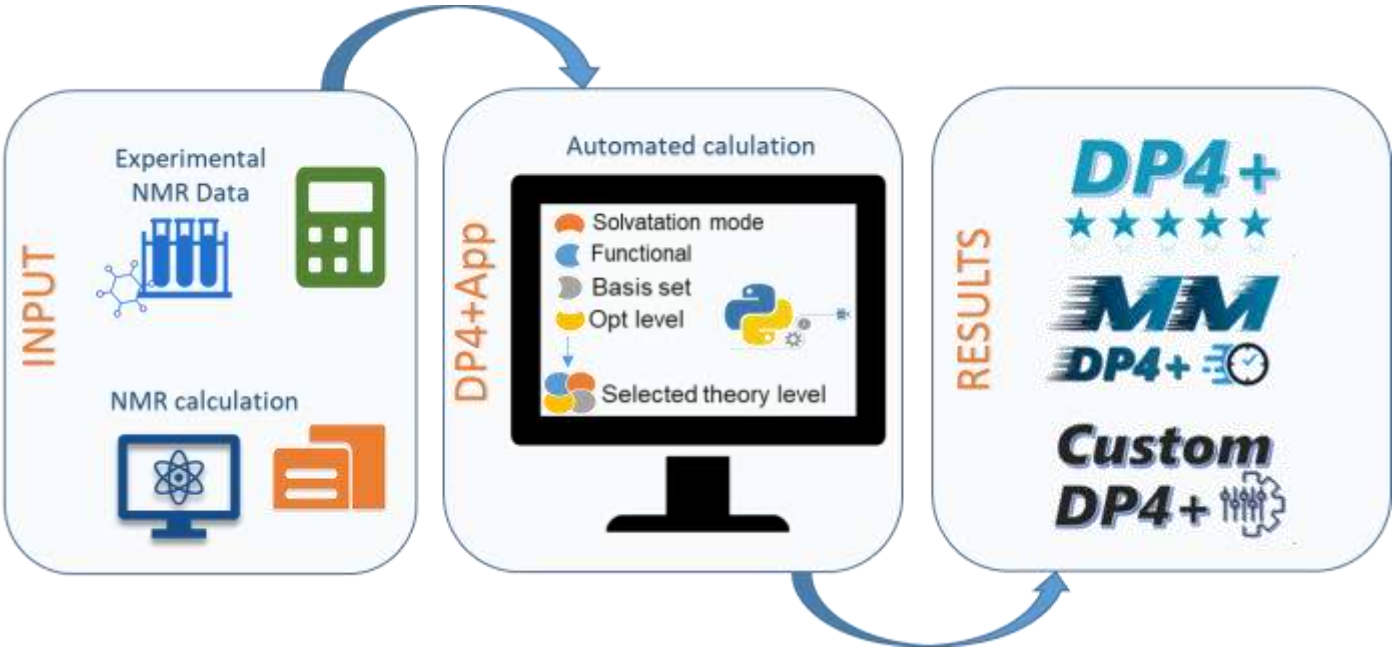
Computational Details

All the DFT calculations were performed using Gaussian 09.[1] For all compounds under study the conformational searches were done in using the MMFFaq force field (implemented in Spartan 14.2).[22] We carried out systematic conformational searches, and all conformers within a 5 kcal/mol window from the global minima were kept for further geometry optimization at DFT level. The choice for the 5 kcal/mol of cutoff was set as a balance between reducing the overall CPU calculation time and minimizing the possibility of losing further contributing conformers. The number of conformations obtained in each case varied significantly with the overall flexibility of the system. The resulting structures were submitted to GIAO NMR calculations at each of the studied levels. The chemical shifts were Boltzmann-averaged and scaled as δs = (δu − b)/m, where m and b are the slope and intercept, respectively, resulting from a linear regression calculation on a plot of δu against δexp. The process of data and file manipulation, such as probability calculation, was automated using the DP4+ app.[3]

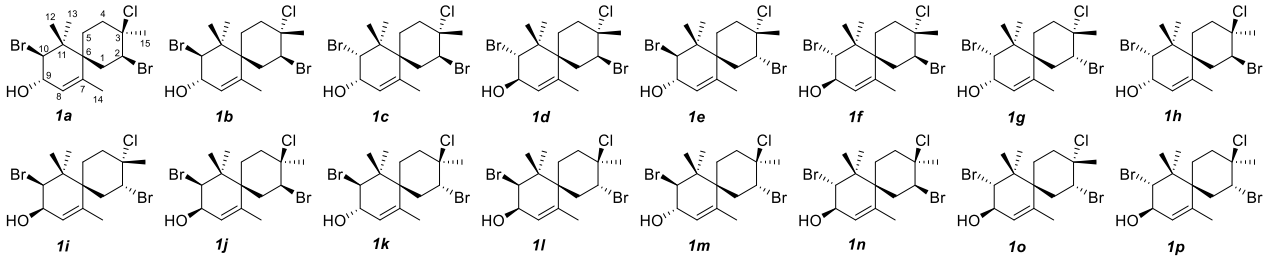


[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., J r., Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Gaussian*, Inc.: Wallingford, CT, **2009**.

[2] Spartan'14; Wavefunction:. Irvine, CA

[3] B. A. Franco, E. R. Luciano, A. M. Sarotti, M. M. Zanardi, *J. Nat. Prod.* **2023**

1. Isomers of 1



X. Q. Yu, C. S. Jiang, Y. Zhang, P. Sun, T. Kurtán, A. Mándi, X. L. Li, L. G. Yao, A. H. Liu, B. Wang, Y. W. Guo, S. C. Mao, *Phytochemistry* **2017**, *136*, 81–93

Table S1.1.1 – *Experimental data of* ***1a*** *and calculated isotropic shielding constants of* ***1a-1p*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory.*

DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Isotropic shielding constants***															
C1	38.2	35.19	36.82	41.38	37.11	33.94	42.05	37.20	40.27	35.69	35.22	36.12	37.54	38.53	39.94	38.42	39.45
C2	60.7	71.63	73.25	73.15	73.47	71.11	72.25	70.57	70.99	71.05	71.16	72.94	73.51	72.14	70.68	70.16	72.07
C3	71.9	78.42	78.13	79.02	78.58	79.95	78.39	80.60	78.79	81.09	78.33	78.70	79.75	79.94	78.36	79.48	79.23
C4	38.7	37.26	38.46	39.11	38.41	38.01	38.85	37.71	39.02	37.66	37.88	38.61	38.75	37.80	37.59	37.68	39.19
C5	30.1	27.96	30.43	25.60	28.27	25.43	24.65	23.07	23.56	23.92	26.36	28.08	24.54	25.00	22.24	22.55	23.53
C6	48.3	50.87	52.50	52.22	53.73	52.27	51.72	51.99	50.95	49.94	53.75	52.31	51.42	50.40	52.05	53.14	51.24
C7	143.4	138.96	138.09	139.24	139.78	137.29	137.84	139.78	139.96	139.51	140.34	136.97	137.00	139.25	138.10	138.15	136.77
C8	123.8	118.49	118.85	120.20	119.81	119.09	119.58	119.95	119.68	120.43	119.41	120.02	122.52	120.44	119.24	118.84	119.86
C9	73.2	70.08	70.00	64.85	65.58	70.00	70.60	64.84	64.43	64.76	65.32	69.71	64.69	65.30	70.04	69.01	69.74
C10	71.7	83.77	83.70	82.36	81.42	85.63	81.61	83.43	83.66	84.64	82.81	84.82	84.96	82.96	83.31	84.95	85.00
C11	45.8	44.60	44.84	43.68	43.23	44.26	45.83	43.20	43.69	42.10	43.64	44.13	42.87	43.96	45.49	44.22	44.25
C12	25.3	22.16	22.71	22.57	23.09	26.69	23.48	25.24	21.48	25.37	22.13	27.35	26.55	24.80	22.32	25.84	24.84
C13	18.1	16.00	15.44	17.95	17.05	16.32	15.41	21.76	17.28	24.33	17.32	16.35	23.03	20.53	15.12	16.73	16.54
C14	25.6	23.98	24.62	25.66	25.91	19.40	25.42	19.95	25.04	19.33	25.44	20.49	18.69	21.85	25.16	19.93	21.13
C15	33.0	28.42	19.94	20.81	22.37	28.40	20.13	28.53	29.00	28.00	28.70	21.21	21.98	24.91	28.18	28.70	24.94
H1a	2.43	2.23	2.19	2.35	2.24	2.54	2.39	2.16	2.65	2.95	2.21	2.32	3.25	2.22	2.67	2.15	2.19
H1b	2.09	2.10	2.08	2.01	2.06	2.16	2.18	1.92	1.87	2.20	2.11	2.25	1.98	1.89	2.06	2.06	1.95
H2	4.57	4.67	4.85	4.70	4.77	4.63	4.79	4.46	4.47	4.65	4.52	4.81	4.90	4.62	4.58	4.48	4.81
H4a	2.19	2.12	2.31	2.43	2.23	2.04	2.42	2.01	2.12	1.94	2.02	2.36	2.17	2.21	2.15	2.11	2.26
H4b	1.93	2.03	2.20	2.19	2.11	2.03	2.21	2.00	2.09	1.94	1.94	2.09	1.99	2.16	2.11	1.99	2.20
H5a	2.51	2.42	2.16	1.87	2.16	1.98	1.86	2.19	2.08	2.06	2.44	1.72	1.79	2.13	2.16	2.42	1.98
H5b	1.62	1.59	1.61	1.69	1.58	1.63	1.59	2.14	1.71	1.55	1.48	1.69	1.57	1.80	1.44	1.68	1.81
H8	5.41	5.54	5.48	5.46	5.41	5.56	5.43	5.53	5.54	5.41	5.51	5.55	5.30	5.48	5.50	5.56	5.57
H9	4.28	4.00	3.94	3.87	3.84	4.07	4.03	4.08	3.96	4.11	3.92	4.02	4.10	3.94	4.03	4.15	4.04
H10	4.41	4.50	4.46	4.78	4.79	4.55	4.52	4.85	4.80	4.57	4.83	4.48	4.47	4.84	4.57	4.63	4.45
Me-12	1.3	1.29	1.17	1.17	1.22	1.28	1.15	1.35	1.30	1.40	1.34	1.31	1.42	1.28	1.30	1.30	1.38
Me-13	0.99	1.13	1.08	1.15	1.19	1.26	1.11	1.17	1.18	1.13	1.25	1.20	1.14	1.23	1.11	1.27	1.16
Me-15	1.96	2.04	2.12	1.99	2.05	1.95	1.99	1.86	1.95	1.83	2.07	1.81	1.66	1.89	1.94	1.89	1.84
Me-15	1.73	1.77	1.77	1.77	1.77	1.75	1.75	1.69	1.71	1.67	1.78	1.81	1.67	1.75	1.79	1.74	1.78

Table S1.1.2 – *Experimental data of* ***1a*** *and scaled chemical shifts of* ***1a-1p*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory.*

DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	35.19	36.82	41.38	37.11	33.94	42.05	37.20	40.27	35.69	35.22	36.12	37.54	38.53	39.94	38.42	39.45
C2	60.7	71.63	73.25	73.15	73.47	71.11	72.25	70.57	70.99	71.05	71.16	72.94	73.51	72.14	70.68	70.16	72.07
C3	71.9	78.42	78.13	79.02	78.58	79.95	78.39	80.60	78.79	81.09	78.33	78.70	79.75	79.94	78.36	79.48	79.23
C4	38.7	37.26	38.46	39.11	38.41	38.01	38.85	37.71	39.02	37.66	37.88	38.61	38.75	37.80	37.59	37.68	39.19
C5	30.1	27.96	30.43	25.60	28.27	25.43	24.65	23.07	23.56	23.92	26.36	28.08	24.54	25.00	22.24	22.55	23.53
C6	48.3	50.87	52.50	52.22	53.73	52.27	51.72	51.99	50.95	49.94	53.75	52.31	51.42	50.40	52.05	53.14	51.24
C7	143.4	138.96	138.09	139.24	139.78	137.29	137.84	139.78	139.96	139.51	140.34	136.97	137.00	139.25	138.10	138.15	136.77
C8	123.8	118.49	118.85	120.20	119.81	119.09	119.58	119.95	119.68	120.43	119.41	120.02	122.52	120.44	119.24	118.84	119.86
C9	71.7	70.08	70.00	64.85	65.58	70.00	70.60	64.84	64.43	64.76	65.32	69.71	64.69	65.30	70.04	69.01	69.74
C10	73.2	83.77	83.70	82.36	81.42	85.63	81.61	83.43	83.66	84.64	82.81	84.82	84.96	82.96	83.31	84.95	85.00
C11	45.8	44.60	44.84	43.68	43.23	44.26	45.83	43.20	43.69	42.10	43.64	44.13	42.87	43.96	45.49	44.22	44.25

C12	25.3	22.16	22.71	22.57	23.09	26.69	23.48	25.24	21.48	25.37	22.13	27.35	26.55	24.80	22.32	25.84	24.84
C13	18.1	16.00	15.44	17.95	17.05	16.32	15.41	21.76	17.28	24.33	17.32	16.35	23.03	20.53	15.12	16.73	16.54
C14	25.6	23.98	24.62	25.66	25.91	19.40	25.42	19.95	25.04	19.33	25.44	20.49	18.69	21.85	25.16	19.93	21.13
C15	33.0	28.42	19.94	20.81	22.37	28.40	20.13	28.53	29.00	28.00	28.70	21.21	21.98	24.91	28.18	28.70	24.94
H1a	2.43	2.23	2.19	2.35	2.24	2.54	2.39	2.16	2.65	2.95	2.21	2.32	3.25	2.22	2.67	2.15	2.19
H1b	2.09	2.10	2.08	2.01	2.06	2.16	2.18	1.92	1.87	2.20	2.11	2.25	1.98	1.89	2.06	2.06	1.95
H2	4.57	4.67	4.85	4.70	4.77	4.63	4.79	4.46	4.47	4.65	4.52	4.81	4.90	4.62	4.58	4.48	4.81
H4a	2.19	2.12	2.31	2.43	2.23	2.04	2.42	2.01	2.12	1.94	2.02	2.36	2.17	2.21	2.15	2.11	2.26
H4b	1.93	2.03	2.20	2.19	2.11	2.03	2.21	2.00	2.09	1.94	1.94	2.09	1.99	2.16	2.11	1.99	2.20
H5a	2.51	2.42	2.16	1.87	2.16	1.98	1.86	2.19	2.08	2.06	2.44	1.72	1.79	2.13	2.16	2.42	1.98
H5b	1.62	1.59	1.61	1.69	1.58	1.63	1.59	2.14	1.71	1.55	1.48	1.69	1.57	1.80	1.44	1.68	1.81
H8	5.41	5.54	5.48	5.46	5.41	5.56	5.43	5.53	5.54	5.41	5.51	5.55	5.30	5.48	5.50	5.56	5.57
H9	4.28	4.00	3.94	3.87	3.84	4.07	4.03	4.08	3.96	4.11	3.92	4.02	4.10	3.94	4.03	4.15	4.04
H10	4.41	4.50	4.46	4.78	4.79	4.55	4.52	4.85	4.80	4.57	4.83	4.48	4.47	4.84	4.57	4.63	4.45
Me-12	1.3	1.29	1.17	1.17	1.22	1.28	1.15	1.35	1.30	1.40	1.34	1.31	1.42	1.28	1.30	1.30	1.38
Me-13	0.99	1.13	1.08	1.15	1.19	1.26	1.11	1.17	1.18	1.13	1.25	1.20	1.14	1.23	1.11	1.27	1.16
Me-14	1.96	2.04	2.12	1.99	2.05	1.95	1.99	1.86	1.95	1.83	2.07	1.81	1.66	1.89	1.94	1.89	1.84
Me-15	1.73	1.77	1.77	1.77	1.77	1.75	1.75	1.69	1.71	1.67	1.78	1.81	1.67	1.75	1.79	1.74	1.78

Table S1.1.3 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, excluding all the signals adjacent to bromine.*

DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	36.70	38.46	43.00	38.62	35.50	43.56	38.64	41.79	37.21	36.63	37.79	39.29	40.06	41.41	39.94	41.13
C3	71.9	80.56	80.40	81.15	80.65	82.26	80.37	82.65	80.88	83.31	80.33	81.07	82.20	82.06	80.37	81.63	81.55
C4	38.7	38.79	40.13	40.69	39.95	39.63	40.31	39.15	40.52	39.21	39.33	40.32	40.52	39.33	39.03	39.19	40.87
C5	30.1	29.36	31.97	27.00	29.67	26.85	25.92	24.30	24.84	25.26	27.65	29.62	26.07	26.34	23.46	23.82	24.95
C6	48.3	52.60	54.38	53.98	55.47	54.13	53.35	53.63	52.63	51.68	55.41	54.24	53.39	52.11	53.69	54.89	53.11
C7	143.4	142.00	141.28	142.22	142.65	140.54	140.59	142.66	142.92	142.63	143.19	140.28	140.39	142.22	140.95	141.21	140.02
C8	123.8	121.23	121.74	122.91	122.42	122.04	122.09	122.55	122.35	123.26	121.98	123.06	125.68	123.14	121.83	121.60	122.83
C10	73.2	72.10	72.15	66.79	67.47	72.15	72.48	66.66	66.31	66.73	67.14	71.93	66.89	67.21	71.93	71.00	71.91
C11	45.8	46.24	46.61	45.33	44.83	45.99	47.38	44.71	45.26	43.72	45.16	45.93	44.71	45.57	47.04	45.83	46.01
C12	25.3	23.47	24.14	23.92	24.42	28.13	24.74	26.51	22.73	26.73	23.36	28.89	28.12	26.14	23.54	27.17	26.29
C13	18.1	17.22	16.75	19.23	18.30	17.59	16.57	22.98	18.47	25.67	18.48	17.71	24.54	21.81	16.24	17.91	17.85
C14	25.6	25.31	26.08	27.05	27.28	20.72	26.71	21.14	26.35	20.59	26.72	21.91	20.13	23.15	26.42	21.16	22.52
C15	33.0	29.82	21.33	22.13	23.69	29.87	21.35	29.84	30.36	29.41	30.02	22.64	23.47	26.25	29.49	30.07	26.38
H1a	2.43	2.24	2.21	2.39	2.28	2.56	2.42	2.18	2.69	2.99	2.24	2.35	3.33	2.25	2.69	2.16	2.21
H1b	2.09	2.11	2.10	2.03	2.09	2.17	2.20	1.94	1.88	2.22	2.13	2.28	2.00	1.90	2.07	2.07	1.96
H4a	2.19	2.13	2.33	2.47	2.27	2.05	2.46	2.03	2.13	1.95	2.03	2.38	2.19	2.24	2.16	2.12	2.28
H4b	1.93	2.04	2.22	2.22	2.14	2.04	2.23	2.01	2.11	1.94	1.95	2.11	2.01	2.19	2.12	1.99	2.22
H5a	2.51	2.43	2.18	1.89	2.19	1.98	1.87	2.21	2.09	2.08	2.47	1.72	1.79	2.16	2.17	2.43	1.99
H5b	1.62	1.59	1.60	1.69	1.57	1.63	1.59	2.16	1.71	1.55	1.47	1.69	1.57	1.81	1.44	1.69	1.81
H8	5.41	5.63	5.64	5.70	5.69	5.65	5.58	5.69	5.67	5.52	5.68	5.71	5.49	5.70	5.58	5.61	5.71
H9	4.28	4.06	4.04	4.01	4.00	4.13	4.13	4.17	4.03	4.18	4.03	4.11	4.23	4.08	4.08	4.18	4.12
Me-12	1.3	1.28	1.15	1.14	1.19	1.27	1.12	1.34	1.29	1.40	1.32	1.29	1.41	1.26	1.29	1.29	1.37
Me-13	0.99	1.11	1.06	1.11	1.16	1.25	1.08	1.16	1.16	1.12	1.23	1.18	1.11	1.20	1.10	1.26	1.14
Me-14	1.96	2.05	2.14	2.01	2.08	1.96	2.00	1.87	1.96	1.83	2.09	1.81	1.66	1.91	1.95	1.90	1.85
Me-15	1.73	1.77	1.77	1.78	1.78	1.75	1.75	1.69	1.71	1.67	1.79	1.82	1.67	1.75	1.79	1.74	1.79

Table S1.1.4 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, excluding signals from nuclei adjacent to bromine and chlorine*

DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	37.27	39.04	43.67	39.22	36.17	44.18	39.38	42.44	37.98	37.19	38.42	40.00	40.78	42.01	40.62	41.82
C4	38.7	39.39	40.72	41.34	40.56	40.36	40.90	39.89	41.15	40.00	39.91	40.97	41.25	40.04	39.61	39.86	41.55
C5	30.1	29.87	32.49	27.52	30.19	27.43	26.39	24.88	25.33	25.88	28.13	30.17	26.64	26.91	23.91	24.34	25.47
C6	48.3	53.32	55.10	54.77	56.22	55.01	54.05	54.54	53.38	52.62	56.14	55.02	54.26	52.95	54.41	55.72	53.92
C7	143.4	143.52	142.76	143.85	144.19	142.35	142.06	144.56	144.51	144.65	144.68	141.87	142.19	144.01	142.43	142.91	141.70
C8	123.8	122.56	123.06	124.36	123.78	123.65	123.40	124.23	123.75	125.05	123.29	124.49	127.32	124.73	123.14	123.10	124.34
C9	73.2	72.99	73.02	67.70	68.33	73.22	73.35	67.71	67.18	67.85	67.97	72.88	67.90	68.21	72.80	71.99	72.90
C11	45.8	46.91	47.26	46.02	45.48	46.78	48.04	45.52	45.94	44.56	45.80	46.63	45.48	46.34	47.69	46.57	46.74
C12	25.3	23.92	24.59	24.41	24.89	28.73	25.20	27.11	23.20	27.37	23.80	29.42	28.71	26.70	23.99	27.72	26.82

C13	18.1	17.62	17.14	19.68	18.72	18.07	16.95	23.54	18.89	26.30	18.88	18.14	25.10	22.33	16.62	18.37	18.30
C14	25.6	25.79	26.55	27.58	27.77	21.24	27.18	21.68	26.85	21.16	27.19	22.38	20.64	23.68	26.89	21.65	23.02
C15	33.0	30.34	21.76	22.61	24.15	30.49	21.77	30.48	30.89	30.08	30.52	23.12	24.01	26.82	29.99	30.65	26.92
H1a	2.43	2.24	2.21	2.39	2.28	2.56	2.42	2.18	2.69	2.99	2.24	2.35	3.33	2.25	2.69	2.16	2.21
H1b	2.09	2.11	2.10	2.03	2.09	2.17	2.20	1.94	1.88	2.22	2.13	2.28	2.00	1.90	2.07	2.07	1.96
H4a	2.19	2.13	2.33	2.47	2.27	2.05	2.46	2.03	2.13	1.95	2.03	2.38	2.19	2.24	2.16	2.12	2.28
H4b	1.93	2.04	2.22	2.22	2.14	2.04	2.23	2.01	2.11	1.94	1.95	2.11	2.01	2.19	2.12	1.99	2.22
H5a	2.51	2.43	2.18	1.89	2.19	1.98	1.87	2.21	2.09	2.08	2.47	1.72	1.79	2.16	2.17	2.43	1.99
H5b	1.62	1.59	1.60	1.69	1.57	1.63	1.59	2.16	1.71	1.55	1.47	1.69	1.57	1.81	1.44	1.69	1.81
H8	5.41	5.63	5.64	5.70	5.69	5.65	5.58	5.69	5.67	5.52	5.68	5.71	5.49	5.70	5.58	5.61	5.71
H9	4.28	4.06	4.04	4.01	4.00	4.13	4.13	4.17	4.03	4.18	4.03	4.11	4.23	4.08	4.08	4.18	4.12
Me-12	1.3	1.28	1.15	1.14	1.19	1.27	1.12	1.34	1.29	1.40	1.32	1.29	1.41	1.26	1.29	1.29	1.37
Me-13	0.99	1.11	1.06	1.11	1.16	1.25	1.08	1.16	1.16	1.12	1.23	1.18	1.11	1.20	1.10	1.26	1.14
Me-14	1.96	2.05	2.14	2.01	2.08	1.96	2.00	1.87	1.96	1.83	2.09	1.81	1.66	1.91	1.95	1.90	1.85
Me-15	1.73	1.77	1.77	1.78	1.78	1.75	1.75	1.69	1.71	1.67	1.79	1.82	1.67	1.75	1.79	1.74	1.79

Table S1.1.5 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	37.27	39.04	43.67	39.22	36.17	44.18	39.38	42.44	37.98	37.19	38.42	40.00	40.78	42.01	40.62	41.82
C4	38.7	39.39	40.72	41.34	40.56	40.36	40.90	39.89	41.15	40.00	39.91	40.97	41.25	40.04	39.61	39.86	41.55
C5	30.1	29.87	32.49	27.52	30.19	27.43	26.39	24.88	25.33	25.88	28.13	30.17	26.64	26.91	23.91	24.34	25.47
C6	48.3	53.32	55.10	54.77	56.22	55.01	54.05	54.54	53.38	52.62	56.14	55.02	54.26	52.95	54.41	55.72	53.92
C7	143.4	143.52	142.76	143.85	144.19	142.35	142.06	144.56	144.51	144.65	144.68	141.87	142.19	144.01	142.43	142.91	141.70
C8	123.8	122.56	123.06	124.36	123.78	123.65	123.40	124.23	123.75	125.05	123.29	124.49	127.32	124.73	123.14	123.10	124.34
C9	73.2	72.99	73.02	67.70	68.33	73.22	73.35	67.71	67.18	67.85	67.97	72.88	67.90	68.21	72.80	71.99	72.90
C11	45.8	46.91	47.26	46.02	45.48	46.78	48.04	45.52	45.94	44.56	45.80	46.63	45.48	46.34	47.69	46.57	46.74
C12	25.3	23.92	24.59	24.41	24.89	28.73	25.20	27.11	23.20	27.37	23.80	29.42	28.71	26.70	23.99	27.72	26.82
C13	18.1	17.62	17.14	19.68	18.72	18.07	16.95	23.54	18.89	26.30	18.88	18.14	25.10	22.33	16.62	18.37	18.30
C14	25.6	25.79	26.55	27.58	27.77	21.24	27.18	21.68	26.85	21.16	27.19	22.38	20.64	23.68	26.89	21.65	23.02
C15	33.0	30.34	21.76	22.61	24.15	30.49	21.77	30.48	30.89	30.08	30.52	23.12	24.01	26.82	29.99	30.65	26.92
H1a	2.43	2.39	2.16	2.65	2.95	2.21	2.32	3.25	2.22	2.67	2.15	2.19	2.39	2.16	2.65	2.95	2.21
H1b	2.09	2.18	1.92	1.87	2.20	2.11	2.25	1.98	1.89	2.06	2.06	1.95	2.18	1.92	1.87	2.20	2.11
H2	4.57	4.79	4.46	4.47	4.65	4.52	4.81	4.90	4.62	4.58	4.48	4.81	4.79	4.46	4.47	4.65	4.52
H4a	2.19	2.42	2.01	2.12	1.94	2.02	2.36	2.17	2.21	2.15	2.11	2.26	2.42	2.01	2.12	1.94	2.02
H4b	1.93	2.21	2.00	2.09	1.94	1.94	2.09	1.99	2.16	2.11	1.99	2.20	2.21	2.00	2.09	1.94	1.94
H5a	2.51	1.86	2.19	2.08	2.06	2.44	1.72	1.79	2.13	2.16	2.42	1.98	1.86	2.19	2.08	2.06	2.44
H5b	1.62	1.59	2.14	1.71	1.55	1.48	1.69	1.57	1.80	1.44	1.68	1.81	1.59	2.14	1.71	1.55	1.48
H8	5.41	5.43	5.53	5.54	5.41	5.51	5.55	5.30	5.48	5.50	5.56	5.57	5.43	5.53	5.54	5.41	5.51
H9	4.28	4.03	4.08	3.96	4.11	3.92	4.02	4.10	3.94	4.03	4.15	4.04	4.03	4.08	3.96	4.11	3.92
H10	4.41	4.52	4.85	4.80	4.57	4.83	4.48	4.47	4.84	4.57	4.63	4.45	4.52	4.85	4.80	4.57	4.83
Me-12	1.3	1.15	1.35	1.30	1.40	1.34	1.31	1.42	1.28	1.30	1.30	1.38	1.15	1.35	1.30	1.40	1.34
Me-13	0.99	1.11	1.17	1.18	1.13	1.25	1.20	1.14	1.23	1.11	1.27	1.16	1.11	1.17	1.18	1.13	1.25
Me-14	1.96	1.99	1.86	1.95	1.83	2.07	1.81	1.66	1.89	1.94	1.89	1.84	1.99	1.86	1.95	1.83	2.07
Me-15	1.73	1.75	1.69	1.71	1.67	1.78	1.81	1.67	1.75	1.79	1.74	1.78	1.75	1.69	1.71	1.67	1.78

Table S1.2.1 – *Experimental data of **1a** and calculated isotropic shielding constants of **1a-1p** at the B3LYP/6-31G**//MMFF level of theory.*

DP4																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Isotropic shielding constants***															
C1	38.2	151.75	150.02	145.57	149.63	152.22	145.41	150.85	147.15	152.10	151.45	150.59	150.22	149.33	147.05	150.35	149.16
C2	60.7	120.98	120.05	120.52	120.12	122.17	120.60	122.53	121.57	122.35	120.98	120.77	121.02	126.69	121.71	122.78	126.02
C3	71.9	117.74	117.42	117.40	117.47	116.99	117.23	116.95	117.85	116.86	117.90	117.08	117.15	117.58	117.68	117.00	117.62
C4	38.7	149.89	148.24	148.12	148.29	149.64	148.09	150.19	149.39	149.59	149.96	148.42	148.30	152.54	149.33	149.81	151.81
C5	30.1	160.04	158.10	162.12	158.45	162.81	162.61	164.84	164.29	163.41	160.31	160.53	161.17	163.86	164.72	165.11	164.24
C6	48.3	135.12	135.45	134.64	134.50	133.11	135.71	132.73	134.34	132.79	134.14	133.58	133.75	137.05	135.31	133.39	137.48
C7	143.4	49.16	49.28	49.56	49.55	50.51	49.33	50.10	49.58	50.12	49.38	51.70	51.64	49.43	49.34	50.66	49.45
C8	123.8	66.64	66.55	66.28	66.70	66.05	66.02	66.05	66.19	66.30	66.89	65.32	64.94	65.63	65.96	65.55	65.64
C9	73.2	117.16	117.13	124.32	124.26	118.77	117.05	123.63	124.27	123.79	124.19	118.68	124.20	124.42	117.02	118.58	117.15
C10	71.7	109.59	109.76	111.82	111.78	106.85	110.19	110.00	111.46	109.84	111.42	107.12	109.93	110.78	109.92	106.92	109.23
C11	45.8	137.68	138.19	140.09	140.33	140.47	138.05	141.59	139.70	141.64	139.90	140.45	141.66	139.89	137.69	140.55	137.82
C12	25.3	166.34	166.55	166.72	166.51	162.21	166.58	162.87	166.63	162.05	166.44	162.00	162.15	165.98	166.52	163.21	165.79

C13	18.1	172.61	172.70	170.60	170.84	170.55	172.41	167.33	170.61	166.93	170.83	170.77	166.37	170.12	172.45	170.49	172.12
C14	25.6	165.23	164.91	164.53	164.72	169.39	164.73	169.38	164.84	169.42	165.00	169.17	169.21	167.24	164.99	169.34	167.66
C15	33.0	157.92	165.79	166.18	165.91	157.84	166.06	157.85	157.82	157.87	157.83	165.43	165.12	159.70	157.83	157.83	160.05
H1a	2.43	29.37	29.46	29.36	29.40	29.11	29.31	29.43	29.08	29.18	29.44	29.34	29.07	29.10	29.04	29.38	29.10
H1b	2.09	29.67	29.59	29.65	29.66	29.55	29.43	29.75	29.86	29.36	29.63	29.41	29.51	29.78	29.64	29.64	29.62
H2	4.57	27.02	26.78	26.90	26.78	26.98	26.89	27.05	27.13	26.98	27.02	26.77	26.75	27.04	27.11	27.02	27.00
H4b	1.93	29.76	29.64	29.65	29.66	29.75	29.63	29.79	29.67	29.77	29.77	29.74	29.75	29.74	29.66	29.77	29.70
H4a	2.19	29.69	29.42	29.28	29.43	29.63	29.27	29.67	29.66	29.67	29.72	29.25	29.33	29.50	29.64	29.69	29.50
H5b	1.62	30.23	30.09	30.05	30.33	30.22	30.11	29.92	30.19	30.32	30.47	30.07	30.16	29.98	30.25	30.06	30.00
H5a	2.51	29.21	29.63	29.94	29.69	29.54	29.89	29.33	29.57	29.57	29.26	29.92	29.98	29.67	29.52	29.28	29.68
H8	5.41	25.96	25.92	25.79	25.81	25.91	25.92	25.82	25.83	25.85	25.85	25.90	25.86	25.81	25.94	25.89	25.92
H9	4.28	27.41	27.41	27.68	27.71	27.47	27.40	27.66	27.68	27.66	27.71	27.47	27.65	27.67	27.39	27.48	27.40
H10	4.41	27.13	27.17	26.95	27.00	27.15	27.14	26.93	26.88	26.99	26.93	27.16	27.01	26.93	27.08	27.10	27.14
Me-12	1.30	30.53	30.67	30.65	30.64	30.58	30.66	30.48	30.55	30.44	30.56	30.46	30.39	30.58	30.53	30.55	30.54
Me-13	0.99	30.73	30.74	30.68	30.70	30.60	30.76	30.59	30.64	30.62	30.62	30.59	30.52	30.59	30.74	30.63	30.70
Me-14	1.96	29.86	29.74	29.77	29.73	29.91	29.78	29.92	29.89	29.92	29.84	30.04	30.05	29.78	29.89	29.93	29.83
Me-15	1.73	30.19	30.11	30.12	30.11	30.17	30.10	30.18	30.19	30.18	30.18	30.04	30.06	30.09	30.18	30.17	30.09

Table S1.2.2 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the B3LYP/6-31G**//MMFF level of theory.*

DP4																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	36.51	38.49	43.36	39.24	36.10	43.13	37.82	41.49	36.34	37.14	37.89	38.37	40.47	41.26	38.20	40.22
C2	60.7	67.46	68.49	68.71	69.19	66.40	67.91	66.62	67.51	66.72	68.21	67.95	68.21	63.21	66.68	65.88	63.21
C3	71.9	70.72	71.13	71.87	71.88	71.63	71.27	72.29	71.30	72.33	71.34	71.67	72.16	72.36	70.72	71.69	71.54
C4	38.7	38.38	40.27	40.77	40.60	38.70	40.46	38.49	39.21	38.89	38.66	40.08	40.33	37.24	38.96	38.74	37.59
C5	30.1	28.17	30.40	26.60	30.30	25.43	25.96	23.59	24.06	24.78	28.12	27.88	27.17	25.87	23.53	23.38	25.25
C6	48.3	53.24	53.07	54.42	54.59	55.37	52.82	56.25	54.52	56.06	54.79	55.03	55.19	52.81	53.03	55.23	51.82
C7	143.4	139.70	139.35	140.55	140.79	138.67	139.07	140.26	140.75	140.50	141.18	137.55	139.11	140.81	139.29	138.29	139.23
C8	123.8	122.12	122.06	123.62	123.39	123.00	122.41	124.04	123.85	123.96	123.33	123.82	125.52	124.54	122.62	123.34	123.15
C9	73.2	71.30	71.42	64.87	64.99	69.83	71.45	65.50	64.77	65.25	64.93	70.05	64.95	65.49	71.39	70.10	72.01
C10	71.7	78.91	78.80	77.52	77.65	81.85	78.31	79.36	77.80	79.50	77.94	81.69	79.54	79.19	78.51	81.80	79.87
C11	45.8	50.66	50.33	48.90	48.69	47.96	50.48	47.23	49.07	47.02	48.92	48.11	47.11	49.95	50.64	48.04	51.48
C12	25.3	21.84	21.93	21.95	22.12	26.03	21.99	25.59	21.68	26.18	21.87	26.40	26.17	23.74	21.72	25.29	23.72
C13	18.1	15.53	15.78	18.01	17.72	17.62	16.17	21.06	17.63	21.19	17.39	17.56	21.86	19.58	15.77	17.98	17.43
C14	25.6	22.95	23.58	24.16	23.93	18.79	23.85	18.97	23.50	18.65	23.34	19.18	18.96	22.47	23.25	19.14	21.86
C15	33.0	30.30	22.70	22.49	22.73	30.43	22.52	30.70	30.64	30.44	30.65	22.94	23.14	30.05	30.44	30.70	29.41
H1a	2.43	2.38	2.28	2.38	2.35	2.60	2.41	2.31	2.65	2.54	2.34	2.37	2.61	2.60	2.68	2.36	2.60
H1b	2.09	2.11	2.16	2.11	2.12	2.21	2.30	2.01	1.93	2.38	2.17	2.30	2.21	1.97	2.13	2.12	2.11
H2	4.57	4.54	4.72	4.62	4.72	4.58	4.63	4.51	4.45	4.57	4.54	4.76	4.76	4.51	4.46	4.54	4.55
H4b	1.93	2.03	2.11	2.11	2.12	2.02	2.11	1.98	2.11	1.99	2.04	2.00	1.98	2.01	2.11	2.00	2.04
H4a	2.19	2.09	2.32	2.45	2.33	2.13	2.44	2.09	2.12	2.09	2.09	2.45	2.38	2.22	2.12	2.07	2.22
H5b	1.62	1.59	1.70	1.74	1.52	1.58	1.67	1.85	1.64	1.49	1.40	1.69	1.61	1.78	1.56	1.73	1.75
H5a	2.51	2.53	2.12	1.84	2.09	2.21	1.87	2.40	2.20	2.18	2.50	1.83	1.77	2.07	2.23	2.46	2.06
H8	5.41	5.52	5.50	5.63	5.59	5.57	5.52	5.66	5.64	5.62	5.60	5.56	5.59	5.66	5.53	5.59	5.56
H9	4.28	4.18	4.15	3.91	3.88	4.12	4.16	3.95	3.94	3.95	3.91	4.10	3.93	3.93	4.20	4.12	4.18
H10	4.41	4.44	4.37	4.58	4.52	4.42	4.41	4.63	4.67	4.56	4.62	4.39	4.53	4.62	4.48	4.47	4.42
Me-12	1.30	1.32	1.17	1.19	1.24	1.25	1.16	1.33	1.30	1.38	1.32	1.33	1.39	1.22	1.30	1.28	1.25
Me-13	0.99	1.13	1.11	1.17	1.18	1.23	1.07	1.24	1.22	1.21	1.26	1.20	1.27	1.21	1.10	1.21	1.10
Me-14	1.96	1.94	2.02	2.00	2.06	1.87	1.98	1.85	1.91	1.86	1.97	1.72	1.71	1.96	1.89	1.86	1.92
Me-15	1.73	1.63	1.69	1.68	1.71	1.63	1.68	1.61	1.64	1.62	1.66	1.72	1.70	1.68	1.63	1.63	1.67

Table S1.2.3 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the B3LYP/6-31G**//MMFF level of theory, excluding all the signals adjacent to bromine.*

DP4																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	37.43	39.49	44.34	40.23	37.12	44.10	38.72	42.39	37.24	38.06	39.04	39.40	41.13	42.13	39.20	40.93
C3	71.9	71.94	72.43	73.08	73.14	73.05	72.48	73.50	72.43	73.56	72.54	73.20	73.52	73.27	71.84	73.06	72.51
C4	38.7	39.32	41.29	41.73	41.60	39.75	41.41	39.40	40.09	39.82	39.59	41.25	41.38	37.88	39.82	39.75	38.28
C5	30.1	29.02	31.33	27.45	31.21	26.32	26.78	24.36	24.82	25.58	28.96	28.91	28.09	26.42	24.26	24.22	25.83
C6	48.3	54.31	54.21	55.49	55.71	56.61	53.87	57.31	55.52	57.14	55.85	56.38	56.39	53.57	54.01	56.42	52.62
C7	143.4	141.53	141.27	142.30	142.61	140.85	140.85	142.08	142.42	142.35	142.95	139.85	141.12	142.25	140.98	140.40	140.77
C8	123.8	123.80	123.82	125.24	125.07	125.00	124.05	125.72	125.39	125.67	124.96	125.97	127.39	125.86	124.16	125.29	124.55
C9	73.2	72.53	72.72	66.02	66.19	71.23	72.66	66.65	65.85	66.42	66.07	71.57	66.24	66.35	72.51	71.45	72.98
C11	45.8	51.71	51.45	49.92	49.75	49.11	51.52	48.22	50.03	48.01	49.93	49.38	48.23	50.68	51.60	49.16	52.28

C12	25.3	22.63	22.79	22.76	22.96	26.94	22.78	26.38	22.42	26.98	22.66	27.40	27.09	24.27	22.44	26.15	24.28
C13	18.1	16.27	16.58	18.79	18.53	18.43	16.92	21.81	18.34	21.95	18.15	18.47	22.73	20.08	16.43	18.76	17.94
C14	25.6	23.75	24.45	24.99	24.80	19.61	24.66	19.70	24.25	19.38	24.15	20.10	19.80	23.00	23.98	19.93	22.41
C15	33.0	31.17	23.56	23.30	23.58	31.38	23.32	31.54	31.45	31.29	31.51	23.91	24.02	30.63	31.23	31.61	30.02
H1a	2.43	2.38	2.29	2.39	2.37	2.61	2.41	2.32	2.67	2.55	2.35	2.38	2.65	2.61	2.67	2.36	2.60
H1b	2.09	2.11	2.16	2.12	2.14	2.21	2.31	2.02	1.94	2.39	2.18	2.32	2.23	1.97	2.12	2.12	2.11
H4b	1.93	2.03	2.11	2.12	2.13	2.02	2.11	1.99	2.12	2.00	2.05	2.00	1.99	2.01	2.10	2.00	2.04
H4a	2.19	2.09	2.33	2.47	2.35	2.13	2.45	2.10	2.12	2.09	2.10	2.47	2.40	2.23	2.12	2.07	2.22
H5b	1.62	1.59	1.70	1.74	1.51	1.58	1.67	1.86	1.64	1.49	1.39	1.69	1.60	1.78	1.56	1.74	1.75
H5a	2.51	2.53	2.13	1.85	2.10	2.22	1.87	2.42	2.21	2.19	2.52	1.83	1.77	2.08	2.23	2.46	2.06
H8	5.41	5.52	5.56	5.74	5.72	5.58	5.55	5.73	5.70	5.69	5.69	5.65	5.74	5.72	5.51	5.60	5.56
H9	4.28	4.18	4.18	3.97	3.95	4.13	4.18	3.99	3.97	3.99	3.96	4.16	4.02	3.96	4.18	4.12	4.18
Me-12	1.30	1.32	1.17	1.18	1.23	1.25	1.16	1.33	1.30	1.38	1.31	1.32	1.38	1.22	1.31	1.28	1.25
Me-13	0.99	1.13	1.10	1.15	1.16	1.23	1.07	1.23	1.22	1.20	1.26	1.19	1.25	1.21	1.11	1.20	1.10
Me-14	1.96	1.94	2.03	2.01	2.07	1.87	1.98	1.85	1.91	1.86	1.98	1.72	1.71	1.97	1.89	1.86	1.91
Me-15	1.73	1.63	1.69	1.68	1.71	1.63	1.68	1.61	1.64	1.62	1.66	1.72	1.70	1.68	1.63	1.63	1.67

Table S1.2.4 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	37.44	39.53	44.42	40.32	37.20	44.15	38.83	42.42	37.35	38.11	39.12	39.51	41.23	42.13	39.28	40.97
C4	38.7	39.32	41.33	41.82	41.69	39.83	41.45	39.51	40.13	39.93	39.64	41.34	41.49	37.97	39.82	39.83	38.32
C5	30.1	29.02	31.36	27.51	31.29	26.39	26.82	24.45	24.85	25.67	29.00	28.98	28.18	26.50	24.26	24.28	25.86
C6	48.3	54.31	54.26	55.59	55.81	56.71	53.92	57.45	55.57	57.29	55.91	56.49	56.53	53.68	54.00	56.52	52.67
C7	143.4	141.54	141.36	142.51	142.83	141.05	140.95	142.36	142.51	142.64	143.06	140.07	141.40	142.49	140.97	140.60	140.88
C8	123.8	123.81	123.91	125.42	125.26	125.18	124.14	125.97	125.48	125.93	125.06	126.17	127.65	126.07	124.16	125.47	124.65
C9	73.2	72.53	72.78	66.13	66.31	71.35	72.72	66.80	65.90	66.58	66.14	71.70	66.40	66.48	72.51	71.57	73.04
C11	45.8	51.71	51.49	50.02	49.85	49.20	51.56	48.34	50.07	48.14	49.98	49.48	48.35	50.80	51.59	49.25	52.33
C12	25.3	22.63	22.82	22.82	23.03	27.00	22.81	26.47	22.45	27.08	22.69	27.48	27.18	24.34	22.43	26.21	24.31
C13	18.1	16.27	16.60	18.85	18.59	18.48	16.94	21.89	18.36	22.03	18.18	18.53	22.82	20.15	16.43	18.81	17.97
C14	25.6	23.75	24.48	25.05	24.86	19.67	24.69	19.78	24.28	19.46	24.18	20.16	19.88	23.07	23.98	19.99	22.44
C15	33.0	31.17	23.59	23.37	23.65	31.45	23.35	31.64	31.48	31.39	31.55	23.98	24.11	30.72	31.22	31.69	30.06
H1a	2.43	2.37	2.28	2.35	2.33	2.59	2.40	2.28	2.60	2.51	2.31	2.37	2.59	2.55	2.65	2.34	2.58
H1b	2.09	2.10	2.16	2.09	2.11	2.20	2.30	2.00	1.92	2.35	2.15	2.30	2.20	1.95	2.11	2.11	2.11
H4b	1.93	2.02	2.11	2.09	2.10	2.01	2.11	1.96	2.09	1.98	2.02	2.00	1.98	1.99	2.10	1.99	2.03
H4a	2.19	2.08	2.32	2.42	2.31	2.12	2.43	2.07	2.09	2.07	2.07	2.45	2.36	2.20	2.11	2.06	2.21
H5b	1.62	1.59	1.70	1.74	1.52	1.58	1.67	1.84	1.64	1.49	1.41	1.69	1.60	1.77	1.56	1.73	1.75
H5a	2.51	2.52	2.12	1.84	2.08	2.20	1.87	2.37	2.17	2.16	2.46	1.83	1.76	2.05	2.22	2.44	2.05
H8	5.41	5.46	5.52	5.50	5.49	5.51	5.50	5.49	5.44	5.48	5.44	5.58	5.53	5.48	5.45	5.50	5.51
H9	4.28	4.41	4.38	4.48	4.44	4.38	4.39	4.50	4.53	4.46	4.50	4.40	4.48	4.49	4.42	4.41	4.39
Me-12	1.30	1.32	1.17	1.21	1.25	1.25	1.17	1.34	1.32	1.39	1.33	1.33	1.39	1.24	1.31	1.28	1.25
Me-13	0.99	1.14	1.11	1.18	1.19	1.24	1.07	1.25	1.24	1.22	1.28	1.20	1.27	1.23	1.12	1.21	1.11
Me-14	1.96	1.93	2.02	1.99	2.04	1.86	1.98	1.84	1.90	1.85	1.96	1.72	1.70	1.95	1.89	1.85	1.91
Me-15	1.73	1.63	1.69	1.68	1.71	1.62	1.68	1.61	1.63	1.62	1.66	1.72	1.69	1.67	1.63	1.63	1.67

Table S1.2.5 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the B3LYP/6-31G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	37.44	39.53	44.42	40.32	37.20	44.15	38.83	42.42	37.35	38.11	39.12	39.51	41.23	42.13	39.28	40.97
C4	38.7	39.32	41.33	41.82	41.69	39.83	41.45	39.51	40.13	39.93	39.64	41.34	41.49	37.97	39.82	39.83	38.32
C5	30.1	29.02	31.36	27.51	31.29	26.39	26.82	24.45	24.85	25.67	29.00	28.98	28.18	26.50	24.26	24.28	25.86
C6	48.3	54.31	54.26	55.59	55.81	56.71	53.92	57.45	55.57	57.29	55.91	56.49	56.53	53.68	54.00	56.52	52.67
C7	143.4	141.54	141.36	142.51	142.83	141.05	140.95	142.36	142.51	142.64	143.06	140.07	141.40	142.49	140.97	140.60	140.88
C8	123.8	123.81	123.91	125.42	125.26	125.18	124.14	125.97	125.48	125.93	125.06	126.17	127.65	126.07	124.16	125.47	124.65
C9	73.2	72.53	72.78	66.13	66.31	71.35	72.72	66.80	65.90	66.58	66.14	71.70	66.40	66.48	72.51	71.57	73.04
C11	45.8	51.71	51.49	50.02	49.85	49.20	51.56	48.34	50.07	48.14	49.98	49.48	48.35	50.80	51.59	49.25	52.33
C12	25.3	22.63	22.82	22.82	23.03	27.00	22.81	26.47	22.45	27.08	22.69	27.48	27.18	24.34	22.43	26.21	24.31
C13	18.1	16.27	16.60	18.85	18.59	18.48	16.94	21.89	18.36	22.03	18.18	18.53	22.82	20.15	16.43	18.81	17.97
C14	25.6	23.75	24.48	25.05	24.86	19.67	24.69	19.78	24.28	19.46	24.18	20.16	19.88	23.07	23.98	19.99	22.44
C15	33.0	31.17	23.59	23.37	23.65	31.45	23.35	31.64	31.48	31.39	31.55	23.98	24.11	30.72	31.22	31.69	30.06
H1a	2.43	2.38	2.28	2.38	2.35	2.60	2.41	2.31	2.65	2.54	2.34	2.37	2.61	2.60	2.68	2.36	2.60
H1b	2.09	2.11	2.16	2.11	2.12	2.21	2.30	2.01	1.93	2.38	2.17	2.30	2.21	1.97	2.13	2.12	2.11

H2	4.57	4.54	4.72	4.62	4.72	4.58	4.63	4.51	4.45	4.57	4.54	4.76	4.76	4.51	4.46	4.54	4.55
H4b	1.93	2.03	2.11	2.11	2.12	2.02	2.11	1.98	2.11	1.99	2.04	2.00	1.98	2.01	2.11	2.00	2.04
H4a	2.19	2.09	2.32	2.45	2.33	2.13	2.44	2.09	2.12	2.09	2.09	2.45	2.38	2.22	2.12	2.07	2.22
H5b	1.62	1.59	1.70	1.74	1.52	1.58	1.67	1.85	1.64	1.49	1.40	1.69	1.61	1.78	1.56	1.73	1.75
H5a	2.51	2.53	2.12	1.84	2.09	2.21	1.87	2.40	2.20	2.18	2.50	1.83	1.77	2.07	2.23	2.46	2.06
H8	5.41	5.52	5.50	5.63	5.59	5.57	5.52	5.66	5.64	5.62	5.60	5.56	5.59	5.66	5.53	5.59	5.56
H9	4.28	4.18	4.15	3.91	3.88	4.12	4.16	3.95	3.94	3.95	3.91	4.10	3.93	3.93	4.20	4.12	4.18
H10	4.41	4.44	4.37	4.58	4.52	4.42	4.41	4.63	4.67	4.56	4.62	4.39	4.53	4.62	4.48	4.47	4.42
Me-12	1.30	1.32	1.17	1.19	1.24	1.25	1.16	1.33	1.30	1.38	1.32	1.33	1.39	1.22	1.30	1.28	1.25
Me-13	0.99	1.13	1.11	1.17	1.18	1.23	1.07	1.24	1.22	1.21	1.26	1.20	1.27	1.21	1.10	1.21	1.10
Me-14	1.96	1.94	2.02	2.00	2.06	1.87	1.98	1.85	1.91	1.86	1.97	1.72	1.71	1.96	1.89	1.86	1.92
Me-15	1.73	1.63	1.69	1.68	1.71	1.63	1.68	1.61	1.64	1.62	1.66	1.72	1.70	1.68	1.63	1.63	1.67

Table S1.3.1 – *Experimental data of* ***1a*** *and calculated isotropic shielding constants of* ***1a-1p*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory*

MM-DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Isotropic shielding constants***															
C1	38.2	158.05	156.41	151.80	156.11	159.03	151.51	156.33	152.91	157.19	158.14	157.41	155.37	155.13	152.93	155.64	154.93
C2	60.7	126.86	125.03	126.83	125.66	128.44	126.90	128.42	127.87	127.88	126.70	126.86	126.12	127.06	127.74	128.20	127.55
C3	71.9	122.72	122.75	123.11	123.04	122.03	122.91	122.07	122.79	121.64	122.67	122.67	122.57	122.91	122.46	122.05	123.08
C4	38.7	156.17	154.90	154.17	155.09	155.98	154.74	156.11	154.34	155.74	156.19	154.09	154.28	154.49	154.91	156.18	154.23
C5	30.1	165.81	163.93	169.39	165.58	168.32	169.39	170.67	171.40	169.43	167.16	166.59	167.68	169.60	171.67	171.34	170.62
C6	48.3	139.90	138.92	139.08	137.71	138.82	140.65	138.71	139.61	139.72	138.50	138.42	139.26	139.11	140.05	138.62	139.67
C7	143.4	47.88	48.48	49.88	48.97	51.15	48.64	50.59	49.43	51.52	48.11	50.51	53.56	50.55	48.74	49.82	50.35
C8	123.8	72.94	72.18	72.84	73.33	71.64	72.26	71.08	72.98	70.19	73.88	71.29	68.88	71.55	72.17	71.25	71.30
C9	73.2	122.24	121.65	129.59	129.00	123.09	121.72	129.44	129.44	129.81	128.88	123.27	130.25	129.11	121.73	123.27	123.00
C10	71.7	117.89	117.71	120.77	121.09	114.94	118.21	118.79	119.85	116.66	119.88	115.67	116.68	119.82	117.82	116.14	117.06
C11	45.8	144.30	144.67	146.59	146.62	145.38	143.97	146.62	146.41	147.35	146.76	145.89	147.23	146.51	143.75	145.37	145.28
C12	25.3	171.63	171.56	171.97	171.38	167.69	171.74	168.54	172.37	168.51	171.82	167.26	167.31	169.40	171.66	168.65	170.02
C13	18.1	178.22	178.46	176.19	176.17	176.08	177.89	171.13	176.22	169.08	176.63	176.57	168.65	172.51	177.99	176.26	177.22
C14	25.6	170.93	170.73	170.59	170.32	175.23	170.42	175.85	170.97	175.14	170.40	174.75	175.36	175.23	170.94	175.66	175.08
C15	33.0	164.11	172.71	172.18	171.32	163.64	172.41	164.15	163.94	164.21	163.90	171.05	170.60	169.70	163.71	163.84	169.01
H1a	2.43	29.47	29.29	29.22	29.29	29.11	29.21	29.34	29.06	29.07	29.45	29.18	28.76	29.36	29.02	29.37	29.33
H1b	2.09	29.51	29.45	29.53	29.51	29.51	29.36	29.55	29.68	29.24	29.46	29.28	29.36	29.55	29.47	29.46	29.57
H2	4.57	26.63	26.43	26.59	26.46	26.64	26.59	26.73	26.76	26.53	26.65	26.41	26.39	26.63	26.75	26.68	26.63
H4b	1.93	29.65	29.42	29.46	29.47	29.78	29.43	29.68	29.63	29.78	29.67	29.64	29.56	29.46	29.62	29.59	29.37
H4a	2.19	29.46	29.25	29.10	29.23	29.35	29.10	29.35	29.26	29.37	29.52	29.07	29.23	29.21	29.35	29.36	29.24
H5b	1.62	30.12	30.03	30.06	30.14	30.02	29.99	29.73	30.08	30.07	30.28	29.94	29.93	29.59	30.10	29.94	29.65
H5a	2.51	29.24	29.40	29.64	29.48	29.50	29.68	29.28	29.53	29.30	29.20	29.71	29.53	29.59	29.52	29.10	29.64
H8	5.41	25.62	25.56	25.47	25.48	25.57	25.61	25.56	25.46	25.57	25.49	25.52	25.62	25.52	25.65	25.50	25.58
H9	4.28	27.44	27.40	27.55	27.62	27.38	27.41	27.47	27.55	27.43	27.57	27.43	27.32	27.52	27.40	27.42	27.44
H10	4.41	26.90	26.91	26.51	26.58	26.92	26.92	26.56	26.51	26.79	26.59	26.89	26.76	26.50	26.85	26.77	26.86
Me-12	1.30	30.46	30.50	30.51	30.50	30.46	30.51	30.36	30.45	30.23	30.46	30.35	30.12	30.38	30.44	30.44	30.37
Me-13	0.99	30.65	30.65	30.62	30.54	30.51	30.66	30.45	30.57	30.48	30.56	30.47	30.40	30.39	30.62	30.53	30.55
Me-14	1.96	29.58	29.46	29.58	29.48	29.72	29.58	29.69	29.65	29.74	29.58	29.75	29.78	29.75	29.65	29.67	29.71
Me-15	1.73	29.99	29.84	29.83	29.82	30.02	29.82	29.99	29.99	29.97	30.04	29.77	29.78	29.82	30.01	29.98	29.81

Table S1.3.2 – *Experimental data of* ***1a*** *and scaled chemical shifts of* ***1a-1p*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory*

MM-DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	36.29	38.03	43.20	38.69	35.26	42.98	38.20	41.77	36.96	36.59	37.05	38.65	39.74	41.20	38.84	39.98
C2	60.7	66.71	68.45	67.90	68.83	65.36	66.86	65.94	66.60	66.23	67.66	66.91	68.04	67.52	65.77	65.56	66.56
C3	71.9	70.75	70.67	71.58	71.42	71.67	70.73	72.25	71.64	72.47	71.65	71.00	71.61	71.64	70.91	71.55	70.90
C4	38.7	38.13	39.50	40.85	39.70	38.27	39.85	38.43	40.35	38.41	38.51	40.29	39.74	40.37	39.27	38.32	40.66
C5	30.1	28.72	30.74	25.79	29.32	26.13	25.64	23.95	23.44	24.73	27.67	28.07	26.28	25.41	22.92	23.56	24.74
C6	48.3	53.99	54.99	55.78	56.90	55.16	53.51	55.72	54.96	54.41	56.00	55.60	54.84	55.60	53.76	55.41	54.79
C7	143.4	143.75	142.67	144.03	144.73	141.41	142.78	143.28	144.39	142.50	145.34	141.55	140.96	143.27	142.80	141.88	141.52
C8	123.8	119.31	119.69	121.32	120.62	121.25	119.87	122.92	121.03	123.85	119.87	121.23	125.56	122.48	119.95	121.01	121.18
C9	73.2	71.22	71.72	65.17	65.52	70.63	71.88	64.92	65.05	64.30	65.50	70.42	63.89	65.50	71.62	70.36	70.98
C10	71.7	75.47	75.55	73.90	73.35	78.65	75.29	75.51	74.55	77.44	74.41	77.85	77.53	74.70	75.44	77.31	76.75
C11	45.8	49.70	49.41	48.35	48.08	48.70	50.30	47.86	48.21	46.79	47.83	48.30	46.83	48.27	50.15	48.85	49.34
C12	25.3	23.04	23.34	23.24	23.57	26.75	23.36	26.07	22.47	25.65	23.07	27.42	26.66	25.61	22.93	26.18	25.32
C13	18.1	16.61	16.65	19.07	18.83	18.50	17.39	23.50	18.66	25.08	18.31	18.31	25.31	22.53	16.75	18.76	18.33
C14	25.6	23.73	24.15	24.60	24.63	19.33	24.64	18.81	23.86	19.03	24.47	20.09	18.56	19.84	23.63	19.35	20.42
C15	33.0	30.38	22.23	23.03	23.63	30.73	22.71	30.44	30.83	29.95	30.90	23.71	23.34	25.32	30.68	30.86	26.31

H1a	2.43	2.17	2.27	2.33	2.27	2.48	2.34	2.22	2.51	2.45	2.19	2.34	2.67	2.17	2.56	2.20	2.22
H1b	2.09	2.14	2.12	2.07	2.08	2.13	2.22	2.04	1.97	2.30	2.18	2.26	2.13	2.00	2.15	2.13	2.01
H2	4.57	4.69	4.80	4.63	4.75	4.67	4.71	4.56	4.51	4.72	4.61	4.83	4.81	4.63	4.59	4.59	4.69
H4b	1.93	2.01	2.15	2.13	2.11	1.88	2.15	1.92	2.02	1.82	2.00	1.94	1.94	2.09	2.02	2.01	2.19
H4a	2.19	2.18	2.30	2.45	2.32	2.27	2.44	2.21	2.33	2.19	2.14	2.44	2.24	2.31	2.26	2.22	2.30
H5b	1.62	1.60	1.61	1.61	1.53	1.67	1.64	1.87	1.62	1.56	1.48	1.67	1.60	1.96	1.59	1.70	1.93
H5a	2.51	2.38	2.16	1.97	2.10	2.13	1.92	2.28	2.09	2.25	2.40	1.87	1.97	1.96	2.11	2.45	1.94
H8	5.41	5.58	5.57	5.60	5.60	5.62	5.59	5.61	5.64	5.58	5.61	5.63	5.51	5.64	5.58	5.64	5.66
H9	4.28	3.97	3.94	3.79	3.73	4.02	3.97	3.90	3.82	3.92	3.82	3.92	3.97	3.83	4.01	3.94	3.96
H10	4.41	4.46	4.37	4.70	4.64	4.42	4.41	4.72	4.73	4.49	4.66	4.40	4.48	4.76	4.51	4.51	4.49
Me-12	1.30	1.30	1.19	1.21	1.21	1.28	1.17	1.31	1.30	1.42	1.32	1.30	1.43	1.25	1.28	1.25	1.27
Me-13	0.99	1.13	1.06	1.12	1.18	1.24	1.04	1.23	1.19	1.20	1.24	1.19	1.18	1.24	1.12	1.17	1.10
Me-14	1.96	2.08	2.11	2.02	2.10	1.93	2.02	1.91	1.99	1.86	2.08	1.83	1.74	1.82	1.99	1.94	1.87
Me-15	1.73	1.71	1.77	1.81	1.81	1.67	1.79	1.64	1.70	1.65	1.68	1.82	1.75	1.76	1.67	1.67	1.78

Table S1.3.3 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

MM-DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	36.95	38.83	43.87	39.38	36.01	43.67	38.82	42.38	37.71	37.25	37.87	39.54	40.42	41.81	39.54	40.73
C3	71.9	71.59	71.66	72.38	72.24	72.71	71.57	73.04	72.39	73.46	72.48	72.08	72.76	72.48	71.67	72.47	71.85
C4	38.7	38.79	40.30	41.51	40.39	39.04	40.53	39.04	40.96	39.16	39.18	41.14	40.64	41.06	39.87	39.02	41.41
C5	30.1	29.34	31.49	26.39	29.97	26.80	26.24	24.49	23.97	25.39	28.29	28.82	27.08	26.02	23.44	24.16	25.39
C6	48.3	54.74	55.89	56.50	57.66	56.06	54.26	56.42	55.63	55.28	56.75	56.57	55.86	56.36	54.44	56.22	55.63
C7	143.4	144.99	144.09	145.14	145.85	143.00	143.99	144.43	145.47	143.99	146.52	143.17	142.64	144.47	143.93	143.27	142.93
C8	123.8	120.41	120.98	122.33	121.64	122.68	120.97	123.97	122.01	125.21	120.92	122.70	127.13	123.57	120.97	122.27	122.46
C9	73.2	72.06	72.72	65.94	66.32	71.65	72.73	65.67	65.77	65.24	66.30	71.50	64.98	66.31	72.39	71.28	71.93
C11	45.8	50.43	50.28	49.05	48.80	49.55	51.03	48.52	48.86	47.60	48.55	49.21	47.79	49.00	50.81	49.62	50.15
C12	25.3	23.62	24.05	23.83	24.20	27.43	23.94	26.62	23.00	26.32	23.67	28.16	27.46	26.22	23.45	26.80	25.97
C13	18.1	17.16	17.32	19.64	19.44	19.11	17.94	24.04	19.17	25.74	18.89	18.99	26.10	23.13	17.24	19.33	18.94
C14	25.6	24.32	24.86	25.20	25.26	19.95	25.23	19.32	24.39	19.65	25.08	20.78	19.30	20.42	24.15	19.92	21.04
C15	33.0	31.01	22.93	23.62	24.26	31.44	23.30	31.01	31.40	30.64	31.53	24.43	24.12	25.93	31.24	31.51	26.97
H1a	2.43	2.18	2.28	2.36	2.30	2.49	2.36	2.24	2.54	2.48	2.21	2.36	2.71	2.19	2.57	2.21	2.24
H1b	2.09	2.15	2.13	2.08	2.10	2.13	2.22	2.05	1.98	2.32	2.20	2.28	2.14	2.02	2.16	2.14	2.01
H4b	1.93	2.02	2.16	2.15	2.13	1.88	2.16	1.93	2.03	1.83	2.01	1.95	1.95	2.11	2.02	2.02	2.20
H4a	2.19	2.19	2.32	2.48	2.35	2.27	2.46	2.23	2.35	2.21	2.15	2.47	2.26	2.34	2.27	2.22	2.32
H5b	1.62	1.60	1.60	1.60	1.52	1.67	1.64	1.88	1.62	1.56	1.47	1.67	1.60	1.98	1.59	1.71	1.94
H5a	2.51	2.40	2.17	1.98	2.12	2.14	1.92	2.30	2.11	2.26	2.43	1.87	1.98	1.98	2.11	2.46	1.95
H8	5.41	5.67	5.66	5.77	5.80	5.67	5.66	5.75	5.77	5.69	5.76	5.75	5.67	5.84	5.63	5.69	5.76
H9	4.28	4.02	4.00	3.88	3.84	4.05	4.01	3.98	3.89	3.99	3.90	3.98	4.06	3.94	4.04	3.97	4.01
Me-12	1.30	1.29	1.18	1.19	1.19	1.27	1.16	1.30	1.29	1.41	1.31	1.29	1.42	1.23	1.28	1.25	1.26
Me-13	0.99	1.12	1.05	1.10	1.15	1.23	1.03	1.21	1.18	1.19	1.22	1.17	1.16	1.22	1.11	1.17	1.09
Me-14	1.96	2.09	2.12	2.04	2.12	1.94	2.02	1.92	2.00	1.87	2.09	1.84	1.74	1.83	1.99	1.94	1.88
Me-15	1.73	1.71	1.78	1.82	1.81	1.67	1.80	1.64	1.70	1.65	1.68	1.82	1.75	1.76	1.67	1.67	1.78

Table S1.3.4 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

MM-DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	36.93	38.81	43.91	39.40	36.06	43.65	38.89	42.42	37.81	37.29	37.88	39.60	40.46	41.79	39.58	40.72
C4	38.7	38.77	40.28	41.55	40.41	39.09	40.50	39.12	40.99	39.27	39.22	41.15	40.70	41.10	39.85	39.06	41.41
C5	30.1	29.32	31.48	26.42	29.99	26.84	26.22	24.55	24.00	25.48	28.33	28.83	27.13	26.06	23.43	24.19	25.38
C6	48.3	54.71	55.87	56.55	57.69	56.13	54.23	56.52	55.68	55.41	56.80	56.58	55.93	56.41	54.42	56.27	55.63
C7	143.4	144.93	144.05	145.22	145.91	143.14	143.93	144.64	145.55	144.27	146.62	143.20	142.79	144.57	143.89	143.37	142.92
C8	123.8	120.36	120.94	122.40	121.69	122.80	120.92	124.15	122.08	125.46	121.01	122.73	127.26	123.66	120.93	122.35	122.45
C9	73.2	72.03	72.70	65.99	66.35	71.73	72.69	65.78	65.81	65.39	66.36	71.52	65.06	66.36	72.37	71.33	71.93
C11	45.8	50.41	50.26	49.09	48.83	49.61	51.01	48.61	48.90	47.72	48.59	49.23	47.86	49.04	50.79	49.66	50.15
C12	25.3	23.61	24.04	23.85	24.22	27.47	23.93	26.69	23.03	26.40	23.70	28.17	27.50	26.26	23.44	26.83	25.97
C13	18.1	17.15	17.31	19.66	19.45	19.15	17.93	24.10	19.19	25.83	18.91	19.00	26.15	23.16	17.23	19.36	18.94
C14	25.6	24.30	24.85	25.22	25.28	19.99	25.21	19.37	24.42	19.73	25.11	20.78	19.34	20.45	24.14	19.95	21.03
C15	33.0	30.99	22.91	23.64	24.28	31.49	23.28	31.08	31.43	30.74	31.57	24.44	24.16	25.96	31.23	31.54	26.96
H1a	2.43	2.16	2.26	2.30	2.24	2.46	2.33	2.20	2.46	2.44	2.17	2.33	2.66	2.15	2.53	2.18	2.21
H1b	2.09	2.13	2.11	2.04	2.06	2.12	2.20	2.02	1.95	2.29	2.16	2.25	2.12	1.99	2.13	2.11	2.00
H4b	1.93	2.00	2.14	2.10	2.09	1.88	2.14	1.91	1.99	1.82	1.98	1.93	1.94	2.07	2.00	2.00	2.17

H4a	2.19	2.17	2.29	2.41	2.29	2.25	2.43	2.19	2.29	2.18	2.11	2.43	2.24	2.28	2.25	2.20	2.29
H5b	1.62	1.60	1.60	1.60	1.53	1.67	1.64	1.86	1.62	1.56	1.48	1.66	1.60	1.95	1.59	1.70	1.93
H5a	2.51	2.37	2.16	1.95	2.08	2.12	1.91	2.25	2.07	2.23	2.37	1.86	1.97	1.95	2.09	2.42	1.93
H8	5.41	5.51	5.53	5.43	5.45	5.56	5.53	5.45	5.43	5.50	5.45	5.60	5.50	5.48	5.47	5.51	5.58
H9	4.28	4.40	4.34	4.56	4.53	4.38	4.37	4.59	4.56	4.44	4.53	4.37	4.46	4.63	4.43	4.42	4.43
Me-12	1.30	1.30	1.19	1.23	1.23	1.28	1.18	1.32	1.32	1.42	1.33	1.30	1.43	1.26	1.29	1.26	1.28
Me-13	0.99	1.14	1.06	1.14	1.19	1.25	1.05	1.24	1.21	1.21	1.25	1.19	1.18	1.25	1.13	1.19	1.11
Me-14	1.96	2.07	2.10	2.00	2.08	1.93	2.01	1.90	1.97	1.85	2.06	1.83	1.73	1.81	1.98	1.93	1.87
Me-15	1.73	1.71	1.77	1.80	1.80	1.67	1.79	1.64	1.69	1.65	1.68	1.81	1.74	1.75	1.67	1.66	1.78

Table S1.3.5 – *Experimental data of* ***1a*** *and scaled chemical shifts of* ***1a-1p*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

MM-DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	36.93	38.81	43.91	39.40	36.06	43.65	38.89	42.42	37.81	37.29	37.88	39.60	40.46	41.79	39.58	40.72
C4	38.7	38.77	40.28	41.55	40.41	39.09	40.50	39.12	40.99	39.27	39.22	41.15	40.70	41.10	39.85	39.06	41.41
C5	30.1	29.32	31.48	26.42	29.99	26.84	26.22	24.55	24.00	25.48	28.33	28.83	27.13	26.06	23.43	24.19	25.38
C6	48.3	54.71	55.87	56.55	57.69	56.13	54.23	56.52	55.68	55.41	56.80	56.58	55.93	56.41	54.42	56.27	55.63
C7	143.4	144.93	144.05	145.22	145.91	143.14	143.93	144.64	145.55	144.27	146.62	143.20	142.79	144.57	143.89	143.37	142.92
C8	123.8	120.36	120.94	122.40	121.69	122.80	120.92	124.15	122.08	125.46	121.01	122.73	127.26	123.66	120.93	122.35	122.45
C9	73.2	72.03	72.70	65.99	66.35	71.73	72.69	65.78	65.81	65.39	66.36	71.52	65.06	66.36	72.37	71.33	71.93
C11	45.8	50.41	50.26	49.09	48.83	49.61	51.01	48.61	48.90	47.72	48.59	49.23	47.86	49.04	50.79	49.66	50.15
C12	25.3	23.61	24.04	23.85	24.22	27.47	23.93	26.69	23.03	26.40	23.70	28.17	27.50	26.26	23.44	26.83	25.97
C13	18.1	17.15	17.31	19.66	19.45	19.15	17.93	24.10	19.19	25.83	18.91	19.00	26.15	23.16	17.23	19.36	18.94
C14	25.6	24.30	24.85	25.22	25.28	19.99	25.21	19.37	24.42	19.73	25.11	20.78	19.34	20.45	24.14	19.95	21.03
C15	33.0	30.99	22.91	23.64	24.28	31.49	23.28	31.08	31.43	30.74	31.57	24.44	24.16	25.96	31.23	31.54	26.96
H1a	2.43	2.17	2.27	2.33	2.27	2.48	2.34	2.22	2.51	2.45	2.19	2.34	2.67	2.17	2.56	2.20	2.22
H1b	2.09	2.14	2.12	2.07	2.08	2.13	2.22	2.04	1.97	2.30	2.18	2.26	2.13	2.00	2.15	2.13	2.01
H2	4.57	4.69	4.80	4.63	4.75	4.67	4.71	4.56	4.51	4.72	4.61	4.83	4.81	4.63	4.59	4.59	4.69
H4b	1.93	2.01	2.15	2.13	2.11	1.88	2.15	1.92	2.02	1.82	2.00	1.94	1.94	2.09	2.02	2.01	2.19
H4a	2.19	2.18	2.30	2.45	2.32	2.27	2.44	2.21	2.33	2.19	2.14	2.44	2.24	2.31	2.26	2.22	2.30
H5b	1.62	1.60	1.61	1.61	1.53	1.67	1.64	1.87	1.62	1.56	1.48	1.67	1.60	1.96	1.59	1.70	1.93
H5a	2.51	2.38	2.16	1.97	2.10	2.13	1.92	2.28	2.09	2.25	2.40	1.87	1.97	1.96	2.11	2.45	1.94
H8	5.41	5.58	5.57	5.60	5.60	5.62	5.59	5.61	5.64	5.58	5.61	5.63	5.51	5.64	5.58	5.64	5.66
H9	4.28	3.97	3.94	3.79	3.73	4.02	3.97	3.90	3.82	3.92	3.82	3.92	3.97	3.83	4.01	3.94	3.96
H10	4.41	4.46	4.37	4.70	4.64	4.42	4.41	4.72	4.73	4.49	4.66	4.40	4.48	4.76	4.51	4.51	4.49
Me-12	1.30	1.30	1.19	1.21	1.21	1.28	1.17	1.31	1.30	1.42	1.32	1.30	1.43	1.25	1.28	1.25	1.27
Me-13	0.99	1.13	1.06	1.12	1.18	1.24	1.04	1.23	1.19	1.20	1.24	1.19	1.18	1.24	1.12	1.17	1.10
Me-14	1.96	2.08	2.11	2.02	2.10	1.93	2.02	1.91	1.99	1.86	2.08	1.83	1.74	1.82	1.99	1.94	1.87
Me-15	1.73	1.71	1.77	1.81	1.81	1.67	1.79	1.64	1.70	1.65	1.68	1.82	1.75	1.76	1.67	1.67	1.78

Table S1.4.1 – *Experimental data of* ***1a*** *and calculated isotropic shielding constants of* ***1a-1p*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

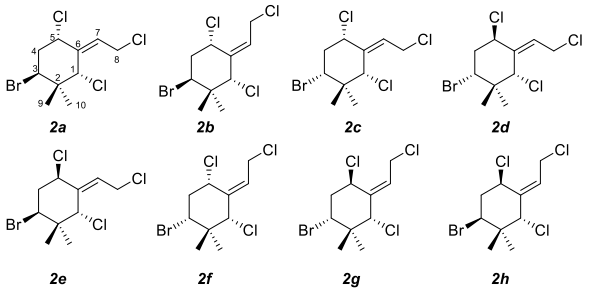
DP4+																	
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Isotropic shielding constants***															
C1	38.2	146.86	145.04	139.77	143.98	146.86	139.24	146.09	141.51	146.45	145.98	145.36	144.70	145.49	140.97	144.97	144.71
C2	60.7	108.94	106.64	107.02	106.33	108.90	107.39	109.86	108.87	109.02	108.62	106.38	106.85	107.74	109.58	110.21	107.81
C3	71.9	100.05	100.13	100.74	100.09	99.68	100.66	98.87	100.13	99.50	100.35	100.39	100.31	99.98	100.07	98.92	100.12
C4	38.7	144.24	143.02	143.01	142.99	144.44	143.00	143.85	144.22	144.05	144.60	143.06	142.80	142.99	144.14	143.47	142.55
C5	30.1	153.71	151.71	156.62	151.87	156.76	157.48	159.03	158.94	158.22	153.66	154.84	155.61	157.91	159.66	159.78	158.85
C6	48.3	130.38	130.65	130.66	130.59	128.68	130.64	129.40	130.40	129.14	130.23	129.19	130.26	130.92	130.30	129.24	130.66
C7	143.4	33.14	32.78	31.71	31.66	34.16	32.34	32.54	32.89	33.08	32.13	35.82	34.35	34.08	32.67	34.45	35.83
C8	123.8	55.23	55.19	54.51	54.60	55.34	54.64	54.56	54.72	55.50	55.33	54.14	54.03	54.09	55.13	53.97	53.69
C9	73.2	111.13	110.71	117.20	117.47	112.36	110.98	116.84	117.07	117.33	117.29	112.23	117.53	117.22	111.05	112.01	111.99
C10	71.7	94.98	95.14	96.10	95.46	93.59	94.67	94.55	96.23	95.49	95.54	93.86	96.04	94.65	95.04	92.69	94.96
C11	45.8	135.22	135.41	137.69	137.64	137.49	135.69	138.83	137.76	138.45	137.71	137.50	138.46	138.47	135.51	138.15	137.24
C12	25.3	161.96	162.93	162.93	163.23	158.08	163.07	159.23	162.29	158.51	162.42	157.79	158.30	160.92	162.13	159.04	160.66
C13	18.1	169.45	169.45	167.34	167.59	167.11	169.09	163.39	167.36	162.99	167.73	167.18	162.36	165.05	169.11	167.16	168.67
C14	25.6	159.16	159.20	159.08	159.51	164.25	159.90	163.83	158.84	164.05	159.41	164.09	163.65	163.63	160.55	164.09	163.73
C15	33.0	153.85	161.54	162.54	162.47	153.73	162.13	153.69	153.52	153.84	153.70	161.77	161.12	158.16	153.55	153.79	157.89
H1a	2.43	29.62	29.63	29.37	29.61	29.23	29.30	29.55	29.02	29.35	29.71	29.39	29.01	29.74	29.13	29.48	29.72
H1b	2.09	29.77	29.77	29.86	29.79	29.62	29.68	29.80	29.96	29.39	29.83	29.46	29.53	30.00	29.85	29.72	29.87
H2	4.57	26.93	26.59	26.80	26.55	27.07	26.81	27.20	27.07	27.07	27.02	26.71	26.67	26.84	27.14	27.15	26.77
H4b	1.93	29.74	29.48	29.47	29.53	29.76	29.45	29.73	29.57	29.82	29.84	29.57	29.56	29.51	29.67	29.76	29.50
H4a	2.19	29.63	29.35	29.16	29.31	29.76	29.19	29.68	29.52	29.78	29.81	29.28	29.29	29.37	29.58	29.66	29.36

H5b	1.62	30.30	30.25	30.11	30.29	30.26	30.21	29.90	30.14	30.31	30.54	30.12	30.11	30.01	30.38	30.13	30.06
H5a	2.51	29.45	29.65	30.00	29.65	29.87	30.06	29.41	29.76	30.03	29.45	30.09	30.03	29.70	29.75	29.33	29.77
H8	5.41	25.92	25.88	25.83	25.77	25.91	25.95	25.80	25.82	25.84	25.79	25.83	25.87	25.78	25.94	25.87	25.89
H9	4.28	27.55	27.54	27.66	27.56	27.49	27.46	27.57	27.57	27.63	27.62	27.51	27.54	27.55	27.51	27.46	27.50
H10	4.41	27.16	27.11	26.77	26.67	27.18	27.23	26.59	26.72	26.78	26.72	27.14	26.81	26.66	27.19	27.02	27.18
Me-12	1.30	30.54	30.60	30.63	30.62	30.53	30.64	30.46	30.50	30.50	30.58	30.45	30.36	30.53	30.55	30.52	30.43
Me-13	0.99	30.75	30.75	30.64	30.63	30.61	30.66	30.58	30.70	30.60	30.70	30.63	30.44	30.54	30.72	30.61	30.71
Me-14	1.96	29.72	29.59	29.68	29.62	29.82	29.69	29.82	29.74	29.87	29.72	29.91	29.94	29.88	29.82	29.85	29.92
Me-15	1.73	29.94	30.00	30.01	30.01	30.01	30.03	30.02	30.03	30.04	30.01	29.90	29.93	29.98	29.95	30.02	29.97

Table S1.4.2 – *Experimental data of **1a** and scaled chemical shifts of **1a-1p** at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory.*

DP4+																
Compound		***1a***	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
Nuclei	***Exp***	***Scaled shifts***															
C1	38.2	35.53	37.42	42.64	38.74	35.67	42.86	36.61	40.75	36.16	36.66	37.19	37.81	37.61	41.08	37.58	38.27
C2	60.7	70.17	72.23	72.33	72.87	70.44	71.53	69.72	70.69	70.68	70.91	72.86	72.74	72.03	69.58	69.17	71.79
C3	71.9	78.29	78.13	78.02	78.53	78.89	77.59	79.76	78.71	79.46	78.48	78.35	78.78	79.10	78.21	79.42	78.78
C4	38.7	37.93	39.25	39.70	39.63	37.88	39.47	38.66	38.26	38.38	37.93	39.29	39.57	39.90	38.20	38.94	40.23
C5	30.1	29.28	31.37	27.37	31.58	26.60	26.44	24.79	24.75	25.31	29.62	28.51	27.74	26.30	24.11	24.13	25.43
C6	48.3	50.59	50.46	50.90	50.88	52.32	50.60	51.86	50.94	52.12	51.10	51.99	51.14	50.90	50.77	51.88	51.04
C7	143.4	139.43	139.19	140.60	140.57	138.89	139.09	140.37	140.39	140.71	141.02	137.45	139.64	139.17	139.42	138.01	137.18
C8	123.8	119.24	118.87	119.93	119.77	119.50	119.02	120.25	120.37	120.04	119.75	120.68	121.48	120.93	119.02	120.27	120.95
C9	71.7	68.18	68.54	63.11	62.77	67.27	68.30	63.34	63.17	63.02	62.96	67.52	62.88	63.39	68.25	67.53	68.00
C10	73.2	82.93	82.66	82.23	82.73	84.46	82.98	83.71	82.29	83.16	82.90	84.33	82.71	83.96	82.78	85.09	83.46
C11	45.8	46.16	46.15	44.53	44.48	44.25	46.05	43.25	44.18	43.54	44.24	44.39	43.57	44.02	46.03	43.78	45.06
C12	25.3	21.73	21.20	21.65	21.28	25.39	21.40	24.60	21.68	25.04	21.59	25.81	25.26	23.56	21.86	24.80	23.79
C13	18.1	14.90	15.29	17.65	17.33	17.12	15.98	20.80	17.03	20.91	16.72	17.22	21.51	19.79	15.53	17.42	16.51
C14	25.6	24.30	24.58	25.14	24.66	19.74	24.25	20.40	24.85	19.93	24.35	20.05	20.32	21.08	23.30	20.21	21.00
C15	33.0	29.15	22.46	22.00	21.98	29.38	22.25	29.67	29.72	29.35	29.58	22.17	22.66	26.07	29.65	29.57	26.30
H1a	2.43	2.17	2.12	2.33	2.12	2.53	2.42	2.17	2.66	2.42	2.13	2.31	2.60	2.01	2.63	2.26	2.05
H1b	2.09	2.03	1.99	1.89	1.96	2.17	2.06	1.95	1.81	2.38	2.03	2.25	2.13	1.78	1.95	2.04	1.91
H2	4.57	4.65	4.86	4.67	4.78	4.55	4.74	4.33	4.44	4.50	4.50	4.79	4.77	4.61	4.50	4.43	4.78
H4a	2.19	2.06	2.25	2.25	2.19	2.03	2.28	2.00	2.16	1.99	2.02	2.15	2.09	2.22	2.12	2.01	2.25
H4b	1.93	2.16	2.37	2.53	2.38	2.03	2.52	2.06	2.21	2.03	2.04	2.41	2.34	2.35	2.21	2.10	2.38
H5a	2.51	1.55	1.56	1.67	1.52	1.57	1.57	1.86	1.64	1.54	1.40	1.63	1.59	1.77	1.46	1.66	1.73
H5b	1.62	2.32	2.10	1.77	2.08	1.94	1.71	2.30	1.99	1.80	2.37	1.66	1.67	2.05	2.05	2.40	2.00
H8	5.41	5.58	5.50	5.55	5.46	5.64	5.54	5.62	5.58	5.61	5.58	5.60	5.51	5.57	5.62	5.62	5.59
H9	4.28	4.07	4.01	3.89	3.91	4.16	4.14	3.99	3.98	3.99	3.97	4.05	3.96	3.97	4.15	4.14	4.10
H10	4.41	4.44	4.39	4.70	4.68	4.45	4.35	4.90	4.75	4.76	4.76	4.39	4.64	4.77	4.45	4.55	4.39
Me-12	1.3	1.32	1.24	1.19	1.24	1.32	1.16	1.34	1.31	1.37	1.37	1.33	1.35	1.31	1.30	1.30	1.40
Me-13	0.99	1.12	1.10	1.18	1.23	1.24	1.15	1.23	1.13	1.28	1.26	1.16	1.28	1.30	1.15	1.21	1.14
Me-14	1.96	2.08	2.15	2.05	2.11	1.98	2.05	1.93	2.01	1.95	2.12	1.83	1.74	1.89	1.98	1.92	1.87
Me-15	1.73	1.88	1.78	1.75	1.77	1.81	1.74	1.74	1.74	1.79	1.87	1.84	1.76	1.80	1.86	1.76	1.82

2. Isomers of 2



C. R. Kaiser, L. F. Pitombo, A. C. Pinto, *Magn. Reson. Chem.* **2001**, *39*, 147–149.

Table S2.1.1 – *Experimental data of **2a-b** and calculated isotropic shielding constants of **2a-2h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory.*

DP4+									
Compound			***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Exp 2b***	***Isotropic shielding constants***							

C8	37.73	37.62	150.42	150.57	150.37	150.46	150.75	150.66	150.87	150.32
C7	131.67	131.89	61.62	61.94	63.85	71.16	70.27	62.75	69.53	68.98
C6	138.22	137.83	57.00	56.82	55.80	54.49	56.75	54.92	55.84	55.09
C5	59.58	50.44	128.08	137.47	131.53	131.21	130.65	140.49	132.38	135.22
C4	41.8	41.32	152.57	153.13	154.87	151.24	151.25	155.62	153.12	154.64
C3	52.72	52.7	127.30	127.30	129.04	123.87	126.74	129.25	124.61	123.51
C2	41.03	41.36	150.61	150.47	151.79	151.09	150.05	152.10	145.77	147.84
C1	60.65	69.98	126.79	117.13	129.53	125.90	122.58	121.66	119.56	120.14
C9	28.6	28.53	167.88	167.58	166.48	167.33	169.35	166.81	167.89	167.64
C10	20.63	20.47	174.89	174.62	168.51	167.79	174.33	167.06	181.11	173.81
H8a	4.16	4.18	27.35	27.33	27.20	27.35	27.40	27.26	27.37	27.23
H8b	4.02	4.04	27.43	27.45	27.39	27.38	27.45	27.33	27.44	27.28
H7	6.03	5.95	25.30	25.31	25.23	25.16	25.21	25.26	25.08	25.18
H5	4.65	4.97	26.81	26.47	26.91	26.02	26.39	26.54	26.25	26.28
H4a	2.65	2.68	29.01	29.02	28.85	29.03	28.98	28.85	29.08	28.87
H4b	2.5	2.53	29.10	29.03	29.00	29.10	29.18	28.86	29.10	29.06
H3	4.83	4.83	26.37	26.32	27.20	27.05	26.73	27.15	26.71	27.00
H1	4.73	4.38	26.71	27.10	26.92	26.72	26.58	27.22	26.54	26.23
Me-9	1.33	1.28	30.28	30.32	30.15	30.20	30.32	30.13	30.19	30.29
Me-10	1.02	1.01	30.52	30.54	30.54	30.50	30.46	30.56	30.51	30.58

Table S2a.1.2 – *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C8	37.73	40.26	40.08	40.38	38.70	39.62	40.24	39.71	39.69
C7	131.67	130.34	130.04	129.84	123.89	124.69	130.28	124.00	124.88
C6	138.22	135.03	135.24	138.17	141.79	138.98	138.31	138.18	139.43
C5	59.58	62.92	53.38	59.86	59.38	60.86	50.65	58.87	55.50
C4	41.8	38.08	37.48	35.73	37.86	39.09	35.16	37.38	35.16
C3	52.72	63.71	63.70	62.44	67.26	65.00	62.17	66.92	67.77
C2	41.03	40.07	40.18	38.92	38.02	40.35	38.76	44.99	42.29
C1	60.65	64.24	74.02	61.94	65.08	69.39	69.94	72.16	71.29
C9	28.6	22.55	22.82	23.73	20.58	19.95	23.69	22.07	21.54
C10	20.63	15.44	15.68	21.62	20.08	14.70	23.44	8.37	15.08
H8a	4.16	4.10	4.12	4.33	4.06	4.03	4.25	4.01	4.11
H8b	4.02	4.02	4.00	4.14	4.03	3.99	4.19	3.95	4.07
H7	6.03	6.02	6.01	6.31	6.11	6.07	6.27	6.11	5.99
H5	4.65	4.60	4.93	4.63	5.30	4.97	4.98	5.04	4.98
H4a	2.65	2.53	2.52	2.68	2.49	2.56	2.65	2.44	2.62
H4b	2.5	2.45	2.52	2.53	2.42	2.37	2.64	2.43	2.44
H3	4.83	5.02	5.07	4.33	4.34	4.65	4.36	4.62	4.32
H1	4.73	4.70	4.34	4.61	4.65	4.79	4.29	4.77	5.02
Me-9	1.33	1.34	1.31	1.37	1.40	1.32	1.36	1.43	1.32
Me-10	1.02	1.12	1.10	0.98	1.11	1.19	0.93	1.14	1.05

Table S2b.1.2 – *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C8	37.62	40.04	40.10	38.44	39.41	40.17	39.57	39.58	40.04
C7	131.89	129.97	130.57	124.42	125.10	130.28	124.21	125.00	129.97
C6	137.83	135.17	138.98	142.49	139.50	138.31	138.45	139.59	135.17
C5	50.44	53.33	59.79	59.31	60.81	50.60	58.81	55.44	53.33
C4	41.32	37.44	35.40	37.59	38.88	35.09	37.23	35.04	37.44
C3	52.7	63.65	62.40	67.27	64.98	62.12	66.89	67.74	63.65
C2	41.36	40.14	38.62	37.75	40.15	38.70	44.87	42.19	40.14
C1	69.98	73.97	61.89	65.07	69.40	69.90	72.15	71.27	73.97
C9	28.53	22.78	23.26	20.15	19.60	23.61	21.86	21.39	22.78
C10	20.47	15.64	21.13	19.65	14.31	23.36	8.10	14.91	15.64
H8a	4.18	4.11	4.33	4.05	4.02	4.24	4.00	4.11	4.11
H8b	4.04	3.99	4.14	4.02	3.98	4.18	3.94	4.06	3.99
H7	5.95	5.99	6.31	6.09	6.06	6.24	6.10	5.99	5.99
H5	4.97	4.91	4.62	5.29	4.96	4.96	5.03	4.98	4.91

H4a	2.68	2.52	2.67	2.49	2.55	2.65	2.44	2.61	2.52
H4b	2.53	2.52	2.52	2.42	2.36	2.64	2.42	2.43	2.52
H3	4.83	5.05	4.33	4.33	4.64	4.35	4.61	4.32	5.05
H1	4.38	4.32	4.61	4.63	4.78	4.28	4.76	5.02	4.32
Me-9	1.28	1.32	1.36	1.40	1.31	1.37	1.42	1.30	1.32
Me-10	1.01	1.11	0.97	1.12	1.18	0.94	1.13	1.04	1.11

Table S2a.1.3 – *Experimental data of **2a** and scaled chemical shifts of **2a-2h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the signals adjacent to bromine.*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C8	37.73	41.62	41.45	41.59	40.51	41.15	41.41	41.47	41.56
C7	131.67	131.08	130.78	130.50	124.93	125.56	130.92	125.01	125.94
C6	138.22	135.73	135.94	138.77	142.66	139.74	138.89	139.06	140.35
C5	59.58	64.13	54.65	60.95	61.00	62.23	51.76	60.46	57.22
C4	41.8	39.46	38.87	36.97	39.68	40.62	36.36	39.17	37.07
C2	41.03	41.43	41.55	40.14	39.84	41.88	39.95	46.71	44.13
C1	60.65	65.43	75.15	63.01	66.66	70.69	70.94	73.63	72.86
C9	28.6	24.04	24.31	25.04	22.56	21.64	24.96	23.99	23.58
C10	20.63	16.97	17.21	22.95	22.06	16.42	24.71	10.42	17.18
H8a	4.16	4.13	4.16	4.25	3.99	4.00	4.18	3.98	4.04
H8b	4.02	4.05	4.04	4.07	3.97	3.96	4.12	3.92	3.99
H7	6.03	6.08	6.08	6.17	5.98	6.02	6.14	6.05	5.86
H5	4.65	4.64	4.98	4.54	5.20	4.93	4.89	4.99	4.88
H4a	2.65	2.55	2.54	2.65	2.46	2.55	2.62	2.43	2.59
H4b	2.5	2.46	2.53	2.50	2.40	2.36	2.62	2.42	2.41
H1	4.73	4.74	4.37	4.53	4.56	4.75	4.22	4.73	4.92
Me-9	1.33	1.34	1.31	1.38	1.40	1.32	1.37	1.43	1.33
Me-10	1.02	1.11	1.09	1.00	1.13	1.19	0.95	1.15	1.07

Table S2b.1.3 – *Experimental data of **2b** and scaled chemical shifts of **2a-2h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the signals adjacent to bromine.*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C8	37.62	41.33	41.40	41.30	40.26	40.94	41.34	41.33	41.45
C7	131.89	131.84	130.72	131.23	125.46	125.97	130.92	125.22	126.07
C6	137.83	136.54	135.88	139.59	143.37	140.27	138.91	139.34	140.52
C5	50.44	64.10	54.60	60.88	60.94	62.17	51.70	60.40	57.16
C4	41.32	39.14	38.82	36.63	39.42	40.41	36.29	39.01	36.95
C2	41.36	41.14	41.50	39.83	39.58	41.67	39.88	46.59	44.03
C1	69.98	65.42	75.10	62.97	66.65	70.70	70.89	73.63	72.84
C9	28.53	23.54	24.26	24.56	22.13	21.28	24.88	23.77	23.42
C10	20.47	16.39	17.16	22.45	21.64	16.02	24.63	10.14	17.00
H8a	4.18	4.13	4.14	4.25	3.98	4.00	4.17	3.97	4.03
H8b	4.04	4.04	4.02	4.06	3.95	3.95	4.10	3.91	3.99
H7	5.95	6.08	6.05	6.17	5.96	6.01	6.11	6.04	5.86
H5	4.97	4.64	4.96	4.53	5.18	4.92	4.87	4.98	4.88
H4a	2.68	2.53	2.54	2.64	2.46	2.54	2.62	2.43	2.58
H4b	2.53	2.45	2.53	2.49	2.40	2.36	2.61	2.41	2.40
H1	4.38	4.74	4.36	4.52	4.55	4.75	4.20	4.72	4.92
Me-9	1.28	1.32	1.31	1.37	1.41	1.31	1.38	1.42	1.31
Me-10	1.01	1.09	1.10	0.99	1.13	1.19	0.96	1.14	1.05

Table S2a.1.4– *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C7	131.67	132.37	132.14	131.05	126.01	127.37	131.33	127.00	127.40
C6	138.22	136.96	137.25	139.24	143.59	141.38	139.24	140.86	141.63
C4	41.8	41.89	41.29	38.42	41.52	43.51	37.53	42.35	39.59
C2	41.03	43.84	43.94	41.56	41.67	44.75	41.09	49.79	46.57
C9	28.6	26.66	26.90	26.60	24.55	24.77	26.23	27.39	26.27
C10	20.63	19.68	19.88	24.53	24.06	19.61	25.98	14.00	19.94
H7	6.03	6.02	6.01	5.99	6.05	6.04	5.97	6.06	5.99
H4a	2.65	2.53	2.52	2.60	2.48	2.55	2.58	2.43	2.62
H4b	2.5	2.45	2.52	2.46	2.41	2.36	2.57	2.41	2.45
Me-9	1.33	1.34	1.31	1.38	1.40	1.31	1.37	1.42	1.33
Me-10	1.02	1.11	1.10	1.01	1.12	1.18	0.96	1.13	1.06

Table S2b.1.4– *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C7	131.89	131.05	126.01	127.37	131.33	127.00	127.40	131.05	126.01
C6	137.83	139.24	143.59	141.38	139.24	140.86	141.63	139.24	143.59
C4	41.32	38.42	41.52	43.51	37.53	42.35	39.59	38.42	41.52
C2	41.36	41.56	41.67	44.75	41.09	49.79	46.57	41.56	41.67
C9	28.53	26.60	24.55	24.77	26.23	27.39	26.27	26.60	24.55
C10	20.47	24.53	24.06	19.61	25.98	14.00	19.94	24.53	24.06
H7	5.95	5.99	6.05	6.04	5.97	6.06	5.99	5.99	6.05
H4a	2.68	2.60	2.48	2.55	2.58	2.43	2.62	2.60	2.48
H4b	2.53	2.46	2.41	2.36	2.57	2.41	2.45	2.46	2.41
Me-9	1.28	1.38	1.40	1.31	1.37	1.42	1.33	1.38	1.40
Me-10	1.01	1.01	1.12	1.18	0.96	1.13	1.06	1.01	1.12

Table S2a.1.5 – *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C7	131.67	132.14	131.05	126.01	127.37	131.33	127.00	127.40	132.14
C6	138.22	137.25	139.24	143.59	141.38	139.24	140.86	141.63	137.25
C4	41.8	41.29	38.42	41.52	43.51	37.53	42.35	39.59	41.29
C2	41.03	43.94	41.56	41.67	44.75	41.09	49.79	46.57	43.94
C9	28.6	26.90	26.60	24.55	24.77	26.23	27.39	26.27	26.90
C10	20.63	19.88	24.53	24.06	19.61	25.98	14.00	19.94	19.88
H8a	4.16	4.11	4.33	4.05	4.02	4.24	4.00	4.11	4.11
H8b	4.02	3.99	4.14	4.02	3.98	4.18	3.94	4.06	3.99
H7	6.03	5.99	6.31	6.09	6.06	6.24	6.10	5.99	5.99
H5	4.65	4.91	4.62	5.29	4.96	4.96	5.03	4.98	4.91
H4a	2.65	2.52	2.67	2.49	2.55	2.65	2.44	2.61	2.52
H4b	2.5	2.52	2.52	2.42	2.36	2.64	2.42	2.43	2.52
H3	4.83	5.05	4.33	4.33	4.64	4.35	4.61	4.32	5.05
H1	4.73	4.32	4.61	4.63	4.78	4.28	4.76	5.02	4.32
Me-9	1.33	1.32	1.36	1.40	1.31	1.37	1.42	1.30	1.32
Me-10	1.02	1.11	0.97	1.12	1.18	0.94	1.13	1.04	1.11

Table S2b.1.5 – *Experimental data of **2b** and scaled chemical shifts of **2a-2h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4+									
Compound		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2b**	**Scaled shifts**							
C7	131.89	132.37	132.14	131.05	126.01	127.37	131.33	127.00	127.40
C6	137.83	136.96	137.25	139.24	143.59	141.38	139.24	140.86	141.63
C4	41.32	41.89	41.29	38.42	41.52	43.51	37.53	42.35	39.59
C2	41.36	43.84	43.94	41.56	41.67	44.75	41.09	49.79	46.57
C9	28.53	26.66	26.90	26.60	24.55	24.77	26.23	27.39	26.27
C10	20.47	19.68	19.88	24.53	24.06	19.61	25.98	14.00	19.94
H8a	4.18	4.10	4.11	4.33	4.05	4.02	4.24	4.00	4.11
H8b	4.04	4.02	3.99	4.14	4.02	3.98	4.18	3.94	4.06
H7	5.95	6.03	5.99	6.31	6.09	6.06	6.24	6.10	5.99
H5	4.97	4.60	4.91	4.62	5.29	4.96	4.96	5.03	4.98
H4a	2.68	2.52	2.52	2.67	2.49	2.55	2.65	2.44	2.61
H4b	2.53	2.44	2.52	2.52	2.42	2.36	2.64	2.42	2.43
H3	4.83	5.02	5.05	4.33	4.33	4.64	4.35	4.61	4.32
H1	4.38	4.70	4.32	4.61	4.63	4.78	4.28	4.76	5.02
Me-9	1.28	1.32	1.32	1.36	1.40	1.31	1.37	1.42	1.30
Me-10	1.01	1.10	1.11	0.97	1.12	1.18	0.94	1.13	1.04

Table S2.2.1 – *Experimental data of **2a-b** and calculated isotropic shielding constants of **2a-2h** at the B3LYP/6-31G**//MMFF level of theory.*

DP4										
Compound			**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2a**	**Exp 2b**	**Isotropic shielding constants**							
C8	37.73	37.62	153.06	153.03	147.59	151.76	153.74	147.94	153.53	149.69
C7	131.67	131.89	63.08	63.08	62.71	65.82	68.15	61.93	67.25	61.73
C6	138.22	137.83	52.51	52.70	56.88	51.87	50.80	57.63	50.75	54.81
C5	59.58	50.44	131.74	140.74	129.11	130.44	131.02	131.91	135.92	134.56
C4	41.8	41.32	147.02	147.37	143.25	145.46	144.85	144.37	147.54	145.88
C3	52.72	52.7	129.25	129.29	124.86	126.73	127.55	125.22	125.63	127.11
C2	41.03	41.36	145.11	144.95	141.73	144.63	144.71	142.01	140.97	144.31
C1	60.65	69.98	127.47	118.06	119.90	125.65	123.24	117.62	118.91	114.68
C10	20.63	20.47	169.50	169.70	175.02	166.80	168.97	174.18	175.92	166.93
C9	28.6	28.53	162.69	162.62	163.92	162.17	163.29	163.51	163.39	164.92
H8b	4.02	4.04	28.06	28.07	27.49	27.76	28.07	27.50	28.09	27.45
H8a	4.16	4.18	27.86	27.82	27.10	27.74	27.94	26.95	27.90	27.45
H7	6.03	5.95	25.90	25.93	25.57	25.61	25.46	25.58	25.41	25.79
H5	4.65	4.97	27.44	27.01	27.86	26.70	26.95	27.73	26.76	26.84
H4b	2.5	2.53	29.38	29.37	29.55	29.40	29.49	29.37	29.36	29.40
H4a	2.65	2.68	29.32	29.28	29.28	29.27	29.23	29.34	29.34	29.28
H3	4.83	4.83	26.72	26.72	27.94	27.44	27.20	27.92	27.14	27.31
H1	4.73	4.38	27.21	27.64	27.74	26.97	26.97	27.85	26.90	27.29
Me-9	1.02	1.01	30.75	30.78	30.58	30.60	30.61	30.68	30.73	30.62
Me-10	1.33	1.28	30.47	30.51	30.57	30.47	30.51	30.61	30.48	30.60

Table S2a.2.2 – *Experimental data of **2a** and scaled shifts of **2a-2h** at the B3LYP/6-31G**//MMFF level of theory*

DP4									
Compound		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2a**	**Scaled shifts**							
C8	37.73	35.19	35.55	38.70	34.84	33.48	38.54	34.81	36.78
C7	131.67	129.15	128.36	129.29	126.88	124.41	130.08	123.97	129.31
C6	138.22	140.19	139.07	135.51	141.81	142.84	134.65	141.02	136.59
C5	59.58	57.46	48.23	58.43	57.68	57.61	55.60	53.01	52.69
C4	41.8	41.50	41.39	43.34	41.58	42.93	42.34	41.00	40.79
C3	52.72	60.05	60.04	62.96	61.64	61.30	62.72	63.65	60.53
C2	41.03	43.49	43.89	44.96	42.48	43.07	44.85	47.79	42.44
C1	60.65	61.92	71.63	68.25	62.80	65.88	70.81	70.59	73.61
C9	20.63	18.03	18.34	9.43	18.74	17.29	10.61	11.68	18.65

C10	28.6	25.14	25.65	21.28	23.70	23.33	21.97	24.62	20.76
H8a	4.02	3.85	3.83	4.53	4.02	3.76	4.49	3.70	4.34
H8b	4.16	4.05	4.08	4.95	4.04	3.89	5.08	3.88	4.34
H7	6.03	6.07	6.01	6.60	6.16	6.33	6.53	6.27	5.99
H5	4.65	4.48	4.91	4.13	5.08	4.86	4.25	4.97	4.94
H4a	2.5	2.48	2.51	2.31	2.39	2.35	2.50	2.49	2.39
H4b	2.65	2.55	2.61	2.60	2.51	2.61	2.54	2.51	2.51
H3	4.83	5.22	5.20	4.05	4.33	4.61	4.04	4.61	4.48
H1	4.73	4.72	4.27	4.26	4.81	4.84	4.11	4.84	4.50
Me-9	1.02	1.07	1.08	1.20	1.19	1.25	1.12	1.17	1.17
Me-10	1.33	1.36	1.35	1.20	1.32	1.35	1.19	1.41	1.20

Table S2b.2.2 – *Experimental data of* ***2b*** *and scaled shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory*

DP4									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C8	37.62	35.19	35.55	38.70	34.84	33.48	38.54	34.81	36.78
C7	131.89	129.15	128.36	129.29	126.88	124.41	130.08	123.97	129.31
C6	137.83	140.19	139.07	135.51	141.81	142.84	134.65	141.02	136.59
C5	50.44	57.46	48.23	58.43	57.68	57.61	55.60	53.01	52.69
C4	41.32	41.50	41.39	43.34	41.58	42.93	42.34	41.00	40.79
C3	52.7	60.05	60.04	62.96	61.64	61.30	62.72	63.65	60.53
C2	41.36	43.49	43.89	44.96	42.48	43.07	44.85	47.79	42.44
C1	69.98	61.92	71.63	68.25	62.80	65.88	70.81	70.59	73.61
C9	28.53	18.03	18.34	9.43	18.74	17.29	10.61	11.68	18.65
C10	20.47	25.14	25.65	21.28	23.70	23.33	21.97	24.62	20.76
H8a	4.18	3.85	3.83	4.53	4.02	3.76	4.49	3.70	4.34
H8b	4.04	4.05	4.08	4.95	4.04	3.89	5.08	3.88	4.34
H7	5.95	6.07	6.01	6.60	6.16	6.33	6.53	6.27	5.99
H5	4.97	4.48	4.91	4.13	5.08	4.86	4.25	4.97	4.94
H4a	2.68	2.48	2.51	2.31	2.39	2.35	2.50	2.49	2.39
H4b	2.53	2.55	2.61	2.60	2.51	2.61	2.54	2.51	2.51
H3	4.83	5.22	5.20	4.05	4.33	4.61	4.04	4.61	4.48
H1	4.38	4.72	4.27	4.26	4.81	4.84	4.11	4.84	4.50
Me-9	1.28	1.07	1.08	1.20	1.19	1.25	1.12	1.17	1.17
Me-10	1.01	1.36	1.35	1.20	1.32	1.35	1.19	1.41	1.20

Table S2a.2.3 – *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

DP4									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C8	37.73	36.13	36.48	39.98	35.98	34.58	39.79	36.21	37.77
C7	131.67	129.66	128.87	129.99	127.50	125.03	130.76	124.76	129.84
C6	138.22	140.65	139.53	136.18	142.35	143.36	135.30	141.69	137.09
C5	59.58	58.29	49.10	59.58	58.69	58.59	56.74	54.28	53.60
C4	41.8	42.41	42.29	44.59	42.69	43.98	43.56	42.35	41.76
C2	41.03	44.39	44.78	46.20	43.57	44.12	46.06	49.09	43.40
C1	60.65	62.73	72.40	69.35	63.78	66.82	71.86	71.74	74.42
C9	28.6	19.05	19.35	10.90	19.97	18.48	12.04	13.23	19.73
C10	20.63	26.13	26.63	22.67	24.90	24.49	23.32	26.09	21.83
H8a	4.16	3.90	3.88	4.40	3.95	3.73	4.36	3.67	4.28
H8b	4.02	4.11	4.14	4.80	3.97	3.86	4.92	3.85	4.28
H7	6.03	6.17	6.11	6.38	6.03	6.26	6.30	6.20	5.89
H5	4.65	4.55	4.99	4.02	4.97	4.82	4.13	4.93	4.87
H4a	2.65	2.50	2.53	2.28	2.37	2.35	2.46	2.47	2.38
H4b	2.5	2.57	2.63	2.56	2.49	2.60	2.50	2.50	2.49
H1	4.73	4.80	4.33	4.14	4.71	4.80	4.00	4.80	4.43
Me-9	1.33	1.06	1.07	1.22	1.20	1.26	1.14	1.18	1.18
Me-10	1.02	1.36	1.35	1.22	1.33	1.35	1.21	1.41	1.21

Table S2b.2.3 – *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

DP4									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C8	37.62	36.13	36.48	39.98	35.98	34.58	39.79	36.21	37.77
C7	131.89	129.66	128.87	129.99	127.50	125.03	130.76	124.76	129.84
C6	137.83	140.65	139.53	136.18	142.35	143.36	135.30	141.69	137.09
C5	50.44	58.29	49.10	59.58	58.69	58.59	56.74	54.28	53.60
C4	41.32	42.41	42.29	44.59	42.69	43.98	43.56	42.35	41.76
C2	41.36	44.39	44.78	46.20	43.57	44.12	46.06	49.09	43.40
C1	69.98	62.73	72.40	69.35	63.78	66.82	71.86	71.74	74.42
C9	28.53	19.05	19.35	10.90	19.97	18.48	12.04	13.23	19.73
C10	20.47	26.13	26.63	22.67	24.90	24.49	23.32	26.09	21.83
H8a	4.18	3.90	3.88	4.40	3.95	3.73	4.36	3.67	4.28
H8b	4.04	4.11	4.14	4.80	3.97	3.86	4.92	3.85	4.28
H7	5.95	6.17	6.11	6.38	6.03	6.26	6.30	6.20	5.89
H5	4.97	4.55	4.99	4.02	4.97	4.82	4.13	4.93	4.87
H4a	2.68	2.50	2.53	2.28	2.37	2.35	2.46	2.47	2.38
H4b	2.53	2.57	2.63	2.56	2.49	2.60	2.50	2.50	2.49
H1	4.38	4.80	4.33	4.14	4.71	4.80	4.00	4.80	4.43
Me-9	1.28	1.06	1.07	1.22	1.20	1.26	1.14	1.18	1.18
Me-10	1.01	1.36	1.35	1.22	1.33	1.35	1.21	1.41	1.21

Table S2a.2.4– *Experimental data of* ***2a*** *and scaled chemcial shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C7	131.67	129.04	129.14	130.81	127.12	125.12	131.75	125.39	130.94
C6	138.22	139.95	139.85	136.90	141.86	143.39	136.24	142.30	138.17
C4	41.8	42.45	42.17	46.72	42.94	44.39	45.53	43.08	43.12
C2	41.03	44.42	44.67	48.30	43.82	44.53	48.00	49.81	44.76
C9	28.6	19.26	19.13	13.54	20.39	18.99	14.36	13.99	21.16
C10	20.63	26.29	26.44	25.14	25.28	24.97	25.52	26.83	23.25
H7	6.03	6.01	5.99	6.08	6.06	6.07	6.04	6.06	6.03
H4a	2.65	2.47	2.49	2.27	2.37	2.29	2.45	2.42	2.43
H4b	2.5	2.53	2.58	2.53	2.49	2.53	2.48	2.44	2.55
Me-9	1.33	1.07	1.06	1.28	1.20	1.23	1.21	1.15	1.21
Me-10	1.02	1.36	1.33	1.29	1.33	1.33	1.28	1.38	1.23

Table S2b.2.4– *Experimental data of* ***2b*** *and scaled chemcial shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C7	131.89	129.04	129.14	130.81	127.12	125.12	131.75	125.39	130.94
C6	137.83	139.95	139.85	136.90	141.86	143.39	136.24	142.30	138.17
C4	41.32	42.45	42.17	46.72	42.94	44.39	45.53	43.08	43.12
C2	41.36	44.42	44.67	48.30	43.82	44.53	48.00	49.81	44.76
C9	28.53	19.26	19.13	13.54	20.39	18.99	14.36	13.99	21.16
C10	20.47	26.29	26.44	25.14	25.28	24.97	25.52	26.83	23.25
H7	5.95	6.01	5.99	6.08	6.06	6.07	6.04	6.06	6.03
H4a	2.68	2.47	2.49	2.27	2.37	2.29	2.45	2.42	2.43
H4b	2.53	2.53	2.58	2.53	2.49	2.53	2.48	2.44	2.55
Me-9	1.28	1.07	1.06	1.28	1.20	1.23	1.21	1.15	1.21
Me-10	1.01	1.36	1.33	1.29	1.33	1.33	1.28	1.38	1.23

Table S2a.2.5 – *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4									
Compound		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2a**	**Scaled shifts**							
C7	131.67	129.04	129.14	130.81	127.12	125.12	131.75	125.39	130.94
C6	138.22	139.95	139.85	136.90	141.86	143.39	136.24	142.30	138.17
C4	41.8	42.45	42.17	46.72	42.94	44.39	45.53	43.08	43.12
C2	41.03	44.42	44.67	48.30	43.82	44.53	48.00	49.81	44.76
C9	28.6	19.26	19.13	13.54	20.39	18.99	14.36	13.99	21.16
C10	20.63	26.29	26.44	25.14	25.28	24.97	25.52	26.83	23.25
H8a	4.16	3.85	3.83	4.53	4.02	3.76	4.49	3.70	4.34
H8b	4.02	4.05	4.08	4.95	4.04	3.89	5.08	3.88	4.34
H7	6.03	6.07	6.01	6.60	6.16	6.33	6.53	6.27	5.99
H5	4.65	4.48	4.91	4.13	5.08	4.86	4.25	4.97	4.94
H4a	2.65	2.48	2.51	2.31	2.39	2.35	2.50	2.49	2.39
H4b	2.5	2.55	2.61	2.60	2.51	2.61	2.54	2.51	2.51
H3	4.83	5.22	5.20	4.05	4.33	4.61	4.04	4.61	4.48
H1	4.73	4.72	4.27	4.26	4.81	4.84	4.11	4.84	4.50
Me-9	1.33	1.07	1.08	1.20	1.19	1.25	1.12	1.17	1.17
Me-10	1.02	1.36	1.35	1.20	1.32	1.35	1.19	1.41	1.20

Table S2b.2.5 – *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4									
Compound		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2b**	**Scaled shifts**							
C7	131.89	129.04	129.14	130.81	127.12	125.12	131.75	125.39	130.94
C6	137.83	139.95	139.85	136.90	141.86	143.39	136.24	142.30	138.17
C4	41.32	42.45	42.17	46.72	42.94	44.39	45.53	43.08	43.12
C2	41.36	44.42	44.67	48.30	43.82	44.53	48.00	49.81	44.76
C9	28.53	19.26	19.13	13.54	20.39	18.99	14.36	13.99	21.16
C10	20.47	26.29	26.44	25.14	25.28	24.97	25.52	26.83	23.25
H8a	4.18	3.85	3.83	4.53	4.02	3.76	4.49	3.70	4.34
H8b	4.04	4.05	4.08	4.95	4.04	3.89	5.08	3.88	4.34
H7	5.95	6.07	6.01	6.60	6.16	6.33	6.53	6.27	5.99
H5	4.97	4.48	4.91	4.13	5.08	4.86	4.25	4.97	4.94
H4a	2.68	2.48	2.51	2.31	2.39	2.35	2.50	2.49	2.39
H4b	2.53	2.55	2.61	2.60	2.51	2.61	2.54	2.51	2.51
H3	4.83	5.22	5.20	4.05	4.33	4.61	4.04	4.61	4.48
H1	4.38	4.72	4.27	4.26	4.81	4.84	4.11	4.84	4.50
Me-9	1.28	1.07	1.08	1.20	1.19	1.25	1.12	1.17	1.17
Me-10	1.01	1.36	1.35	1.20	1.32	1.35	1.19	1.41	1.20

Table S2.3.1 – *Experimental data of* ***2a-b*** *and calculated isotropic shielding constants of* ***2a-2h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory.*

MM-DP4+										
Compound			**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2a**	**Exp 2b**	**Isotropic shielding constants**							
C8	37.73	37.62	153.06	153.03	147.59	151.76	153.74	147.94	153.53	149.69
C7	131.67	131.89	63.08	63.08	62.71	65.82	68.15	61.93	67.25	61.73
C6	138.22	137.83	52.51	52.70	56.88	51.87	50.80	57.63	50.75	54.81
C5	59.58	50.44	131.74	140.74	129.11	130.44	131.02	131.91	135.92	134.56
C4	41.8	41.32	147.02	147.37	143.25	145.46	144.85	144.37	147.54	145.88
C3	52.72	52.7	129.25	129.29	124.86	126.73	127.55	125.22	125.63	127.11
C2	41.03	41.36	145.11	144.95	141.73	144.63	144.71	142.01	140.97	144.31
C1	60.65	69.98	127.47	118.06	119.90	125.65	123.24	117.62	118.91	114.68
C10	20.63	20.47	169.50	169.70	175.02	166.80	168.97	174.18	175.92	166.93
C9	28.6	28.53	162.69	162.62	163.92	162.17	163.29	163.51	163.39	164.92
H8b	4.02	4.04	28.06	28.07	27.49	27.76	28.07	27.50	28.09	27.45
H8a	4.16	4.18	27.86	27.82	27.10	27.74	27.94	26.95	27.90	27.45
H7	6.03	5.95	25.90	25.93	25.57	25.61	25.46	25.58	25.41	25.79
H5	4.65	4.97	27.44	27.01	27.86	26.70	26.95	27.73	26.76	26.84

H4b	2.5	2.53	29.38	29.37	29.55	29.40	29.49	29.37	29.36	29.40
H4a	2.65	2.68	29.32	29.28	29.28	29.27	29.23	29.34	29.34	29.28
H3	4.83	4.83	26.72	26.72	27.94	27.44	27.20	27.92	27.14	27.31
H1	4.73	4.38	27.21	27.64	27.74	26.97	26.97	27.85	26.90	27.29
Me-9	1.02	1.01	30.75	30.78	30.58	30.60	30.61	30.68	30.73	30.62
Me-10	1.33	1.28	30.47	30.51	30.57	30.47	30.51	30.61	30.48	30.60

Table S2a.3.2 – *Experimental data of **2a** and scaled chemical shifts of **2a-2h** at the SMD/wB97XD/6-31+G**//MMFF level of theory.*

MM-DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C8	37.73	36.35	36.46	37.07	33.82	34.69	36.90	35.48	35.69
C7	131.67	130.26	130.46	130.49	124.69	124.73	131.09	124.56	125.92
C6	138.22	138.68	138.30	141.46	144.68	142.42	141.20	141.24	142.13
C5	59.58	56.58	48.23	53.66	55.69	57.68	45.28	52.72	50.52
C4	41.8	41.92	41.35	39.94	42.29	42.85	39.43	41.44	38.89
C3	52.72	59.32	59.42	56.98	60.43	60.35	56.78	62.36	62.18
C2	41.03	43.76	43.90	43.28	42.03	43.15	42.95	47.35	44.62
C1	60.65	60.51	69.27	57.20	60.25	63.90	65.06	69.09	67.54
C9	20.63	19.44	19.20	25.57	23.66	18.99	26.70	13.30	19.55
C10	28.6	25.80	26.04	26.99	25.11	23.86	27.23	25.09	25.59
H8a	4.02	3.85	3.87	3.96	3.83	3.80	3.95	3.76	3.85
H8b	4.16	4.00	3.99	4.11	3.86	3.89	4.11	3.86	3.91
H7	6.03	6.18	6.18	6.44	6.29	6.26	6.40	6.22	6.18
H5	4.65	4.59	4.87	4.66	5.25	4.91	5.03	4.97	4.98
H4a	2.5	2.45	2.53	2.52	2.51	2.36	2.62	2.40	2.42
H4b	2.65	2.60	2.57	2.73	2.57	2.64	2.74	2.53	2.66
H3	4.83	5.00	4.99	4.34	4.29	4.55	4.34	4.59	4.32
H1	4.73	4.73	4.43	4.71	4.79	4.91	4.36	4.94	5.09
Me-9	1.02	1.16	1.15	1.05	1.17	1.25	1.00	1.17	1.12
Me-10	1.33	1.37	1.33	1.40	1.37	1.33	1.36	1.47	1.38

Table S2b.3.2 – *Experimental data of **2b** and scaled chemical shifts of **2a-2h** at the SMD/wB97XD/6-31+G**//MMFF level of theory.*

MM-DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C8	37.62	36.04	36.42	36.77	33.49	34.41	36.84	35.36	35.58
C7	131.89	130.92	130.39	131.18	125.28	125.25	131.08	124.67	126.01
C6	137.83	139.42	138.23	142.26	145.47	143.09	141.20	141.39	142.25
C5	50.44	56.48	48.19	53.53	55.58	57.60	45.22	52.65	50.45
C4	41.32	41.67	41.31	39.67	42.04	42.63	39.37	41.34	38.79
C3	52.7	59.25	59.37	56.88	60.37	60.29	56.73	62.32	62.14
C2	41.36	43.53	43.86	43.04	41.79	42.94	42.89	47.27	44.53
C1	69.98	60.45	69.21	57.10	60.19	63.88	65.01	69.06	67.51
C9	28.53	18.97	19.16	25.14	23.23	18.57	26.63	13.13	19.41
C10	20.47	25.39	26.00	26.58	24.69	23.48	27.16	24.95	25.46
H8a	4.18	3.84	3.86	3.96	3.82	3.80	3.94	3.75	3.85
H8b	4.04	3.99	3.98	4.10	3.85	3.88	4.10	3.85	3.91
H7	5.95	6.19	6.17	6.44	6.28	6.27	6.38	6.23	6.19
H5	4.97	4.59	4.86	4.66	5.24	4.91	5.02	4.97	4.98
H4a	2.68	2.43	2.53	2.51	2.50	2.35	2.62	2.39	2.41
H4b	2.53	2.58	2.57	2.72	2.56	2.63	2.74	2.52	2.65
H3	4.83	5.00	4.98	4.34	4.28	4.55	4.33	4.59	4.32
H1	4.38	4.73	4.42	4.71	4.78	4.91	4.35	4.94	5.09
Me-9	1.28	1.14	1.15	1.03	1.17	1.24	1.00	1.15	1.10
Me-10	1.01	1.35	1.33	1.39	1.37	1.32	1.37	1.45	1.36

Table S2a.3.3 – *Experimental data of **2a** and scaled chemical shifts of **2a-2h** at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

MM-DP4+								
Compound	***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***

Nuclei	Exp 2a	Scaled shifts							
C8	37.73	36.87	37.26	37.30	34.48	35.38	37.35	36.59	36.78
C7	131.67	131.36	130.84	131.46	125.83	125.80	131.35	125.35	126.68
C6	138.22	139.83	138.65	142.51	145.92	143.55	141.45	141.98	142.83
C5	59.58	57.23	48.98	54.01	56.46	58.46	45.71	53.77	51.56
C4	41.8	42.48	42.14	40.19	42.99	43.56	39.87	42.53	39.97
C2	41.03	44.33	44.67	43.55	42.73	43.87	43.39	48.42	45.68
C1	60.65	61.18	69.92	57.58	61.04	64.71	65.45	70.08	68.52
C9	28.6	19.87	20.08	25.70	24.26	19.61	27.17	14.48	20.70
C10	20.63	26.26	26.89	27.14	25.72	24.50	27.70	26.23	26.72
H8a	4.16	3.87	3.88	3.89	3.75	3.76	3.87	3.72	3.78
H8b	4.02	4.02	4.00	4.03	3.78	3.85	4.03	3.82	3.84
H7	6.03	6.23	6.21	6.30	6.12	6.19	6.24	6.16	6.05
H5	4.65	4.62	4.89	4.57	5.12	4.85	4.92	4.92	4.88
H4a	2.65	2.44	2.54	2.48	2.48	2.34	2.59	2.38	2.39
H4b	2.5	2.59	2.58	2.69	2.53	2.62	2.71	2.51	2.62
H1	4.73	4.76	4.44	4.62	4.68	4.85	4.27	4.89	4.98
Me-9	1.33	1.14	1.15	1.05	1.18	1.25	1.02	1.16	1.12
Me-10	1.02	1.35	1.33	1.39	1.38	1.32	1.38	1.46	1.37

Table S2b.3.3 – *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

MM-DP4+									
Compound		2a	2b	2c	2d	2e	2f	2g	2h
Nuclei	Exp 2b	Scaled shifts							
C8	37.62	36.87	37.26	37.30	34.48	35.38	37.35	36.59	36.78
C7	131.89	131.36	130.84	131.46	125.83	125.80	131.35	125.35	126.68
C6	137.83	139.83	138.65	142.51	145.92	143.55	141.45	141.98	142.83
C5	50.44	57.23	48.98	54.01	56.46	58.46	45.71	53.77	51.56
C4	41.32	42.48	42.14	40.19	42.99	43.56	39.87	42.53	39.97
C2	41.36	44.33	44.67	43.55	42.73	43.87	43.39	48.42	45.68
C1	69.98	61.18	69.92	57.58	61.04	64.71	65.45	70.08	68.52
C9	28.53	19.87	20.08	25.70	24.26	19.61	27.17	14.48	20.70
C10	20.47	26.26	26.89	27.14	25.72	24.50	27.70	26.23	26.72
H8a	4.18	3.87	3.88	3.89	3.75	3.76	3.87	3.72	3.78
H8b	4.04	4.02	4.00	4.03	3.78	3.85	4.03	3.82	3.84
H7	5.95	6.23	6.21	6.30	6.12	6.19	6.24	6.16	6.05
H5	4.97	4.62	4.89	4.57	5.12	4.85	4.92	4.92	4.88
H4a	2.68	2.44	2.54	2.48	2.48	2.34	2.59	2.38	2.39
H4b	2.53	2.59	2.58	2.69	2.53	2.62	2.71	2.51	2.62
H1	4.38	4.76	4.44	4.62	4.68	4.85	4.27	4.89	4.98
Me-9	1.28	1.14	1.15	1.05	1.18	1.25	1.02	1.16	1.12
Me-10	1.01	1.35	1.33	1.39	1.38	1.32	1.38	1.46	1.37

Table S2a.3.4– *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

MM-DP4+									
Compound		2a	2b	2c	2d	2e	2f	2g	2h
Nuclei	Exp 2a	Scaled shifts							
C7	131.67	130.38	130.68	129.55	124.68	125.54	130.09	125.65	126.49
C6	138.22	138.78	138.51	140.53	144.73	143.19	140.23	142.25	142.64
C4	41.8	42.23	41.76	38.84	42.04	43.78	38.14	42.97	39.77
C2	41.03	44.06	44.31	42.18	41.78	44.09	41.67	48.85	45.48
C9	28.6	19.80	19.66	24.44	23.36	19.97	25.37	14.97	20.50
C10	20.63	26.14	26.48	25.87	24.81	24.83	25.90	26.70	26.52
H7	6.03	6.04	6.02	6.01	6.04	6.06	5.98	6.07	6.02
H4a	2.65	2.39	2.47	2.41	2.43	2.30	2.50	2.34	2.37
H4b	2.5	2.54	2.52	2.60	2.49	2.57	2.62	2.47	2.60
Me-9	1.33	1.14	1.13	1.05	1.15	1.23	1.01	1.14	1.10
Me-10	1.02	1.34	1.31	1.38	1.34	1.30	1.35	1.43	1.35

Table S2b.3.4– *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

MM-DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C7	131.89	130.38	130.68	129.55	124.68	125.54	130.09	125.65	126.49
C6	137.83	138.78	138.51	140.53	144.73	143.19	140.23	142.25	142.64
C4	41.32	42.23	41.76	38.84	42.04	43.78	38.14	42.97	39.77
C2	41.36	44.06	44.31	42.18	41.78	44.09	41.67	48.85	45.48
C9	28.53	19.80	19.66	24.44	23.36	19.97	25.37	14.97	20.50
C10	20.47	26.14	26.48	25.87	24.81	24.83	25.90	26.70	26.52
H7	5.95	6.04	6.02	6.01	6.04	6.06	5.98	6.07	6.02
H4a	2.68	2.39	2.47	2.41	2.43	2.30	2.50	2.34	2.37
H4b	2.53	2.54	2.52	2.60	2.49	2.57	2.62	2.47	2.60
Me-9	1.28	1.14	1.13	1.05	1.15	1.23	1.01	1.14	1.10
Me-10	1.01	1.34	1.31	1.38	1.34	1.30	1.35	1.43	1.35

Table S2a.3.5 – *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

MM-DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2a***	***Scaled shifts***							
C7	131.67	130.47	130.78	129.64	124.75	125.62	130.18	125.74	126.58
C6	138.22	138.87	138.61	140.62	144.79	143.26	140.32	142.34	142.72
C4	41.8	42.32	41.85	38.93	42.14	43.88	38.23	43.06	39.87
C2	41.03	44.16	44.40	42.27	41.88	44.18	41.76	48.94	45.57
C9	28.6	19.89	19.75	24.53	23.46	20.07	25.46	15.07	20.59
C10	20.63	26.23	26.57	25.96	24.92	24.93	26.00	26.80	26.61
H8a	4.16	3.85	3.87	3.96	3.83	3.80	3.95	3.76	3.85
H8b	4.02	4.00	3.99	4.11	3.86	3.89	4.11	3.86	3.91
H7	6.03	6.18	6.18	6.44	6.29	6.26	6.40	6.22	6.18
H5	4.65	4.59	4.87	4.66	5.25	4.91	5.03	4.97	4.98
H4a	2.65	2.45	2.53	2.52	2.51	2.36	2.62	2.40	2.42
H4b	2.5	2.60	2.57	2.73	2.57	2.64	2.74	2.53	2.66
H3	4.83	5.00	4.99	4.34	4.29	4.55	4.34	4.59	4.32
H1	4.73	4.73	4.43	4.71	4.79	4.91	4.36	4.94	5.09
Me-9	1.33	1.16	1.15	1.05	1.17	1.25	1.00	1.17	1.12
Me-10	1.02	1.37	1.33	1.40	1.37	1.33	1.36	1.47	1.38

Table S2b.3.5 – *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

MM-DP4+									
Compound		***2a***	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
Nuclei	***Exp 2b***	***Scaled shifts***							
C7	131.89	130.38	130.68	129.55	124.68	125.54	130.09	125.65	126.49
C6	137.83	138.78	138.51	140.53	144.73	143.19	140.23	142.25	142.64
C4	41.32	42.23	41.76	38.84	42.04	43.78	38.14	42.97	39.77
C2	41.36	44.06	44.31	42.18	41.78	44.09	41.67	48.85	45.48
C9	28.53	19.80	19.66	24.44	23.36	19.97	25.37	14.97	20.50
C10	20.47	26.14	26.48	25.87	24.81	24.83	25.90	26.70	26.52
H8a	4.18	3.84	3.86	3.96	3.82	3.80	3.94	3.75	3.85
H8b	4.04	3.99	3.98	4.10	3.85	3.88	4.10	3.85	3.91
H7	5.95	6.19	6.17	6.44	6.28	6.27	6.38	6.23	6.19
H5	4.97	4.59	4.86	4.66	5.24	4.91	5.02	4.97	4.98
H4a	2.68	2.43	2.53	2.51	2.50	2.35	2.62	2.39	2.41
H4b	2.53	2.58	2.57	2.72	2.56	2.63	2.74	2.52	2.65
H3	4.83	5.00	4.98	4.34	4.28	4.55	4.33	4.59	4.32
H1	4.38	4.73	4.42	4.71	4.78	4.91	4.35	4.94	5.09
Me-9	1.28	1.14	1.15	1.03	1.17	1.24	1.00	1.15	1.10
Me-10	1.01	1.35	1.33	1.39	1.37	1.32	1.37	1.45	1.36

Table S2.4.1 – *Experimental data of* ***2a-b*** *and calculated isotropic shielding constants of* ***2a-2h*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory.*

DP4+										
Compound			**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2a**	**Exp 2b**	**Isotropic shielding constants**							
C8	37.73	37.62	139.23	139.17	138.94	139.51	139.70	139.12	139.82	138.82
C7	131.67	131.89	44.19	44.02	47.77	53.62	53.66	46.17	52.66	51.09
C6	138.22	137.83	39.30	39.18	39.60	37.76	39.23	37.98	38.28	38.76
C5	59.58	50.44	115.37	125.47	118.42	118.27	118.20	128.38	120.37	121.97
C4	41.8	41.32	142.56	143.04	142.61	140.92	140.79	144.57	142.86	143.22
C3	52.72	52.7	115.17	115.11	115.27	111.57	114.11	117.26	111.91	111.85
C2	41.03	41.36	140.07	139.72	138.95	139.05	138.99	140.11	135.12	137.37
C1	60.65	69.98	114.72	104.36	114.24	113.47	109.89	109.21	106.90	104.72
C9	28.6	28.53	166.22	166.67	163.98	160.27	165.64	159.95	172.57	163.79
C10	20.63	20.47	158.70	158.72	158.54	158.28	159.78	158.29	158.55	160.48
H8a	4.16	4.18	27.57	27.60	27.42	27.48	27.59	27.43	27.54	27.26
H8b	4.02	4.04	27.53	27.50	27.23	27.47	27.58	27.32	27.51	27.23
H7	6.03	5.95	25.42	25.47	25.35	25.31	25.32	25.40	25.19	25.42
H5	4.65	4.97	26.94	26.65	27.11	26.31	26.60	26.74	26.43	26.51
H4a	2.65	2.68	29.24	29.28	29.25	29.27	29.40	29.05	29.32	29.25
H4b	2.5	2.53	29.22	29.14	29.05	29.20	29.11	28.98	29.23	29.10
H3	4.83	4.83	26.71	26.64	27.58	27.32	27.00	27.46	26.98	27.25
H1	4.73	4.38	26.91	27.25	27.18	26.86	26.76	27.40	26.70	26.68
Me-9	1.33	1.28	30.74	30.72	30.58	30.62	30.64	30.68	30.74	30.67
Me-10	1.02	1.01	30.41	30.44	30.37	30.37	30.43	30.31	30.33	30.47

Table S2a.4.2 – *Experimental data of* ***2a*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

DP4+									
Compound		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2a**	**Scaled shifts**							
C8	37.73	40.83	40.95	40.87	39.09	39.87	41.16	40.12	40.16
C7	131.67	130.39	130.32	128.95	124.72	124.69	130.05	124.20	125.83
C6	138.22	135.00	134.87	136.85	140.53	138.90	137.88	138.07	137.87
C5	59.58	63.32	53.82	60.70	60.26	61.06	51.44	58.88	56.61
C4	41.8	37.70	37.32	37.32	37.69	38.80	35.96	37.19	35.86
C3	52.72	63.51	63.55	63.73	66.95	65.10	62.07	67.04	66.49
C2	41.03	40.05	40.44	40.86	39.55	40.57	40.22	44.65	41.57
C1	60.65	63.93	73.65	64.74	65.05	69.26	69.77	71.88	73.46
C9	28.6	15.40	15.12	16.68	18.40	14.31	21.25	8.53	15.77
C10	20.63								
H8a	4.16	4.07	4.04	4.29	4.10	4.02	4.25	4.01	4.27
H8b	4.02	4.10	4.13	4.49	4.11	4.02	4.36	4.03	4.30
H7	6.03	6.08	6.05	6.39	6.15	6.13	6.31	6.14	5.99
H5	4.65	4.66	4.94	4.60	5.21	4.94	4.95	5.02	4.97
H4a	2.65	2.49	2.45	2.44	2.41	2.32	2.60	2.39	2.41
H4b	2.5	2.51	2.58	2.64	2.48	2.59	2.68	2.47	2.55
H3	4.83	4.87	4.94	4.13	4.26	4.57	4.22	4.52	4.28
H1	4.73	4.69	4.37	4.54	4.69	4.79	4.28	4.77	4.81
Me-9	1.33	1.08	1.08	1.09	1.14	1.17	0.95	1.10	1.08
Me-10	1.02	1.38	1.35	1.30	1.37	1.36	1.33	1.47	1.27

Table S2b.4.2 – *Experimental data of* ***2b*** *and scaled chemical shifts of* ***2a-2h*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

DP4+									
Compound		**2a**	**2b**	**2c**	**2d**	**2e**	**2f**	**2g**	**2h**
Nuclei	**Exp 2b**	**Scaled shifts**							
C8	37.62	40.54	40.90	40.62	38.83	39.66	41.09	39.98	40.07
C7	131.89	131.17	130.29	129.58	125.28	125.11	130.08	124.42	125.91
C6	137.83	135.84	134.83	137.56	141.25	139.44	137.93	138.36	137.98
C5	50.44	63.29	53.77	60.64	60.21	61.01	51.38	58.82	56.55
C4	41.32	37.37	37.27	37.04	37.41	38.58	35.88	37.04	35.76
C3	52.7	63.49	63.50	63.71	66.95	65.08	62.02	67.02	66.45
C2	41.36	39.74	40.39	40.60	39.29	40.37	40.15	44.53	41.49

C1	69.98	63.91	73.60	64.72	65.04	69.27	69.73	71.88	73.44
C9	28.53	14.80	15.06	16.19	17.93	13.91	21.15	8.26	15.63
C10	20.47	21.98	22.53	21.49	19.94	19.72	22.74	21.84	18.86
H8a	4.18	4.06	4.03	4.28	4.09	4.01	4.24	4.00	4.26
H8b	4.04	4.10	4.12	4.49	4.10	4.02	4.35	4.02	4.29
H7	5.95	6.09	6.03	6.39	6.14	6.13	6.28	6.14	5.98
H5	4.97	4.65	4.92	4.60	5.19	4.94	4.94	5.01	4.96
H4a	2.68	2.48	2.45	2.43	2.41	2.32	2.60	2.38	2.40
H4b	2.53	2.49	2.57	2.63	2.48	2.59	2.68	2.46	2.54
H3	4.83	4.87	4.93	4.12	4.25	4.56	4.21	4.51	4.27
H1	4.38	4.68	4.35	4.53	4.68	4.78	4.27	4.77	4.80
Me-9	1.28	1.06	1.09	1.08	1.14	1.16	0.96	1.09	1.08
Me-10	1.01	1.37	1.36	1.29	1.37	1.35	1.33	1.47	1.26

3. Isomers of 3

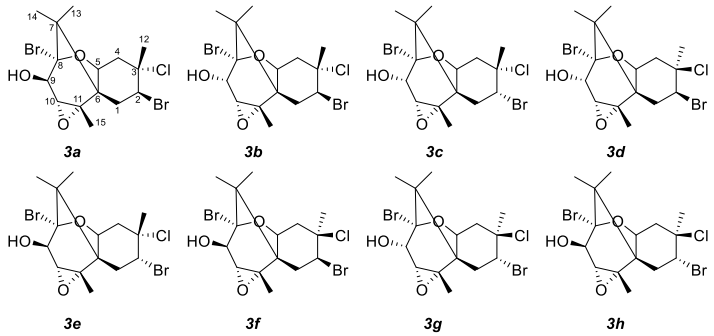


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Table S3.1.1 – *Experimental data of* ***3a*** *and calculated isotropic shielding constants of* ***3a-3h*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory.*

DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Isotropic shielding constants***							
C1	33.6	159.58	159.20	159.76	159.35	158.69	160.44	159.14	159.23
C2	58.1	121.46	121.51	122.62	125.40	122.37	125.20	122.01	120.99
C3	68.0	116.16	115.88	115.59	114.74	115.51	114.69	116.00	116.15
C4	45.2	148.63	148.44	149.04	148.27	148.55	148.26	148.37	148.00
C5	74.2	119.46	119.78	119.05	120.00	118.37	120.19	119.15	118.54
C6	50.4	141.02	141.14	143.26	140.20	142.34	140.19	142.77	143.07
C7	49.3	143.09	142.96	142.11	142.01	142.73	144.31	140.90	143.53
C8	112.6	63.61	72.82	71.99	72.93	62.72	65.79	71.77	63.75
C9	73.8	118.77	119.36	119.96	119.03	118.96	119.04	119.01	119.11
C10	61.0	131.71	133.29	130.87	133.22	129.95	132.35	130.57	130.54
C11	61.0	131.86	129.31	126.90	128.78	129.20	131.08	126.73	129.30
C12	31.0	165.38	165.29	163.86	164.74	163.53	164.75	171.88	172.22
C13	24.6	170.00	169.85	167.63	169.37	168.39	169.87	167.96	167.53
C14	18.2	176.81	178.35	178.68	177.63	177.46	176.48	177.66	176.78
C15	21.5	173.48	173.95	174.34	173.40	174.12	172.89	174.69	174.41
H1a	2.92	29.45	29.42	28.83	29.06	28.89	29.07	29.16	29.11
H1b	2.13	29.52	29.53	29.33	29.64	29.34	29.61	29.27	29.15
H2	4.22	26.91	26.91	26.86	27.43	26.86	27.46	26.57	26.65
H4a	2.45	29.03	29.04	28.89	28.84	28.81	28.91	28.79	28.83
H4b	2.23	29.14	29.14	29.58	28.94	29.53	28.96	29.17	29.25
H5	4.58	26.82	26.89	26.91	27.27	26.69	27.17	27.12	27.01
H8	4.00	27.49	27.58	27.72	27.55	27.56	27.68	27.70	27.66
H10	3.16	28.32	28.43	28.45	28.45	28.40	28.33	28.60	28.49
Me-12	1.64	29.84	29.83	29.85	29.85	29.84	29.86	29.82	29.83
Me-13	1.20	30.34	30.34	30.28	30.21	30.32	30.34	30.16	30.21
Me-14	1.11	30.48	30.47	30.53	30.53	30.41	30.44	30.61	30.42
Me-15	1.35	30.16	30.15	30.15	30.11	30.17	30.11	30.24	30.19

Table S3.1.2 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory.*

DP4+									
Compound		**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**3g**	**3h**
Nuclei	**Exp**	**Scaled shifts**							
C1	33.6	34.34	34.35	33.60	33.96	34.74	33.53	34.63	34.99
C2	58.1	66.94	68.28	66.89	64.75	65.62	64.21	67.35	67.26
C3	68.0	71.47	73.34	73.19	74.41	71.46	73.36	72.65	71.34
C4	45.2	43.70	44.04	43.21	44.00	43.36	44.13	44.12	44.47
C5	74.2	68.65	69.84	70.09	69.65	69.02	68.58	69.87	69.33
C6	50.4	50.21	50.61	48.39	51.32	48.64	51.16	49.06	48.63
C7	49.3	48.44	48.97	49.42	49.69	48.31	47.57	50.70	48.24
C8	112.6	116.41	112.11	112.27	112.34	116.34	115.94	111.63	115.56
C9	73.8	69.24	70.21	69.27	70.53	68.52	69.57	70.00	68.84
C10	61.0	58.17	57.67	59.49	57.65	59.17	57.99	59.81	59.20
C11	61.0	58.05	61.26	63.05	61.69	59.81	59.10	63.19	60.25
C12	31.0	29.38	28.87	29.92	29.07	30.63	29.78	23.40	24.03
C13	24.6	25.43	24.76	26.54	24.86	26.49	25.32	26.86	27.99
C14	18.2	19.61	17.11	16.64	17.38	18.78	19.56	18.31	20.18
C15	21.5	22.45	21.07	20.53	21.21	21.62	22.69	20.93	22.18
H1a	2.92	2.11	2.15	2.70	2.51	2.59	2.50	2.36	2.37
H1b	2.13	2.04	2.05	2.21	1.88	2.17	1.92	2.25	2.33
H2	4.22	4.54	4.60	4.61	4.27	4.50	4.23	4.91	4.81
H4a	2.45	2.51	2.52	2.64	2.74	2.67	2.67	2.73	2.65
H4b	2.23	2.41	2.42	1.97	2.64	2.00	2.62	2.35	2.24
H5	4.58	4.63	4.62	4.56	4.44	4.66	4.55	4.37	4.46
H8	4.00	3.98	3.95	3.78	4.14	3.85	4.00	3.80	3.81
H10	3.16	3.20	3.11	3.07	3.17	3.05	3.30	2.91	2.99
Me-12	1.64	1.74	1.75	1.70	1.65	1.70	1.65	1.71	1.66
Me-13	1.20	1.26	1.25	1.29	1.26	1.25	1.14	1.38	1.29
Me-14	1.11	1.13	1.13	1.05	0.91	1.16	1.02	0.93	1.08
Me-15	1.35	1.43	1.44	1.42	1.37	1.39	1.38	1.29	1.30

Table S3.1.3 – *Experimental data of **3a** and scaled chemical of **3a-3h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the signals adjacent to bromine.*

DP4+									
Compound		**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**3g**	**3h**
Nuclei	**Exp**	**Scaled shifts**							
C1	33.6	34.38	34.89	34.04	34.30	34.75	33.43	35.17	35.18
C3	68.0	74.46	74.56	74.27	75.24	74.20	75.83	73.50	73.95
C4	45.2	44.48	44.75	43.81	44.46	44.01	44.72	44.74	45.29
C5	74.2	71.42	70.99	71.12	70.42	71.58	70.74	70.70	71.80
C6	50.4	51.51	51.43	49.07	51.87	49.69	52.20	49.72	49.73
C7	49.3	49.60	49.76	50.12	50.21	49.34	48.38	51.38	49.32
C9	73.8	72.05	71.37	70.30	71.31	71.05	71.80	70.83	71.28
C10	61.0	60.11	58.62	60.36	58.28	61.01	59.47	60.55	61.01
C11	61.0	59.97	62.26	63.97	62.36	61.69	60.65	63.97	62.12
C12	31.0	29.03	29.31	30.30	29.35	30.33	29.44	23.85	23.49
C13	24.6	24.76	25.13	26.87	25.09	25.89	24.69	27.33	27.72
C14	18.2	18.48	17.35	16.81	17.52	17.60	18.56	18.72	19.39
C15	21.5	21.55	21.38	20.76	21.40	20.66	21.90	21.36	21.52
H1a	2.92	2.13	2.17	2.75	2.52	2.63	2.50	2.42	2.42
H1b	2.13	2.06	2.06	2.24	1.88	2.18	1.92	2.30	2.38
H4a	2.45	2.55	2.56	2.69	2.75	2.70	2.67	2.83	2.73
H4b	2.23	2.44	2.46	1.98	2.65	2.00	2.62	2.41	2.28
H5	4.58	4.76	4.78	4.72	4.46	4.77	4.56	4.65	4.69
H8	4.00	4.09	4.07	3.89	4.16	3.93	4.01	4.01	3.99
H10	3.16	3.26	3.19	3.14	3.18	3.10	3.30	3.03	3.10
Me-12	1.64	1.74	1.75	1.70	1.65	1.70	1.65	1.70	1.65
Me-13	1.20	1.24	1.22	1.26	1.25	1.23	1.14	1.34	1.24
Me-14	1.11	1.10	1.09	1.01	0.90	1.14	1.02	0.84	1.02
Me-15	1.35	1.42	1.42	1.40	1.37	1.38	1.38	1.24	1.26

Table S3.1.4 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.6	34.55	35.08	34.20	34.48	34.92	33.59	35.34	35.36
C4	45.2	45.01	45.29	44.30	45.06	44.50	45.37	45.19	45.80
C5	74.2	72.90	72.49	72.56	72.05	73.02	72.53	71.94	73.18
C6	50.4	52.29	52.21	49.74	52.76	50.37	53.18	50.32	50.39
C7	49.3	50.31	50.49	50.83	51.04	50.01	49.19	52.03	49.96
C9	73.8	73.56	72.88	71.70	72.98	72.46	73.63	72.07	72.65
C10	61.0	61.19	59.66	61.42	59.43	62.08	60.77	61.49	62.03
C11	61.0	61.05	63.44	65.16	63.67	62.78	62.00	65.00	63.18
C12	31.0	29.00	29.30	30.33	29.33	30.35	29.43	23.67	23.29
C13	24.6	24.58	24.97	26.77	24.91	25.76	24.47	27.26	27.65
C14	18.2	18.08	16.91	16.36	17.03	17.19	18.08	18.38	19.05
C15	21.5	21.26	21.08	20.45	21.06	20.35	21.56	21.10	21.26
H1a	2.92	2.13	2.17	2.75	2.52	2.63	2.50	2.42	2.42
H1b	2.13	2.06	2.06	2.24	1.88	2.18	1.92	2.30	2.38
H4a	2.45	2.55	2.56	2.69	2.75	2.70	2.67	2.83	2.73
H4b	2.23	2.44	2.46	1.98	2.65	2.00	2.62	2.41	2.28
H5	4.58	4.76	4.78	4.72	4.46	4.77	4.56	4.65	4.69
H8	4.00	4.09	4.07	3.89	4.16	3.93	4.01	4.01	3.99
H10	3.16	3.26	3.19	3.14	3.18	3.10	3.30	3.03	3.10
Me-12	1.64	1.74	1.75	1.70	1.65	1.70	1.65	1.70	1.65
Me-13	1.20	1.24	1.22	1.26	1.25	1.23	1.14	1.34	1.24
Me-14	1.11	1.10	1.09	1.01	0.90	1.14	1.02	0.84	1.02
Me-15	1.35	1.42	1.42	1.40	1.37	1.38	1.38	1.24	1.26

Table S3.1.5 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.6	34.55	35.08	34.20	34.48	34.92	33.59	35.34	35.36
C4	45.2	45.01	45.29	44.30	45.06	44.50	45.37	45.19	45.80
C5	74.2	72.90	72.49	72.56	72.05	73.02	72.53	71.94	73.18
C6	50.4	52.29	52.21	49.74	52.76	50.37	53.18	50.32	50.39
C7	49.3	50.31	50.49	50.83	51.04	50.01	49.19	52.03	49.96
C9	73.8	73.56	72.88	71.70	72.98	72.46	73.63	72.07	72.65
C10	61.0	61.19	59.66	61.42	59.43	62.08	60.77	61.49	62.03
C11	61.0	61.05	63.44	65.16	63.67	62.78	62.00	65.00	63.18
C12	31.0	29.00	29.30	30.33	29.33	30.35	29.43	23.67	23.29
C13	24.6	24.58	24.97	26.77	24.91	25.76	24.47	27.26	27.65
C14	18.2	18.08	16.91	16.36	17.03	17.19	18.08	18.38	19.05
C15	21.5	21.26	21.08	20.45	21.06	20.35	21.56	21.10	21.26
H1a	2.92	2.11	2.15	2.70	2.51	2.59	2.50	2.36	2.37
H1b	2.13	2.04	2.05	2.21	1.88	2.17	1.92	2.25	2.33
H2	4.22	4.54	4.60	4.61	4.27	4.50	4.23	4.91	4.81
H4a	2.45	2.51	2.52	2.64	2.74	2.67	2.67	2.73	2.65
H4b	2.23	2.41	2.42	1.97	2.64	2.00	2.62	2.35	2.24
H5	4.58	4.63	4.62	4.56	4.44	4.66	4.55	4.37	4.46
H8	4.00	3.98	3.95	3.78	4.14	3.85	4.00	3.80	3.81
H10	3.16	3.20	3.11	3.07	3.17	3.05	3.30	2.91	2.99
Me-12	1.64	1.74	1.75	1.70	1.65	1.70	1.65	1.71	1.66
Me-13	1.20	1.26	1.25	1.29	1.26	1.25	1.14	1.38	1.29
Me-14	1.11	1.13	1.13	1.05	0.91	1.16	1.02	0.93	1.08
Me-15	1.35	1.43	1.44	1.42	1.37	1.39	1.38	1.29	1.30

Table S3.2.1 – *Experimental data of **3a** and calculated isotropic shielding constants of **3a-3h** at the B3LYP/6-31G**//MMFF level of theory.*

DP4

Compound		3a	3b	3c	3d	3e	3f	3g	3h
Nuclei	**Exp**	**Isotropic shielding constants**							
C1	33.60	153.99	154.03	154.38	155.02	154.36	154.99	153.61	153.41
C2	58.10	122.98	123.22	121.85	125.82	121.61	125.57	120.92	120.64
C3	68.00	120.55	120.60	120.09	117.95	119.96	117.85	118.85	118.68
C4	45.20	142.74	142.92	142.21	141.89	141.88	141.66	140.95	140.60
C5	74.20	118.32	118.67	117.55	118.59	117.06	118.25	116.77	116.21
C6	50.40	135.69	135.66	136.72	135.08	136.43	135.10	137.18	136.89
C7	49.30	138.37	136.97	136.38	136.99	138.05	138.36	136.40	138.14
C8	112.60	61.17	70.22	69.81	69.92	61.37	61.03	70.32	61.85
C9	73.80	116.20	113.38	113.63	113.33	115.92	116.18	113.77	116.04
C10	61.00	132.85	132.51	129.64	132.50	130.26	132.85	129.49	130.06
C11	61.00	130.86	128.70	126.78	128.79	128.57	130.84	127.21	129.04
C12	31.00	159.58	159.65	157.84	158.34	157.82	158.32	166.30	166.26
C14	18.20	171.83	172.64	173.08	172.72	172.07	171.80	173.15	172.08
C13	24.60	166.11	166.18	165.16	166.11	165.13	166.05	164.91	164.90
C15	21.50	170.60	170.89	171.85	170.84	171.62	170.53	171.70	171.42
H1b	2.13	29.70	29.73	29.74	29.79	29.67	29.76	29.54	29.48
H1a	2.92	29.63	29.67	29.15	29.26	29.13	29.24	29.46	29.44
H2	4.22	27.25	27.28	27.31	27.68	27.32	27.66	27.11	27.09
H4b	2.23	29.74	29.70	29.89	29.27	29.96	29.31	29.53	29.58
H4a	2.45	29.35	29.31	29.10	29.26	29.12	29.30	29.10	29.12
H5	4.58	26.86	26.97	26.94	27.43	26.82	27.34	27.24	27.13
H9	4.00	27.61	27.69	27.85	27.70	27.63	27.66	27.85	27.66
H10	3.16	28.91	29.06	29.11	29.08	28.96	28.93	29.11	28.96
Me-12	1.64	30.20	30.19	30.21	30.20	30.22	30.21	30.14	30.14
Me-13	1.11	30.54	30.67	30.68	30.66	30.60	30.50	30.70	30.53
Me-14	1.20	30.52	30.53	30.57	30.43	30.52	30.45	30.47	30.50
Me-15	1.35	30.42	30.45	30.54	30.46	30.50	30.43	30.59	30.55

Table S3.2.2 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the B3LYP/6-31G**//MMFF level of theory.*

DP4									
Compound		3a	3b	3c	3d	3e	3f	3g	3h
Nuclei	**Exp**	**Scaled shifts**							
C1	33.60	36.09	35.58	34.82	34.55	35.28	35.08	36.08	36.61
C2	58.10	63.99	64.59	65.19	61.97	64.57	61.49	66.12	65.47
C3	68.00	66.17	67.06	66.83	69.36	66.04	68.43	68.02	67.20
C4	45.20	46.21	46.04	46.18	46.88	46.44	47.05	47.71	47.89
C5	74.20	68.19	68.89	69.20	68.76	68.64	68.07	69.93	69.37
C6	50.40	52.56	52.88	51.30	53.27	51.31	52.94	51.18	51.16
C7	49.30	50.14	51.64	51.62	51.48	49.86	50.01	51.89	50.06
C8	112.60	119.61	114.52	113.78	114.47	118.44	119.47	112.60	117.25
C9	73.80	70.09	73.87	72.87	73.70	69.65	69.93	72.68	69.52
C10	61.00	55.11	55.84	57.91	55.70	56.83	54.96	58.24	57.18
C11	61.00	56.90	59.44	60.59	59.18	58.34	56.77	60.34	58.07
C12	31.00	31.06	30.28	31.59	31.43	32.18	32.08	24.43	25.30
C14	18.20	20.04	18.05	17.36	17.93	19.43	19.97	18.13	20.17
C13	24.60	25.18	24.13	24.75	24.13	25.64	25.13	25.70	26.49
C15	21.50	21.15	19.69	18.51	19.70	19.84	21.12	19.46	20.75
H1b	2.13	2.13	2.14	2.12	2.02	2.15	2.02	2.28	2.29
H1a	2.92	2.20	2.20	2.69	2.59	2.65	2.58	2.36	2.33
H2	4.22	4.46	4.50	4.44	4.29	4.34	4.26	4.70	4.62
H4b	2.23	2.09	2.17	1.98	2.58	1.88	2.50	2.29	2.20
H4a	2.45	2.47	2.54	2.73	2.59	2.66	2.51	2.72	2.65
H5	4.58	4.83	4.80	4.79	4.56	4.80	4.60	4.57	4.58
H9	4.00	4.12	4.11	3.92	4.27	4.05	4.26	3.96	4.06
H10	3.16	2.88	2.79	2.73	2.78	2.81	2.90	2.71	2.80
Me-12	1.64	1.66	1.70	1.68	1.58	1.63	1.54	1.69	1.65
Me-13	1.11	1.33	1.23	1.22	1.09	1.29	1.23	1.13	1.26
Me-14	1.20	1.36	1.37	1.33	1.33	1.36	1.28	1.35	1.30
Me-15	1.35	1.45	1.45	1.36	1.30	1.38	1.31	1.24	1.25

Table S3.2.3 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

DP4

Compound		3a	3b	3c	3d	3e	3f	3g	3h
Nuclei	**Exp**	**Scaled shifts**							
C1	33.60	35.84	35.75	35.06	34.55	35.07	34.58	36.50	36.69
C3	68.00	69.67	68.61	68.17	70.62	69.10	71.77	69.04	69.99
C4	45.20	47.22	46.67	46.81	47.33	47.42	47.93	48.35	48.97
C5	74.20	71.94	70.51	70.61	70.00	71.98	71.37	70.99	72.37
C6	50.40	54.36	53.81	52.10	53.95	52.81	54.49	51.88	52.53
C7	49.30	51.64	52.52	52.43	52.10	51.21	51.23	52.61	51.33
C9	73.80	74.08	75.71	74.40	75.12	73.10	73.45	73.79	72.53
C10	61.00	57.23	56.90	58.94	56.47	58.91	56.74	59.08	59.08
C11	61.00	59.24	60.65	61.71	60.08	60.59	58.76	61.22	60.06
C12	31.00	30.19	30.22	31.72	31.33	31.64	31.24	24.63	24.37
C14	18.20	17.79	17.46	17.00	17.33	17.55	17.74	18.21	18.79
C13	24.60	23.57	23.81	24.65	23.76	24.41	23.49	25.92	25.67
C15	21.50	19.03	19.17	18.19	19.16	17.99	19.01	19.57	19.42
H1b	2.13	2.15	2.16	2.13	2.03	2.15	2.02	2.32	2.32
H1a	2.92	2.22	2.22	2.72	2.60	2.67	2.58	2.40	2.36
H4b	2.23	2.11	2.18	1.99	2.59	1.88	2.50	2.33	2.22
H4a	2.45	2.49	2.57	2.76	2.60	2.67	2.52	2.79	2.70
H5	4.58	4.93	4.92	4.88	4.59	4.85	4.61	4.77	4.74
H9	4.00	4.20	4.20	3.99	4.30	4.09	4.27	4.11	4.19
H10	3.16	2.92	2.83	2.76	2.79	2.83	2.91	2.78	2.86
Me-12	1.64	1.66	1.70	1.67	1.58	1.63	1.54	1.68	1.64
Me-13	1.20	1.34	1.36	1.32	1.33	1.35	1.28	1.32	1.27
Me-14	1.11	1.32	1.21	1.20	1.08	1.28	1.23	1.08	1.24
Me-15	1.35	1.44	1.43	1.35	1.30	1.37	1.30	1.20	1.22

Table S3.2.4 – *Experimental data of* ***3a*** *and scaled chemical shifts of* ***3a-3h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

DP4									
Compound		3a	3b	3c	3d	3e	3f	3g	3h
Nuclei	**Exp**	**Scaled shifts**							
C1	33.6	35.90	35.77	35.06	34.62	35.11	34.68	36.54	36.77
C4	45.2	47.38	46.73	46.82	47.58	47.53	48.30	48.46	49.18
C5	74.2	72.32	70.65	70.65	70.57	72.23	72.22	71.22	72.82
C6	50.4	54.58	53.89	52.12	54.30	52.95	55.00	52.01	52.78
C7	49.3	51.84	52.59	52.45	52.42	51.34	51.67	52.74	51.56
C9	73.8	74.48	75.86	74.44	75.77	73.36	74.34	74.04	72.99
C10	61.0	57.48	56.99	58.97	56.85	59.08	57.30	59.25	59.40
C11	61.0	59.51	60.75	61.74	60.51	60.77	59.36	61.39	60.39
C12	31.0	30.19	30.23	31.72	31.35	31.66	31.27	24.60	24.31
C14	18.2	17.68	17.42	16.99	17.15	17.47	17.49	18.15	18.67
C13	24.6	23.51	23.79	24.64	23.68	24.38	23.36	25.90	25.63
C15	21.5	18.93	19.14	18.18	19.01	17.93	18.79	19.51	19.31
H1b	2.13	2.15	2.16	2.13	2.03	2.15	2.02	2.32	2.32
H1a	2.92	2.22	2.22	2.72	2.60	2.67	2.58	2.40	2.36
H4b	2.23	2.11	2.18	1.99	2.59	1.88	2.50	2.33	2.22
H4a	2.45	2.49	2.57	2.76	2.60	2.67	2.52	2.79	2.70
H5	4.58	4.93	4.92	4.88	4.59	4.85	4.61	4.77	4.74
H9	4.00	4.20	4.20	3.99	4.30	4.09	4.27	4.11	4.19
H10	3.16	2.92	2.83	2.76	2.79	2.83	2.91	2.78	2.86
Me-12	1.64	1.66	1.70	1.67	1.58	1.63	1.54	1.68	1.64
Me-13	1.20	1.34	1.36	1.32	1.33	1.35	1.28	1.32	1.27
Me-14	1.11	1.32	1.21	1.20	1.08	1.28	1.23	1.08	1.24
Me-15	1.35	1.44	1.43	1.35	1.30	1.37	1.30	1.20	1.22

Table S3.2.5 – *Experimental data of* ***3a*** *and scaled chemical shifts of* ***3a-3h*** *at the B3LYP/6-31G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

DP4									
Compound		3a	3b	3c	3d	3e	3f	3g	3h
Nuclei	**Exp**	**Scaled shifts**							
C1	33.6	35.90	35.77	35.06	34.62	35.11	34.68	36.54	36.77
C4	45.2	47.38	46.73	46.82	47.58	47.53	48.30	48.46	49.18
C5	74.2	72.32	70.65	70.65	70.57	72.23	72.22	71.22	72.82
C6	50.4	54.58	53.89	52.12	54.30	52.95	55.00	52.01	52.78
C7	49.3	51.84	52.59	52.45	52.42	51.34	51.67	52.74	51.56

C9	73.8	74.48	75.86	74.44	75.77	73.36	74.34	74.04	72.99
C10	61.0	57.48	56.99	58.97	56.85	59.08	57.30	59.25	59.40
C11	61.0	59.51	60.75	61.74	60.51	60.77	59.36	61.39	60.39
C12	31.0	30.19	30.23	31.72	31.35	31.66	31.27	24.60	24.31
C14	18.2	17.68	17.42	16.99	17.15	17.47	17.49	18.15	18.67
C13	24.6	23.51	23.79	24.64	23.68	24.38	23.36	25.90	25.63
C15	21.5	18.93	19.14	18.18	19.01	17.93	18.79	19.51	19.31
H1b	2.13	2.13	2.14	2.12	2.02	2.15	2.02	2.28	2.29
H1a	2.92	2.20	2.20	2.69	2.59	2.65	2.58	2.36	2.33
H2	4.22	4.46	4.50	4.44	4.29	4.34	4.26	4.70	4.62
H4b	2.23	2.09	2.17	1.98	2.58	1.88	2.50	2.29	2.20
H4a	2.45	2.47	2.54	2.73	2.59	2.66	2.51	2.72	2.65
H5	4.58	4.83	4.80	4.79	4.56	4.80	4.60	4.57	4.58
H9	4.00	4.12	4.11	3.92	4.27	4.05	4.26	3.96	4.06
H10	3.16	2.88	2.79	2.73	2.78	2.81	2.90	2.71	2.80
Me-12	1.64	1.66	1.70	1.68	1.58	1.63	1.54	1.69	1.65
Me-13	1.11	1.33	1.23	1.22	1.09	1.29	1.23	1.13	1.26
Me-14	1.20	1.36	1.37	1.33	1.33	1.36	1.28	1.35	1.30
Me-15	1.35	1.45	1.45	1.36	1.30	1.38	1.31	1.24	1.25

Table S3.3.1 – *Experimental data of* ***3a*** *and calculated isotropic shielding constants of* ***3a-3h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory.*

MM-DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Isotropic shielding constants***							
C1	33.60	159.90	159.78	160.76	159.72	159.82	160.15	159.62	159.55
C2	58.10	129.60	129.70	129.02	132.43	128.44	132.16	127.98	127.04
C3	68.00	126.11	125.96	124.70	123.53	124.70	123.54	124.42	124.60
C4	45.20	148.23	148.39	148.81	148.16	148.60	147.85	147.82	147.72
C5	74.20	123.29	123.61	122.25	123.78	121.47	123.56	122.58	122.02
C6	50.40	140.96	140.73	143.01	140.15	142.55	140.38	142.82	142.54
C7	49.30	144.76	143.59	142.39	142.96	143.97	144.90	142.99	144.86
C8	112.60	71.11	78.94	79.25	78.89	70.56	72.27	78.23	72.11
C9	73.80	120.74	117.49	118.06	118.79	120.53	121.42	118.65	121.41
C10	61.00	136.28	137.02	136.13	137.72	135.26	137.08	135.68	134.58
C11	61.00	135.34	132.81	130.83	132.08	132.30	134.54	129.91	131.60
C12	31.00	165.61	165.41	163.71	164.36	164.12	164.31	172.12	172.50
C14	18.20	176.53	178.06	178.59	177.64	177.31	176.40	177.50	176.24
C13	24.60	171.61	171.48	169.88	171.37	170.32	171.55	169.82	169.94
C15	21.50	176.17	176.62	176.94	175.86	177.19	175.54	177.51	177.19
H1b	2.13	29.48	29.48	29.32	29.60	29.22	29.54	29.22	29.16
H1a	2.92	29.29	29.27	29.05	29.01	29.04	28.98	29.09	29.05
H2	4.22	27.05	27.03	26.70	27.33	26.73	27.32	26.55	26.60
H4b	2.23	29.29	29.24	29.45	29.07	29.47	29.12	29.21	29.33
H4a	2.45	29.15	29.10	28.96	28.94	28.95	29.00	28.80	28.91
H5	4.58	26.84	26.87	26.90	27.26	26.79	27.21	27.11	27.08
H9	4.00	27.47	27.53	27.64	27.53	27.38	27.59	27.69	27.61
H10	3.16	28.66	28.75	28.66	28.67	28.66	28.65	28.77	28.68
Me-12	1.64	29.91	29.89	30.00	29.90	29.98	29.90	29.86	29.87
Me-13	1.11	30.54	30.61	30.49	30.60	30.38	30.51	30.63	30.46
Me-14	1.20	30.35	30.32	30.30	30.25	30.30	30.28	30.20	30.21
Me-15	1.35	30.21	30.22	30.32	30.26	30.27	30.22	30.32	30.26

Table S3.3.2 – *Experimental data of* ***3a*** *and scaled chemical shifts of* ***3a-3h*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory.*

MM-DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.60	35.45	35.17	33.93	34.95	35.21	34.98	35.58	35.90
C2	58.10	63.35	63.88	64.18	61.21	63.70	61.07	65.11	65.35
C3	68.00	66.56	67.45	68.29	69.77	67.09	69.11	68.42	67.56
C4	45.20	46.20	46.04	45.32	46.07	45.40	46.44	46.59	46.61
C5	74.20	69.16	69.70	70.62	69.54	70.02	69.09	70.14	69.90
C6	50.40	52.90	53.35	50.84	53.79	50.89	53.41	51.25	51.31
C7	49.30	49.40	50.62	51.43	51.08	49.60	49.19	51.10	49.20
C8	112.60	117.20	112.34	111.60	112.75	116.24	116.89	111.52	115.11
C9	73.80	71.51	75.54	74.61	74.34	70.87	71.08	73.81	70.45

C10	61.00	57.20	56.90	57.40	56.12	57.50	56.48	57.92	58.52
C11	61.00	58.07	60.91	62.45	61.55	60.19	58.85	63.31	61.22
C12	31.00	30.20	29.80	31.12	30.48	31.31	31.11	23.92	24.17
C14	18.20	20.15	17.72	16.95	17.70	19.34	19.83	18.90	20.78
C13	24.60	24.68	23.99	25.24	23.73	25.68	24.36	26.07	26.49
C15	21.50	20.48	19.09	18.51	19.42	19.45	20.63	18.89	19.92
H1b	2.13	2.14	2.14	2.26	1.99	2.32	2.04	2.33	2.36
H1a	2.92	2.32	2.34	2.52	2.61	2.48	2.63	2.45	2.47
H2	4.22	4.48	4.52	4.74	4.37	4.63	4.38	4.92	4.88
H4b	2.23	2.32	2.37	2.15	2.55	2.08	2.48	2.33	2.20
H4a	2.45	2.46	2.51	2.61	2.68	2.56	2.61	2.73	2.61
H5	4.58	4.68	4.68	4.54	4.44	4.57	4.50	4.38	4.40
H9	4.00	4.07	4.03	3.85	4.16	4.02	4.09	3.81	3.88
H10	3.16	2.93	2.85	2.88	2.96	2.83	2.98	2.77	2.83
Me-12	1.64	1.72	1.74	1.62	1.68	1.61	1.67	1.70	1.66
Me-13	1.11	1.12	1.05	1.16	0.94	1.24	1.02	0.95	1.09
Me-14	1.20	1.30	1.33	1.34	1.31	1.31	1.26	1.37	1.33
Me-15	1.35	1.44	1.42	1.32	1.30	1.34	1.32	1.25	1.28

Table S3.3.3 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine.*

MM-DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.60	35.48	34.32	35.09	35.17	34.72	36.02	36.09	35.48
C3	68.00	68.08	68.69	70.24	69.21	71.27	68.91	69.47	68.08
C4	45.20	46.46	45.71	46.32	46.05	47.00	47.04	47.38	46.46
C5	74.20	70.35	71.02	70.01	72.33	71.25	70.63	71.94	70.35
C6	50.40	53.84	51.23	54.10	51.91	54.46	51.72	52.33	53.84
C7	49.30	51.09	51.83	51.37	50.53	49.94	51.56	50.11	51.09
C9	73.80	76.26	75.01	74.85	73.25	73.38	74.30	72.52	76.26
C10	61.00	57.43	57.79	56.46	58.97	57.75	58.39	59.94	57.43
C11	61.00	61.48	62.84	61.94	61.84	60.28	63.79	62.78	61.48
C12	31.00	30.05	31.51	30.58	31.00	30.57	24.34	23.71	30.05
C14	18.20	17.85	17.33	17.68	18.22	18.49	19.31	20.14	17.85
C13	24.60	24.19	25.62	23.77	24.99	23.34	26.49	26.16	24.19
C15	21.50	19.24	18.89	19.41	18.34	19.35	19.30	19.23	19.24
H1b	2.13	2.16	2.30	2.00	2.35	2.05	2.39	2.42	2.16
H1a	2.92	2.37	2.58	2.63	2.52	2.65	2.52	2.54	2.37
H4b	2.23	2.40	2.17	2.56	2.10	2.50	2.39	2.24	2.40
H4a	2.45	2.54	2.67	2.70	2.61	2.63	2.83	2.69	2.54
H5	4.58	4.80	4.76	4.49	4.74	4.56	4.66	4.66	4.80
H9	4.00	4.13	4.00	4.21	4.15	4.14	4.03	4.09	4.13
H10	3.16	2.89	2.97	2.98	2.90	3.00	2.87	2.94	2.89
Me-12	1.64	1.74	1.61	1.68	1.60	1.67	1.70	1.65	1.74
Me-13	1.20	1.02	1.11	0.93	1.20	1.01	0.87	1.02	1.02
Me-14	1.11	1.31	1.30	1.30	1.28	1.25	1.32	1.29	1.31
Me-15	1.35	1.41	1.29	1.29	1.31	1.31	1.20	1.23	1.41

Table S3.3.4 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the signals adjacent to bromine and chlorine.*

MM-DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.6	35.35	35.48	34.34	35.15	35.20	34.81	36.05	36.14
C4	45.2	47.04	46.47	45.77	46.52	46.15	47.30	47.13	47.52
C5	74.2	72.02	70.37	71.17	70.49	72.61	71.99	70.83	72.27
C6	50.4	54.33	53.85	51.31	54.40	52.05	54.90	51.82	52.51
C7	49.3	50.52	51.10	51.91	51.63	50.67	50.30	51.66	50.27
C9	73.8	74.58	76.28	75.18	75.40	73.53	74.16	74.52	72.85
C10	61.0	59.01	57.44	57.89	56.78	59.16	58.25	58.53	60.18
C11	61.0	59.95	61.49	62.96	62.33	62.05	60.83	63.95	63.04
C12	31.0	29.64	30.05	31.51	30.59	31.01	30.58	24.31	23.66
C14	18.2	18.70	17.85	17.28	17.53	18.14	18.30	19.26	20.06
C13	24.6	23.63	24.19	25.61	23.70	24.96	23.23	26.48	26.13
C15	21.5	19.06	19.23	18.85	19.29	18.26	19.17	19.25	19.15

H1b	2.13	2.16	2.16	2.30	2.00	2.35	2.05	2.39	2.42
H1a	2.92	2.35	2.37	2.58	2.63	2.52	2.65	2.52	2.54
H4b	2.23	2.34	2.40	2.17	2.56	2.10	2.50	2.39	2.24
H4a	2.45	2.48	2.54	2.67	2.70	2.61	2.63	2.83	2.69
H5	4.58	4.78	4.80	4.76	4.49	4.74	4.56	4.66	4.66
H9	4.00	4.15	4.13	4.00	4.21	4.15	4.14	4.03	4.09
H10	3.16	2.97	2.89	2.97	2.98	2.90	3.00	2.87	2.94
Me-12	1.64	1.72	1.74	1.61	1.68	1.60	1.67	1.70	1.65
Me-13	1.20	1.10	1.02	1.11	0.93	1.20	1.01	0.87	1.02
Me-14	1.11	1.28	1.31	1.30	1.30	1.28	1.25	1.32	1.29
Me-15	1.35	1.43	1.41	1.29	1.29	1.31	1.31	1.20	1.23

Table S3.3.5 – *Experimental data of **3a** and scaled chemical shifts of **3a-3h** at the SMD/wB97XD/6-31+G**//MMFF level of theory, after excluding all the carbon signals adjacent to bromine and chlorine.*

MM-DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.6	35.35	35.48	34.34	35.15	35.20	34.81	36.05	36.14
C4	45.2	47.04	46.47	45.77	46.52	46.15	47.30	47.13	47.52
C5	74.2	72.02	70.37	71.17	70.49	72.61	71.99	70.83	72.27
C6	50.4	54.33	53.85	51.31	54.40	52.05	54.90	51.82	52.51
C7	49.3	50.52	51.10	51.91	51.63	50.67	50.30	51.66	50.27
C9	73.8	74.58	76.28	75.18	75.40	73.53	74.16	74.52	72.85
C10	61.0	59.01	57.44	57.89	56.78	59.16	58.25	58.53	60.18
C11	61.0	59.95	61.49	62.96	62.33	62.05	60.83	63.95	63.04
C12	31.0	29.64	30.05	31.51	30.59	31.01	30.58	24.31	23.66
C14	18.2	18.70	17.85	17.28	17.53	18.14	18.30	19.26	20.06
C13	24.6	23.63	24.19	25.61	23.70	24.96	23.23	26.48	26.13
C15	21.5	19.06	19.23	18.85	19.29	18.26	19.17	19.25	19.15
H1b	2.13	2.14	2.14	2.26	1.99	2.32	2.04	2.33	2.36
H1a	2.92	2.32	2.34	2.52	2.61	2.48	2.63	2.45	2.47
H2	4.22	4.48	4.52	4.74	4.37	4.63	4.38	4.92	4.88
H4b	2.23	2.32	2.37	2.15	2.55	2.08	2.48	2.33	2.20
H4a	2.45	2.46	2.51	2.61	2.68	2.56	2.61	2.73	2.61
H5	4.58	4.68	4.68	4.54	4.44	4.57	4.50	4.38	4.40
H9	4.00	4.07	4.03	3.85	4.16	4.02	4.09	3.81	3.88
H10	3.16	2.93	2.85	2.88	2.96	2.83	2.98	2.77	2.83
Me-12	1.64	1.72	1.74	1.62	1.68	1.61	1.67	1.70	1.66
Me-13	1.11	1.12	1.05	1.16	0.94	1.24	1.02	0.95	1.09
Me-14	1.20	1.30	1.33	1.34	1.31	1.31	1.26	1.37	1.33
Me-15	1.35	1.44	1.42	1.32	1.30	1.34	1.32	1.25	1.28

Table S3.4.1 – *Experimental data of **3a** and calculated isotropic shielding constants of **3a-3h** at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory.*

DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Isotropic shielding constants***							
C1	33.6	149.76	149.83	149.42	151.24	149.87	151.14	149.21	149.13
C2	58.1	109.82	110.02	109.58	114.68	109.58	114.76	107.52	107.84
C3	68.0	103.03	102.78	102.46	101.92	102.27	101.89	102.67	102.72
C4	45.2	138.15	138.24	138.49	138.40	138.72	138.36	137.69	137.41
C5	74.2	108.75	108.90	106.93	109.01	106.64	108.88	106.65	106.24
C6	50.4	130.77	131.18	131.70	130.12	131.83	130.32	132.09	131.69
C7	49.3	132.15	130.51	129.68	130.31	131.64	131.04	130.11	131.02
C8	112.6	50.08	59.23	58.13	59.18	49.16	50.17	59.47	50.02
C9	73.8	108.70	109.54	109.48	109.68	108.54	108.54	110.14	108.86
C10	61.0	122.79	123.61	120.72	123.15	120.20	122.28	120.63	119.92
C11	61.0	122.51	119.49	117.72	119.17	120.16	121.91	118.48	120.87
C12	31.0	155.88	155.98	153.80	155.24	153.83	155.23	162.40	162.28
C13	24.6	167.76	168.81	169.58	169.70	168.40	168.20	170.45	168.97
C14	18.2	162.63	162.56	160.23	162.05	160.21	162.26	159.98	160.71
C15	21.5	164.58	164.65	165.31	164.81	165.08	164.85	165.05	164.92
H1a	2.92	29.70	29.74	29.59	29.83	29.57	29.78	29.57	29.44
H1b	2.13	29.61	29.59	29.12	29.15	29.14	29.14	29.46	29.38
H2	4.22	27.24	27.26	27.19	27.81	27.35	27.81	27.00	27.02
H4a	2.45	29.39	29.34	29.77	29.20	29.72	29.22	29.35	29.38
H4b	2.23	29.21	29.19	29.04	29.04	28.99	29.10	28.95	28.98

H5	4.58	27.05	27.12	27.21	27.65	27.05	27.52	27.44	27.38
H8	4.00	27.76	27.84	28.02	27.88	27.79	27.87	28.00	27.86
H10	3.16	28.57	28.65	28.69	28.63	28.63	28.58	28.75	28.65
Me-12	1.64	30.01	30.01	29.98	30.03	30.00	30.04	30.01	30.03
Me-13	1.20	30.68	30.71	30.75	30.77	30.63	30.69	30.80	30.62
Me-14	1.11	30.51	30.49	30.50	30.40	30.55	30.52	30.44	30.48
Me-15	1.35	30.38	30.37	30.40	30.36	30.40	30.35	30.47	30.43

Table S3.4.2 – *Experimental data of* ***3a*** *and scaled chemical shifts of* ***3a-3h*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory.*

DP4+									
Compound		***3a***	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
Nuclei	***Exp***	***Scaled shifts***							
C1	33.6	34.69	34.20	34.02	33.21	34.15	33.72	34.90	35.31
C2	58.1	67.50	68.57	68.12	64.71	66.95	63.56	70.23	68.52
C3	68.0	73.09	74.82	74.20	75.71	72.91	74.12	74.34	72.64
C4	45.2	44.23	44.21	43.37	44.28	43.23	44.20	44.67	44.74
C5	74.2	68.38	69.54	70.38	69.60	69.34	68.39	70.96	69.81
C6	50.4	50.30	50.31	49.19	51.41	48.84	50.80	49.41	49.34
C7	49.3	49.16	50.89	50.92	51.25	49.00	50.21	51.09	49.88
C8	112.6	116.58	112.42	112.15	112.53	116.15	116.54	110.94	115.03
C9	73.8	68.42	68.98	68.20	69.02	67.80	68.67	68.01	67.70
C10	61.0	56.85	56.84	58.58	57.42	58.31	57.40	59.12	58.81
C11	61.0	57.08	60.39	61.15	60.84	58.34	57.70	60.94	58.04
C12	31.0	29.67	28.90	30.27	29.77	30.93	30.37	23.73	24.74
C13	24.6	19.91	17.82	16.77	17.31	19.07	19.73	16.91	19.35
C14	18.2	24.12	23.22	24.77	23.90	25.73	24.60	25.78	26.00
C15	21.5	22.52	21.41	20.42	21.53	21.77	22.48	21.48	22.61
H1a	2.92	2.07	2.04	2.18	1.90	2.17	1.96	2.19	2.28
H1b	2.13	2.16	2.19	2.65	2.67	2.59	2.67	2.30	2.33
H2	4.22	4.48	4.51	4.59	4.19	4.36	4.15	4.82	4.74
H4a	2.45	2.37	2.43	2.00	2.61	2.02	2.58	2.42	2.33
H4b	2.23	2.55	2.58	2.73	2.80	2.75	2.72	2.82	2.74
H5	4.58	4.67	4.66	4.57	4.38	4.65	4.47	4.37	4.37
H8	4.00	3.97	3.94	3.75	4.12	3.92	4.08	3.80	3.89
H10	3.16	3.17	3.12	3.08	3.26	3.10	3.29	3.03	3.08
Me-12	1.64	1.76	1.77	1.79	1.67	1.75	1.67	1.74	1.67
Me-13	1.20	1.11	1.06	1.02	0.83	1.13	0.95	0.93	1.07
Me-14	1.11	1.28	1.29	1.27	1.25	1.20	1.14	1.30	1.22
Me-15	1.35	1.40	1.41	1.36	1.30	1.35	1.32	1.27	1.27

4. Results:

Table S4.1.1 – *DP4+ results calculated for example* ***1a*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory*

	1a	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
sDP4+ (H data)	80.54	0.06	0.00	0.03	1.98	0.08	0.00	0.01	0.05	0.26	0.00	0.00	0.01	2.15	14.82	0.00
sDP4+ (C data)	82.75	3.01	0.03	1.78	0.01	0.62	0.01	2.58	0.00	4.54	0.03	0.00	0.37	4.05	0.14	0.10
sDP4+ (all data)	99.82	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.13	0.03	0.00
uDP4+ (H data)	78.88	0.00	0.00	0.00	2.30	0.00	0.02	0.02	0.01	0.07	0.00	0.00	0.00	2.10	16.58	0.00
uDP4+ (C data)	99.88	0.01	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.02	0.01	0.00
uDP4+ (all data)	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DP4+ (H data)	96.14	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07	3.72	0.00
DP4+ (C data)	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DP4+ (all data)	100.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4.2.1 – *DP4 results calculated for example* ***1a*** *at the B3LYP/6-31G**//MMFF level of theory*

	1a	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
sDP4+ (H data)	91.61	0.23	0.00	0.01	0.64	0.02	0.03	0.00	0.01	0.12	0.00	0.00	0.00	1.08	5.28	0.97
sDP4+ (C data)	10.19	0.10	0.00	0.02	0.12	0.00	0.02	0.11	0.01	4.53	0.00	0.00	10.31	0.71	0.26	73.64
sDP4+ (all data)	92.66	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.08	0.14	7.06

Table S4.3.1 – *MM-DP4+ results calculated for example* ***1a*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory*

	1a	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
sDP4+ (H data)	39.85	0.25	0.00	0.00	13.62	0.06	0.13	0.05	0.67	0.14	0.00	0.06	0.00	18.36	26.80	0.00
sDP4+ (C data)	82.70	1.32	0.00	0.47	1.04	0.10	0.07	0.24	0.02	8.32	0.05	0.00	0.00	4.14	1.43	0.11
sDP4+ (all data)	96.21	0.01	0.00	0.00	0.41	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00	2.22	1.12	0.00
uDP4+ (H data)	48.41	0.16	0.00	0.00	12.21	0.03	1.44	0.03	0.59	0.06	0.00	0.00	0.00	14.07	22.98	0.01
uDP4+ (C data)	87.11	0.34	0.01	0.68	0.79	0.03	0.01	0.09	0.00	10.03	0.04	0.00	0.00	0.57	0.23	0.07
uDP4+ (all data)	99.44	0.00	0.00	0.00	0.23	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.19	0.12	0.00
DP4+ (H data)	64.95	0.00	0.00	0.00	5.60	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	8.69	20.73	0.00
DP4+ (C data)	98.80	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	1.14	0.00	0.00	0.00	0.03	0.00	0.00
DP4+ (all data)	99.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4.4.1 – *DP4+ results calculated for example* ***1a*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

	1a	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***	***1i***	***1j***	***1k***	***1l***	***1m***	***1n***	***1o***	***1p***
sDP4+ (H data)	13.78	0.01	0.00	0.00	5.78	0.05	0.00	0.01	0.01	0.00	0.01	0.00	0.00	1.09	79.26	0.00
sDP4+ (C data)	60.92	0.72	0.01	0.06	0.14	0.01	0.01	1.09	0.01	35.42	0.01	0.00	0.01	1.28	0.24	0.07
sDP4+ (all data)	97.53	0.00	0.00	0.00	0.09	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.16	2.19	0.00
uDP4+ (H data)	2.02	0.00	0.00	0.00	0.95	0.00	0.09	0.00	0.00	0.00	0.00	0.00	0.00	0.69	96.25	0.00
uDP4+ (C data)	86.20	0.00	0.00	0.00	3.61	0.00	0.01	0.07	0.02	9.74	0.01	0.00	0.00	0.05	0.29	0.01
uDP4+ (all data)	84.78	0.00	0.00	0.00	1.67	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	13.53	0.00
DP4+ (H data)	0.36	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	99.56	0.00
DP4+ (C data)	93.82	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	6.17	0.00	0.00	0.00	0.00	0.00	0.00
DP4+ (all data)	99.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.36	0.00

Table S4.1.2 – *DP4+ results calculated for example* ***2a*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	98.87	0.32	0.15	0.01	0.50	0.00	0.05	0.11

sDP4+ (C data)	0.02	0.00	99.98	0.00	0.00	0.00	0.00	0.00
sDP4+ (all data)	10.56	0.00	89.44	0.00	0.00	0.00	0.00	0.00
uDP4+ (H data)	54.60	0.59	22.68	1.01	17.91	0.02	3.15	0.05
uDP4+ (C data)	1.22	0.10	98.48	0.03	0.16	0.00	0.00	0.01
uDP4+ (all data)	2.90	0.00	96.97	0.00	0.12	0.00	0.00	0.00
DP4+ (H data)	99.77	0.00	0.06	0.00	0.16	0.00	0.00	0.00
DP4+ (C data)	0.00	0.00	100.00	0.00	0.00	0.00	0.00	0.00
DP4+ (all data)	0.35	0.00	99.65	0.00	0.00	0.00	0.00	0.00

Table S4.2.2 – *DP4 results calculated for example* ***2a*** *at the B3LYP/6-31G**//MMFF level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	94.88	2.54	0.00	0.83	0.97	0.00	0.50	0.29
sDP4+ (C data)	98.76	0.00	0.00	1.24	0.00	0.00	0.00	0.00
sDP4+ (all data)	99.99	0.00	0.00	0.01	0.00	0.00	0.00	0.00

Table S4.3.2 – *MM-DP4+ results calculated for example* ***2a*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	89.50	1.81	8.64	0.00	0.03	0.01	0.00	0.01
sDP4+ (C data)	99.55	0.01	0.43	0.00	0.01	0.00	0.00	0.00
sDP4+ (all data)	99.96	0.00	0.04	0.00	0.00	0.00	0.00	0.00
uDP4+ (H data)	33.89	1.24	64.23	0.03	0.25	0.08	0.21	0.06
uDP4+ (C data)	97.08	0.06	2.42	0.08	0.31	0.04	0.00	0.00
uDP4+ (all data)	95.48	0.00	4.51	0.00	0.00	0.00	0.00	0.00
DP4+ (H data)	84.49	0.06	15.45	0.00	0.00	0.00	0.00	0.00
DP4+ (C data)	99.99	0.00	0.01	0.00	0.00	0.00	0.00	0.00
DP4+ (all data)	100.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4.4.2 – *DP4+ results calculated for example* ***2a*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	99.16	0.77	0.00	0.00	0.06	0.00	0.01	0.00
sDP4+ (C data)	6.57	0.00	91.95	1.02	0.01	0.45	0.00	0.00
sDP4+ (all data)	100.0 0	0.00	0.00	0.00	0.00	0.00	0.00	0.00
uDP4+ (H data)	82.64	8.53	0.23	0.05	8.23	0.00	0.30	0.01
uDP4+ (C data)	0.78	0.17	97.48	0.04	0.01	1.52	0.00	0.00

uDP4+ (all data)	73.04	1.61	25.23	0.00	0.12	0.00	0.00	0.00
DP4+ (H data)	99.91	0.08	0.00	0.00	0.01	0.00	0.00	0.00
DP4+ (C data)	0.06	0.00	99.94	0.00	0.00	0.01	0.00	0.00
DP4+ (all data)	100.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S4.1.3 – *DP4+ results calculated for example* ***2b*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	0.30	97.95	0.01	0.01	0.28	0.70	0.02	0.73
sDP4+ (C data)	0.00	0.08	0.00	0.00	0.00	99.92	0.00	0.00
sDP4+ (all data)	0.00	10.34	0.00	0.00	0.00	89.66	0.00	0.00
uDP4+ (H data)	2.35	74.28	0.38	0.04	11.48	11.03	0.37	0.07
uDP4+ (C data)	0.92	9.98	0.18	0.01	1.06	87.74	0.00	0.10
uDP4+ (all data)	0.13	43.03	0.00	0.00	0.71	56.13	0.00	0.00
DP4+ (H data)	0.01	99.84	0.00	0.00	0.04	0.11	0.00	0.00
DP4+ (C data)	0.00	0.01	0.00	0.00	0.00	99.99	0.00	0.00
DP4+ (all data)	0.00	8.12	0.00	0.00	0.00	91.88	0.00	0.00

Table S4.2.3 – *DP4 results calculated for example* ***2b*** *at the B3LYP/6-31G**//MMFF level of theory*

	3a	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***
sDP4+ (H data)	0.12	93.07	0.00	0.19	0.02	0.00	0.04
sDP4+ (C data)	0.02	96.35	0.00	0.00	0.00	0.00	0.00
sDP4+ (all data)	0.00	99.73	0.00	0.00	0.00	0.00	0.00

Table S4.3.3 – *MM-DP4+ results calculated for example* ***2b*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	0.11	88.14	0.06	0.00	0.01	11.67	0.00	0.01
sDP4+ (C data)	0.03	99.81	0.01	0.00	0.00	0.14	0.00	0.02
sDP4+ (all data)	0.00	99.98	0.00	0.00	0.00	0.02	0.00	0.00
uDP4+ (H data)	0.21	58.03	0.49	0.01	0.29	40.82	0.06	0.10
uDP4+ (C data)	0.05	98.23	0.07	0.00	0.00	0.37	0.00	1.27
uDP4+ (all data)	0.00	99.73	0.00	0.00	0.00	0.27	0.00	0.00
DP4+ (H data)	0.00	91.48	0.00	0.00	0.00	8.52	0.00	0.00
DP4+ (C data)	0.00	100.0	0.00	0.00	0.00	0.00	0.00	0.00
DP4+ (all data)	0.00	100.0	0.00	0.00	0.00	0.00	0.00	0.00

Table S4.4.3 – *DP4+ results calculated for example* ***2b*** *at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

	2a	***2b***	***2c***	***2d***	***2e***	***2f***	***2g***	***2h***
sDP4+ (H data)	0.25	99.70	0.00	0.00	0.01	0.03	0.00	0.01
sDP4+ (C data)	0.00	0.00	0.00	0.00	0.00	100.0	0.00	0.00
sDP4+ (all data)	0.00	11.13	0.00	0.00	0.00	88.87	0.00	0.00
uDP4+ (H data)	6.45	91.12	0.00	0.00	2.27	0.11	0.04	0.01
uDP4+ (C data)	0.10	0.02	8.64	0.00	0.00	91.23	0.00	0.00
uDP4+ (all data)	4.98	16.88	0.23	0.00	0.02	77.89	0.00	0.00
DP4+ (H data)	0.02	99.98	0.00	0.00	0.00	0.00	0.00	0.00
DP4+ (C data)	0.00	0.00	0.00	0.00	0.00	100.0	0.00	0.00
DP4+ (all data)	0.00	2.64	0.00	0.00	0.00	97.36	0.00	0.00

Table S4.1.4 – *DP4+ results calculated for example* ***3a*** *at the PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* level of theory*

	3a	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
sDP4+ (H data)	29.2	12.29	5.96	0.9	16.82	34.51	0	0.32
sDP4+ (C data)	0.12	18.35	2.75	76.84	1.31	0.58	0.04	0
sDP4+ (all data)	1.01	63.25	4.6	19.34	6.16	5.64	0	0
uDP4+ (H data)	5.51	44.32	22.9	1.79	9.99	14.69	0.01	0.79
uDP4+ (C data)	4.37	9.3	1.29	18.99	0.12	65.93	0	0
uDP4+ (all data)	1.64	28.05	2	2.31	0.08	65.92	0	0
DP4+ (H data)	10.59	35.86	8.99	0.11	11.06	33.37	0	0.02
DP4+ (C data)	0.03	10.2	0.21	87.25	0.01	2.3	0	0
DP4+ (all data)	0.08	80.57	0.42	2.03	0.02	16.88	0	0

Table S4.2.4 – *DP4 results calculated for example* ***3a*** *at the B3LYP/6-31G**//MMFF level of theory*

	3a	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
sDP4+ (H data)	0.37	0.24	6.19	9.47	9.64	73.38	0.10	0.63
sDP4+ (C data)	0.00	7.23	59.07	32.80	0.06	0.02	0.80	0.00
sDP4+ (all data)	0.00	0.25	53.75	45.66	0.09	0.23	0.01	0.00

Table S4.3.4 – *MM-DP4+ results calculated for example* ***3a*** *at the SMD/wB97XD/6-31+G**//MMFF level of theory*

	1a	***1b***	***1c***	***1d***	***1e***	***1f***	***1g***	***1h***
sDP4+ (H data)	22.69	2.24	0.79	0.58	1.12	72.57	0.00	0.02
sDP4+ (C data)	0.25	8.67	60.71	21.42	7.22	1.56	0.13	0.03

sDP4+ (all data)	2.73	9.42	23.16	5.97	3.91	54.83	0.00	0.00
uDP4+ (H data)	4.02	0.66	1.47	3.03	0.01	90.77	0.00	0.03
uDP4+ (C data)	14.88	7.53	16.40	7.24	23.93	29.73	0.06	0.22
uDP4+ (all data)	2.13	0.18	0.86	0.78	0.01	96.04	0.00	0.00
DP4+ (H data)	1.37	0.02	0.02	0.03	0.00	98.57	0.00	0.00
DP4+ (C data)	0.26	4.54	69.20	10.78	12.01	3.22	0.00	0.00
DP4+ (all data)	0.11	0.03	0.37	0.09	0.00	99.40	0.00	0.00

Table S4.4.4 – *DP4+ results calculated for example **3a** at the PCM/mPW1PW91/6-311+G**// B3LYP/6-31G* level of theory*

	3a	***3b***	***3c***	***3d***	***3e***	***3f***	***3g***	***3h***
sDP4+ (H data)	20.40	1.73	0.67	0.09	74.59	2.42	0.00	0.11
sDP4+ (C data)	0.03	3.44	20.52	73.35	0.99	1.63	0.04	0.01
sDP4+ (all data)	0.49	5.68	13.09	6.39	70.57	3.78	0.00	0.00
uDP4+ (H data)	11.60	8.52	5.77	0.10	70.07	3.73	0.01	0.20
uDP4+ (C data)	2.68	15.07	0.36	74.13	0.15	7.61	0.00	0.00
uDP4+ (all data)	14.93	61.73	1.01	3.67	5.00	13.66	0.00	0.00
DP4+ (H data)	4.31	0.27	0.07	0.00	95.19	0.16	0.00	0.00
DP4+ (C data)	0.00	0.94	0.14	98.70	0.00	0.23	0.00	0.00
DP4+ (all data)	0.92	43.90	1.65	2.94	44.13	6.46	0.00	0.00

Table S4.5*- MAE and MaxErr obtained for ^{1}H and ^{13}C by using the three DP4 methods under analysis.*

	DP4	**MM-DP4+**	**DP4+**	**DP4**	**MM-DP4+**	**DP4+**
	Unscaled ^{13}C MAE			Scaled ^{13}C MAE		
1	4.1	5.0	4.8	3.2	2.6	4.3
2a	3.5	4.3	5.6	2.5	2.0	4.1
2b	3.6	4.4	5.7	2.6	1.9	4.1
3	4.3	4.9	5.7	2.9	2.3	2.7
	Unscaled ^{13}C MaxErr			Scaled ^{13}C MaxErr		
1	11.1	11.2	17.2	7.2	6.0	12.1
2a	10.4	10.8	16.6	7.4	6.6	11.0
2b	10.4	11.0	16.6	7.3	6.7	11.0
3	18.7	15.1	20.4	7.0	5.3	8.8
	Unscaled ^{1}H MAE			Scaled ^{1}H MAE		
1	0.13	0.17	0.14	0.06	0.11	0.10
2a	0.15	0.12	0.12	0.11	0.10	0.06
2b	0.14	0.14	0.12	0.11	0.12	0.08
3	0.21	0.20	0.17	0.19	0.14	0.15
	Unscaled ^{1}H MaxErr			Scaled ^{1}H MaxErr		
1	0.46	0.66	0.50	0.14	0.31	0.28
2a	0.28	0.40	0.36	0.39	0.17	0.19

2b	0.28	0.48	0.41	0.37	0.22	0.22
3	0.71	0.51	0.81	0.72	0.60	0.81

5. Study of the dependence of magnetic isotropic shielding constants calculation and calculated bond distance

Table 5.1 *- Carbon-Halogen bond distances (Å) and associated ^{13}C unscaled errors (UE_C) with B3LYP/6-31G* optimized geometries (OPTB) and Molecular Mechanics (MMFF) Optimized Geometries. NMR calculations at PCM/mPW1PW91/6-31+G** level of theory*

	Nuclei	***OPTB***		***MMFF***	
		UE_C	**C-X dist**	**UE_C**	**C-X dist**
1	***C2-Br***	15.93	2.00	11.25	1.96
	C3-Cl	11.59	1.85	4.19	1.81
	C10-Br	17.20	2.02	9.23	1.98
2a	***C1-Cl***	8.95	1.85	1.20	1.79
	C3-Br	16.59	2.00	10.83	1.97
	C5-Cl	9.17	1.85	4.11	1.80
	C8-Cl	8.46	1.84	2.56	1.77
2b	***C1-Cl***	8.70	1.85	2.02	1.79
	C3-Br	16.61	2.00	11.04	1.97
	C5-Cl	9.50	1.85	3.70	1.80
	C8-Cl	8.62	1.83	2.96	1.77
3	***C2-Br***	17.05	1.99	11.01	1.96
	C3-Cl	12.45	1.85	4.85	1.81
	C8-Br	20.40	2.01	7.27	1.97

Table S5.2 *– Impact of solvation on the C-Halogen bond distance for geometries optimized at the B3LYP/6-31G* theory level. Carbon-Halogen bond distances (Å) and associated ^{13}C unscaled errors (UE_C) with B3LYP/6-31G* optimized geometries in vacuum (OPTB) and PCM/B3LYP/6-31G* Optimized Geometries (OPTB/PCM). NMR calculations at PCM/mPW1PW91/6-31+G** level of theory*

	Nuclei	***OPTB***		***OPTB/PCM***	
		UE_C	**C-X dist**	**UE_C**	**C-X dist**
1	***C2-Br***	15.93	2.00	16.69	2.00
	C3-Cl	11.59	1.85	13.04	1.86
	C10-Br	17.20	2.02	17.45	2.02
2a	***C1-Cl***	8.95	1.85	9.06	1.86
	C3-Br	16.59	2.00	17.00	2.00
	C5-Cl	9.17	1.85	10.15	1.86
	C8-Cl	8.46	1.84	10.20	1.84
2b	***C1-Cl***	8.70	1.85	9.02	1.86
	C3-Br	16.61	2.00	16.80	2.00
	C5-Cl	9.50	1.85	9.80	1.86
	C8-Cl	8.62	1.83	10.74	1.84

3	**C2-Br**	17.05	1.99	17.28	2.00
	C3-Cl	12.45	1.85	13.91	1.87
	C8-Br	20.40	2.01	20.61	2.02
4	**C-Br**	17.57	2.00	19.12	2.01
5	**C-Cl**	10.28	1.84	11.96	1.85

Table S5.3 *– ^{13}C and ^{1}H unscaled errors (UE) for nuclei adjacent to Br and Cl, with associated Carbon-Halogen bond distances for each geometry. A: NMR Calculations with PCM/mPW1PW91/6-31+G** level. B: NMR Calculations with B3LYP/6-31G* level.*

	UE α Br ^{13}C	**UE α Br ^{1}H**	**Dist C-Br Calc**	**UE α Cl ^{13}C**	**UE α Cl ^{1}H**	**Dist C-Cl Calc**
B//MMFF	5.60	-0.229	1.9463	0.07	-0.344	1.7827
A//MMFF	7.12	0.008	1.9463	0.70	-0.222	1.7827
B//UFF	5.89	-0.428	1.9475	-0.261	-0.4802	1.7897
A//UFF	7.16	-0.186	1.9475	0.3693	-0.3533	1.7897
B//RHF_Am1	5.33	-0.315	1.9373	-2.7066	-0.4645	1.7611
A//RHF_Am1	6.35	-0.119	1.9373	-2.4906	-0.379	1.7611
B//RHF_321G	15.47	-0.075	2.0023	19.293	0.2685	1.9081
A//RHF_321G	18.05	0.178	2.0023	22.2025	0.4445	1.9081
B// B3LYP/6-31G*	14.86	0.049	2.0021	8.74	-0.116	1.8378
A// B3LYP/6-31G*	17.57	0.301	2.0021	10.28	0.010	1.8378
B// B3LYP/6-311++G**	15.73	0.119	2.0075	9.1556	-0.071	1.8393
A// B3LYP/6-311++G**	18.41	0.362	2.0075	10.5875	0.0493	1.8393
B// B3LYP/6-311++G(3df,2pd)	14.73	0.101	1.9989	7.3018	-0.1269	1.8246
A// B3LYP/6-311++G(3df,2pd)	17.26	0.338	1.9989	8.4974	-0.0148	1.8246
B// B3LYP/cc-PVTZ	14.63	0.082	1.9996	8.1386	-0.105	1.832
A// B3LYP/cc-PVTZ	17.18	0.321	1.9996	9.4722	0.0123	1.832
B//M062X/6-31G*	10.54	-0.121	1.969	4.9861	-0.2443	1.8109
A//M062X/6-31G*	12.44	0.111	1.969	5.9443	-0.1315	1.8109
B//MO62X/6-311++G**	11.49	-0.058	1.9757	5.3615	-0.2092	1.8129

A//M062X/6-311++G**	13.51	0.170	1.9757	6.3659	-0.0997	1.8129
B//M062X/6-311++G(3df,2pd)	10.55	-0.084	1.9671	3.8182	-0.2601	1.7998
A//M062X/6-311++G(3df,2pd)	12.43	0.139	1.9671	4.6308	-0.1573	1.7998
B//M062X/cc-PVTZ	10.59	-0.092	1.9684	4.4344	-0.2432	1.8057
A//M062X/cc-PVTZ	12.49	0.133	1.9684	5.3443	-0.1366	1.8057
B//MP2 /6-31G*	12.01	-0.024	1.9784	3.6086	-0.2703	1.8016
A//MP2/6-31G*	14.08	0.218	1.9784	4.4327	-0.159	1.8016
B//MP2/6-311++G**	10.28	-0.138	1.9641	3.3904	-0.2969	1.7984
A//MP2/6-311++G**	9.38	0.089	1.9641	1.5357	-0.189	1.7984
B//MP2/6-311++G(3df,2pd)	9.14	-0.126	1.9535	2.7856	-0.2746	1.7907
A//MP2/6-311++G(3df,2pd)	10.71	0.095	1.9535	3.4347	-0.1717	1.7907
B//MP2/cc-PVTZ	8.10	-0.190	1.948	3.7151	-0.2614	1.7989
A//MP2/cc-PVTZ	9.60	0.029	1.948	4.4995	-0.1625	1.7989

Table S5.4 *– Impact of the C-Cl bond distance on the unscaled error in ^{13}C NMR at levels: PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* (OPTB_DP4+), B3LYP/6-31G*//B3LYP/6-31G* (OPTB_DP4), PCM/mPW1PW91/6-31+G**//MMFF (MMFF_DP4+), and B3LYP/6-31G*//MMFF (MMFF_DP4)*

System	**exo-2-Chloronorbornane**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.7	-11.2745	-11.1649	-11.5019	-11.4075
1.71	-9.9133	-9.874	-10.1411	-10.1142
1.72	-8.5191	-8.5554	-8.7478	-8.7939
1.73	-7.0925	-7.2101	-7.3225	-7.4469
1.74	-4.1438	-5.8384	-5.8658	-6.0742
1.75	-2.6229	-3.0191	-4.3779	-4.6761
1.76	-1.0716	-1.5728	-2.8594	-3.2534
1.77	0.5093	-0.1032	-1.3107	-1.807
1.78	2.1194	1.3892	0.267	-0.337
1.79	3.758	2.9036	1.8737	1.1556
1.8	5.4243	4.4391	3.5085	2.6699
1.81	7.1181	5.9949	5.1713	4.2049
1.82	8.8379	7.5706	6.8608	5.7604
1.83	10.5837	9.1651	8.5765	7.3354

1.84	12.3546	10.7777	10.3178	8.9291
1.85	14.1497	12.4071	12.084	10.5408
1.86	15.9686	14.0531	13.8744	12.1696
1.87	17.8103	15.7145	15.6883	13.8148
1.88	19.6743	17.3908	17.5251	15.4754
1.89	21.5598	19.081	19.3838	17.1507
1.9	23.4657	20.784	21.2641	18.84
1.91	25.3918	22.4994	23.1651	20.5424
1.92	27.3369	24.2261	25.086	22.2571
1.93	29.3006	25.9634	27.0261	23.9832
1.94	31.2819	27.7105	28.9846	25.72
1.95	33.2799	29.4663	30.9608	27.4665
1.96	35.294	31.2302	32.954	29.2221
1.97	37.3235	33.0014	34.9633	30.9858
1.98	39.3674	34.7789	36.9879	32.7568
1.99	41.425	36.5621	39.0271	34.5344

System	**1-Chloropropane**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.7	-9.1963	-9.867	-7.7425	-8.3251
1.71	-7.9679	-8.7394	-6.5121	-7.1903
1.72	-6.7106	-7.5878	-5.2531	-6.0316
1.73	-5.4249	-6.4127	-3.9659	-4.8497
1.74	-4.1113	-5.2149	-2.6511	-3.6452
1.75	-2.7702	-3.9949	-1.309	-2.4186
1.76	-1.4024	-2.7534	0.0596	-1.1707
1.77	-0.0082	-1.491	1.4545	0.098
1.78	1.4116	-0.2086	2.8749	1.3868
1.79	2.8566	1.0934	4.3203	2.6951
1.8	4.3262	2.4141	5.7903	4.0222
1.81	5.8197	3.753	7.2842	5.3675
1.82	7.3366	5.1093	8.8015	6.7303
1.83	8.8763	6.4823	10.3416	8.11
1.84	10.4381	7.8714	11.9038	9.5058
1.85	12.0215	9.2758	13.4876	10.9171
1.86	13.6257	10.6948	15.0923	12.3433
1.87	15.2501	12.1276	16.7173	13.7835
1.88	16.894	13.5737	18.362	15.2372
1.89	18.5569	15.0323	20.0259	16.7036
1.9	20.238	16.5027	21.7082	18.182
1.91	21.9367	17.9841	23.4084	19.6718
1.92	23.6523	19.476	25.1258	21.1724
1.93	25.3843	20.9775	26.8599	22.6829
1.94	27.1319	22.488	28.61	24.2028
1.95	28.8945	24.0068	30.3756	25.7314
1.96	30.6716	25.5332	32.1559	27.2679
1.97	32.4623	27.0666	33.9502	28.8118

1.98	34.266	28.6062	35.758	30.3623
1.99	36.082	30.1514	37.5785	31.9188

System	**Chlorociclohexane**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.7	-15.2637	-15.8626	-14.8616	-15.3822
1.71	-13.7871	-14.4685	-13.3925	-13.9908
1.72	-12.2798	-13.0486	-11.8931	-12.5739
1.73	-10.7422	-11.6035	-10.3641	-11.1324
1.74	-9.1751	-10.1341	-8.8057	-9.6668
1.75	-7.5789	-8.641	-7.2186	-8.1777
1.76	-5.9541	-7.125	-5.6034	-6.6659
1.77	-4.3015	-5.5868	-3.9604	-5.1321
1.78	-2.6216	-4.0271	-2.2904	-3.5768
1.79	-0.9151	-2.4467	-0.5939	-2.0009
1.8	0.8173	-0.8462	1.1284	-0.4051
1.81	2.575	0.7734	2.876	1.21
1.82	4.3573	2.4114	4.6483	2.8436
1.83	6.1635	4.067	6.4445	4.495
1.84	7.9929	5.7395	8.264	6.1633
1.85	9.8449	7.428	10.1063	7.8478
1.86	11.7187	9.1317	11.9707	9.5478
1.87	13.6138	10.8497	13.8565	11.2624
1.88	15.5293	12.5814	15.763	12.991
1.89	17.4647	14.3259	17.6898	14.7327
1.9	19.4192	16.0824	19.6359	16.4868
1.91	21.3921	17.8502	21.6009	18.2526
1.92	23.3826	19.6284	23.5839	20.0292
1.93	25.3901	21.4163	25.5844	21.816
1.94	27.4137	23.213	27.6015	23.6122
1.95	29.4528	25.0179	29.6346	25.417
1.96	31.5064	26.8302	31.6829	27.2298
1.97	33.574	28.649	33.7456	29.0497
1.98	35.6546	30.4736	35.8222	30.876
1.99	37.7476	32.3033	37.9118	32.7079

System	**1-Chloropropene**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.7	-10.5233	-11.1078	-9.9596	-10.4305
1.71	-9.8095	-10.303	-9.2425	-9.6229
1.72	-9.0739	-9.4805	-8.5034	-8.7972
1.73	-8.3168	-8.6405	-7.7424	-7.9536
1.74	-7.5382	-7.7833	-6.9596	-7.0925
1.75	-6.7383	-6.9092	-6.1551	-6.2141
1.76	-5.9172	-6.0185	-5.3288	-5.3185
1.77	-5.0748	-5.1113	-4.4809	-4.406

1.78	-4.2112	-4.1879	-3.6113	-3.4769
1.79	-3.3265	-3.2484	-2.7203	-2.5313
1.8	-2.4211	-2.2932	-1.8082	-1.5695
1.81	-1.4951	-1.3224	-0.8751	-0.5918
1.82	-0.5486	-0.3362	0.0792	0.4018
1.83	0.4185	0.6653	1.0547	1.4111
1.84	1.4061	1.6819	2.0514	2.4357
1.85	2.4143	2.7133	3.0693	3.4757
1.86	3.4432	3.7595	4.1083	4.5306
1.87	4.4925	4.8202	5.1682	5.6004
1.88	5.5623	5.8953	6.2489	6.6847
1.89	6.6523	6.9844	7.3501	7.7835

System	**Chlorobenzene**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.7	0.593	-1.1412	0.5942	-1.1176
1.71	1.3663	-0.2724	1.37	-0.2475
1.72	2.1605	0.6147	2.1666	0.6409
1.73	2.9756	1.5199	2.9839	1.5473
1.74	3.8115	2.4432	3.822	2.4716
1.75	4.6683	3.3841	4.6808	3.4135
1.76	5.5459	4.3426	5.5602	4.3729
1.77	6.4443	5.3183	6.4604	5.3496
1.78	7.3634	6.3112	7.3812	6.3433
1.79	8.3031	7.3208	8.3224	7.3537
1.8	9.2633	8.3469	9.284	8.3807
1.81	10.2438	9.3894	10.2659	9.424
1.82	11.2446	10.4478	11.268	10.4833
1.83	12.2654	11.5219	12.2901	11.5583
1.84	13.3062	12.6114	13.3322	12.6487
1.85	14.3668	13.716	14.3941	13.7542
1.86	15.4471	14.8354	15.4758	14.8746
1.87	16.5471	15.9692	16.5771	16.0096
1.88	17.6664	17.1171	17.6979	17.1587
1.89	18.805	18.2789	18.838	18.3218

System	**3-Chlorotoluene**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.7	0.5404	-1.0306	1.2775	-0.2928
1.71	1.3265	-0.1641	2.068	0.579
1.72	2.1336	0.721	2.8796	1.4693
1.73	2.9618	1.6243	3.7123	2.3778
1.74	3.811	2.5457	4.566	3.3043
1.75	4.6811	3.485	5.4406	4.2487
1.76	5.5722	4.442	6.336	5.2107
1.77	6.484	5.4163	7.252	6.1901

1.78	7.4165	6.4078	8.1886	7.1868
1.79	8.3695	7.4163	9.1456	8.2003
1.8	9.3428	8.4414	10.123	9.2306
1.81	10.3363	9.4829	11.1205	10.2773
1.82	11.3499	10.5404	12.1382	11.3402
1.83	12.3833	11.6138	13.1758	12.419
1.84	13.4364	12.7027	14.2332	13.5134
1.85	14.5091	13.8067	15.3104	14.623
1.86	15.6013	14.9256	16.4071	15.7477
1.87	16.7127	16.0591	17.5232	16.8871
1.88	17.8432	17.2068	18.6585	18.0408
1.89	18.9927	18.3683	19.813	19.2086

Table S5.5 *— Impact of the C-Br bond distance on the unscaled error in ^{13}C NMR at levels: PCM/mPW1PW91/6-31+G**// B3LYP/6-31G* (OPTB_DP4+), B3LYP/6-31G*//B3LYP/6-31G* (OPTB_DP4), PCM/mPW1PW91/6-31+G**//MMFF (MMFF_DP4+), and B3LYP/6-31G*//MMFF (MMFF_DP4)*

System	**exo-2-Bromonorbornane**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.80	-13.87	-13.66	-14.35	-14.10
1.81	-12.57	-12.45	-13.06	-12.91
1.82	-11.24	-11.21	-11.75	-11.69
1.83	-9.88	-9.95	-10.41	-10.44
1.84	-8.49	-8.66	-9.04	-9.18
1.85	-7.07	-7.35	-7.64	-7.88
1.86	-5.63	-6.02	-6.22	-6.57
1.87	-4.16	-4.67	-4.77	-5.24
1.88	-2.67	-3.29	-3.30	-3.88
1.89	-1.15	-1.90	-1.80	-2.51
1.90	0.40	-0.49	-0.27	-1.11
1.91	1.97	0.95	1.28	0.30
1.92	3.56	2.40	2.85	1.74
1.93	5.18	3.87	4.45	3.19
1.94	6.82	5.36	6.07	4.66
1.95	8.49	6.86	7.72	6.14
1.96	10.17	8.38	9.38	7.64
1.97	11.88	9.92	11.07	9.16
1.98	13.61	11.47	12.78	10.69
1.99	15.36	13.03	14.50	12.23
2.00	17.12	14.61	16.25	13.79
2.01	18.91	16.19	18.02	15.36
2.02	20.71	17.80	19.80	16.94
2.03	22.54	19.41	21.60	18.53
2.04	24.38	21.03	23.42	20.13
2.05	26.23	22.66	25.26	21.75

System	Bromoethane			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.80	-8.1426	-8.4857	-6.4914	-6.7132
1.81	-7.0167	-7.4798	-5.3623	-5.6994
1.82	-5.8655	-6.4527	-4.2082	-4.6645
1.83	-4.6893	-5.4047	-3.0296	-3.6091
1.84	-3.4887	-4.3367	-1.8267	-2.5338
1.85	-2.2641	-3.2491	-0.6	-1.4391
1.86	-1.016	-2.1425	0.6498	-0.3256
1.87	0.2551	-1.0175	1.9224	0.8061
1.88	1.5487	0.1251	3.2175	1.9555
1.89	2.8646	1.2852	4.5345	3.1219
1.90	4.2021	2.4618	5.873	4.3049
1.91	5.5608	3.6544	7.2326	5.5039
1.92	6.9402	4.8626	8.6128	6.7183
1.93	8.3399	6.0855	10.0131	7.9475
1.94	9.7593	7.3228	11.4332	9.1910
1.95	11.1978	8.5738	12.8722	10.4482
1.96	12.655	9.8377	14.33	11.7184
1.97	14.1305	11.1142	15.8058	13.0012
1.98	15.6236	12.4026	17.2993	14.2958
1.99	17.1339	13.7023	18.8099	15.6019
2.00	18.6607	15.0128	20.337	16.9188
2.01	20.2036	16.3334	21.8803	18.2458
2.02	21.7621	17.6636	23.439	19.5825
2.03	23.3355	19.0027	25.0128	20.9282
2.04	24.9233	20.3501	26.6014	22.2826
2.05	26.5252	21.7055	28.2038	23.6448

System	Bromociclohexane			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.80	-17.8939	-13.3688	-18.8958	-18.9903
1.81	-16.4609	-12.0371	-17.4994	-17.6937
1.82	-15.0009	-10.6826	-16.0764	-16.3747
1.83	-13.5144	-9.3058	-14.6272	-15.0339
1.84	-12.0023	-7.9076	-13.1525	-13.6717
1.85	-10.4648	-6.4885	-11.6526	-12.289
1.86	-8.9023	-5.049	-10.128	-10.8861
1.87	-7.3158	-3.59	-8.5793	-9.4639
1.88	-5.7054	-2.1121	-7.0069	-8.023
1.89	-4.0716	-0.6156	-5.4114	-6.5639
1.90	-2.4152	0.8983	-3.7932	-5.0873
1.91	-0.7366	2.4292	-2.1529	-3.5939
1.92	0.9639	3.9767	-0.4909	-2.0842
1.93	2.6853	5.5398	1.1922	-0.5588

1.94	4.4275	7.118	2.896	0.9816
1.95	6.1895	8.7105	4.6196	2.5363
1.96	7.9709	10.3167	6.3626	4.1046
1.97	9.7711	11.9359	8.1245	5.686
1.98	11.5896	13.5677	9.9045	7.2798
1.99	13.4254	15.2109	11.7023	8.8853
2.00	15.2784	16.8654	13.5171	10.5018
2.01	17.1476	18.53	15.3486	12.129
2.02	19.0326	20.2042	17.1958	13.7657
2.03	20.9328	21.8876	19.0585	15.4116
2.04	22.8475	23.5792	20.9359	17.0659
2.05	24.7762	25.2785	22.8276	18.7282

System	**1-Bromopropene**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.80	6.7128	6.9379	8.1819	8.5577
1.81	7.3147	7.6227	8.7864	9.2479
1.82	7.9361	8.3239	9.4103	9.9546
1.83	8.5767	9.0411	10.0536	10.6774
1.84	9.2365	9.7743	10.716	11.4162
1.85	9.9154	10.5232	11.3975	12.1708
1.86	10.6133	11.2877	12.0981	12.941
1.87	11.3302	12.0676	12.8178	13.7268
1.88	12.0659	12.8625	13.5565	14.5278
1.89	12.8205	13.6725	14.3142	15.3439
1.90	13.5938	14.4972	15.091	16.175
1.91	14.3859	15.3365	15.8868	17.0208
1.92	15.1965	16.1901	16.7015	17.8813
1.93	16.0258	17.058	17.5351	18.7561
1.94	16.8734	17.9397	18.3873	19.6451
1.95	17.7395	18.8353	19.2582	20.5482
1.96	18.6238	19.7443	20.1476	21.4651
1.97	19.5261	20.6667	21.0553	22.3956
1.98	20.4462	21.602	21.9813	23.3395
1.99	21.3842	22.5504	22.9253	24.2966
2.00	22.3397	23.5112	23.8874	25.2667

System	**Bromobenzene**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.80	6.3191	5.1059	6.366	5.2015
1.81	7.0123	5.8891	7.0578	5.9828
1.82	7.7239	6.6886	7.7678	6.7802
1.83	8.4538	7.504	8.4959	7.5933
1.84	9.2018	8.3351	9.2422	8.4221
1.85	9.9679	9.1816	10.0063	9.2662
1.86	10.7519	10.0434	10.7882	10.1254

1.87	11.5537	10.9201	11.5878	10.9995
1.88	12.3732	11.8115	12.4051	11.8883
1.89	13.2103	12.7173	13.2398	12.7914
1.90	14.0648	13.6374	14.0919	13.7087
1.91	14.9368	14.5714	14.9613	14.6399
1.92	15.8259	15.5192	15.8478	15.5848
1.93	16.7322	16.4804	16.7514	16.5432
1.94	17.6554	17.4548	17.672	17.5148
1.95	18.5955	18.4422	18.6093	18.4995
1.96	19.5523	19.4423	19.5633	19.4968
1.97	20.5255	20.4548	20.5339	20.5066
1.98	21.5151	21.4795	21.5208	21.5286
1.99	22.5209	22.5161	22.5239	22.5626
2.00	23.5428	23.5642	23.5431	23.6083

System	**3-Bromotoluene**			
Bond distance (Å)	OPTB_DP4+	OPTB_DP4	MMFF_DP4+	MMFF_DP4
1.80	2.682	2.1985	2.2934	1.9245
1.81	3.3919	2.9851	3.0013	2.708
1.82	4.1205	3.7885	3.7279	3.5082
1.83	4.8678	4.6084	4.4731	4.3248
1.84	5.6337	5.4446	5.2368	5.1577
1.85	6.418	6.2968	6.019	6.0066
1.86	7.2207	7.1647	6.8195	6.8712
1.87	8.0417	8.0483	7.6383	7.7514
1.88	8.8809	8.9471	8.4752	8.6469
1.89	9.7381	9.8611	9.3302	9.5575
1.90	10.6133	10.79	10.2031	10.483
1.91	11.5064	11.7335	11.0939	11.4232
1.92	12.4173	12.6914	12.0025	12.3777
1.93	13.3459	13.6635	12.9288	13.3465
1.94	14.2922	14.6496	13.8728	14.3293
1.95	15.2559	15.6493	14.8343	15.3259
1.96	16.2371	16.6625	15.8133	16.3359
1.97	17.2356	17.689	16.8096	17.3593
1.98	18.2512	18.7283	17.8231	18.3957
1.99	19.2839	19.7804	18.8539	19.4448
2.00	20.3337	20.845	19.9016	20.5065

Table S5.6 *–Results obtained by removing conflicting signals. Strategy A: Removing bromine attached nucleus. Strategy B: Removing bromine and chlorine attached signals. Strategy C: Removing carbon atoms attached to bromine and chlorine*

Strategy A

	DP4			MM-DP4+			DP4+		
	H data	**C data**	**All**	**H data**	**C data**	**All**	**H data**	**C data**	**All**
1	89.6	88.2	99.9	66.6	99.8	100.0	89.5	100.0	100.0
2a	94.1	95.5	99.8	15.2	100.0	100.0	96.9	0.0	0.3
2b	95.6	95.8	99.8	12.9	100.0	100.0	99.5	0.7	58.4
3	0.6	2.8	0.1	3.8	1.8	25.5	1.3	84.4	69.4

Strategy B

	DP4			MM-DP4+			DP4+		
	H data	**C data**	**All**	**H data**	**C data**	**All**	**H data**	**C data**	**All**
1	81.7	85.2	99.6	74.5	99.8	100.0	89.5	100.0	100.0
2a	25.5	37.0	30.6	2.7	28.7	17.1	4.2	37.2	48.1
2b	51.4	40.1	66.9	6.6	72.6	89.1	13.8	72.6	89.4
3	0.6	3.3	0.2	3.8	0.7	2.9	1.3	28.3	68.3

Strategy C

	DP4			MM-DP4+			DP4+		
	H data	**C data**	**All**	**H data**	**C data**	**All**	**H data**	**C data**	**All**
1	92.6	85.2	100.0	65.0	99.8	100.0	96.1	100.0	100.0
2a	94.9	37.0	97.0	84.5	28.7	99.8	99.8	37.2	100.0
2b	93.1	40.1	96.3	91.5	72.6	100.0	99.8	72.6	100.0
3	0.4	3.3	0.1	1.4	0.7	0.4	10.6	28.3	11.2

Table S5.7 *– Dependence of diamagnetic (σ^D), paramagnetic (σ^P), and spin-orbit (σ^{SO}) contributions of the isotropic shielding values of the Cα with the bond distance, computed for* ***4*** *and* ***5*** *at the ZORA/mPW1PW/TZP//B3LYP/6-31G* level of theory.*

Compound	*C-X distance (Å)*	σ^D	σ^P	σ^{SO}	σ
4	1.85	-125.355	236.705	236.654	2.969
4	1.90	-134.412	236.927	236.875	2.996
4	1.95	-143.791	237.071	237.018	3.028
4	2.00	-153.415	237.153	237.101	3.066
5	1.90	-104.497	234.703	234.944	10.073
5	1.95	-112.359	234.765	234.976	10.075
5	2.00	-121.139	234.876	235.057	10.076
5	2.05	-129.637	235.007	235.165	10.081

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

1a_C001

MMFF Geometry

C	-1.411469	-0.551993	-0.419796
C	-3.042312	1.438797	-0.195702
C	-0.156313	0.424780	-0.013521
C	-2.695685	0.019135	0.257662
H	-3.597241	1.435309	-1.141897
H	-2.602490	-0.016269	1.349653
C	-1.841338	2.303534	-0.379545
H	-2.077964	3.343087	-0.603036
C	-0.553539	1.903533	-0.326929
O	-3.866884	2.080982	0.775707
H	-4.668655	1.535044	0.864068
Br	-4.310976	-1.093444	-0.032093
C	-1.200608	-2.018709	0.057696
H	-1.893478	-2.705537	-0.442071
H	-1.373333	-2.129375	1.133121
H	-0.199914	-2.398492	-0.157003
C	-1.565617	-0.608948	-1.967481
H	-2.453621	-1.173252	-2.269161
H	-0.713561	-1.115819	-2.433333
H	-1.643093	0.382730	-2.421892
C	0.492790	2.954255	-0.607522
H	0.050662	3.940737	-0.791167
H	1.062504	2.704859	-1.507144
H	1.172478	3.081160	0.235697
C	0.108132	0.322919	1.526016
H	-0.648601	0.893153	2.080631
H	-0.011022	-0.708773	1.865223
C	1.121101	-0.008823	-0.813098
H	1.042463	0.351749	-1.848186
H	1.148402	-1.098316	-0.903655
C	1.483092	0.783260	2.016960
H	1.545653	1.874613	1.952286
H	1.559625	0.556167	3.089286
C	2.477223	0.433342	-0.241548
H	2.635912	1.498975	-0.421852
C	2.660133	0.142198	1.258218
Cl	2.660962	-1.633550	1.600550
C	3.971370	0.722522	1.810927
H	4.855115	0.240102	1.381073
H	4.032852	0.596491	2.898461

H	4.043771	1.796016	1.602250
Br	3.892419	-0.372862	-1.359346

SCF Energy (SMD/wB97XD/6-31+G) = -6264.267312**
SCF Energy (B3LYP/6-31G) = -6264.30343407**

1a_C002

MMFF Geometry

C	-1.423275	-0.573731	-0.398244
C	-3.047174	1.437529	-0.234541
C	-0.165107	0.419473	-0.045591
C	-2.708323	0.026245	0.258128
H	-3.642271	1.400912	-1.154540
H	-2.613735	0.021802	1.350580
C	-1.844132	2.280212	-0.504292
H	-2.080904	3.299713	-0.808499
C	-0.558057	1.878090	-0.444207
O	-3.827771	2.132939	0.738131
H	-3.264428	2.282253	1.516268
Br	-4.318041	-1.102574	0.004116
C	-1.209405	-2.016339	0.148683
H	-1.908983	-2.725578	-0.308487
H	-1.369432	-2.073188	1.230197
H	-0.212872	-2.410408	-0.058458
C	-1.583665	-0.704342	-1.940869
H	-2.463782	-1.295583	-2.212375
H	-0.726442	-1.219692	-2.387359
H	-1.679229	0.263935	-2.439969
C	0.489320	2.899343	-0.816481
H	0.048942	3.871970	-1.066300
H	1.046520	2.581873	-1.702307
H	1.179849	3.083960	0.007419
C	0.096656	0.406713	1.496932
H	-0.663157	1.004525	2.017258
H	-0.018565	-0.604646	1.894078
C	1.113868	-0.063790	-0.815221
H	1.037360	0.231544	-1.870838
H	1.141355	-1.156488	-0.838334
C	1.469286	0.902965	1.959023
H	1.528288	1.987966	1.821627
H	1.544683	0.747109	3.044028
C	2.469991	0.411466	-0.270278
H	2.630577	1.463170	-0.517924
C	2.649593	0.216670	1.245459
Cl	2.651568	-1.533109	1.700796
C	3.958584	0.833251	1.762973
H	4.844027	0.326238	1.366179
H	4.017999	0.776429	2.856420
H	4.029552	1.891522	1.486930
Br	3.886360	-0.465213	-1.331344

SCF Energy (SMD/wB97XD/6-31+G) = -6264.265277**
SCF Energy (B3LYP/6-31G) = --6264.29822701**

1a_C003

MMFF Geometry

C	-1.418844	-0.574649	-0.398621
C	-3.046214	1.430678	-0.189917
C	-0.162739	0.415835	-0.036800
C	-2.700923	0.012363	0.274593
H	-3.660169	1.407600	-1.098681
H	-2.606192	-0.015293	1.366764
C	-1.847257	2.279891	-0.460919
H	-2.076672	3.305958	-0.743255
C	-0.559943	1.877719	-0.419321
O	-3.802470	2.088359	0.826731
H	-4.195573	2.882098	0.427327
Br	-4.313500	-1.113509	-0.006913
C	-1.200027	-2.025098	0.125251
H	-1.902632	-2.727941	-0.337086
H	-1.352039	-2.098364	1.206904
H	-0.205049	-2.415695	-0.095326
C	-1.585637	-0.681938	-1.942429
H	-2.461484	-1.276785	-2.219675
H	-0.726143	-1.182556	-2.401102
H	-1.692397	0.293216	-2.425585
C	0.485018	2.904747	-0.781547
H	0.042956	3.879559	-1.019524
H	1.040890	2.598564	-1.672169
H	1.176767	3.080894	0.043205
C	0.101516	0.384817	1.505211
H	-0.659053	0.974045	2.034076
H	-0.010236	-0.631817	1.889757
C	1.116415	-0.055193	-0.813550
H	1.037885	0.251905	-1.865641
H	1.147272	-1.147399	-0.849148
C	1.473075	0.879031	1.971894
H	1.528603	1.965867	1.847853
H	1.550349	0.709835	3.054756
C	2.471616	0.417949	-0.264556
H	2.628662	1.473023	-0.499615
C	2.654271	0.205360	1.248341
Cl	2.664595	-1.550160	1.681454
C	3.961990	0.820399	1.771061

H	4.848579	0.321664	1.366406
H	4.023641	0.750265	2.863613
H	4.028547	1.882264	1.508013
Br	3.889535	-0.440392	-1.339160

SCF Energy (SMD/wB97XD/6-31+G) = -6264.264476**

SCF Energy (B3LYP/6-31G) = -6264.29725926**

C	4.091677	1.185954	-0.342560
H	4.719346	0.289032	-0.349359
H	4.623255	1.945722	0.242782
H	4.026217	1.554107	-1.372785
Br	2.686867	-1.798917	-0.871313

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258552**

SCF Energy (B3LYP/6-31G) = -6264.29410042**

1a_C004

MMFF Geometry

C	-1.720293	0.770091	1.009501
C	-3.073912	0.221229	-1.163194
C	-0.411044	1.067490	0.087315
C	-2.766293	-0.150280	0.296073
H	-3.181683	-0.662020	-1.803004
H	-3.700523	-0.123893	0.873468
C	-2.087476	1.133318	-1.814468
H	-2.405727	1.494011	-2.792130
C	-0.911283	1.551562	-1.303751
O	-4.330839	0.905517	-1.221147
H	-5.022077	0.248045	-1.031032
Br	-2.366147	-2.082087	0.386247
C	-2.467096	2.115669	1.313357
H	-3.399036	1.929379	1.861200
H	-2.731631	2.670688	0.409136
H	-1.866988	2.781081	1.942968
C	-1.385729	0.200960	2.418758
H	-2.307127	-0.058760	2.955260
H	-0.866009	0.929119	3.048832
H	-0.767593	-0.698056	2.393613
C	-0.118744	2.537271	-2.125910
H	-0.625573	2.796028	-3.063144
H	0.853854	2.132347	-2.409227
H	0.016711	3.477806	-1.584602
C	0.486072	2.134111	0.806312
H	0.026587	3.127575	0.729969
H	0.526423	1.919199	1.877634
C	0.425542	-0.230915	-0.148813
H	-0.086859	-0.873118	-0.875714
H	0.480834	-0.814247	0.773862
C	1.946591	2.259231	0.349915
H	1.993033	2.783803	-0.608978
H	2.469547	2.922387	1.053239
C	1.857878	-0.020438	-0.652942
H	1.837320	0.354578	-1.680461
C	2.693080	0.918663	0.235342
Cl	2.909142	0.253098	1.903845

1a_C005

MMFF Geometry

C	-1.71247	0.71572	1.03378
C	-3.19127	0.23092	-1.05901
C	-0.43726	1.03078	0.06544
C	-2.78060	-0.20440	0.35400
H	-3.44047	-0.63121	-1.68774
H	-3.67593	-0.22751	0.99034
C	-2.19056	1.07597	-1.78116
H	-2.51571	1.40609	-2.76658
C	-0.98287	1.47088	-1.32696
O	-4.39230	1.00571	-0.95941
H	-4.68799	1.20328	-1.86379
Br	-2.31995	-2.12323	0.32245
C	-2.45066	2.05588	1.38023
H	-3.38272	1.86013	1.92428
H	-2.70928	2.64055	0.49305
H	-1.84490	2.69834	2.02840
C	-1.32570	0.12989	2.42301
H	-2.22759	-0.09135	3.00785
H	-0.73904	0.83165	3.02287
H	-0.75356	-0.79758	2.36688
C	-0.18823	2.39464	-2.21836
H	-0.70510	2.60563	-3.16208
H	0.77466	1.96303	-2.49246
H	-0.03330	3.36315	-1.73457
C	0.43668	2.14922	0.73450
H	-0.05020	3.12608	0.61859
H	0.48586	1.98235	1.81405
C	0.43700	-0.24610	-0.15957
H	-0.05558	-0.90479	-0.88514
H	0.50353	-0.82180	0.76659
C	1.89116	2.29559	0.26713
H	1.92012	2.77999	-0.71356
H	2.39771	3.00122	0.94043
C	1.86824	-0.01414	-0.65751
H	1.84885	0.32605	-1.69656
C	2.67312	0.97253	0.20528

Cl	2.89268	0.36770	1.89542
C	4.06888	1.25653	-0.37170
H	4.71916	0.37625	-0.34474
H	4.57660	2.04832	0.19200
H	4.00207	1.58912	-1.41386
Br	2.74460	-1.77697	-0.81632

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256829**

SCF Energy (B3LYP/6-31G) = -6264.29262637**

C	2.693080	0.918663	0.235342
Cl	2.909142	0.253098	1.903845
C	4.091677	1.185954	-0.342560
H	4.719346	0.289032	-0.349359
H	4.623255	1.945722	0.242782
H	4.026217	1.554107	-1.372785
Br	2.686867	-1.798917	-0.871313

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258938**

SCF Energy (B3LYP/6-31G) = -6264.29458446**

1a_C006

MMFF Geometry

C	-1.720293	0.770091	1.009501
C	-3.073912	0.221229	-1.163194
C	-0.411044	1.067490	0.087315
C	-2.766293	-0.150280	0.296073
H	-3.181683	-0.662020	-1.803004
H	-3.700523	-0.123893	0.873468
C	-2.087476	1.133318	-1.814468
H	-2.405727	1.494011	-2.792130
C	-0.911283	1.551562	-1.303751
O	-4.330839	0.905517	-1.221147
H	-5.022077	0.248045	-1.031032
Br	-2.366147	-2.082087	0.386247
C	-2.467096	2.115669	1.313357
H	-3.399036	1.929379	1.861200
H	-2.731631	2.670688	0.409136
H	-1.866988	2.781081	1.942968
C	-1.385729	0.200960	2.418758
H	-2.307127	-0.058760	2.955260
H	-0.866009	0.929119	3.048832
H	-0.767593	-0.698056	2.393613
C	-0.118744	2.537271	-2.125910
H	-0.625573	2.796028	-3.063144
H	0.853854	2.132347	-2.409227
H	0.016711	3.477806	-1.584602
C	0.486072	2.134111	0.806312
H	0.026587	3.127575	0.729969
H	0.526423	1.919199	1.877634
C	0.425542	-0.230915	-0.148813
H	-0.086859	-0.873118	-0.875714
H	0.480834	-0.814247	0.773862
C	1.946591	2.259231	0.349915
H	1.993033	2.783803	-0.608978
H	2.469547	2.922387	1.053239
C	1.857878	-0.020438	-0.652942
H	1.837320	0.354578	-1.680461

1a_C007

MMFF Geometry

C	-1.399319	0.731199	1.016352
C	-3.087517	0.207723	-1.137410
C	-0.179224	1.048085	0.079648
C	-2.722776	-0.189687	0.307575
H	-3.572633	-0.672298	-1.773284
H	-2.675661	-0.187199	0.902657
C	-1.902579	1.105110	-1.808576
H	-2.149876	1.440293	-2.796828
C	-0.612462	1.523113	-1.310548
O	-4.000049	0.892548	-1.153388
H	-4.788075	1.810621	-0.874676
Br	-4.300396	-2.115973	0.351285
C	-1.162414	2.071986	1.349446
H	-1.864813	1.877645	1.862941
H	-1.291768	2.666861	0.460785
H	-0.166662	2.706446	2.020080
C	-1.514689	0.145936	2.414646
H	-2.389897	-0.104608	2.967093
H	-0.650320	0.860154	3.039681
H	-1.588650	-0.762305	2.371676
C	0.433330	2.488672	-2.155319
H	-0.012946	2.731013	-3.095841
H	1.112580	2.075869	-2.433764
H	1.010704	3.439156	-1.632760
C	0.157321	2.135254	0.787121
H	0.525858	3.120950	0.699585
H	-0.746032	1.933689	1.860968
C	1.108246	-0.237054	-0.158781
H	1.094136	-0.882813	-0.890835
H	1.117990	-0.823355	0.761495
C	1.213940	2.277018	0.330436
H	1.373195	2.790590	-0.634758
H	0.791725	2.955937	1.026604
C	2.406564	-0.010182	-0.654025

H	2.442275	0.356515	-1.684345
C	2.564982	0.946395	0.232500
Cl	3.093506	0.297509	1.907445
C	3.626928	1.228668	-0.338170
H	4.611530	0.340582	-0.333647
H	3.739652	2.000313	0.244684
H	3.348757	1.587843	-1.371677
Br	3.916331	-1.778123	-0.854847

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259884**
SCF Energy (B3LYP/6-31G) = -6264.29675105**

1a_C008

MMFF Geometry

C	-1.403649	-0.390999	-0.482641
C	-3.097012	1.445909	0.196886
C	-0.184740	0.465095	0.182694
C	-2.727640	-0.038779	0.271466
H	-3.635403	1.675381	-0.730709
H	-2.679847	-0.363542	1.316617
C	-1.911897	2.348505	0.295214
H	-2.151566	3.407607	0.371722
C	-0.620005	1.963302	0.293990
O	-3.955916	1.771342	1.290379
H	-4.376335	2.622632	1.083276
Br	-4.296503	-1.071939	-0.379723
C	-1.156265	-1.917602	-0.385177
H	-1.855719	-2.483562	-1.010284
H	-1.282235	-2.279355	0.640223
H	-0.159564	-2.203265	-0.729766
C	-1.528999	-0.049937	-1.998813
H	-2.389825	-0.543118	-2.460597
H	-0.654988	-0.390706	-2.563414
H	-1.634366	1.023439	-2.180705
C	0.426326	3.046493	0.443283
H	-0.020595	4.044329	0.522899
H	1.094306	3.076820	-0.421558
H	1.015392	2.899325	1.352393
C	0.152432	0.010548	1.648104
H	0.523383	0.860367	2.236448
H	-0.750677	-0.312957	2.175054
C	1.103893	0.332397	-0.704879
H	1.090365	1.093732	-1.495838
H	1.115111	-0.620776	-1.242797
C	1.207314	-1.095881	1.774271
H	1.365179	-1.294738	2.842744
H	0.784702	-2.026638	1.386893
C	2.401459	0.411187	0.104584

H	2.435970	1.348087	0.665854
C	2.559315	-0.771842	1.086490
Cl	3.090720	-2.293157	0.253007
C	3.619280	-0.448959	2.152637
H	4.604398	-0.265626	1.710869
H	3.731655	-1.272195	2.868090
H	3.339394	0.444010	2.723179
Br	3.912431	0.629569	-1.133231

SCF Energy (SMD/wB97XD/6-31+G) = -6264.257043**
SCF Energy (B3LYP/6-31G) = -6264.29042194**

1a_C009

MMFF Geometry

C	-1.407949	-0.383649	-0.489082
C	-3.096645	1.463433	0.172736
C	-0.187156	0.469347	0.179745
C	-2.734646	-0.023648	0.256947
H	-3.615908	1.694845	-0.764394
H	-2.686825	-0.339023	1.304912
C	-1.907836	2.359526	0.280082
H	-2.153797	3.419471	0.341713
C	-0.618179	1.968770	0.292622
O	-3.978530	1.822793	1.237556
H	-3.485605	1.738783	2.071202
Br	-4.301465	-1.059854	-0.379901
C	-1.166063	-1.910785	-0.386933
H	-1.864942	-2.475951	-1.013414
H	-1.296740	-2.269560	0.638924
H	-0.168987	-2.200238	-0.727340
C	-1.526409	-0.046288	-2.006537
H	-2.392273	-0.531139	-2.467830
H	-0.655199	-0.398767	-2.568300
H	-1.619046	1.027638	-2.192123
C	0.430573	3.049605	0.443121
H	-0.014435	4.048366	0.522004
H	1.100230	3.077976	-0.420478
H	1.017644	2.901103	1.353328
C	0.146345	0.013052	1.645223
H	0.517978	0.861689	2.234864
H	-0.758664	-0.308802	2.170041
C	1.102205	0.333403	-0.706344
H	1.091646	1.095109	-1.496988
H	1.111055	-0.619672	-1.244521
C	1.198839	-1.095503	1.773132
H	1.355614	-1.293278	2.841979
H	0.773893	-2.025789	1.387074

C	2.399344	0.407827	0.104207
H	2.435963	1.344324	0.666079
C	2.552434	-0.776258	1.085637
Cl	3.077396	-2.299357	0.251977
C	3.613358	-0.458113	2.152246
H	4.599421	-0.278832	1.710933
H	3.722005	-1.281994	2.867536
H	3.336995	0.435879	2.722904
Br	3.912127	0.621576	-1.131613

SCF Energy (SMD/wB97XD/6-31+G) = -6264.257843**
SCF Energy (B3LYP/6-31G) = -6264.291669**

H	1.573963	1.752457	2.518531
C	2.421319	0.057946	-0.373272
H	2.622454	0.907518	-1.030006
C	2.612417	0.476758	1.094650
Cl	4.169256	1.384400	1.280961
C	2.647585	-0.696264	2.088732
H	1.774447	-1.347567	1.988944
H	2.664292	-0.333392	3.123466
H	3.536733	-1.322303	1.959662
Br	3.771107	-1.253087	-0.976180

SCF Energy (SMD/wB97XD/6-31+G) = -6264.267337**
SCF Energy (B3LYP/6-31G) = -6264.30200231**

1b_C001

MMFF Geometry

C	-1.513234	-0.715304	-0.088626
C	-3.049661	1.240560	-0.791003
C	-0.207315	0.276376	-0.169011
C	-2.756599	0.163357	0.255067
H	-3.627674	0.838673	-1.632234
H	-2.641937	0.620088	1.245304
C	-1.815590	1.864366	-1.348814
H	-2.010336	2.698436	-2.022065
C	-0.545988	1.466834	-1.122110
O	-3.819183	2.293654	-0.213174
H	-4.649762	1.892657	0.099650
Br	-4.425177	-0.879316	0.498950
C	-1.358071	-1.814761	1.002253
H	-2.099706	-2.611879	0.875516
H	-1.499088	-1.414745	2.011492
H	-0.385532	-2.309655	0.974577
C	-1.702847	-1.460027	-1.441929
H	-2.619690	-2.057740	-1.454385
H	-0.882580	-2.161985	-1.627292
H	-1.749089	-0.779604	-2.296783
C	0.537820	2.216331	-1.859165
H	0.133891	3.027452	-2.476684
H	1.072484	1.551923	-2.543875
H	1.244360	2.684135	-1.173151
C	0.086942	0.869597	1.249998
H	-0.642531	1.652530	1.494493
H	-0.045048	0.104098	2.018579
C	1.035309	-0.534493	-0.678016
H	0.950592	-0.688892	-1.762658
H	1.016186	-1.542209	-0.253850
C	1.483672	1.455957	1.464474
H	1.577590	2.386675	0.895507

1b_C002

MMFF Geometry

C	-1.520657	-0.721269	-0.084925
C	-3.049583	1.268736	-0.737164
C	-0.213605	0.265497	-0.173266
C	-2.761253	0.157708	0.277313
H	-3.688900	0.902466	-1.549765
H	-2.646712	0.583504	1.281384
C	-1.818890	1.857924	-1.345598
H	-2.006297	2.676516	-2.038563
C	-0.551181	1.443516	-1.141057
O	-3.745721	2.330519	-0.084794
H	-4.074279	2.930117	-0.775263
Br	-4.429188	-0.900091	0.491208
C	-1.358448	-1.825232	1.001548
H	-2.110747	-2.613991	0.886686
H	-1.477003	-1.425816	2.013809
H	-0.393347	-2.332788	0.956747
C	-1.723050	-1.460283	-1.439584
H	-2.627835	-2.076083	-1.439265
H	-0.894123	-2.145939	-1.645649
H	-1.800008	-0.775258	-2.288437
C	0.530362	2.158640	-1.914895
H	0.126700	2.956272	-2.549872
H	1.049072	1.469829	-2.587542
H	1.250242	2.638130	-1.250616
C	0.079342	0.875591	1.238168
H	-0.653833	1.657122	1.475920
H	-0.046509	0.117383	2.015122
C	1.030794	-0.552007	-0.669375
H	0.946902	-0.724787	-1.751183
H	1.014565	-1.552485	-0.229307
C	1.472949	1.473805	1.438748

H	1.560626	2.392815	0.849565
H	1.563546	1.791901	2.486403
C	2.416041	0.047216	-0.373877
H	2.616671	0.885013	-1.045624
C	2.605654	0.492621	1.086349
Cl	4.158734	1.410157	1.255302
C	2.645947	-0.662663	2.100759
H	1.776769	-1.320822	2.010709
H	2.658865	-0.281726	3.129021
H	3.538944	-1.285644	1.983954
Br	3.768544	-1.271376	-0.953462

SCF Energy (SMD/wB97XD/6-31+G) = -6264.264626**
SCF Energy (B3LYP/6-31G) = -6264.29607249**

C	1.469668	1.495622	1.413548
H	1.560341	2.405209	0.810421
H	1.558923	1.829969	2.456264
C	2.413723	0.038053	-0.374371
H	2.616968	0.864451	-1.059341
C	2.601562	0.506940	1.078787
Cl	4.154864	1.425511	1.235980
C	2.638261	-0.631542	2.112138
H	1.768181	-1.289681	2.031376
H	2.649944	-0.233792	3.134032
H	3.530492	-1.257726	2.007244
Br	3.764372	-1.292463	-0.929123

SCF Energy (SMD/wB97XD/6-31+G) = -6264.265441**
SCF Energy (B3LYP/6-31G) = -6264.29704547**

1b_C003

MMFF Geometry

C	-1.525431	-0.719609	-0.078914
C	-3.051788	1.249821	-0.791250
C	-0.216215	0.264858	-0.181695
C	-2.768963	0.166799	0.255560
H	-3.669971	0.856683	-1.606816
H	-2.654234	0.622603	1.246249
C	-1.816544	1.831319	-1.396161
H	-2.011534	2.631372	-2.110402
C	-0.549608	1.427960	-1.169043
O	-3.775639	2.331679	-0.204647
H	-3.173094	2.797701	0.399567
Br	-4.433363	-0.881447	0.503267
C	-1.368519	-1.799621	1.032035
H	-2.116398	-2.593980	0.927100
H	-1.497827	-1.379115	2.034444
H	-0.400600	-2.303232	1.006629
C	-1.721139	-1.488122	-1.418032
H	-2.630950	-2.096492	-1.411678
H	-0.895570	-2.184434	-1.600683
H	-1.784723	-0.822206	-2.283060
C	0.534724	2.131583	-1.949910
H	0.132975	2.919553	-2.598059
H	1.055991	1.432670	-2.610043
H	1.252169	2.621254	-1.290486
C	0.075020	0.897532	1.219877
H	-0.657157	1.684350	1.442909
H	-0.053817	0.152759	2.009200
C	1.027563	-0.563045	-0.662159
H	0.944957	-0.753247	-1.741164
H	1.008170	-1.556214	-0.205700

1b_C004

MMFF Geometry

C	-1.474702	-0.437817	-0.519655
C	-3.050328	1.479019	0.197760
C	-0.186615	0.356563	0.100758
C	-2.745647	-0.017732	0.286166
H	-3.565712	1.736673	-0.735325
H	-2.663125	-0.323236	1.334963
C	-1.821989	2.316398	0.294558
H	-2.018131	3.382071	0.406377
C	-0.550471	1.869576	0.253745
O	-3.900594	1.872954	1.274244
H	-4.715910	1.346580	1.191902
Br	-4.394225	-0.975086	-0.264407
C	-1.303735	-1.975571	-0.437493
H	-2.074279	-2.501858	-1.011451
H	-1.374434	-2.333897	0.594410
H	-0.351432	-2.311885	-0.855193
C	-1.642553	-0.086979	-2.028889
H	-2.555613	-0.518836	-2.450251
H	-0.818715	-0.486865	-2.629425
H	-1.680025	0.991394	-2.208103
C	0.545031	2.902454	0.398708
H	0.145118	3.915372	0.524716
H	1.179609	2.930759	-0.491344
H	1.159272	2.702494	1.280692
C	0.196409	-0.145505	1.538920
H	0.600760	0.676334	2.143635
H	-0.690861	-0.480719	2.084807
C	1.053294	0.172185	-0.847411
H	1.013610	0.918386	-1.652240
H	1.013734	-0.795970	-1.357664

C	1.234180	-1.272072	1.565057
H	1.381823	-1.594417	2.604388
H	0.817341	-2.149695	1.063862
C	2.401542	0.238269	-0.119320
H	2.498633	1.206151	0.376184
C	2.587794	-0.900317	0.910352
Cl	3.693309	-0.294160	2.216136
C	3.210164	-2.196696	0.364161
H	2.647471	-2.571194	-0.498301
H	3.202911	-2.986432	1.125690
H	4.254066	-2.069255	0.059496
Br	3.831315	0.332929	-1.464581

SCF Energy (SMD/wB97XD/6-31+G) = -6264.261829**
SCF Energy (B3LYP/6-31G) = -6264.29840831**

H	-0.327602	0.898200	0.866866
C	-1.958500	-2.112312	0.605676
H	-2.079743	-2.646248	-0.341387
H	-2.470023	-2.740148	1.348449
C	-1.826461	0.138633	-0.449482
H	-1.888814	-0.257139	-1.467601
C	-2.636897	-0.734582	0.523635
Cl	-4.303667	-1.013392	-0.129508
C	-2.793534	-0.141246	1.934327
H	-1.828526	0.088791	2.395710
H	-3.307066	-0.844900	2.600716
H	-3.384223	0.780602	1.932875
Br	-2.576520	1.955194	-0.644700

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258315**
SCF Energy (B3LYP/6-31G) = -6264.29299537**

1b_C005

MMFF Geometry

C	1.804310	-0.787058	1.023011
C	3.062540	-0.361178	-1.232340
C	0.432174	-1.041823	0.182323
C	2.851406	0.063897	0.229096
H	3.183761	0.498065	-1.901776
H	3.813311	0.009104	0.756942
C	1.995886	-1.234513	-1.805128
H	2.239316	-1.631949	-2.790126
C	0.830026	-1.579677	-1.221175
O	4.276118	-1.114838	-1.332621
H	5.011306	-0.488132	-1.218968
Br	2.542690	2.013497	0.285069
C	2.501891	-2.160079	1.321209
H	3.472254	-2.006681	1.809266
H	2.685620	-2.750397	0.419327
H	1.908305	-2.778651	2.002659
C	1.577169	-0.168711	2.432921
H	2.538649	0.057014	2.911314
H	1.058268	-0.854725	3.109264
H	1.003278	0.759385	2.417925
C	-0.057725	-2.537200	-1.977415
H	0.382304	-2.840856	-2.934711
H	-1.021675	-2.085960	-2.216787
H	-0.211897	-3.458534	-1.408773
C	-0.471374	-2.047705	0.978229
H	-0.063314	-3.063382	0.902680
H	-0.444532	-1.804536	2.043985
C	-0.356182	0.289552	-0.040421
H	0.140143	0.887271	-0.814944

1b_C006

MMFF Geometry

C	1.801289	-0.725210	1.052715
C	3.178191	-0.383420	-1.135569
C	0.457953	-1.008034	0.169941
C	2.870409	0.118687	0.281306
H	3.433070	0.443504	-1.807757
H	3.800968	0.119646	0.865374
C	2.097266	-1.199891	-1.769211
H	2.346903	-1.576390	-2.760151
C	0.900300	-1.518782	-1.233996
O	4.343467	-1.214391	-1.073494
H	4.570883	-1.466954	-1.984053
Br	2.496639	2.055038	0.207890
C	2.493851	-2.088334	1.403842
H	3.464733	-1.921377	1.886094
H	2.671267	-2.714140	0.524816
H	1.897451	-2.678127	2.108321
C	1.524846	-0.076439	2.440252
H	2.468921	0.120301	2.964083
H	0.943073	-0.729423	3.097269
H	0.993359	0.874925	2.384324
C	0.009924	-2.426538	-2.048640
H	-0.165843	-3.370205	-1.524551
H	0.460853	-2.693549	-3.011787
H	-0.943558	-1.953033	-2.283686
C	-0.428104	-2.058544	0.928640
H	0.005273	-3.061429	0.823778
H	-0.412181	-1.849547	2.001923
C	-0.367329	0.302526	-0.051254

H	0.110721	0.910515	-0.828996
H	-0.350200	0.912275	0.855072
C	-1.910698	-2.148569	0.546033
H	-2.014280	-2.654513	-0.418533
H	-2.409876	-2.811574	1.266287
C	-1.836968	0.126499	-0.452926
H	-1.899032	-0.245399	-1.479501
C	-2.621725	-0.786302	0.503390
Cl	-4.285084	-1.088902	-0.148021
C	-2.783287	-0.229735	1.928072
H	-1.821298	0.017365	2.386922
H	-3.271548	-0.962350	2.582075
H	-3.399275	0.675135	1.951766
Br	-2.630845	1.929342	-0.604185

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256731**
SCF Energy (B3LYP/6-31G) = -6264.29166748**

C	-0.357791	0.296440	-0.049333
H	0.127461	0.896313	-0.829119
H	-0.333452	0.909688	0.854737
C	-1.926583	-2.127829	0.592059
H	-2.041133	-2.654964	-0.359707
H	-2.429307	-2.768677	1.329715
C	-1.828790	0.129594	-0.450189
H	-1.892875	-0.260358	-1.470173
C	-2.623292	-0.758716	0.521981
Cl	-4.289006	-1.056499	-0.125007
C	-2.780500	-0.175044	1.936478
H	-3.385234	0.737644	1.943179
H	-1.816313	0.067703	2.393058
H	-3.279124	-0.889842	2.602304
Br	-2.603089	1.937362	-0.631755

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258687**
SCF Energy (B3LYP/6-31G) = -6264.29348712**

1b_C007

MMFF Geometry

C	1.812360	-0.747609	1.031056
C	3.109527	-0.356113	-1.207940
C	0.450707	-1.023013	0.177104
C	2.866238	0.100394	0.239006
H	3.269151	0.496349	-1.876688
H	3.819268	0.070968	0.784498
C	2.037485	-1.213708	-1.799274
H	2.277090	-1.587202	-2.795181
C	0.865784	-1.556429	-1.225898
O	4.326550	-1.110878	-1.262700
H	4.125985	-2.025719	-1.003113
Br	2.518646	2.045442	0.245586
C	2.506251	-2.114837	1.360982
H	3.491971	-1.955034	1.814413
H	2.651212	-2.743559	0.478809
H	1.925791	-2.700822	2.082008
C	1.566104	-0.108897	2.429409
H	2.521703	0.109108	2.923003
H	1.023454	-0.778061	3.103770
H	1.006867	0.827438	2.393721
C	-0.025866	-2.495384	-2.002037
H	0.416033	-2.785637	-2.962642
H	-0.986708	-2.036342	-2.237383
H	-0.186162	-3.425251	-1.449111
C	-0.440633	-2.046514	0.964762
H	-0.018886	-3.056139	0.880945
H	-0.416611	-1.812249	2.032598

1b_C008

MMFF Geometry

C	-1.484679	-0.471501	-0.493469
C	-3.056024	1.493094	0.119837
C	-0.194490	0.364204	0.064896
C	-2.757693	-0.000919	0.284951
H	-3.609175	1.689318	-0.805862
H	-2.675636	-0.251522	1.348189
C	-1.824372	2.335145	0.113742
H	-2.019084	3.407535	0.116171
C	-0.554245	1.885040	0.095812
O	-3.868582	1.959659	1.197998
H	-3.331761	1.928570	2.008125
Br	-4.398718	-0.997557	-0.215365
C	-1.310665	-2.000208	-0.303967
H	-2.079942	-2.567219	-0.839469
H	-1.380917	-2.284934	0.750685
H	-0.358204	-2.364844	-0.696305
C	-1.656489	-0.226400	-2.023091
H	-2.561078	-0.701343	-2.415229
H	-0.825418	-0.652122	-2.595116
H	-1.712885	0.836499	-2.274789
C	0.544189	2.924661	0.129508
H	0.146607	3.945640	0.166385
H	1.168526	2.869832	-0.766381
H	1.167725	2.805317	1.019638
C	0.185086	-0.021367	1.538657
H	0.591966	0.845903	2.074707

H	-0.703597	-0.308559	2.108928
C	1.046885	0.100031	-0.863748
H	1.010313	0.777869	-1.727014
H	1.006127	-0.905768	-1.294545
C	1.218875	-1.145745	1.655153
H	1.361534	-1.388461	2.716590
H	0.801928	-2.057792	1.219814
C	2.394661	0.221554	-0.141678
H	2.493639	1.227109	0.271564
C	2.576085	-0.827543	0.980020
Cl	3.670836	-0.111513	2.238570
C	3.203990	-2.163544	0.548241
H	2.647614	-2.609805	-0.283644
H	3.192694	-2.886985	1.372951
H	4.249752	-2.059711	0.240982
Br	3.826633	0.201126	-1.487070

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259869**
SCF Energy (B3LYP/6-31G) = -6264.29373224**

H	0.599189	0.821749	2.087818
H	-0.695305	-0.333984	2.112739
C	1.048622	0.114637	-0.859003
H	1.010069	0.805485	-1.711796
H	1.009861	-0.884303	-1.305525
C	1.226915	-1.164366	1.645957
H	1.374411	-1.415471	2.704761
H	0.808058	-2.073114	1.205602
C	2.396132	0.227946	-0.135558
H	2.492606	1.226329	0.295442
C	2.580857	-0.840318	0.967047
Cl	3.689089	-0.150820	2.228635
C	3.199935	-2.171243	0.507260
H	2.635485	-2.600846	-0.327924
H	3.192023	-2.908772	1.319439
H	4.243686	-2.066400	0.193617
Br	3.827548	0.234473	-1.482197

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258978**
SCF Energy (B3LYP/6-31G) = -6264.29224323**

1b_C009

MMFF Geometry

C	-1.479318	-0.470717	-0.491629
C	-3.057478	1.475658	0.162859
C	-0.192204	0.361888	0.074687
C	-2.750947	-0.018624	0.299396
H	-3.626827	1.683047	-0.751292
H	-2.669963	-0.291967	1.357169
C	-1.830055	2.324909	0.161073
H	-2.018076	3.396756	0.191217
C	-0.557702	1.880755	0.124220
O	-3.852181	1.894196	1.272921
H	-4.202521	2.775792	1.062540
Br	-4.392778	-1.008469	-0.229035
C	-1.298570	-2.001390	-0.325832
H	-2.066321	-2.563367	-0.868768
H	-1.366558	-2.302410	0.724441
H	-0.345067	-2.356249	-0.724486
C	-1.656836	-0.202499	-2.016879
H	-2.556729	-0.680674	-2.415699
H	-0.822583	-0.610009	-2.597419
H	-1.725219	0.863704	-2.251022
C	0.537906	2.922846	0.171057
H	0.137844	3.942248	0.221672
H	1.161475	2.881870	-0.726110
H	1.162912	2.793507	1.058722
C	0.191664	-0.039936	1.543316

1c_C001

MMFF Geometry

C	-1.596885	0.300492	0.825215
C	-2.747025	0.518585	-1.494378
C	-0.174077	0.798757	0.171260
C	-2.424786	-0.392451	-0.304674
H	-3.000541	-0.091938	-2.368951
H	-1.862594	-1.258249	-0.674128
C	-1.616871	1.429089	-1.838303
H	-1.797927	2.030474	-2.728657
C	-0.477835	1.601516	-1.134434
O	-3.857701	1.379915	-1.247119
H	-4.566243	0.823883	-0.875519
Br	-4.101345	-1.232990	0.315384
C	-2.358637	1.512467	1.432579
H	-3.375593	1.244309	1.735855
H	-2.434140	2.355194	0.739993
H	-1.858696	1.882683	2.334672
C	-1.388592	-0.711130	1.990547
H	-2.300640	-0.826369	2.587708
H	-0.612659	-0.398296	2.692005
H	-1.124282	-1.709175	1.626184
C	0.473822	2.658096	-1.643321
H	0.575418	3.470725	-0.918490
H	0.119963	3.121736	-2.571905
H	1.455749	2.242990	-1.871133

C	0.600640	1.668135	1.220558
H	0.155112	2.669815	1.278248
H	0.477564	1.248617	2.222646
C	0.689497	-0.446163	-0.229177
H	0.280665	-0.903798	-1.140345
H	0.606297	-1.220514	0.538163
C	2.112885	1.834038	1.016502
H	2.300514	2.538797	0.201117
H	2.526027	2.323716	1.909303
C	2.183612	-0.184001	-0.448245
H	2.330246	0.392235	-1.365748
C	2.856080	0.513627	0.748013
Cl	4.563310	0.953299	0.329185
C	2.906382	-0.330006	2.033238
H	3.537373	-1.217817	1.922073
H	1.914178	-0.670245	2.343061
H	3.320677	0.249784	2.866978
Br	3.026762	-1.914732	-0.891801

SCF Energy (SMD/wB97XD/6-31+G) = -6264.262769**
SCF Energy (B3LYP/6-31G) = -6264.30018434**

H	0.585350	3.484928	-0.848241
C	0.593030	1.638607	1.259579
H	0.147193	2.638490	1.341776
H	0.470046	1.194356	2.251136
C	0.683667	-0.436546	-0.247544
H	0.276626	-0.865952	-1.173140
H	0.599665	-1.234495	0.494885
C	2.105046	1.809769	1.059599
H	2.292450	2.533788	0.261185
H	2.517971	2.278072	1.963894
C	2.178717	-0.170427	-0.454962
H	2.329143	0.427738	-1.357430
C	2.848904	0.496603	0.759585
Cl	4.556549	0.947868	0.353879
C	2.898046	-0.379381	2.022790
H	1.905933	-0.729815	2.321051
H	3.308941	0.179780	2.872138
H	3.531343	-1.262652	1.890466
Br	3.022674	-1.889417	-0.941067

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259235**
SCF Energy (B3LYP/6-31G) = -6264.29240701**

1c_C002

MMFF Geometry

C	-1.599959	0.273732	0.837637
C	-2.781372	0.590980	-1.452699
C	-0.182464	0.795433	0.189721
C	-2.438347	-0.373427	-0.311678
H	-3.076923	0.015365	-2.337941
H	-1.866456	-1.209471	-0.731812
C	-1.638511	1.492430	-1.793674
H	-1.803946	2.108772	-2.676017
C	-0.491481	1.633519	-1.095071
O	-3.869487	1.450703	-1.117776
H	-4.118251	1.937951	-1.920262
Br	-4.079201	-1.288929	0.289236
C	-2.355773	1.461325	1.497635
H	-3.376392	1.185679	1.781773
H	-2.419672	2.336747	0.845511
H	-1.857963	1.785266	2.418611
C	-1.380590	-0.779033	1.964077
H	-2.284545	-0.910087	2.570336
H	-0.592715	-0.493935	2.664191
H	-1.126733	-1.765183	1.561764
C	0.471796	2.687632	-1.588191
H	0.119850	3.173551	-2.506053
H	1.447856	2.266525	-1.828311

1c_C003

MMFF Geometry

C	1.4853510	-0.8006290	-1.0252070
C	3.2508740	-1.3221590	0.7735550
C	0.3862750	-0.3525480	0.1115520
C	2.9627340	-0.6052130	-0.5510690
H	3.4353080	-2.3811120	0.5546850
H	3.6550020	-0.9978600	-1.3075410
C	2.1219570	-1.2863680	1.7482210
H	2.3821550	-1.6809910	2.7305130
C	0.8524890	-0.8998190	1.4995710
O	4.4283110	-0.8631620	1.4262140
H	4.3787230	0.1103840	1.4377870
Br	3.5498370	1.2764820	-0.4682080
C	1.2872780	-0.1120510	-2.4050700
H	2.0136080	-0.4977360	-3.1316710
H	1.4233830	0.9705910	-2.3815680
H	0.2955580	-0.3031750	-2.8245400
C	1.3315760	-2.3312010	-1.3349970
H	2.1620840	-2.6905910	-1.9548070
H	0.4148420	-2.5446850	-1.8952950
H	1.3100260	-2.9450490	-0.4297290
C	-0.1301270	-1.0623560	2.6357100
H	0.3553670	-1.4017140	3.5585300

H	-0.8799400	-1.8197820	2.3906510
H	-0.6235000	-0.1242290	2.8860390
C	0.2818150	1.2059390	0.2215020
H	1.0959600	1.5943850	0.8429580
H	0.4050680	1.6668280	-0.7603040
C	-1.0121570	-0.9434890	-0.2965860
H	-1.0379550	-2.0152600	-0.0550240
H	-1.1177890	-0.8946380	-1.3851700
C	-1.0089160	1.7969640	0.7977590
H	-1.0322410	1.6322740	1.8795280
H	-0.9675010	2.8887200	0.6790520
C	-2.2625980	-0.2818640	0.3010580
H	-2.3674750	-0.5483120	1.3557430
C	-2.2835500	1.2456660	0.1422540
Cl	-3.6831840	1.9469170	1.0535370
C	-2.3923900	1.7358650	-1.3108300
H	-1.6088230	1.3161600	-1.9483600
H	-2.3001000	2.8273650	-1.3642030
H	-3.3550990	1.4770500	-1.7637970
Br	-3.8376280	-1.1550910	-0.5111590

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259102**
SCF Energy (B3LYP/6-31G) = -6264.29634869**

H	0.357977	-1.554622	3.494070
H	-0.871742	-1.926562	2.305183
H	-0.625016	-0.253380	2.876170
C	0.277622	1.200480	0.279833
H	1.089373	1.563016	0.919922
H	0.400270	1.706450	-0.679567
C	-1.007222	-0.928883	-0.335845
H	-1.028710	-2.010404	-0.142044
H	-1.113294	-0.832591	-1.421136
C	-1.016017	1.759993	0.880450
H	-1.039881	1.546831	1.953716
H	-0.978858	2.856133	0.810944
C	-2.260358	-0.299230	0.289751
H	-2.364640	-0.612656	1.331500
C	-2.287492	1.233665	0.199157
Cl	-3.691476	1.887159	1.139265
C	-2.396935	1.787654	-1.230698
H	-1.610690	1.400378	-1.885245
H	-2.309660	2.880856	-1.235201
H	-3.357901	1.544798	-1.696034
Br	-3.831725	-1.142563	-0.560581

SCF Energy (SMD/wB97XD/6-31+G) = -6264.255197**
SCF Energy (B3LYP/6-31G) = -6264.28782875**

1c_C004

MMFF Geometry

C	1.488131	-0.742862	-1.057458
C	3.261252	-1.332827	0.713340
C	0.388906	-0.350899	0.098376
C	2.965092	-0.553795	-0.575472
H	3.436641	-2.380300	0.436471
H	3.657552	-0.909603	-1.350074
C	2.130859	-1.348076	1.693759
H	2.375114	-1.787707	2.659389
C	0.858462	-0.959312	1.460370
O	4.463349	-0.911131	1.346295
H	4.518481	-1.333727	2.218150
Br	3.530532	1.329616	-0.432579
C	1.281353	-0.000158	-2.408216
H	2.015503	-0.343377	-3.148154
H	1.398294	1.082733	-2.339948
H	0.294069	-0.190219	-2.838566
C	1.344923	-2.260317	-1.431145
H	2.177936	-2.587514	-2.065227
H	0.429566	-2.456355	-2.000075
H	1.326822	-2.912126	-0.552793
C	-0.126434	-1.177030	2.585679

1c_C005

MMFF Geometry

C	1.5774410	0.5517120	-0.7421180
C	2.6570420	0.0935640	1.5775030
C	0.1485230	0.8540020	-0.0004040
C	2.3581960	-0.4518070	0.1702420
H	2.8233240	-0.7405950	2.2689220
H	1.7694360	-1.3705890	0.2711810
C	1.5688090	0.9702910	2.1087880
H	1.7608860	1.3550290	3.1097810
C	0.4628170	1.3652500	1.4419110
O	3.8303680	0.9074010	1.6124380
H	4.5211330	0.4257330	1.1225210
Br	4.0313520	-1.1470080	-0.6124520
C	2.3910830	1.8657650	-0.9467600
H	3.4205850	1.6576370	-1.2558600
H	2.4406010	2.4861470	-0.0483570
H	1.9627960	2.4883000	-1.7390840
C	1.3885010	-0.0424600	-2.1613850
H	2.3452450	-0.1585210	-2.6822580
H	0.8001900	0.6209960	-2.8001540
H	0.9142290	-1.0266380	-2.1488610

C	-0.4480920	2.3498310	2.1383430
H	-0.1811740	2.4829180	3.1932030
H	-1.4897570	2.0278620	2.1248820
H	-0.3730780	3.3356380	1.6681370
C	-0.7256500	1.8742490	-0.8137560
H	-1.2731460	2.5581250	-0.1602220
H	-0.1042260	2.5269180	-1.4313450
C	-0.6787140	-0.4780680	0.1790560
H	-0.3096950	-1.0338550	1.0517020
H	-0.5309000	-1.1500820	-0.6719610
C	-1.7752740	1.2116010	-1.7137310
H	-2.2687290	1.9838040	-2.3187560
H	-1.2699850	0.5634560	-2.4363240
C	-2.1858360	-0.2448510	0.3296460
H	-2.3565150	0.3863500	1.2040310
C	-2.8237030	0.3797020	-0.9348650
Cl	-4.1455980	1.4999950	-0.3971160
C	-3.4548390	-0.6068160	-1.9317980
H	-2.7353910	-1.3760860	-2.2344730
H	-3.7794150	-0.0899400	-2.8435010
H	-4.3407490	-1.1069480	-1.5265290
Br	-3.0220740	-1.9317510	0.8961880

SCF Energy (SMD/wB97XD/6-31+G) = -6264.254522**
SCF Energy (B3LYP/6-31G) = -6264.29333385**

H	-1.179824	-2.591267	1.386953
C	0.102883	-1.536412	-2.322720
H	-0.391352	-2.086205	-3.132386
H	0.915417	-2.176188	-1.966454
H	0.519897	-0.635946	-2.779633
C	-0.138544	1.143546	-0.559025
H	0.099252	1.125133	-1.628634
H	-1.045217	1.740223	-0.496234
C	1.030874	-0.826628	0.530481
H	1.054469	-1.923677	0.484750
H	1.150004	-0.569769	1.589674
C	0.977313	1.931303	0.137837
H	0.982672	2.959849	-0.246792
H	0.730172	2.032257	1.198650
C	2.246625	-0.237856	-0.198305
H	2.184005	-0.473392	-1.261911
C	2.377570	1.289611	-0.003028
Cl	3.165500	1.976648	-1.486042
C	3.219021	1.743344	1.201578
H	2.858378	1.285696	2.129636
H	3.162441	2.831202	1.331993
H	4.280572	1.498497	1.091511
Br	3.844529	-1.247299	0.340011

SCF Energy (SMD/wB97XD/6-31+G) = -6264.254929**
SCF Energy (B3LYP/6-31G) = -6264.29320097**

1c_C006

MMFF Geometry

C	-1.457309	-0.385650	1.212762
C	-3.180549	-1.583182	-0.277768
C	-0.362032	-0.308815	-0.001709
C	-2.940813	-0.436173	0.709951
H	-3.239949	-2.526106	0.277980
H	-3.623779	-0.567882	1.559505
C	-2.086659	-1.733567	-1.277467
H	-2.342539	-2.374321	-2.121067
C	-0.849037	-1.203460	-1.192439
O	-4.419843	-1.476356	-0.969668
H	-4.460475	-0.570216	-1.327508
Br	-3.618956	1.256829	-0.041589
C	-1.303114	0.746304	2.256445
H	-2.049387	0.643105	3.053834
H	-1.435470	1.742516	1.827929
H	-0.321540	0.719268	2.740348
C	-1.259154	-1.710532	2.031616
H	-2.099133	-1.878059	2.716889
H	-0.360873	-1.681428	2.657030

1d_C001

MMFF Geometry

C	-1.537371	-0.577715	-0.198187
C	-3.044337	1.538003	-0.150760
C	-0.206172	0.359127	0.028328
C	-2.753862	0.158347	0.450004
H	-3.649308	2.125565	0.549734
H	-2.561327	0.281553	1.522401
C	-1.798855	2.289881	-0.478438
H	-1.982745	3.304085	-0.831564
C	-0.535540	1.816129	-0.431522
O	-3.771543	1.467165	-1.376416
H	-4.511050	0.850240	-1.228894
Br	-4.428630	-0.888791	0.456380
C	-1.389443	-1.981902	0.458520
H	-2.145233	-2.680938	0.081904
H	-1.513021	-1.942123	1.545647
H	-0.424639	-2.449215	0.251802
C	-1.762309	-0.828907	-1.716167
H	-2.724383	-1.313227	-1.910937

H	-0.995994	-1.496998	-2.125062
H	-1.732402	0.091106	-2.306305
C	0.551361	2.753977	-0.900451
H	0.157353	3.738277	-1.180346
H	1.045358	2.360350	-1.793277
H	1.291014	2.937942	-0.120961
C	0.148136	0.411557	1.553004
H	-0.548983	1.072462	2.083977
H	0.016558	-0.572061	2.010296
C	0.996646	-0.246189	-0.777705
H	0.875092	-0.012187	-1.844446
H	0.958557	-1.338232	-0.728574
C	1.567822	0.860188	1.905342
H	1.672936	1.929538	1.695333
H	1.697947	0.766531	2.992292
C	2.408548	0.176785	-0.339594
H	2.616355	1.198237	-0.666524
C	2.655632	0.053064	1.173825
Cl	4.242795	0.812579	1.605872
C	2.686586	-1.393594	1.695035
H	1.792395	-1.954371	1.408062
H	2.744697	-1.415135	2.789932
H	3.553023	-1.949965	1.322347
Br	3.699818	-0.865926	-1.411601

SCF Energy (SMD/wB97XD/6-31+G) = -6264.264346**
SCF Energy (B3LYP/6-31G) = -6264.30040321**

H	-2.721633	-1.013313	-2.095660
H	-0.993374	-1.193850	-2.321755
H	-1.701787	0.415713	-2.283077
C	0.548448	2.865437	-0.436831
H	0.157262	3.882919	-0.555737
H	1.055803	2.624848	-1.375372
H	1.276352	2.917627	0.372660
C	0.138898	0.167485	1.597061
H	-0.556732	0.742300	2.221878
H	0.002152	-0.873680	1.898565
C	0.991753	-0.119567	-0.807220
H	0.872580	0.280796	-1.823627
H	0.953275	-1.205757	-0.931742
C	1.559564	0.547422	2.019314
H	1.669501	1.635996	1.985567
H	1.686392	0.279596	3.077360
C	2.402455	0.227805	-0.304341
H	2.610397	1.288452	-0.463200
C	2.646840	-0.135567	1.170317
Cl	4.234568	0.543370	1.719691
C	2.674862	-1.646493	1.455242
H	1.779055	-2.152529	1.084239
H	2.733880	-1.841699	2.532764
H	3.539593	-2.138541	0.997796
Br	3.696467	-0.629194	-1.526740

SCF Energy (SMD/wB97XD/6-31+G) = -6264.260800**
SCF Energy (B3LYP/6-31G) = -6264.29264414**

1d_C002

MMFF Geometry

C	-1.540361	-0.545910	-0.288891
C	-3.057945	1.535820	0.032477
C	-0.213343	0.350896	0.081101
C	-2.763279	0.090086	0.447588
H	-3.698905	2.006732	0.787285
H	-2.564818	0.078438	1.526078
C	-1.808703	2.338242	-0.141077
H	-1.980028	3.399562	-0.314255
C	-0.544488	1.863503	-0.147658
O	-3.745055	1.605161	-1.215653
H	-3.996733	2.531395	-1.363825
Br	-4.422237	-0.972329	0.346398
C	-1.391325	-2.030330	0.157920
H	-2.136744	-2.670784	-0.327909
H	-1.529481	-2.150727	1.237357
H	-0.420137	-2.456646	-0.101346
C	-1.753565	-0.577517	-1.828603

1d_C003

MMFF Geometry

C	-1.712975	0.935724	1.113398
C	-3.337107	0.761433	-0.876265
C	-0.419282	1.070355	0.109213
C	-2.905596	0.158197	0.466066
H	-3.983866	1.622972	-0.669239
H	-3.772783	0.173339	1.139448
C	-2.211098	1.275271	-1.709388
H	-2.515329	1.583447	-2.709803
C	-0.932252	1.455579	-1.315975
O	-4.124906	-0.116654	-1.670579
H	-3.660729	-0.973979	-1.682525
Br	-2.615988	-1.785604	0.297300
C	-2.265275	2.363799	1.456658
H	-3.226815	2.296334	1.980068
H	-2.420134	2.981764	0.567336
H	-1.590593	2.913505	2.121897

C	-1.378704	0.315178	2.499318
H	-2.269825	0.309712	3.139742
H	-0.614058	0.885307	3.034349
H	-1.032274	-0.718550	2.448536
C	-0.007734	2.100635	-2.321961
H	0.310031	3.087897	-1.975210
H	-0.496147	2.260743	-3.290623
H	0.866383	1.484323	-2.527267
C	0.539413	2.170287	0.689899
H	0.138953	3.168515	0.469371
H	0.559808	2.102864	1.781844
C	0.355438	-0.286763	-0.012460
H	-0.159394	-0.938351	-0.728128
H	0.330763	-0.814486	0.943241
C	2.005888	2.148991	0.244556
H	2.086315	2.508494	-0.785904
H	2.556405	2.885513	0.846108
C	1.825768	-0.224766	-0.448480
H	1.889065	0.006046	-1.514874
C	2.666001	0.767344	0.369310
Cl	4.324140	0.918043	-0.344436
C	2.838141	0.389517	1.849747
H	3.432753	-0.520968	1.977992
H	1.878529	0.224785	2.348412
H	3.354467	1.185333	2.400015
Br	2.543519	-2.065617	-0.376630

SCF Energy (SMD/wB97XD/6-31+G) = -6264.257817**
SCF Energy (B3LYP/6-31G) = -6264.29620463**

1d_C004

MMFF Geometry

C	-1.503916	-0.245666	-0.519297
C	-3.048825	1.226356	0.964542
C	-0.189240	0.250942	0.321024
C	-2.746469	-0.177212	0.428608
H	-3.703169	1.151209	1.841208
H	-2.584464	-0.843502	1.282969
C	-1.807021	1.957591	1.342229

1d_C005

MMFF Geometry

C	-1.50850	-0.24896	-0.52843
C	-3.05835	1.25620	0.91353
C	-0.19701	0.25041	0.31541
C	-2.75581	-0.16050	0.41220
H	-3.74657	1.19901	1.76539
H	-2.58728	-0.79961	1.28615
H	-1.990222	2.897962	1.860444
C	-0.540855	1.570755	1.084512
O	-3.712333	2.058896	0.016509
H	-4.450291	1.536781	-0.346559
Br	-4.407974	-0.913993	-0.346914
C	-1.340492	-1.695119	-1.044089
H	-2.133048	-1.962682	-1.751592
H	-1.377574	-2.425959	-0.230038
H	-0.404953	-1.835501	-1.591701
C	-1.709019	0.654389	-1.773069
H	-2.670294	0.463560	-2.260224
H	-0.943216	0.464740	-2.533155
H	-1.664187	1.721116	-1.536266
C	0.565331	2.475592	1.580497
H	0.176854	3.349837	2.115865
H	1.159974	2.863328	0.748819
H	1.216580	1.949683	2.283718
C	0.251463	-0.779335	1.422220
H	0.680761	-0.261999	2.289832
H	-0.612565	-1.319194	1.821480
C	1.010870	0.475387	-0.669891
H	0.939058	1.478332	-1.111437
H	0.947967	-0.213273	-1.519213
C	1.288513	-1.806166	0.956544
H	1.476803	-2.515585	1.773400
H	0.851937	-2.415997	0.161191
C	2.388680	0.267395	-0.029290
H	2.509000	0.961463	0.804532
C	2.615554	-1.182805	0.457504
Cl	3.767095	-1.125260	1.859842
C	3.219833	-2.146745	-0.577744
H	2.626369	-2.158404	-1.498831
H	3.242112	-3.173429	-0.191626
H	4.251601	-1.892110	-0.841223
Br	3.761875	0.907299	-1.281280

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258715**
SCF Energy (B3LYP/6-31G) = -6264.29670572**

C	-1.81354	1.97210	1.32405
H	-1.98484	2.90251	1.86288
C	-0.54821	1.57207	1.08099
O	-3.67988	2.06475	-0.08205
H	-3.87949	2.92674	0.31834
Br	-4.40430	-0.94974	-0.33109
C	-1.34647	-1.70403	-1.03810
H	-2.13433	-1.97537	-1.74947

H	-1.39130	-2.42748	-0.21792
H	-0.40757	-1.85129	-1.57832
C	-1.70222	0.63619	-1.79412
H	-2.67099	0.45761	-2.27135
H	-0.94521	0.41946	-2.55590
H	-1.63186	1.70510	-1.57360
C	0.56243	2.45918	1.60018
H	0.17737	3.33117	2.14166
H	1.16853	2.85067	0.77850
H	1.20195	1.91960	2.30363
C	0.24020	-0.78187	1.41747
H	0.66525	-0.26663	2.28813
H	-0.62540	-1.32254	1.81238
C	1.00586	0.47429	-0.67192
H	0.93598	1.47800	-1.11210
H	0.94419	-0.21398	-1.52175
C	1.27978	-1.80840	0.95619
H	1.46677	-2.51571	1.77521
H	0.84593	-2.42117	0.16175
C	2.38199	0.26450	-0.02862
H	2.50121	0.95798	0.80574
C	2.60743	-1.18553	0.45865
Cl	3.75700	-1.12725	1.86296
C	3.21336	-2.14959	-0.57544
H	2.62129	-2.16142	-1.49742
H	3.23515	-3.17619	-0.18909
H	4.24549	-1.89490	-0.83743
Br	3.75858	0.90537	-1.27638

SCF Energy (SMD/wB97XD/6-31+G) = -6264.255105**
SCF Energy (B3LYP/6-31G) = -6264.28894811**

H	-2.133806	-1.972491	-1.746230
H	-1.392988	-2.424691	-0.213388
H	-0.407447	-1.849300	-1.572183
C	-1.702776	0.638884	-1.789148
H	-2.684034	0.488233	-2.249407
H	-0.964644	0.397287	-2.562254
H	-1.594226	1.705294	-1.576218
C	0.563787	2.473671	1.582598
H	0.178645	3.348788	2.118951
H	1.164210	2.860511	0.754596
H	1.208735	1.941307	2.286627
C	0.240248	-0.773204	1.423302
H	0.667861	-0.253753	2.290329
H	-0.625617	-1.310176	1.822596
C	1.005175	0.472548	-0.672436
H	0.936639	1.474733	-1.116246
H	0.941482	-0.217880	-1.520290
C	1.277450	-1.803693	0.965473
H	1.464320	-2.507478	1.787542
H	0.841402	-2.419348	0.174453
C	2.381833	0.262979	-0.029721
H	2.502883	0.960062	0.801450
C	2.605623	-1.185363	0.463366
Cl	3.757266	-1.122630	1.865333
C	3.208300	-2.154737	-0.567590
H	2.614648	-2.169582	-1.488509
H	3.229170	-3.179707	-0.176886
H	4.240361	-1.902721	-0.832423
Br	3.756703	0.896721	-1.282809

SCF Energy (SMD/wB97XD/6-31+G) = -6264.257404**
SCF Energy (B3LYP/6-31G) = -6264.29112375**

1d_C006

MMFF Geometry

C	-1.510171	-0.245562	-0.523570
C	-3.058161	1.242706	0.951980
C	-0.197046	0.254094	0.317044
C	-2.759296	-0.163623	0.416823
H	-3.706373	1.155386	1.831922
H	-2.591697	-0.819946	1.278307
C	-1.811048	1.967848	1.339817
H	-1.990070	2.894830	1.884342
C	-0.546955	1.578693	1.076819
O	-3.753675	2.067118	0.019019
H	-3.112867	2.632387	-0.441841
Br	-4.406131	-0.938661	-0.343624
C	-1.347088	-1.701250	-1.033574

1e_C001

MMFF Geometry

C	-1.296819	-0.526981	-0.228204
C	-3.131017	1.275625	-0.549970
C	-0.148938	0.635533	-0.030113
C	-2.672989	0.055809	0.248374
H	-3.550692	0.997450	-1.523972
H	-2.642543	0.295434	1.317558
C	-2.022549	2.239782	-0.771864
H	-2.342221	3.213490	-1.141214
C	-0.714338	2.005704	-0.552022
O	-4.145989	1.980244	0.165434
H	-4.877116	1.351383	0.301907
Br	-4.169770	-1.252161	0.188243

C	-1.021000	-1.814668	0.582978
H	-1.690012	-2.631299	0.288885
H	-1.172343	-1.656768	1.655171
H	-0.020528	-2.208960	0.425455
C	-1.379067	-0.955557	-1.720570
H	-2.242966	-1.596843	-1.920006
H	-0.501306	-1.543041	-2.011998
H	-1.448432	-0.098969	-2.397728
C	0.233665	3.164176	-0.801683
H	-0.295710	4.122248	-0.861214
H	0.760551	3.030295	-1.751879
H	0.968324	3.268372	0.000982
C	0.202928	0.859562	1.480778
H	0.576076	1.879797	1.631291
H	-0.701944	0.814681	2.096870
C	1.176255	0.335496	-0.821501
H	1.739417	1.263269	-0.965845
H	0.953580	0.019853	-1.846227
C	1.248862	-0.080285	2.099142
H	1.491495	0.294221	3.103586
H	0.807887	-1.065311	2.273591
C	2.158087	-0.638551	-0.166897
H	1.763808	-1.654825	-0.193735
C	2.540059	-0.243639	1.273944
Cl	3.435551	1.328375	1.330301
C	3.423812	-1.302659	1.951895
H	2.947897	-2.289370	1.918773
H	3.596257	-1.058396	3.006880
H	4.406431	-1.391898	1.477551
Br	3.731368	-0.800274	-1.353643

SCF Energy (SMD/wB97XD/6-31+G) = -6264.262315**

SCF Energy (B3LYP/6-31G) = -6264.30095356**

Br	-4.171799	-1.269433	0.194140
C	-1.025146	-1.818045	0.577372
H	-1.693306	-2.638412	0.291980
H	-1.170476	-1.654318	1.649420
H	-0.025068	-2.210897	0.416109
C	-1.402668	-0.973131	-1.729227
H	-2.267833	-1.615497	-1.919000
H	-0.527862	-1.563260	-2.023863
H	-1.477084	-0.121021	-2.411335
C	0.236100	3.124112	-0.917555
H	-0.286173	4.083493	-1.009886
H	0.753327	2.949134	-1.866326
H	0.977185	3.252754	-0.124081
C	0.185946	0.885136	1.447990
H	0.560400	1.908550	1.574048
H	-0.721659	0.857481	2.060752
C	1.172125	0.302034	-0.834862
H	1.735153	1.225398	-1.004304
H	0.954426	-0.044422	-1.850508
C	1.225953	-0.042169	2.094079
H	1.458566	0.351265	3.093610
H	0.784300	-1.024546	2.281392
C	2.155967	-0.649436	-0.149430
H	1.770428	-1.669206	-0.154619
C	2.525002	-0.218239	1.284137
Cl	3.411064	1.359953	1.310124
C	3.408655	-1.255976	1.994154
H	2.937776	-2.245570	1.981562
H	3.572005	-0.985305	3.044124
H	4.395199	-1.351755	1.529331
Br	3.739525	-0.827886	-1.320537

SCF Energy (SMD/wB97XD/6-31+G) = -6264.26018**

SCF Energy (B3LYP/6-31G) = -6264.29611489**

1e_C002

MMFF Geometry

C	-1.309061	-0.535576	-0.239627
C	-3.143670	1.278451	-0.542325
C	-0.157757	0.625574	-0.058365
C	-2.684436	0.048588	0.244459
H	-3.609395	0.996724	-1.493535
H	-2.646005	0.280814	1.314842
C	-2.027262	2.221712	-0.822803
H	-2.342549	3.179153	-1.237393
C	-0.718624	1.984553	-0.612950
O	-4.119953	2.009450	0.202160
H	-3.676982	2.385270	0.981934

1e_C003

MMFF Geometry

C	-1.304958	-0.534173	-0.235685
C	-3.144558	1.281290	-0.498155
C	-0.155340	0.625623	-0.045088
C	-2.677977	0.040901	0.265403
H	-3.625735	1.011543	-1.445916
H	-2.639434	0.251459	1.340310
C	-2.031482	2.230463	-0.774426
H	-2.340519	3.199921	-1.161489
C	-0.720247	1.989598	-0.582433
O	-4.103071	1.986182	0.292074

H	-4.531744	2.638301	-0.286886
Br	-4.166349	-1.281878	0.184931
C	-1.015450	-1.827536	0.561945
H	-1.684477	-2.644504	0.269020
H	-1.155226	-1.678866	1.636904
H	-0.016051	-2.217369	0.389969
C	-1.405184	-0.950591	-1.731096
H	-2.268293	-1.593989	-1.926145
H	-0.529799	-1.533026	-2.038962
H	-1.486795	-0.089003	-2.400351
C	0.232555	3.134291	-0.873663
H	0.977046	3.251972	-0.081712
H	-0.290095	4.094832	-0.950146
H	0.745939	2.973316	-1.827013
C	0.193035	0.868861	1.463112
H	0.566547	1.891250	1.599590
H	-0.712490	0.833105	2.078505
C	1.172664	0.313264	-0.829235
H	1.733840	1.239358	-0.989707
H	0.952643	-0.021696	-1.848205
C	1.236336	-0.063897	2.095536
H	1.471674	0.318686	3.098624
H	0.796445	-1.048885	2.273155
C	2.159818	-0.644467	-0.157569
H	1.776056	-1.664729	-0.173233
C	2.532873	-0.229302	1.279595
Cl	3.419086	1.348606	1.320083
C	3.419489	-1.274604	1.974794
H	2.949053	-2.264245	1.952639
H	3.586329	-1.015726	3.027188
H	4.404461	-1.364653	1.505507
Br	3.739815	-0.807869	-1.336298

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259270**
SCF Energy (B3LYP/6-31G) = -6264.29457507**

O	-3.804182	2.207405	0.379680
H	-4.601256	1.730988	0.672671
Br	-4.260702	-1.106452	0.443296
C	-1.091393	-1.938398	0.492159
H	-1.850335	-2.711926	0.330410
H	-1.043957	-1.764741	1.570501
H	-0.146027	-2.386080	0.174508
C	-1.697351	-1.098927	-1.769306
H	-2.598713	-1.716663	-1.835009
H	-0.889672	-1.718105	-2.170663
H	-1.833253	-0.261120	-2.458134
C	0.362649	2.601370	-1.700093
H	-0.072104	3.566657	-1.984248
H	0.708987	2.126144	-2.623368
H	1.224916	2.825649	-1.072856
C	0.090265	0.860398	1.245694
H	-0.674677	1.567249	1.592184
H	0.016366	0.000761	1.918666
C	1.132838	-0.189970	-0.841250
H	1.627806	0.490276	-1.539318
H	0.907871	-1.066046	-1.454203
C	1.457820	1.503861	1.499599
H	1.478756	2.482624	1.010436
H	1.525686	1.736115	2.570889
C	2.152662	-0.587413	0.233995
H	1.705916	-1.332712	0.901246
C	2.651952	0.613899	1.068730
Cl	3.791759	1.666958	0.132930
C	3.408325	0.133391	2.319216
H	2.767279	-0.499737	2.943315
H	3.735603	0.978165	2.937049
H	4.302013	-0.446321	2.066057
Br	3.600422	-1.611621	-0.618740

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256992**
SCF Energy (B3LYP/6-31G) = -6264.29404647**

1e_C004

MMFF Geometry

C	-1.414762	-0.646548	-0.302528
C	-3.086566	1.317204	-0.472736
C	-0.182766	0.428546	-0.244623
C	-2.667378	0.061468	0.304165
H	-3.749188	1.064219	-1.309766
H	-2.499325	0.305746	1.359253
C	-1.935230	2.086314	-1.036963
H	-2.220273	2.999924	-1.556748
C	-0.637574	1.715469	-0.995990

1e_C005

MMFF Geometry

C	-1.421644	-0.653809	-0.300536
C	-3.081082	1.337604	-0.398535
C	-0.190881	0.419330	-0.256023
C	-2.668018	0.048026	0.330603
H	-3.816113	1.121520	-1.183546
H	-2.494528	0.251492	1.393715
C	-1.942875	2.077581	-1.033773
H	-2.227242	2.974829	-1.580509

C	-0.649224	1.691857	-1.026868
O	-3.698923	2.224424	0.533762
H	-4.043547	2.981272	0.031122
Br	-4.262931	-1.127535	0.431536
C	-1.082890	-1.947487	0.486160
H	-1.849753	-2.717523	0.347998
H	-1.003088	-1.772214	1.562316
H	-0.149167	-2.401106	0.143158
C	-1.725049	-1.100949	-1.764997
H	-2.585530	-1.776232	-1.811108
H	-0.894241	-1.658416	-2.206389
H	-1.942229	-0.263724	-2.433322
C	0.341715	2.540874	-1.786744
H	-0.090757	3.499292	-2.096316
H	0.661958	2.028418	-2.699471
H	1.219813	2.779049	-1.186003
C	0.081898	0.874823	1.227300
H	-0.685812	1.582446	1.565777
H	0.015533	0.025157	1.913862
C	1.127131	-0.207744	-0.841184
H	1.624075	0.461058	-1.548607
H	0.904554	-1.094028	-1.440265
C	1.446148	1.532315	1.459882
H	1.462255	2.492690	0.934737
H	1.515167	1.801506	2.522290
C	2.145399	-0.585978	0.242494
H	1.697550	-1.320399	0.921176
C	2.641434	0.631255	1.056519
Cl	3.789035	1.665056	0.108463
C	3.387556	0.173823	2.321512
H	2.740106	-0.444252	2.954018
H	3.713776	1.029777	2.924304
H	4.280697	-0.414095	2.085901
Br	3.596263	-1.622665	-0.589356

SCF Energy (SMD/wB97XD/6-31+G) = -6264.254615**
SCF Energy (B3LYP/6-31G) = -6264.28854513**

H	3.0881240	-1.5572500	-2.4100480
C	1.2797740	-1.4164060	-1.3455210
O	4.4029460	-1.4306200	0.0022510
H	4.7683540	-1.9612580	-0.7254540
Br	2.4359960	2.1121900	-0.0576340
C	2.0289920	-1.7386730	1.8599740
H	2.8588730	-1.4683660	2.5243050
H	2.3922540	-2.5177160	1.1831070
H	1.2606600	-2.1848690	2.5012660
C	0.8664140	0.3937010	2.2060540
H	1.6217050	0.6444750	2.9623810
H	0.0615300	-0.1090460	2.7430050
H	0.4831460	1.3452940	1.8341520
C	0.5810320	-2.1602330	-2.4718150
H	0.4345500	-3.2111270	-2.2021950
H	1.1683600	-2.1467220	-3.3974580
H	-0.3881900	-1.7227040	-2.7207030
C	-0.4279910	-2.1987450	0.3398670
H	-0.8666570	-2.6710290	-0.5449050
H	0.1801620	-2.9991230	0.7727600
C	-0.5342240	0.1605860	-0.5543780
H	-0.9168450	-0.0781790	-1.5536540
H	-0.0000930	1.0992030	-0.7056980
C	-1.6097360	-1.9040410	1.2643890
H	-2.1547430	-2.8423530	1.4378120
H	-1.2455140	-1.6042540	2.2501010
C	-1.7574220	0.4178980	0.3426660
H	-1.4590980	0.9147270	1.2660900
C	-2.5721440	-0.8405470	0.6968400
Cl	-3.3944030	-1.5389640	-0.7578360
C	-3.6583880	-0.5531620	1.7451490
H	-3.2249940	-0.1023300	2.6452140
H	-4.1649920	-1.4753580	2.0537430
H	-4.4286500	0.1287070	1.3705440
Br	-2.8514250	1.8235610	-0.5144480

SCF Energy (SMD/wB97XD/6-31+G) = -6264.254898**
SCF Energy (B3LYP/6-31G) = -6264.29143804**

1e_C006

MMFF Geometry

C	1.4845140	-0.4877590	1.0933180
C	3.5034170	-0.4782090	-0.5669280
C	0.4536380	-0.9664810	-0.0875780
C	2.7578800	0.2596830	0.5447540
H	4.1277010	0.2144750	-1.1431540
H	3.4542800	0.4248870	1.3782370
C	2.5994690	-1.1982790	-1.5053580

1e_C007

MMFF Geometry

C	-1.427240	-0.650548	-0.300745
C	-3.087182	1.334532	-0.445392
C	-0.192592	0.420482	-0.256297
C	-2.678191	0.060151	0.312504
H	-3.794525	1.098329	-1.249069
H	-2.507125	0.287989	1.370904

C	-1.939549	2.074687	-1.060790
H	-2.228708	2.967571	-1.614554
C	-0.644897	1.694973	-1.028822
O	-3.748691	2.241998	0.435932
H	-3.072070	2.646970	1.004647
Br	-4.268238	-1.113854	0.438533
C	-1.098029	-1.938467	0.499205
H	-1.860754	-2.711217	0.353024
H	-1.036176	-1.756562	1.575467
H	-0.158008	-2.391821	0.173737
C	-1.720057	-1.110065	-1.763571
H	-2.599901	-1.759453	-1.814647
H	-0.899132	-1.699305	-2.182010
H	-1.899534	-0.276678	-2.447673
C	0.352310	2.547898	-1.776766
H	-0.078582	3.507127	-2.086169
H	0.681435	2.039566	-2.688606
H	1.224593	2.784852	-1.167479
C	0.079393	0.875281	1.226904
H	-0.686640	1.585663	1.563356
H	0.008526	0.026007	1.913381
C	1.123715	-0.211086	-0.840214
H	1.621321	0.455025	-1.549735
H	0.898634	-1.098117	-1.437178
C	1.445678	1.527054	1.464529
H	1.464711	2.491398	0.946887
H	1.513952	1.788701	2.528911
C	2.142239	-0.590008	0.243093
H	1.693948	-1.323423	0.922505
C	2.640265	0.626470	1.056739
Cl	3.784304	1.661375	0.106405
C	3.390214	0.168687	2.319379
H	2.745114	-0.450785	2.952922
H	3.716910	1.024476	2.922159
H	4.283525	-0.417863	2.081046
Br	3.591335	-1.628375	-0.589011

SCF Energy (SMD/wB97XD/6-31+G) = -6264.255465**

SCF Energy (B3LYP/6-31G) = -6264.28918930**

H	3.4627860	0.3960380	1.3313620
C	2.5672610	-1.2384930	-1.5218340
H	3.0600100	-1.6356900	-2.4084830
C	1.2536190	-1.4716260	-1.3377950
O	4.4272860	-1.4049090	-0.1164060
H	5.1659600	-0.8894650	0.2493650
Br	2.4211050	2.1079830	-0.0446900
C	2.0600020	-1.7653660	1.8262720
H	2.9018870	-1.4932210	2.4745930
H	2.4152440	-2.5375460	1.1373360
H	1.3086860	-2.2202080	2.4814910
C	0.8881680	0.3568240	2.2084320
H	1.6563560	0.6066780	2.9520420
H	0.0968170	-0.1531650	2.7576520
H	0.4931680	1.3087660	1.8509240
C	0.5530160	-2.2617270	-2.4296360
H	0.4175470	-3.3034480	-2.1214900
H	1.1316740	-2.2763240	-3.3606920
H	-0.4217490	-1.8386200	-2.6835500
C	-0.4534780	-2.2080870	0.3727550
H	-0.9005310	-2.6937070	-0.5004720
H	0.1467390	-3.0058970	0.8209380
C	-0.5331990	0.1344120	-0.5669260
H	-0.9259330	-0.1222280	-1.5584600
H	0.0129970	1.0615510	-0.7436250
C	-1.6316990	-1.8834030	1.2919180
H	-2.1903910	-2.8114030	1.4772770
H	-1.2647620	-1.5772080	2.2742900
C	-1.7452300	0.4258640	0.3337760
H	-1.4318470	0.9294850	1.2484080
C	-2.5787700	-0.8136550	0.7105040
Cl	-3.4171150	-1.5214560	-0.7300610
C	-3.6567060	-0.4926570	1.7577240
H	-3.2132250	-0.0337240	2.6487370
H	-4.1759990	-1.4019100	2.0831950
H	-4.4180700	0.1944920	1.3746750
Br	-2.8201600	1.8378280	-0.5360090

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256795**

SCF Energy (B3LYP/6-31G) = -6264.29301789**

1e_C008

MMFF Geometry

C	1.4903910	-0.5132640	1.0786310
C	3.4746940	-0.4727550	-0.6291660
C	0.4412080	-0.9950890	-0.0836500
C	2.7488490	0.2432220	0.5103980
H	4.0434910	0.2321630	-1.2471790

1e_C009

MMFF Geometry

C	-1.588990	0.674210	1.057698
C	-3.115111	0.166523	-1.022727
C	-0.448918	1.202237	0.027150
C	-2.627032	-0.277792	0.367800

H	-3.099061	-0.651980	-1.751389
H	-3.497348	-0.379618	1.030699
C	-2.375679	1.315333	-1.625114
H	-2.858369	1.754696	-2.497015
C	-1.207317	1.824686	-1.186273
O	-4.480776	0.586073	-0.926347
H	-5.015989	-0.216107	-0.798613
Br	-2.064030	-2.171143	0.281562
C	-2.439437	1.895401	1.578052
H	-3.282316	1.549115	2.189731
H	-2.863189	2.503451	0.774679
H	-1.855085	2.560976	2.220667
C	-1.076175	0.032007	2.367449
H	-1.911924	-0.387391	2.942984
H	-0.611225	0.767578	3.028948
H	-0.370043	-0.779759	2.211957
C	-0.603481	2.983325	-1.944370
H	-0.581055	3.881359	-1.318987
H	-1.179054	3.235255	-2.842217
H	0.412023	2.747260	-2.276757
C	0.514848	2.245673	0.694505
H	0.994384	2.860589	-0.073883
H	-0.037299	2.966453	1.303560
C	0.451068	0.106963	-0.638103
H	0.908329	0.536157	-1.542691
H	-0.157544	-0.708377	-1.035586
C	1.669913	1.672297	1.529203
H	2.302875	2.508503	1.857675
H	1.288410	1.233200	2.452961
C	1.591485	-0.454560	0.213207
H	1.194948	-1.067895	1.022577
C	2.526893	0.628641	0.784487
Cl	3.443914	1.487957	-0.519274
C	3.557210	0.047311	1.765232
H	3.062536	-0.513580	2.566416
H	4.146030	0.842079	2.238474
H	4.264051	-0.629350	1.274219
Br	2.551742	-1.799428	-0.868681

SCF Energy (SMD/wB97XD/6-31+G) = -6264.255881**
SCF Energy (B3LYP/6-31G) = -6264.29175814**

1e_C010

MMFF Geometry

C	-1.559880	-0.352772	-0.711996
C	-2.836368	1.436426	0.641663
C	-0.125625	0.159626	-0.073472
C	-2.682277	-0.052709	0.331203
H	-3.455336	1.944689	-0.107818
H	-2.509346	-0.617381	1.255206
C	-1.530206	2.149551	0.710133
H	-1.612742	3.185549	1.037167
C	-0.320654	1.641296	0.390808
O	-3.471702	1.613859	1.906611
H	-4.347501	1.193293	1.840047
Br	-4.471720	-0.718117	-0.205208
C	-1.562792	-1.876578	-1.029463
H	-2.423402	-2.154337	-1.648769
H	-1.619419	-2.488558	-0.124334
H	-0.687016	-2.197382	-1.595564
C	-1.836864	0.377774	-2.060434
H	-2.824731	0.129577	-2.461436
H	-1.116279	0.085454	-2.831336
H	-1.789155	1.466529	-1.971686
C	0.849619	2.577199	0.529222
H	0.564693	3.536133	0.978820
H	1.262729	2.816694	-0.453012
H	1.617044	2.162608	1.181678
C	0.198834	-0.659685	1.218648
H	-0.342644	-0.245908	2.080407
H	-0.174226	-1.682521	1.132611
C	1.008909	0.006094	-1.166454
H	1.031074	0.904036	-1.797883
H	0.706023	-0.781581	-1.862058
C	1.672971	-0.758941	1.608844
H	2.041681	0.217208	1.937791
H	1.744604	-1.410317	2.490722
C	2.444207	-0.413014	-0.766253
H	2.878254	-0.950863	-1.620401
C	2.543760	-1.314046	0.479108
Cl	4.237186	-1.476294	1.103564
C	2.124571	-2.751738	0.111652
H	1.129075	-2.795026	-0.334211
H	2.116399	-3.403024	0.993606
H	2.814422	-3.191219	-0.619059
Br	3.626235	1.159590	-0.731741

SCF Energy (SMD/wB97XD/6-31+G) = -6264.249437**
SCF Energy (B3LYP/6-31G) = -6264.28673508**

1e_C011

MMFF Geometry

C	1.6128550	-0.3383850	1.1741730
C	3.4074510	-0.6425830	-0.6893270

C	0.4494810	-0.9631390	0.2145160
C	2.8204830	0.2785400	0.3844940
H	3.9171580	-0.0632470	-1.4677000
H	3.6144970	0.5269220	1.1019980
C	2.4049330	-1.5358510	-1.3402230
H	2.7898380	-2.0872360	-2.1968950
C	1.1153930	-1.7010900	-0.9845670
O	4.4121560	-1.4737130	-0.1020690
H	4.7271500	-2.0834160	-0.7902520
Br	2.4920390	2.0459650	-0.4196610
C	2.2350410	-1.4757740	2.0591150
H	3.1323050	-1.1233030	2.5821070
H	2.5183140	-2.3535540	1.4707740
H	1.5461770	-1.8158790	2.8395940
C	1.0709360	0.6975360	2.1935560
H	1.8855590	1.0952950	2.8111920
H	0.3453130	0.2533680	2.8819830
H	0.5845220	1.5523920	1.7180200
C	0.2923080	-2.6536060	-1.8233120
H	0.0514740	-3.5560450	-1.2541760
H	0.8278540	-2.9844280	-2.7208400
H	-0.6292410	-2.1838170	-2.1749640
C	-0.4235910	-1.9624270	1.0675510
H	0.0886740	-2.9294590	1.1551830
H	-0.5261750	-1.5871430	2.0920660
C	-0.5032220	0.1313300	-0.3795840
H	-0.7684510	-0.0973880	-1.4194110
H	0.0051520	1.0901310	-0.4487420
C	-1.8572710	-2.2216200	0.5829870
H	-1.8259960	-2.8217550	-0.3295480
H	-2.3418970	-2.8806440	1.3161720
C	-1.7962910	0.3113350	0.4214900
H	-1.5530760	0.5504830	1.4616150
C	-2.7014190	-0.9381670	0.3821890
Cl	-3.5548510	-1.1172790	-1.2086690
C	-3.7871620	-0.8592630	1.4685550
H	-3.3370060	-0.7752390	2.4643390
H	-4.4180850	-1.7560930	1.4690990
H	-4.4490900	0.0018610	1.3296820
Br	-2.6945900	1.9554820	-0.1779690

SCF Energy (SMD/wB97XD/6-31+G) = -6264.249742**
SCF Energy (B3LYP/6-31G) = -6264.28589068**

1e_C012

MMFF Geometry

C	-1.714507	-0.761519	1.119792
C	-2.523789	1.486963	-0.010331
C	-0.213341	-0.167523	0.914070
C	-2.765473	-0.021543	0.215074
H	-2.367879	1.741158	-1.065079
H	-3.765228	-0.171492	0.644344
C	-1.375888	2.059954	0.752672
H	-1.446006	3.126937	0.958590
C	-0.322203	1.353212	1.211594
O	-3.688156	2.208590	0.404365
H	-4.386781	2.012407	-0.243909
Br	-3.036981	-0.853311	-1.566726
C	-2.183899	-0.528463	2.599444
H	-3.190678	-0.936439	2.754452
H	-2.229603	0.528834	2.874749
H	-1.529442	-1.031649	3.318292
C	-1.811835	-2.304692	0.949907
H	-2.859423	-2.630326	0.970146
H	-1.318789	-2.840437	1.767856
H	-1.373033	-2.670723	0.019821
C	0.663293	2.072574	2.100113
H	1.655756	2.125408	1.655330
H	0.732867	1.592843	3.080213
H	0.359841	3.108857	2.291297
C	0.785047	-0.904117	1.867272
H	0.629261	-0.596723	2.907545
H	0.579572	-1.977800	1.862654
C	0.252038	-0.376236	-0.576616
H	-0.271554	0.319014	-1.243164
H	-0.064776	-1.370875	-0.902405
C	2.278078	-0.757295	1.544285
H	2.617938	0.255677	1.772324
H	2.837794	-1.406144	2.232073
C	1.755932	-0.314379	-0.892525
H	1.905806	-0.707444	-1.906641
C	2.620100	-1.120031	0.094267
Cl	4.389916	-0.840615	-0.162696
C	2.413007	-2.630956	-0.143846
H	3.006810	-3.229574	0.557173
H	1.369645	-2.936395	-0.023313
H	2.713262	-2.915781	-1.159379
Br	2.297894	1.559503	-1.120791

SCF Energy (SMD/wB97XD/6-31+G) = -6264.253967**
SCF Energy (B3LYP/6-31G) = -6264.28758627**

1e_C013

MMFF Geometry

C	-1.572366	-0.348200	-0.712068
C	-2.833926	1.433200	0.679062
C	-0.135272	0.161295	-0.079158
C	-2.695099	-0.052895	0.335752
H	-3.489195	1.944876	-0.035460
H	-2.526370	-0.637280	1.248242
C	-1.529197	2.156597	0.703047
H	-1.612659	3.202401	0.999258
C	-0.323991	1.647046	0.372758
O	-3.421812	1.591029	1.970728
H	-2.762332	1.317687	2.630936
Br	-4.482056	-0.707720	-0.221399
C	-1.575435	-1.872520	-1.031612
H	-2.438578	-2.150902	-1.646973
H	-1.626727	-2.485076	-0.126525
H	-0.702874	-2.193765	-1.602182
C	-1.853200	0.385147	-2.058142
H	-2.833225	0.121588	-2.468377
H	-1.122286	0.110359	-2.825655
H	-1.826981	1.474001	-1.962614
C	0.845843	2.588838	0.471496
H	0.564490	3.557722	0.901602
H	1.246732	2.805647	-0.520983
H	1.621097	2.190314	1.125164
C	0.186107	-0.648796	1.218578
H	-0.355990	-0.228591	2.076837
H	-0.187479	-1.672063	1.139250
C	0.998868	-0.005790	-1.171936
H	1.024124	0.886125	-1.811589
H	0.693320	-0.797253	-1.861644
C	1.660042	-0.743621	1.609461
H	2.028760	0.237485	1.924168
H	1.731853	-1.383080	2.499960
C	2.433129	-0.426828	-0.768941
H	2.864454	-0.975329	-1.617647
C	2.529679	-1.314542	0.486228
Cl	4.221501	-1.474417	1.114653
C	2.106126	-2.754731	0.133857
H	1.111867	-2.799242	-0.315020
H	2.092736	-3.395866	1.023137
H	2.796611	-3.205046	-0.589628
Br	3.621192	1.141632	-0.750872

SCF Energy (SMD/wB97XD/6-31+G) = -6264.247660**

SCF Energy (B3LYP/6-31G) = -6264.28191406**

1e_C014

MMFF Geometry

C	-1.567226	-0.362675	-0.706879
C	-2.832032	1.415895	0.687335
C	-0.132690	0.155796	-0.078781
C	-2.688579	-0.068633	0.342252
H	-3.503862	1.922172	-0.016491
H	-2.522598	-0.655929	1.253474
C	-1.531641	2.148850	0.698304
H	-1.606714	3.194139	0.993761
C	-0.326065	1.644944	0.358910
O	-3.399120	1.541316	1.991403
H	-3.617779	2.478659	2.124619
Br	-4.478772	-0.719184	-0.223890
C	-1.564926	-1.888728	-1.018678
H	-2.429846	-2.174242	-1.628192
H	-1.609095	-2.496848	-0.110244
H	-0.693880	-2.209480	-1.591831
C	-1.852858	0.363413	-2.055877
H	-2.827764	0.086274	-2.469269
H	-1.115971	0.095915	-2.820205
H	-1.841254	1.452759	-1.963091
C	0.841342	2.590696	0.446229
H	0.558685	3.563025	0.867544
H	1.239464	2.799292	-0.549143
H	1.619198	2.200418	1.101749
C	0.190807	-0.641466	1.226569
H	-0.353202	-0.215618	2.080797
H	-0.179306	-1.666684	1.156105
C	1.002372	-0.017544	-1.169485
H	1.025794	0.868905	-1.816737
H	0.699533	-0.815263	-1.853037
C	1.664760	-0.727300	1.619322
H	2.030144	0.258087	1.924369
H	1.738365	-1.357744	2.516065
C	2.437218	-0.431421	-0.761856
H	2.869658	-0.987654	-1.604976
C	2.536080	-1.306412	0.501970
Cl	4.228963	-1.455501	1.131028
C	2.116604	-2.751155	0.163210
H	1.122919	-2.802594	-0.286375
H	2.104026	-3.383610	1.058688
H	2.808978	-3.206708	-0.555182
Br	3.622375	1.139760	-0.761436

SCF Energy (SMD/wB97XD/6-31+G) = -6264.246776**

SCF Energy (B3LYP/6-31G) = -6264.28087953**

1e_C015

MMFF Geometry

C	1.609008	-0.374314	1.159250
C	3.370348	-0.657672	-0.746220
C	0.432597	-0.989123	0.210405
C	2.810671	0.241591	0.360923
H	3.822989	-0.070393	-1.553847
H	3.619480	0.461151	1.071283
C	2.368888	-1.575913	-1.354993
H	2.761590	-2.154268	-2.190586
C	1.085595	-1.745591	-0.981054
O	4.414121	-1.487421	-0.230540
H	5.183524	-0.914511	-0.071661
Br	2.505559	2.037436	-0.385686
C	2.238186	-1.520668	2.027648
H	3.133563	-1.170236	2.555295
H	2.528372	-2.387592	1.426744
H	1.551381	-1.875980	2.803049
C	1.082671	0.656794	2.191488
H	1.906503	1.052108	2.798407
H	0.367642	0.211024	2.889709
H	0.589036	1.512952	1.725712
C	0.262709	-2.724002	-1.788303
H	0.797748	-3.083481	-2.675047
H	-0.657584	-2.261948	-2.154115
H	0.019585	-3.607985	-1.191914
C	-0.452486	-1.967236	1.075805
H	0.044435	-2.941652	1.169692
H	-0.544866	-1.583520	2.097948
C	-0.504036	0.111307	-0.394792
H	-0.781112	-0.132080	-1.428516
H	0.021837	1.059078	-0.484235
C	-1.891861	-2.205915	0.597099
H	-1.872554	-2.809600	-0.313449
H	-2.385076	-2.854078	1.334178
C	-1.788326	0.324243	0.411897
H	-1.534490	0.570113	1.447838
C	-2.715575	-0.909627	0.392959
Cl	-3.588579	-1.088091	-1.187058
C	-3.788226	-0.801331	1.489738
H	-3.326252	-0.717433	2.480106
H	-4.435774	-1.686100	1.504498
H	-4.435206	0.070989	1.350188
Br	-2.659927	1.977852	-0.199402

SCF Energy (SMD/wB97XD/6-31+G) = -6264.251707**

SCF Energy (B3LYP/6-31G) = -6264.28760761**

1e_C016

MMFF Geometry

C	-1.553284	-0.450445	-0.649644
C	-2.817100	1.520402	0.439252
C	-0.130636	0.080967	-0.019747
C	-2.709781	0.000191	0.301442
H	-3.348237	1.969884	-0.408395
H	-2.611316	-0.457254	1.291481
C	-1.483716	2.177175	0.550790
H	-1.527502	3.233682	0.812333
C	-0.287216	1.587421	0.351502
O	-3.543227	1.858519	1.620448
H	-4.423836	1.452403	1.531887
Br	-4.496188	-0.665982	-0.245664
C	-1.563312	-1.997866	-0.783920
H	-2.416788	-2.346576	-1.375516
H	-1.625031	-2.491816	0.190821
H	-0.674178	-2.379348	-1.292424
C	-1.773174	0.134856	-2.078830
H	-2.768761	-0.099541	-2.467772
H	-1.069175	-0.282523	-2.805568
H	-1.660595	1.222451	-2.108163
C	0.943883	2.442684	0.532490
H	0.701545	3.436692	0.926243
H	1.451210	2.602713	-0.421318
H	1.633895	1.993177	1.244553
C	0.193305	-0.676434	1.309875
H	0.504934	0.029187	2.089980
H	-0.702354	-1.139130	1.734049
C	1.009681	-0.104556	-1.087998
H	1.065069	0.782602	-1.732146
H	0.683364	-0.885138	-1.783954
C	1.253198	-1.772916	1.195920
H	1.366523	-2.253282	2.177075
H	0.899665	-2.559808	0.519059
C	2.416318	-0.589014	-0.678024
H	2.662261	-1.362272	-1.420963
C	2.605496	-1.235243	0.710150
Cl	3.253366	-0.114364	1.971796
C	3.608716	-2.400293	0.625331
H	3.267879	-3.164958	-0.082328
H	3.734558	-2.893295	1.596599
H	4.595997	-2.059216	0.294206
Br	3.782623	0.735292	-1.163061

SCF Energy (SMD/wB97XD/6-31+G) = -6264.248933**

SCF Energy (B3LYP/6-31G) = -6264.28664050**

1e_C017

MMFF Geometry

C	-1.73340	-0.74462	1.12265
C	-2.61964	1.45854	-0.02413
C	-0.23887	-0.13327	0.91004
C	-2.78809	-0.06201	0.18018
H	-2.57184	1.73101	-1.08433
H	-3.79276	-0.26799	0.57371
C	-1.44216	2.07079	0.66651
H	-1.50414	3.14546	0.82746
C	-0.36978	1.39857	1.13432
O	-3.78799	2.10048	0.50123
H	-3.77118	3.02298	0.19456
Br	-2.95036	-0.91006	-1.60764
C	-2.22159	-0.46718	2.58797
H	-3.22935	-0.87250	2.74316
H	-2.27125	0.59766	2.83118
H	-1.57496	-0.94687	3.32975
C	-1.80587	-2.29436	1.00343
H	-2.84912	-2.63392	1.02088
H	-1.31554	-2.79550	1.84451
H	-1.35143	-2.68557	0.09144
C	0.62316	2.17359	1.96791
H	0.31557	3.21706	2.10598
H	1.60974	2.20864	1.50990
H	0.70829	1.74952	2.97224
C	0.75433	-0.81024	1.91202
H	0.58182	-0.45008	2.93273
H	0.55787	-1.88446	1.96144
C	0.25399	-0.39579	-0.56259
H	-0.26034	0.27557	-1.26060
H	-0.05399	-1.40286	-0.85615
C	2.25043	-0.66784	1.60185
H	2.58078	0.35728	1.78520
H	2.80497	-1.27836	2.32791
C	1.76177	-0.34585	-0.86054
H	1.92560	-0.79033	-1.85109
C	2.61507	-1.09807	0.17621
Cl	4.38721	-0.82176	-0.06784
C	2.41805	-2.61971	0.00830
H	1.37396	-2.92361	0.12650
H	3.00267	-3.18087	0.74699
H	2.73597	-2.95195	-0.98726
Br	2.30253	1.51436	-1.18343

SCF Energy (SMD/wB97XD/6-31+G) = -6264.251811**

SCF Energy (B3LYP/6-31G) = -6264.28520980**

1e_C018

MMFF Geometry

C	-1.747164	-0.707854	1.119320
C	-2.671105	1.457529	-0.060625
C	-0.254423	-0.089676	0.901081
C	-2.801954	-0.065301	0.148655
H	-2.674903	1.731928	-1.120603
H	-3.807071	-0.291110	0.530071
C	-1.477529	2.096046	0.574846
H	-1.542747	3.180070	0.666894
C	-0.397445	1.450111	1.060178
O	-3.824177	2.094923	0.505974
H	-3.731320	2.066185	1.473580
Br	-2.915214	-0.937109	-1.626594
C	-2.245269	-0.394000	2.573722
H	-3.261094	-0.779056	2.727011
H	-2.275881	0.675479	2.797790
H	-1.613761	-0.870557	3.330688
C	-1.808144	-2.261219	1.041993
H	-2.849222	-2.606866	1.069764
H	-1.313137	-2.736923	1.894820
H	-1.353791	-2.674652	0.139969
C	0.604609	2.271382	1.836992
H	0.699354	1.904682	2.862947
H	0.298299	3.321178	1.918520
H	1.586938	2.279757	1.369898
C	0.728412	-0.713830	1.946481
H	0.544079	-0.301153	2.945262
H	0.531516	-1.784053	2.049853
C	0.260558	-0.406069	-0.553410
H	-0.240101	0.244112	-1.281007
H	-0.048948	-1.420781	-0.816566
C	2.227784	-0.586689	1.646718
H	2.556774	0.446149	1.783818
H	2.773462	-1.161242	2.408016
C	1.772475	-0.379463	-0.833729
H	1.945298	-0.872842	-1.799352
C	2.608367	-1.086055	0.248103
Cl	4.385021	-0.830873	0.015575
C	2.404561	-2.612838	0.149515
H	2.735315	-2.993713	-0.824205
H	1.356895	-2.904951	0.265744
H	2.974499	-3.141479	0.922847
Br	2.330506	1.457761	-1.242759

SCF Energy (SMD/wB97XD/6-31+G) = -6264.252714**

SCF Energy (B3LYP/6-31G) = -6264.28673196**

1f_C001

MMFF Geometry

C	1.595495	0.606692	-0.795182
C	2.761672	0.321102	1.493968
C	0.169469	0.897281	-0.035792
C	2.451713	-0.309174	0.134648
H	3.630756	0.988190	1.439486
H	1.963202	-1.281189	0.271690
C	1.622968	1.109188	2.047166
H	1.797357	1.485499	3.054587
C	0.471955	1.407561	1.408921
O	3.065084	-0.691904	2.451131
H	3.838869	-1.175533	2.110755
Br	4.183554	-0.854291	-0.661897
C	2.323929	1.948983	-1.094732
H	3.320238	1.787598	-1.518226
H	2.448451	2.571219	-0.204119
H	1.774603	2.542430	-1.833645
C	1.404339	-0.106595	-2.165367
H	2.317079	-0.062025	-2.770680
H	0.622140	0.346885	-2.776980
H	1.160610	-1.167178	-2.046068
C	-0.504235	2.287695	2.151992
H	-0.146500	2.547173	3.155547
H	-1.466448	1.795263	2.294094
H	-0.648767	3.236320	1.627294
C	-0.655177	1.946327	-0.857123
H	-0.247425	2.952644	-0.695186
H	-0.537384	1.765675	-1.928660
C	-0.640330	-0.438398	0.090510
H	-0.196389	-1.068811	0.873121
H	-0.543862	-1.020706	-0.829907
C	-2.167948	2.003104	-0.603514
H	-2.364237	2.502158	0.349995
H	-2.616323	2.661428	-1.360586
C	-2.138063	-0.290193	0.379400
H	-2.287092	0.063264	1.403293
C	-2.857783	0.627683	-0.625680
Cl	-4.571601	0.897846	-0.102875
C	-2.901684	0.087594	-2.065425
H	-1.903780	-0.136572	-2.453090
H	-3.351980	0.820654	-2.745712
H	-3.498254	-0.826783	-2.147377
Br	-2.911732	-2.107105	0.435824

SCF Energy (SMD/wB97XD/6-31+G) = -6264.265515**

SCF Energy (B3LYP/6-31G) = -6264.30146369**

1f_C002

MMFF Geometry

C	1.613611	0.645091	-0.760025
C	2.735349	0.199715	1.533813
C	0.180344	0.899077	-0.002295
C	2.459331	-0.330034	0.122264
H	3.630536	0.832464	1.547622
H	1.972213	-1.310840	0.177326
C	1.608243	0.996338	2.104130
H	1.785965	1.342440	3.122416
C	0.470655	1.341143	1.466637
O	2.976913	-0.881536	2.433966
H	2.139771	-1.361730	2.552707
Br	4.201671	-0.810166	-0.692828
C	2.350110	1.999387	-0.973761
H	3.343820	1.860541	-1.410998
H	2.482418	2.560779	-0.044735
H	1.802810	2.643282	-1.670619
C	1.433268	0.012487	-2.171513
H	2.354440	0.080044	-2.761607
H	0.665829	0.508611	-2.768217
H	1.175481	-1.049947	-2.115490
C	-0.495492	2.215523	2.230028
H	-0.619815	3.183070	1.735724
H	-0.141260	2.435668	3.244163
H	-1.466966	1.734539	2.348703
C	-0.640236	1.983525	-0.782011
H	-0.232873	2.981768	-0.575840
H	-0.518357	1.849323	-1.859604
C	-0.629320	-0.440071	0.055918
H	-0.186944	-1.108982	0.806839
H	-0.532354	-0.975961	-0.892377
C	-2.154632	2.030726	-0.534238
H	-2.355346	2.491791	0.437294
H	-2.599031	2.719081	-1.266548
C	-2.126566	-0.301234	0.351800
H	-2.272907	0.012640	1.389156
C	-2.845235	0.657716	-0.614776
Cl	-4.558835	0.905668	-0.081625
C	-2.887772	0.178113	-2.075674
H	-3.480472	-0.734614	-2.195298
H	-1.889097	-0.025162	-2.472940
H	-3.341534	0.937094	-2.724505
Br	-2.900568	-2.117690	0.338855

SCF Energy (SMD/wB97XD/6-31+G) = -6264.26381**

SCF Energy (B3LYP/6-31G) = -6264.29665693**

1f_C003

MMFF Geometry

C	1.608399	0.640803	-0.767332
C	2.724542	0.175205	1.526965
C	0.177623	0.896205	-0.007853
C	2.449774	-0.341060	0.110869
H	3.633801	0.788250	1.551768
H	1.965524	-1.323983	0.154436
C	1.605829	0.984344	2.098206
H	1.773339	1.328283	3.117574
C	0.472662	1.341863	1.458937
O	2.928838	-0.935552	2.399494
H	3.268801	-0.587350	3.240495
Br	4.201289	-0.806637	-0.703058
C	2.348789	1.993676	-0.976917
H	3.338375	1.854540	-1.423246
H	2.490963	2.547638	-0.044908
H	1.798902	2.644761	-1.664949
C	1.425986	0.012949	-2.180737
H	2.348978	0.074304	-2.768614
H	0.664338	0.516732	-2.778371
H	1.159583	-1.047479	-2.128059
C	-0.489706	2.220986	2.221222
H	-0.133419	2.443366	3.234129
H	-1.462307	1.742922	2.342768
H	-0.611993	3.187557	1.724510
C	-0.644420	1.979718	-0.787268
H	-0.235774	2.978149	-0.584691
H	-0.526497	1.843256	-1.864923
C	-0.632818	-0.442908	0.054677
H	-0.188740	-1.111295	0.804992
H	-0.539031	-0.979845	-0.893370
C	-2.157767	2.028547	-0.534599
H	-2.355314	2.491980	0.436407
H	-2.603981	2.715674	-1.266984
C	-2.128742	-0.302714	0.355612
H	-2.271392	0.012660	1.393071
C	-2.849410	0.655873	-0.610158
Cl	-4.561656	0.907676	-0.072771
C	-2.897048	0.174270	-2.070409
H	-1.899853	-0.031116	-2.470356
H	-3.351501	0.933084	-2.718963
H	-3.491631	-0.737590	-2.187167
Br	-2.908029	-2.117280	0.345581

SCF Energy (SMD/wB97XD/6-31+G) = -6264.26274**

SCF Energy (B3LYP/6-31G) = -6264.29535543**

1f_C004

MMFF Geometry

C	1.56564	-0.60912	-0.98734
C	3.30949	-1.02243	0.90570
C	0.40421	-0.34064	0.12843
C	3.00856	-0.34883	-0.43928
H	4.01553	-0.43205	1.50032
H	3.73375	-0.70645	-1.18310
C	2.10996	-1.32289	1.74643
H	2.33982	-1.82026	2.68760
C	0.82051	-1.06291	1.44531
O	3.96122	-2.27143	0.64711
H	4.19124	-2.66515	1.50537
Br	3.51904	1.55439	-0.33076
C	1.36355	0.17506	-2.31661
H	2.19279	-0.02502	-3.00706
H	1.31826	1.25762	-2.18737
H	0.45162	-0.12251	-2.84222
C	1.53210	-2.11465	-1.42696
H	2.38494	-2.35276	-2.07424
H	0.63191	-2.34995	-2.00506
H	1.56388	-2.80553	-0.57990
C	-0.21718	-1.53239	2.43694
H	0.23408	-2.01429	3.31238
H	-0.87525	-2.28009	1.98525
H	-0.81158	-0.70376	2.82251
C	0.26880	1.18236	0.45413
H	1.07306	1.49751	1.12869
H	0.38499	1.77968	-0.45244
C	-0.96305	-0.87744	-0.43098
H	-0.97645	-1.97443	-0.37326
H	-1.02916	-0.64918	-1.49893
C	-1.04099	1.64025	1.10176
H	-1.07828	1.28033	2.13537
H	-1.02042	2.73604	1.17989
C	-2.24838	-0.34090	0.21781
H	-2.39174	-0.78920	1.20390
C	-2.29062	1.19128	0.32757
Cl	-3.72365	1.70348	1.31027
C	-2.37554	1.92410	-1.02170
H	-1.57952	1.61965	-1.70786
H	-2.28691	3.00860	-0.88508
H	-3.32911	1.74649	-1.52989
Br	-3.77639	-1.07633	-0.79591

SCF Energy (SMD/wB97XD/6-31+G) = -6264.258190**

SCF Energy (B3LYP/6-31G) = -6264.29237052**

1f_C005

MMFF Geometry

C	1.566743	-0.628378	-0.973567
C	3.277608	-0.965678	0.976346
C	0.389875	-0.376562	0.125946
C	2.997861	-0.351042	-0.403263
H	3.880897	-0.305473	1.609852
H	3.736487	-0.736636	-1.119241
C	2.067939	-1.361577	1.755797
H	2.298504	-1.903991	2.672335
C	0.779403	-1.142372	1.422497
O	4.043490	-2.164490	0.813071
H	4.939314	-1.897284	0.544529
Br	3.517220	1.553585	-0.367379
C	1.367945	0.152810	-2.304904
H	2.230008	0.004682	-2.967626
H	1.252882	1.229474	-2.169212
H	0.494464	-0.194077	-2.865125
C	1.562284	-2.133767	-1.414506
H	2.407040	-2.347847	-2.080712
H	0.656230	-2.391629	-1.973110
H	1.634264	-2.825623	-0.570825
C	-0.270845	-1.701714	2.350602
H	0.169983	-2.233414	3.202192
H	-0.901780	-2.429436	1.832553
H	-0.891756	-0.911799	2.775505
C	0.273716	1.136200	0.498393
H	1.088985	1.425351	1.171715
H	0.383848	1.759691	-0.391514
C	-0.977339	-0.867500	-0.472222
H	-1.005325	-1.965404	-0.472819
H	-1.031629	-0.581193	-1.526640
C	-1.027015	1.572846	1.178048
H	-1.062396	1.155963	2.190551
H	-0.995103	2.662552	1.314220
C	-2.260929	-0.348003	0.194935
H	-2.418362	-0.846688	1.154142
C	-2.284427	1.177179	0.386064
Cl	-3.709227	1.652602	1.398504
C	-2.365596	1.980840	-0.922834
H	-1.580132	1.698304	-1.630283
H	-2.256918	3.055061	-0.730768
H	-3.325703	1.846878	-1.432160
Br	-3.790883	-1.008027	-0.866926

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259879**

SCF Energy (B3LYP/6-31G) = -6264.29380652**

1f_C006

MMFF Geometry

C	1.572771	-0.618945	-0.975927
C	3.293333	-0.981691	0.961321
C	0.399890	-0.364155	0.128871
C	3.009867	-0.350919	-0.410506
H	3.924127	-0.332930	1.578294
H	3.745858	-0.729255	-1.132906
C	2.084548	-1.347330	1.760573
H	2.317803	-1.857246	2.695602
C	0.796310	-1.120470	1.431731
O	4.054249	-2.181986	0.778023
H	3.435212	-2.904772	0.580526
Br	3.520993	1.557062	-0.353945
C	1.375890	0.168956	-2.304368
H	2.227408	0.002521	-2.976356
H	1.286707	1.247844	-2.167444
H	0.488299	-0.156246	-2.855147
C	1.549367	-2.121554	-1.424365
H	2.413761	-2.355631	-2.057426
H	0.659062	-2.353749	-2.019095
H	1.563283	-2.818086	-0.582234
C	-0.252713	-1.644724	2.382483
H	0.189567	-2.160517	3.243072
H	-0.894734	-2.378407	1.886868
H	-0.862503	-0.839176	2.793116
C	0.278003	1.151512	0.489420
H	1.088806	1.446712	1.165434
H	0.392468	1.768236	-0.404493
C	-0.967055	-0.868062	-0.459365
H	-0.991010	-1.966103	-0.442818
H	-1.023606	-0.598968	-1.518225
C	-1.026664	1.596270	1.156341
H	-1.065036	1.197508	2.175797
H	-0.997489	2.688216	1.274378
C	-2.251736	-0.342561	0.200770
H	-2.405934	-0.825942	1.168365
C	-2.280666	1.185206	0.367152
Cl	-3.709503	1.671679	1.368242
C	-2.360361	1.967542	-0.954491
H	-1.569960	1.678505	-1.653751
H	-2.258569	3.045254	-0.778926
H	-3.317327	1.819912	-1.465922
Br	-3.779374	-1.026627	-0.848593

SCF Energy (SMD/wB97XD/6-31+G) = -6264.260372**

SCF Energy (B3LYP/6-31G) = -6264.29443055**

1f_C007

MMFF Geometry

C	-1.584901	-0.977066	-0.363547
C	-2.662560	0.542924	1.431318
C	-0.151665	-0.838072	0.412023
C	-2.387438	0.329938	-0.064784
H	-3.584597	0.035153	1.740876
H	-1.873013	1.201977	-0.484647
C	-1.569091	0.048353	2.323131
H	-1.750873	0.211948	3.384385
C	-0.458335	-0.607845	1.924902
O	-2.831779	1.930756	1.710536
H	-3.597406	2.230220	1.188810
Br	-4.129879	0.437473	-1.000404
C	-2.371659	-2.231763	0.128538
H	-3.372660	-2.277794	-0.312712
H	-2.499880	-2.263316	1.213468
H	-1.877960	-3.163156	-0.164403
C	-1.409178	-1.166583	-1.891327
H	-2.369248	-1.324784	-2.394264
H	-0.819637	-2.058520	-2.119736
H	-0.939717	-0.305554	-2.372886
C	0.476875	-1.109874	2.999639
H	0.204707	-0.731627	3.991830
H	1.507866	-0.800166	2.825034
H	0.437246	-2.202379	3.057852
C	0.766348	-2.089620	0.175481
H	1.336069	-2.355985	1.069412
H	0.175728	-2.981078	-0.047367
C	0.621984	0.447607	-0.080057
H	0.224265	1.340328	0.421376
H	0.454818	0.621470	-1.147751
C	1.793626	-1.898788	-0.946414
H	2.319620	-2.847436	-1.117399
H	1.266298	-1.692206	-1.883135
C	2.135338	0.371273	0.147716
H	2.322005	0.241250	1.215798
C	2.805136	-0.758775	-0.671660
Cl	4.163164	-1.438871	0.321099
C	3.406717	-0.347723	-2.026140
H	2.661804	0.157121	-2.651622
H	3.756102	-1.225905	-2.583318
H	4.271101	0.316121	-1.919565
Br	2.905898	2.151246	-0.172336

SCF Energy (SMD/wB97XD/6-31+G) = -6264.257858**

SCF Energy (B3LYP/6-31G) = -6264.29480000**

1f_C008

MMFF Geometry

C	-1.604574	-0.985011	-0.314273
C	-2.628512	0.672376	1.398977
C	-0.164576	-0.821076	0.440542
C	-2.394074	0.347071	-0.087132
H	-3.575576	0.241274	1.744541
H	-1.883205	1.181652	-0.581170
C	-1.553546	0.173571	2.315194
H	-1.741481	0.366874	3.371011
C	-0.459899	-0.524166	1.943080
O	-2.723312	2.083526	1.588850
H	-1.828213	2.454543	1.507042
Br	-4.150871	0.390058	-1.001252
C	-2.401583	-2.201518	0.252460
H	-3.391024	-2.285024	-0.208991
H	-2.558682	-2.149719	1.332776
H	-1.900221	-3.151215	0.044802
C	-1.438050	-1.261766	-1.830265
H	-2.401709	-1.433728	-2.321436
H	-0.861089	-2.172839	-2.010960
H	-0.957852	-0.435113	-2.359326
C	0.458362	-1.020299	3.035052
H	0.192668	-0.607539	4.015137
H	1.497248	-0.740255	2.854385
H	0.391113	-2.109434	3.123156
C	0.746619	-2.086483	0.248272
H	1.318206	-2.322592	1.149376
H	0.150880	-2.982497	0.060108
C	0.611729	0.437431	-0.111324
H	0.217612	1.354171	0.347388
H	0.445172	0.561581	-1.186216
C	1.771608	-1.943868	-0.883563
H	2.292997	-2.900666	-1.019492
H	1.241456	-1.771083	-1.825794
C	2.124204	0.363071	0.122702
H	2.306637	0.268570	1.195663
C	2.788877	-0.798510	-0.655058
Cl	4.146220	-1.444197	0.360297
C	3.388031	-0.439622	-2.025049
H	2.642846	0.043521	-2.667105
H	3.734060	-1.338756	-2.549922
H	4.253978	0.225917	-1.945094
Br	2.900792	2.127607	-0.255988

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256601**

SCF Energy (B3LYP/6-31G) = -6264.29037842**

1f_C009

MMFF Geometry

C	-1.601629	-0.996124	-0.288926
C	-2.606807	0.747377	1.352373
C	-0.163177	-0.807324	0.459862
C	-2.384785	0.347028	-0.117162
H	-3.568871	0.366839	1.716843
H	-1.878867	1.154927	-0.658730
C	-1.545986	0.262384	2.294143
H	-1.726155	0.489118	3.343412
C	-0.462072	-0.465581	1.951398
O	-2.647231	2.170481	1.448276
H	-2.865998	2.396438	2.367586
Br	-4.155486	0.345382	-1.012606
C	-2.404286	-2.186072	0.324378
H	-3.382386	-2.301317	-0.154219
H	-2.587267	-2.076701	1.396325
H	-1.893438	-3.142243	0.180148
C	-1.433525	-1.332042	-1.792749
H	-2.397322	-1.511865	-2.280713
H	-0.864957	-2.255003	-1.936770
H	-0.942678	-0.530955	-2.350661
C	0.447277	-0.938872	3.060241
H	0.180104	-0.498779	4.027914
H	1.488948	-0.670655	2.876703
H	0.371847	-2.024814	3.176666
C	0.749008	-2.077625	0.307103
H	1.319693	-2.286567	1.215423
H	0.154304	-2.979320	0.144494
C	0.613581	0.434844	-0.129671
H	0.217720	1.365630	0.298200
H	0.450154	0.524194	-1.208595
C	1.774961	-1.967774	-0.827196
H	2.296914	-2.927869	-0.934735
H	1.245541	-1.822662	-1.774606
C	2.124855	0.367947	0.112412
H	2.302694	0.302885	1.188492
C	2.791291	-0.815795	-0.630017
Cl	4.147437	-1.432289	0.405761
C	3.392627	-0.497102	-2.009082
H	2.648657	-0.032274	-2.665895
H	3.738752	-1.411291	-2.507214
H	4.259002	0.169805	-1.947348
Br	2.908544	2.118502	-0.313094

SCF Energy (SMD/wB97XD/6-31+G) = -6264.255444**

SCF Energy (B3LYP/6-31G) = -6264.28931000**

1g_C001

MMFF Geometry

C	-1.380965	0.102840	0.743087
C	-2.961581	0.864045	-1.187615
C	-0.130556	0.947824	0.082732
C	-2.357913	-0.310938	-0.414472
H	-3.388976	0.502750	-2.130715
H	-1.819425	-0.950543	-1.123207
C	-1.942307	1.904315	-1.483042
H	-2.277399	2.668169	-2.183364
C	-0.701090	1.973980	-0.963052
O	-4.005077	1.528089	-0.480327
H	-4.621936	0.836866	-0.179525
Br	-3.845956	-1.491611	0.143416
C	-2.118307	0.965457	1.804264
H	-3.071628	0.521170	2.106773
H	-2.326058	1.978826	1.448607
H	-1.525689	1.054074	2.721996
C	-0.934027	-1.185628	1.473605
H	-1.749394	-1.622560	2.061383
H	-0.139043	-1.006986	2.194083
H	-0.606610	-1.956848	0.769646
C	0.174321	3.114038	-1.449486
H	0.219953	3.909782	-0.699120
H	-0.212961	3.564261	-2.370915
H	1.189906	2.778392	-1.675080
C	0.691240	1.754963	1.151351
H	1.236689	2.572489	0.670896
H	0.032018	2.274351	1.853304
C	0.853483	0.023820	-0.719330
H	1.366577	0.615381	-1.488436
H	0.286966	-0.718066	-1.294302
C	1.756854	0.989702	1.937658
H	2.309515	1.710726	2.556467
H	1.280628	0.319102	2.657010
C	1.934809	-0.698958	0.099847
H	1.493673	-1.510269	0.681241
C	2.742930	0.211938	1.042470
Cl	3.739531	1.408935	0.120842
C	3.697525	-0.584539	1.946023
H	3.154729	-1.352135	2.509369
H	4.189680	0.069212	2.675939
H	4.488043	-1.086016	1.378465
Br	3.074894	-1.702271	-1.164458

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259789**

SCF Energy (B3LYP/6-31G) = -6264.29924075**

1g_C002

MMFF Geometry

C	-1.464549	0.072897	0.791883
C	-2.880825	0.968245	-1.195299
C	-0.144926	0.869995	0.231685
C	-2.387084	-0.262651	-0.426637
H	-3.243520	0.662002	-2.183781
H	-1.842469	-0.906640	-1.125804
C	-1.806914	1.987304	-1.363248
H	-2.073073	2.803171	-2.033908
C	-0.599198	1.981978	-0.763076
O	-3.955310	1.642635	-0.544994
H	-4.611386	0.961596	-0.311035
Br	-3.952100	-1.383051	0.018784
C	-2.217249	0.946740	1.836863
H	-3.189260	0.520062	2.102902
H	-2.388825	1.967576	1.484042
H	-1.655481	1.023589	2.774336
C	-1.072468	-1.241299	1.520198
H	-1.930921	-1.695647	2.026704
H	-0.329364	-1.075969	2.304316
H	-0.674729	-1.989586	0.827735
C	0.343546	3.112266	-1.104198
H	-0.052446	3.757236	-1.897224
H	1.300157	2.729986	-1.468918
H	0.509602	3.754163	-0.234479
C	0.640010	1.481518	1.448009
H	0.165600	2.418163	1.768900
H	0.575299	0.815222	2.314547
C	0.806763	-0.083787	-0.572318
H	1.207296	0.420925	-1.461378
H	0.245961	-0.929475	-0.982640
C	2.138845	1.743332	1.240287
H	2.264036	2.612522	0.589441
H	2.551774	2.075109	2.202751
C	1.983483	-0.600208	0.260019
H	1.608793	-1.129976	1.140694
C	2.939433	0.525524	0.710123
Cl	3.969277	1.128479	-0.656831
C	3.896359	0.024173	1.805016
H	3.337076	-0.337959	2.675283
H	4.560586	0.824555	2.152301
H	4.533067	-0.795052	1.455196
Br	2.873405	-2.044576	-0.736205

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256943**

SCF Energy (B3LYP/6-31G) = -6264.29519147**

1g_C003

MMFF Geometry

C	1.188382	-0.346895	-1.089868
C	3.154049	-1.589437	0.034597
C	0.345660	-0.287746	0.321644
C	2.742810	-0.426106	-0.870076
H	3.045211	-2.534527	-0.508514
H	3.260918	-0.536898	-1.831688
C	2.317600	-1.674820	1.260505
H	2.748583	-2.277385	2.059503
C	1.101438	-1.117179	1.426281
O	4.524435	-1.528667	0.417191
H	4.669758	-0.637182	0.784798
Br	3.552163	1.252133	-0.199740
C	0.911931	0.808647	-2.081759
H	1.514899	0.688625	-2.991228
H	1.166186	1.789747	-1.675805
H	-0.127260	0.836710	-2.412885
C	0.820117	-1.639327	-1.889885
H	1.492350	-1.779085	-2.745469
H	-0.193060	-1.586401	-2.302448
H	0.885515	-2.543106	-1.276277
C	0.430750	-1.367076	2.767586
H	1.149895	-1.694463	3.527800
H	-0.320299	-2.158433	2.679222
H	-0.048446	-0.473250	3.170758
C	0.145597	1.173441	0.859696
H	-0.073736	1.152407	1.931830
H	1.070342	1.746927	0.797407
C	-1.087401	-0.926260	0.197525
H	-1.495778	-1.115368	1.196813
H	-1.030500	-1.929097	-0.240393
C	-0.973947	2.013829	0.220907
H	-1.076721	2.941476	0.801648
H	-0.670650	2.350354	-0.773133
C	-2.126606	-0.074986	-0.534486
H	-1.851635	0.039171	-1.584750
C	-2.338352	1.306078	0.117992
Cl	-3.016253	1.169199	1.791568
C	-3.293323	2.194784	-0.694277
H	-2.954769	2.286862	-1.732594
H	-3.344107	3.207181	-0.276110
H	-4.315064	1.802003	-0.711952
Br	-3.793679	-1.123705	-0.656231

SCF Energy (SMD/wB97XD/6-31+G) = -6264.259289**

SCF Energy (B3LYP/6-31G) = -6264.29719469**

1g_C004

MMFF Geometry

C	-1.385459	0.083035	0.748392
C	-2.993549	0.890513	-1.138287
C	-0.141979	0.939349	0.088791
C	-2.376479	-0.304543	-0.406692
H	-3.466282	0.543592	-2.065050
H	-1.836938	-0.912494	-1.142485
C	-1.961877	1.915471	-1.461485
H	-2.280647	2.672496	-2.176063
C	-0.714153	1.970230	-0.954866
O	-3.996777	1.546045	-0.368062
H	-4.340859	2.284123	-0.897360
Br	-3.828753	-1.536520	0.122916
C	-2.109285	0.922451	1.836251
H	-3.062510	0.474367	2.134118
H	-2.313493	1.945707	1.507831
H	-1.508295	0.986097	2.750743
C	-0.929269	-1.218813	1.449760
H	-1.737554	-1.667618	2.038421
H	-0.127232	-1.051922	2.165585
H	-0.607639	-1.976168	0.728224
C	0.173574	3.095050	-1.456820
H	-0.211306	3.538744	-2.382404
H	1.185710	2.748767	-1.680507
H	0.228855	3.898583	-0.715400
C	0.676705	1.746291	1.159151
H	1.218991	2.567541	0.681453
H	0.015667	2.261417	1.862625
C	0.844905	0.019595	-0.717018
H	1.352531	0.611889	-1.488653
H	0.279552	-0.725118	-1.289721
C	1.742700	0.980013	1.943497
H	2.290616	1.698840	2.568988
H	1.266313	0.302183	2.656154
C	1.933479	-0.698640	0.097044
H	1.500894	-1.518603	0.672636
C	2.734371	0.212923	1.045217
Cl	3.723996	1.421518	0.130405
C	3.693467	-0.581978	1.945329
H	3.155104	-1.355399	2.504945
H	4.181528	0.071282	2.678420
H	4.487059	-1.076108	1.375624
Br	3.082276	-1.682967	-1.175204

SCF Energy (SMD/wB97XD/6-31+G) = -6264.256128**

SCF Energy (B3LYP/6-31G) = -6264.29139704**

1g_C005

MMFF Geometry

C	-1.390259	0.090655	0.744155
C	-2.982915	0.878258	-1.170197
C	-0.142075	0.940742	0.085711
C	-2.377821	-0.307223	-0.411397
H	-3.421006	0.515444	-2.107543
H	-1.835287	-0.928838	-1.133535
C	-1.949144	1.904564	-1.486339
H	-2.268139	2.650720	-2.213712
C	-0.709297	1.968967	-0.963027
O	-4.031677	1.527629	-0.454787
H	-3.702605	2.374410	-0.111322
Br	-3.835327	-1.526530	0.130707
C	-2.116851	0.938158	1.823437
H	-3.080492	0.504754	2.108461
H	-2.300045	1.964895	1.495796
H	-1.526265	0.992316	2.745451
C	-0.937108	-1.206543	1.456938
H	-1.747257	-1.649977	2.047083
H	-0.136677	-1.035070	2.173353
H	-0.614103	-1.969686	0.742152
C	0.180245	3.093448	-1.463127
H	0.231345	3.898345	-0.722891
H	-0.200473	3.535444	-2.391232
H	1.193580	2.746937	-1.681093
C	0.676004	1.748073	1.156632
H	1.217672	2.569891	0.679275
H	0.014657	2.262364	1.860369
C	0.843979	0.016168	-0.715746
H	1.353135	0.604973	-1.489146
H	0.277887	-0.729528	-1.286375
C	1.742649	0.983235	1.941950
H	2.291332	1.703629	2.564998
H	1.266906	0.307666	2.657147
C	1.930789	-0.701250	0.101398
H	1.495878	-1.517452	0.680702
C	2.733408	0.212965	1.045460
Cl	3.721630	1.418703	0.125867
C	3.693227	-0.579000	1.947326
H	3.155380	-1.350807	2.509657
H	4.181664	0.076583	2.678090
H	4.486576	-1.074675	1.378629
Br	3.077699	-1.692860	-1.166273

SCF Energy (SMD/wB97XD/6-31+G) = -6264.257636**

SCF Energy (B3LYP/6-31G) = -6264.29307963**

1g_C006

MMFF Geometry

C	-1.470669	0.061891	0.799786
C	-2.908624	0.989031	-1.154921
C	-0.154961	0.865129	0.239047
C	-2.401130	-0.255968	-0.417759
H	-3.310301	0.691977	-2.131161
H	-1.849050	-0.871264	-1.137066
C	-1.821967	1.995670	-1.347463
H	-2.070046	2.804256	-2.032946
C	-0.609542	1.979557	-0.756308
O	-3.953881	1.652331	-0.448643
H	-4.254330	2.396030	-0.996279
Br	-3.930441	-1.428824	0.002231
C	-2.216672	0.921593	1.860690
H	-3.195167	0.500348	2.111879
H	-2.372553	1.952474	1.530324
H	-1.657979	0.971033	2.801941
C	-1.072520	-1.259266	1.512610
H	-1.926057	-1.716248	2.025169
H	-0.321263	-1.100570	2.290386
H	-0.682896	-2.002690	0.810449
C	0.345240	3.096045	-1.111434
H	-0.045332	3.736746	-1.910573
H	1.297859	2.701712	-1.473084
H	0.518075	3.745178	-0.248396
C	0.629671	1.475605	1.455623
H	0.153375	2.410659	1.778409
H	0.566425	0.806841	2.320498
C	0.797702	-0.087101	-0.567242
H	1.193422	0.416549	-1.458872
H	0.238100	-0.934892	-0.975059
C	2.127925	1.741093	1.249429
H	2.251779	2.615598	0.605446
H	2.539914	2.066640	2.214454
C	1.979135	-0.599849	0.260799
H	1.610030	-1.134083	1.141023
C	2.931454	0.528965	0.710802
Cl	3.951805	1.142427	-0.659113
C	3.896508	0.028571	1.799019
H	3.343456	-0.340270	2.670449
H	4.557845	0.831318	2.146378
H	4.536234	-0.785555	1.442885
Br	2.873856	-2.036533	-0.743038

SCF Energy (SMD/wB97XD/6-31+G) = -6264.253251**

SCF Energy (B3LYP/6-31G) = -6264.28722580**

1g_C007

MMFF Geometry

C	1.592537	0.802606	0.462128
C	2.509940	-1.597328	0.034896
C	0.067101	0.188118	0.580511
C	2.411540	-0.152065	-0.469211
H	2.719791	-2.270842	-0.803978
H	1.941301	-0.165911	-1.459311
C	1.277985	-2.050566	0.743372
H	1.340946	-3.073996	1.112379
C	0.197703	-1.298265	1.044828
O	3.560655	-1.772074	0.987439
H	4.350095	-1.336935	0.617981
Br	4.226162	0.496909	-0.904783
C	2.234006	0.922250	1.873746
H	3.289511	1.207167	1.816402
H	2.179111	-0.005680	2.448876
H	1.737822	1.697763	2.467892
C	1.616450	2.238876	-0.141575
H	2.587005	2.722553	0.019960
H	0.880413	2.905116	0.311213
H	1.446420	2.238711	-1.222619
C	-0.816165	-1.931318	1.971574
H	-0.863539	-1.394097	2.923180
H	-0.557841	-2.967397	2.221392
H	-1.811332	-1.969943	1.537992
C	-0.760992	1.035492	1.601373
H	-0.476026	0.778866	2.629410
H	-0.508803	2.094694	1.512852
C	-0.613357	0.220103	-0.844019
H	-0.235195	-0.607933	-1.458113
H	-0.280196	1.120258	-1.367222
C	-2.288506	0.947694	1.488687
H	-2.642100	-0.023026	1.844752
H	-2.719272	1.678726	2.186951
C	-2.146530	0.270673	-0.948484
H	-2.400882	0.610259	-1.961557
C	-2.808547	1.214345	0.071585
Cl	-4.611192	1.050619	0.086767
C	-2.542229	2.680160	-0.330758
H	-1.475067	2.907251	-0.400437
H	-2.975568	3.378134	0.395376
H	-2.979697	2.907465	-1.310374
Br	-2.861234	-1.555760	-0.988631

SCF Energy (SMD/wB97XD/6-31+G) = -6264.254364**

SCF Energy (B3LYP/6-31G) = -6264.29238729**

1g_C008

MMFF Geometry

C	-1.474027	0.066988	0.793990
C	-2.895687	0.976665	-1.188784
C	-0.154938	0.866075	0.235449
C	-2.403382	-0.258769	-0.423497
H	-3.255751	0.661931	-2.175382
H	-1.851040	-0.889669	-1.129126
C	-1.809399	1.986882	-1.369740
H	-2.058049	2.786041	-2.067730
C	-0.605697	1.979704	-0.762061
O	-3.988147	1.635153	-0.550320
H	-3.657441	2.425528	-0.093496
Br	-3.939846	-1.416255	0.010455
C	-2.219305	0.931601	1.850615
H	-3.210289	0.530391	2.083796
H	-2.346077	1.968513	1.529391
H	-1.673068	0.961233	2.800199
C	-1.078762	-1.252469	1.512983
H	-1.933508	-1.705770	2.026763
H	-0.327777	-1.092568	2.290725
H	-0.689711	-1.999308	0.814087
C	0.349187	3.097727	-1.112913
H	-0.039404	3.738695	-1.912803
H	1.303542	2.704456	-1.471157
H	0.518042	3.746371	-0.248717
C	0.628216	1.476600	1.453112
H	0.153203	2.413024	1.773766
H	0.561504	0.809497	2.318934
C	0.797572	-0.088770	-0.567783
H	1.195403	0.413292	-1.459424
H	0.237257	-0.936184	-0.975344
C	2.127504	1.739025	1.250083
H	2.254182	2.613763	0.606888
H	2.538002	2.063378	2.216153
C	1.977140	-0.602273	0.262636
H	1.605786	-1.134628	1.143078
C	2.930377	0.525800	0.712535
Cl	3.951444	1.137763	-0.657151
C	3.894509	0.025345	1.801507
H	3.340736	-0.342875	2.672741
H	4.556030	0.827907	2.148948
H	4.534081	-0.789220	1.446109
Br	2.871135	-2.041396	-0.737686

SCF Energy (SMD/wB97XD/6-31+G) = -6264.254966**

SCF Energy (B3LYP/6-31G) = -6264.28907022**

1g_C009

MMFF Geometry

C	1.191140	-0.318368	-1.090111
C	3.156230	-1.572570	0.017522
C	0.349284	-0.273410	0.322094
C	2.747146	-0.393456	-0.868581
H	3.015865	-2.507826	-0.536149
H	3.265006	-0.490863	-1.831887
C	2.330932	-1.655666	1.255265
H	2.757182	-2.245707	2.064070
C	1.112511	-1.101774	1.424043
O	4.542062	-1.537674	0.342364
H	4.721385	-2.245842	0.981737
Br	3.538982	1.285839	-0.184832
C	0.909970	0.844230	-2.072967
H	1.515132	0.735023	-2.982336
H	1.157377	1.823652	-1.658859
H	-0.128962	0.868856	-2.405584
C	0.825972	-1.604305	-1.902391
H	1.500639	-1.735877	-2.757338
H	-0.186252	-1.548858	-2.316940
H	0.889483	-2.513661	-1.297024
C	0.447605	-1.347988	2.769505
H	1.169426	-1.675801	3.526996
H	-0.304971	-2.138397	2.686063
H	-0.028167	-0.453559	3.174869
C	0.135194	1.184582	0.865353
H	-0.084465	1.158506	1.937055
H	1.054365	1.767152	0.805568
C	-1.077862	-0.924055	0.195891
H	-1.484630	-1.119901	1.194532
H	-1.012112	-1.924986	-0.245117
C	-0.992228	2.017203	0.230213
H	-1.104223	2.940973	0.815424
H	-0.691858	2.361664	-0.761995
C	-2.123745	-0.079367	-0.534408
H	-1.848219	0.042078	-1.583750
C	-2.349530	1.296825	0.123409
Cl	-3.028125	1.145896	1.795680
C	-3.312435	2.179512	-0.686058
H	-2.973905	2.279196	-1.723681
H	-3.373461	3.189616	-0.263735
H	-4.330278	1.776859	-0.706297
Br	-3.780521	-1.143824	-0.662990

SCF Energy (SMD/wB97XD/6-31+G) = -6264.255292**

SCF Energy (B3LYP/6-31G) = -6264.28891489**

1g_C010

MMFF Geometry

C	-1.598881	-0.793227	0.483032
C	-2.539762	1.592558	0.040994
C	-0.075920	-0.170148	0.588736
C	-2.423971	0.146935	-0.457959
H	-2.789499	2.250626	-0.799545
H	-1.938839	0.166638	-1.440855
C	-1.293471	2.072344	0.713501
H	-1.337243	3.107759	1.047964
C	-0.207223	1.329012	1.017321
O	-3.574591	1.730205	1.015907
H	-3.701518	2.679438	1.177886
Br	-4.212139	-0.538134	-0.934341
C	-2.236538	-0.896322	1.897344
H	-3.296342	-1.166046	1.843903
H	-2.164667	0.033480	2.467678
H	-1.748916	-1.675311	2.494196
C	-1.616395	-2.239065	-0.098070
H	-2.581005	-2.728469	0.081351
H	-0.869848	-2.891429	0.357727
H	-1.456963	-2.254701	-1.180659
C	0.821579	1.987143	1.909964
H	0.569233	3.030830	2.132673
H	1.810602	2.010260	1.462412
H	0.880741	1.478129	2.876371
C	0.752529	-0.991076	1.630653
H	0.468544	-0.706357	2.651640
H	0.498671	-2.052018	1.570763
C	0.606069	-0.234163	-0.834714
H	0.231622	0.582954	-1.465472
H	0.269049	-1.142788	-1.340230
C	2.279971	-0.908377	1.514526
H	2.635343	0.070816	1.844692
H	2.710087	-1.621310	2.231669
C	2.138827	-0.295553	-0.939797
H	2.389537	-0.665127	-1.943284
C	2.799238	-1.213016	0.104858
Cl	4.602341	-1.051759	0.116637
C	2.530803	-2.688299	-0.259097
H	1.463376	-2.914575	-0.325474
H	2.960913	-3.367767	0.486238
H	2.969968	-2.942425	-1.231342
Br	2.862510	1.525653	-1.036463

SCF Energy (SMD/wB97XD/6-31+G) = -6264.251113**

SCF Energy (B3LYP/6-31G) = -6264.28510752**

1g_C011

MMFF Geometry

C	-1.33480	-1.09810	-0.63774
C	-3.35201	0.36371	-1.30902
C	-0.37740	0.22450	-0.50631
C	-2.84536	-0.76272	-0.39453
H	-3.63327	-0.08914	-2.26825
H	-3.45890	-1.65247	-0.58988
C	-2.33917	1.41192	-1.63359
H	-2.73475	2.23657	-2.22650
C	-1.02167	1.37491	-1.34215
O	-4.52954	1.00457	-0.83585
H	-4.37373	1.21622	0.10266
Br	-3.31987	-0.42738	1.48822
C	-0.90019	-2.28327	0.26103
H	-1.60175	-3.12061	0.15801
H	-0.85719	-2.03936	1.32369
H	0.08296	-2.66750	-0.02838
C	-1.26985	-1.68249	-2.09550
H	-2.08759	-2.39319	-2.26826
H	-0.34810	-2.24412	-2.27859
H	-1.34074	-0.91024	-2.86667
C	-0.17290	2.50814	-1.87532
H	-0.78333	3.34298	-2.23904
H	0.43058	2.16658	-2.72229
H	0.48817	2.92351	-1.11637
C	-0.29226	0.74226	0.97741
H	-1.14458	1.39377	1.20378
H	-0.34487	-0.08962	1.68379
C	1.08470	-0.10164	-0.99081
H	1.53045	0.74044	-1.52812
H	1.08721	-0.90481	-1.72959
C	0.97217	1.52713	1.35160
H	0.95580	2.48458	0.82471
H	0.89851	1.80355	2.41210
C	2.02594	-0.45307	0.16593
H	1.60148	-1.27366	0.75178
C	2.28932	0.75424	1.09354
Cl	3.45387	1.94087	0.37015
C	2.88954	0.28886	2.43034
H	2.21514	-0.40953	2.93895
H	3.05830	1.13341	3.10895
H	3.85155	-0.21673	2.29602
Br	3.65967	-1.26829	-0.56015

SCF Energy (SMD/wB97XD/6-31+G) = -6264.248586**

SCF Energy (B3LYP/6-31G) = -6264.28667575**

1h_C001

MMFF Geometry

C	-1.510970	0.218247	0.819227
C	-2.736916	0.614213	-1.437065
C	-0.131195	0.841301	0.181654
C	-2.343386	-0.394805	-0.352098
H	-2.989339	0.081653	-2.361485
H	-1.758575	-1.195435	-0.820231
C	-1.657137	1.604759	-1.716922
H	-1.890784	2.283417	-2.536537
C	-0.506351	1.757490	-1.027918
O	-3.875792	1.396946	-1.079846
H	-4.542328	0.777898	-0.730621
Br	-3.966582	-1.362406	0.223818
C	-2.303585	1.328649	1.565348
H	-3.298275	0.986377	1.867827
H	-2.436420	2.231281	0.962697
H	-1.791742	1.630190	2.486108
C	-1.223998	-0.894819	1.870045
H	-2.109112	-1.104492	2.481877
H	-0.433630	-0.623646	2.572866
H	-0.937656	-1.840704	1.398680
C	0.383915	2.902420	-1.447965
H	-0.015662	3.441063	-2.315498
H	1.376192	2.557978	-1.739810
H	0.471674	3.641082	-0.646265
C	0.637293	1.636374	1.291731
H	0.156560	2.609821	1.455095
H	0.551507	1.121026	2.252076
C	0.768209	-0.318274	-0.366929
H	0.351039	-0.697087	-1.309971
H	0.737501	-1.170583	0.317238
C	2.137332	1.881128	1.073626
H	2.280281	2.676104	0.335585
H	2.556036	2.289385	2.004166
C	2.242454	0.029738	-0.596734
H	2.337716	0.705266	-1.450925
C	2.932261	0.636386	0.639248
Cl	2.963146	-0.521913	2.028478
C	4.382282	1.058382	0.354275
H	5.033100	0.203126	0.145835
H	4.815174	1.590457	1.209814
H	4.431829	1.732346	-0.508568
Br	3.147054	-1.598642	-1.252744

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2594737**

SCF Energy (B3LYP/6-31G) = -6264.30169607**

1h_C002

MMFF Geometry

C	-1.513166	0.185758	0.830413
C	-2.772881	0.686271	-1.384219
C	-0.139959	0.836687	0.205788
C	-2.357078	-0.374963	-0.358907
H	-3.067403	0.192176	-2.317788
H	-1.763780	-1.136914	-0.878515
C	-1.681254	1.671300	-1.656002
H	-1.900425	2.369315	-2.462377
C	-0.521811	1.791528	-0.974314
O	-3.887756	1.456166	-0.936966
H	-4.190777	1.997558	-1.684020
Br	-3.940990	-1.419069	0.182759
C	-2.299416	1.261352	1.631665
H	-3.297854	0.910385	1.911464
H	-2.421516	2.196022	1.077400
H	-1.788434	1.510299	2.568576
C	-1.213285	-0.968906	1.831851
H	-2.088910	-1.199249	2.449987
H	-0.409890	-0.727463	2.530938
H	-0.938268	-1.896550	1.319202
C	0.379485	2.936229	-1.372323
H	0.479312	3.654063	-0.553283
H	-0.019170	3.500482	-2.223855
H	1.366276	2.589523	-1.678550
C	0.628981	1.598904	1.338394
H	0.147475	2.566792	1.530361
H	0.543447	1.055174	2.283170
C	0.762451	-0.301632	-0.383839
H	0.347049	-0.645539	-1.340945
H	0.731312	-1.178902	0.267692
C	2.128741	1.850963	1.127746
H	2.271164	2.666932	0.412828
H	2.546920	2.232426	2.069814
C	2.237743	0.052020	-0.597670
H	2.336681	0.752902	-1.430475
C	2.924893	0.620075	0.657706
Cl	2.954231	-0.580091	2.010252
C	4.375292	1.051245	0.388330
H	5.026826	0.203074	0.154677
H	4.806528	1.556807	1.260624
H	4.426063	1.751565	-0.453195
Br	3.143992	-1.554921	-1.302759

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2594737**

SCF Energy (B3LYP/6-31G) = -6264.29374580**

1h_C003

MMFF Geometry

C	1.361344	-0.328605	-1.235136
C	3.200101	-1.562262	0.074203
C	0.331991	-0.397327	0.044091
C	2.864554	-0.352149	-0.806241
H	3.339387	-2.432544	-0.578745
H	3.508924	-0.388074	-1.694534
C	2.126607	-1.930737	1.042710
H	2.428521	-2.696297	1.757410
C	0.857516	-1.470324	1.053489
O	4.424550	-1.427494	0.786090
H	4.414601	-0.540154	1.189890
Br	3.500878	1.315435	0.034755
C	1.110123	0.875763	-2.185926
H	1.778357	0.821900	-3.054712
H	1.288926	1.848092	-1.723466
H	0.088977	0.887959	-2.577244
C	1.155522	-1.587945	-2.148713
H	1.947543	-1.657248	-2.904351
H	0.209234	-1.544076	-2.698707
H	1.160263	-2.524541	-1.583372
C	-0.065500	-2.077149	2.083344
H	0.460366	-2.761124	2.760142
H	-0.846933	-2.669182	1.598795
H	-0.520014	-1.318514	2.719360
C	0.266263	0.973518	0.797193
H	1.110384	1.061995	1.490189
H	0.371848	1.800231	0.092598
C	-1.095432	-0.774372	-0.494620
H	-1.128942	-1.851564	-0.709968
H	-1.254512	-0.287080	-1.462051
C	-0.989622	1.284850	1.619266
H	-0.971725	0.702702	2.546155
H	-0.933435	2.332648	1.946260
C	-2.300535	-0.419315	0.387174
H	-2.353600	-1.088769	1.249194
C	-2.310546	1.037643	0.874306
Cl	-2.422132	2.207293	-0.498895
C	-3.475349	1.331349	1.832596
H	-4.449536	1.268990	1.337019
H	-3.394485	2.339377	2.256603
H	-3.482232	0.624575	2.670222
Br	-3.935573	-0.905462	-0.607915

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2588513**

SCF Energy (B3LYP/6-31G) = -6264.29774312**

1h_C004

MMFF Geometry

C	-1.364229	-0.291603	1.234886
C	-3.209600	-1.543656	-0.046297
C	-0.335430	-0.387738	-0.042175
C	-2.867886	-0.311496	0.802406
H	-3.330392	-2.396250	0.634059
H	-3.511798	-0.325102	1.691876
C	-2.138486	-1.931861	-1.016394
H	-2.426739	-2.708330	-1.722788
C	-0.867344	-1.475138	-1.034269
O	-4.460519	-1.422018	-0.713164
H	-4.569611	-2.185037	-1.302730
Br	-3.482879	1.351801	-0.059044
C	-1.104924	0.925859	2.167290
H	-1.775907	0.891363	3.034950
H	-1.273328	1.892653	1.689723
H	-0.084754	0.935189	2.561310
C	-1.166429	-1.536734	2.169907
H	-1.961935	-1.591057	2.923080
H	-0.222302	-1.486896	2.723179
H	-1.170855	-2.482582	1.620234
C	0.054259	-2.096206	-2.057352
H	-0.473097	-2.786101	-2.726907
H	0.833631	-2.685286	-1.565968
H	0.511028	-1.346206	-2.701810
C	-0.259172	0.970515	-0.817282
H	-1.099968	1.051725	-1.515230
H	-0.363393	1.808959	-0.126541
C	1.089077	-0.766171	0.503757
H	1.115403	-1.840403	0.734397
H	1.250221	-0.266383	1.464426
C	1.001164	1.264297	-1.638919
H	0.982796	0.670711	-2.558520
H	0.951973	2.308146	-1.979424
C	2.297597	-0.431107	-0.381064
H	2.347067	-1.112030	-1.234244
C	2.318456	1.019076	-0.887253
Cl	2.435500	2.205602	0.470647
C	3.487374	1.292316	-1.846682
H	4.460019	1.230369	-1.348025
H	3.414002	2.295054	-2.284382
H	3.491622	0.574311	-2.674722
Br	3.928034	-0.916601	0.622045

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2549295**

SCF Energy (B3LYP/6-31G) = -6264.28900332**

1i_C001

MMFF Geometry

C	-1.331320	-0.418331	-0.207107
C	-3.140953	1.453906	-0.030918
C	-0.151836	0.652487	0.213778
C	-2.682993	0.067722	0.427761
H	-3.916972	1.827815	0.647823
H	-2.577599	0.082735	1.518884
C	-2.011855	2.418989	-0.055403
H	-2.316353	3.455952	-0.190165
C	-0.703831	2.116793	0.059376
O	-3.692393	1.460860	-1.344344
H	-4.354831	0.747362	-1.373045
Br	-4.204464	-1.175872	0.184520
C	-1.065165	-1.858230	0.294853
H	-1.759720	-2.578532	-0.152259
H	-1.185963	-1.937297	1.379660
H	-0.077923	-2.225462	0.025951
C	-1.449177	-0.514433	-1.752554
H	-2.347918	-1.055211	-2.064855
H	-0.603893	-1.066910	-2.178748
H	-1.473877	0.468634	-2.231647
C	0.264344	3.285504	0.043963
H	-0.241436	4.239610	0.232667
H	0.750054	3.368626	-0.933571
H	1.031978	3.187182	0.815965
C	0.265507	0.506601	1.718055
H	0.672044	1.455997	2.087185
H	-0.615082	0.333094	2.346408
C	1.135316	0.531146	-0.681736
H	1.718643	1.455594	-0.620270
H	0.867028	0.477829	-1.742265
C	1.309931	-0.569710	2.051402
H	1.604342	-0.443793	3.102889
H	0.849667	-1.560535	2.014588
C	2.110976	-0.591281	-0.323418
H	1.683696	-1.562993	-0.573510
C	2.560971	-0.558989	1.151472
Cl	3.505383	0.936191	1.539476
C	3.438119	-1.766631	1.518100
H	2.931654	-2.707180	1.273047
H	3.658791	-1.784596	2.592056
H	4.398410	-1.759855	0.992469
Br	3.632026	-0.497083	-1.583129

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2590807**

SCF Energy (B3LYP/6-31G) = -6264.29888838**

1i_C002

MMFF Geometry

C	-1.333384	-0.419893	-0.225872
C	-3.144810	1.445888	-0.027012
C	-0.159843	0.636886	0.245393
C	-2.692713	0.049082	0.406291
H	-3.956161	1.784324	0.628657
H	-2.589404	0.048308	1.498065
C	-2.018566	2.418259	0.037604
H	-2.315686	3.463971	-0.021820
C	-0.712832	2.108980	0.161886
O	-3.638076	1.472850	-1.362923
H	-3.887631	2.388644	-1.568689
Br	-4.201735	-1.203507	0.157149
C	-1.070955	-1.875569	0.231914
H	-1.758811	-2.581789	-0.246970
H	-1.203224	-1.990515	1.312213
H	-0.079992	-2.232350	-0.038497
C	-1.431703	-0.469482	-1.774336
H	-2.331190	-0.993762	-2.112243
H	-0.584514	-1.014984	-2.205968
H	-1.441591	0.527386	-2.224577
C	0.256022	3.275865	0.237045
H	-0.252758	4.215592	0.481546
H	0.753743	3.422638	-0.726909
H	1.015215	3.128459	1.009184
C	0.255318	0.417569	1.742530
H	0.654941	1.348394	2.162041
H	-0.626290	0.207562	2.358413
C	1.127929	0.563277	-0.653164
H	1.709156	1.484908	-0.545891
H	0.860783	0.562127	-1.715379
C	1.305783	-0.667530	2.025602
H	1.601778	-0.586860	3.081128
H	0.850226	-1.658077	1.947118
C	2.103172	-0.575307	-0.349569
H	1.674615	-1.533935	-0.644754
C	2.554915	-0.611634	1.124840
Cl	3.495889	0.866801	1.581517
C	3.435918	-1.832624	1.433278
H	2.931948	-2.761994	1.144366
H	3.657580	-1.900695	2.505022
H	4.395761	-1.798186	0.907929
Br	3.623178	-0.420213	-1.604720

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2552897**

SCF Energy (B3LYP/6-31G) = -6264.29112421**

1i_C003

MMFF Geometry

C	1.378547	-0.646447	1.204367
C	3.490650	-0.900562	-0.260316
C	0.389536	-1.013495	-0.058054
C	2.746916	-0.022343	0.747896
H	3.908461	-1.774157	0.251977
H	3.402341	0.138417	1.613946
C	2.601975	-1.397254	-1.343588
H	3.127712	-1.768793	-2.222698
C	1.255873	-1.455205	-1.296684
O	4.605578	-0.238334	-0.848554
H	4.272542	0.610794	-1.193844
Br	2.601243	1.821256	0.042926
C	1.761234	-1.943943	1.989942
H	2.553217	-1.743479	2.722105
H	2.123258	-2.739474	1.331351
H	0.912300	-2.338667	2.558548
C	0.771351	0.284556	2.280587
H	1.496029	0.469556	3.084163
H	-0.105809	-0.151027	2.762019
H	0.495123	1.265723	1.889367
C	0.570309	-2.029232	-2.526290
H	1.231207	-2.023192	-3.401190
H	-0.317636	-1.464217	-2.815128
H	0.282207	-3.070920	-2.352984
C	-0.571324	-2.217065	0.259532
H	-0.994745	-2.613400	-0.669072
H	-0.023515	-3.071839	0.668940
C	-0.521387	0.187439	-0.505630
H	-0.868545	0.024174	-1.531497
H	0.061936	1.105927	-0.577783
C	-1.769519	-1.905551	1.157333
H	-2.363787	-2.822558	1.271945
H	-1.424302	-1.661897	2.165842
C	-1.773701	0.460381	0.347004
H	-1.496517	0.901357	1.304899
C	-2.659449	-0.772818	0.605347
Cl	-3.451422	-1.361150	-0.912631
C	-3.773706	-0.483784	1.623282
H	-3.357624	-0.098735	2.561264
H	-4.335412	-1.393947	1.864940
H	-4.494708	0.252365	1.253354
Br	-2.762329	1.954348	-0.488231

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2596971**

SCF Energy (B3LYP/6-31G) = -6264.29733199**

1i_C004

MMFF Geometry

C	-1.338261	-0.417905	-0.222362
C	-3.147084	1.456433	-0.023305
C	-0.160647	0.640648	0.234255
C	-2.696943	0.057353	0.408147
H	-3.935567	1.802689	0.655392
H	-2.590949	0.058544	1.499716
C	-2.015332	2.424874	0.019529
H	-2.317988	3.469748	-0.044890
C	-0.709501	2.112857	0.130231
O	-3.697307	1.489609	-1.338173
H	-3.062914	1.918317	-1.935872
Br	-4.205120	-1.196427	0.164858
C	-1.075846	-1.869016	0.250960
H	-1.764477	-2.580184	-0.219383
H	-1.206469	-1.972156	1.332644
H	-0.085423	-2.229112	-0.016692
C	-1.439313	-0.484882	-1.769694
H	-2.347749	-0.996878	-2.101830
H	-0.601394	-1.049766	-2.194748
H	-1.430094	0.505431	-2.232567
C	0.262886	3.278257	0.183968
H	-0.242279	4.223204	0.415469
H	0.757328	3.408581	-0.784028
H	1.024406	3.140251	0.955588
C	0.252954	0.442382	1.734821
H	0.652881	1.378962	2.141190
H	-0.629348	0.242142	2.352901
C	1.127099	0.548694	-0.663040
H	1.708745	1.471933	-0.573784
H	0.859911	0.527082	-1.724973
C	1.302027	-0.639419	2.034918
H	1.595956	-0.544523	3.089820
H	0.845801	-1.630609	1.968470
C	2.102729	-0.584445	-0.338995
H	1.675048	-1.548123	-0.618489
C	2.552967	-0.596367	1.136044
Cl	3.491158	0.890498	1.569006
C	3.434924	-1.811081	1.465460
H	2.932363	-2.745652	1.191251
H	3.655405	-1.861296	2.538430
H	4.395335	-1.784133	0.940705
Br	3.622957	-0.449576	-1.595934

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2568555**

SCF Energy (B3LYP/6-31G) = -6264.29287061**

1i_C005

MMFF Geometry

C	-1.437998	-0.534639	-0.249062
C	-3.078615	1.476063	-0.148664
C	-0.176399	0.499332	-0.091832
C	-2.664863	0.126220	0.460320
H	-3.648510	2.053403	0.588567
H	-2.423274	0.280900	1.517838
C	-1.912078	2.284898	-0.617714
H	-2.183734	3.258578	-1.023894
C	-0.621217	1.888597	-0.642580
O	-3.910975	1.328402	-1.299322
H	-4.590808	0.668563	-1.072455
Br	-4.256650	-1.032706	0.592928
C	-1.132064	-1.917316	0.384531
H	-1.902623	-2.654532	0.132219
H	-1.080805	-1.875188	1.475876
H	-0.194183	-2.337241	0.012123
C	-1.751273	-0.812058	-1.751134
H	-2.718235	-1.309495	-1.877151
H	-1.014301	-1.482894	-2.204335
H	-1.770642	0.096526	-2.358629
C	0.382219	2.841645	-1.249097
H	-0.033957	3.847187	-1.380717
H	0.688476	2.493364	-2.240609
H	1.268044	2.956583	-0.625539
C	0.163355	0.717235	1.430637
H	-0.567828	1.388038	1.899760
H	0.090348	-0.224190	1.983262
C	1.099288	-0.060750	-0.819950
H	1.584255	0.696787	-1.441144
H	0.827466	-0.840948	-1.535092
C	1.556787	1.287690	1.717329
H	1.586277	2.326075	1.373126
H	1.669876	1.362510	2.807258
C	2.149968	-0.620953	0.147528
H	1.711903	-1.441980	0.725381
C	2.710807	0.443799	1.117288
Cl	3.838039	1.595102	0.288415
C	3.504273	-0.218860	2.256761
H	2.873471	-0.920677	2.814292
H	3.875472	0.526189	2.970630
H	4.373413	-0.773885	1.888836
Br	3.538589	-1.545666	-0.895907

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2534548**

SCF Energy (B3LYP/6-31G) = -6264.29210537**

1i_C006

MMFF Geometry

C	-1.533759	0.436843	1.334270
C	-3.441294	0.979985	-0.305691
C	-0.398353	0.998135	0.293797
C	-2.828515	-0.079460	0.618032
H	-3.960261	1.728605	0.303882
H	-3.584115	-0.365034	1.361596
C	-2.426019	1.705617	-1.119605
H	-2.844592	2.277555	-1.947421
C	-1.097693	1.742684	-0.887715
O	-4.434583	0.452914	-1.178457
H	-4.038188	-0.326248	-1.610728
Br	-2.614952	-1.780987	-0.356396
C	-2.023040	1.593599	2.275674
H	-2.910739	1.288898	2.843417
H	-2.282275	2.500804	1.721291
H	-1.268315	1.869419	3.019634
C	-0.995937	-0.650618	2.298619
H	-1.787852	-0.992059	2.976520
H	-0.186297	-0.268314	2.928301
H	-0.617764	-1.536304	1.783191
C	-0.268986	2.575118	-1.841701
H	-0.838338	2.874806	-2.729418
H	0.600270	2.026845	-2.210775
H	0.060075	3.497518	-1.354539
C	0.553947	1.982654	1.074449
H	0.079187	2.967817	1.170543
H	0.702774	1.619800	2.098252
C	0.484691	-0.149668	-0.313688
H	0.691638	0.026757	-1.375945
H	-0.051882	-1.095444	-0.311850
C	1.964703	2.185699	0.503809
H	1.900258	2.766052	-0.419581
H	2.509812	2.844938	1.193006
C	1.817358	-0.346006	0.416483
H	1.626559	-0.547929	1.475455
C	2.756212	0.871714	0.287640
Cl	3.515467	0.980770	-1.355698
C	3.903485	0.786855	1.308403
H	3.512694	0.742237	2.331429
H	4.559305	1.663462	1.246372
H	4.530282	-0.097515	1.153590
Br	2.629542	-2.035069	-0.181557

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2538368**

SCF Energy (B3LYP/6-31G) = -6264.29102182**

1i_C007

MMFF Geometry

C	1.379590	-0.611328	1.208896
C	3.498630	-0.877428	-0.240289
C	0.397283	-0.997089	-0.052775
C	2.745841	0.017493	0.747317
H	3.887762	-1.753843	0.290344
H	3.395649	0.194643	1.614529
C	2.616686	-1.373197	-1.334356
H	3.130661	-1.740034	-2.220524
C	1.269946	-1.437576	-1.288876
O	4.646979	-0.228920	-0.776748
H	5.011834	-0.788862	-1.480748
Br	2.578350	1.850878	0.024822
C	1.766735	-1.897581	2.011033
H	2.557002	-1.684579	2.741487
H	2.132163	-2.700405	1.363384
H	0.918758	-2.289010	2.583325
C	0.763080	0.326834	2.274094
H	1.485310	0.527026	3.076229
H	-0.110767	-0.111205	2.759553
H	0.478157	1.301107	1.872085
C	0.587131	-2.012291	-2.520376
H	1.250007	-2.007072	-3.393785
H	-0.300131	-1.448566	-2.813084
H	0.299191	-3.054035	-2.347252
C	-0.550140	-2.209503	0.270778
H	-0.969518	-2.614755	-0.655800
H	0.007076	-3.056338	0.683976
C	-0.528145	0.191117	-0.507316
H	-0.873948	0.018278	-1.531789
H	0.044064	1.116075	-0.585094
C	-1.750499	-1.906100	1.168513
H	-2.333753	-2.829235	1.290231
H	-1.406799	-1.651307	2.174803
C	-1.783989	0.454703	0.343002
H	-1.512882	0.906712	1.297477
C	-2.654327	-0.787619	0.610331
Cl	-3.441136	-1.396457	-0.902613
C	-3.770924	-0.505421	1.627686
H	-3.358505	-0.109213	2.562635
H	-4.321303	-1.420702	1.875990
H	-4.501198	0.219495	1.253791
Br	-2.792828	1.929032	-0.503661

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2556294**

SCF Energy (B3LYP/6-31G) = -6264.28888645**

1i_C008

MMFF Geometry

C	1.576772	-0.306969	0.619464
C	2.828584	1.306595	-0.982382
C	0.125054	0.137740	-0.035266
C	2.672493	-0.132605	-0.482022
H	3.331231	1.306187	-1.956706
H	2.419830	-0.772625	-1.335908
C	1.517988	2.004814	-1.103679
H	1.594644	2.999402	-1.542054
C	0.315459	1.544706	-0.695367
O	3.609768	2.118978	-0.107639
H	4.411898	1.609422	0.106658
Br	4.456522	-0.813976	0.023385
C	1.581839	-1.785861	1.106377
H	2.452021	-1.994294	1.739615
H	1.621689	-2.496457	0.275352
H	0.714229	-2.036197	1.718815
C	1.886874	0.562628	1.873258
H	2.911390	0.411546	2.228055
H	1.232943	0.303238	2.712866
H	1.757082	1.632674	1.690375
C	-0.852375	2.470073	-0.907656
H	-0.577844	3.361311	-1.484929
H	-1.226314	2.836005	0.050989
H	-1.646637	1.986271	-1.474683
C	-0.253457	-0.836269	-1.199064
H	0.260880	-0.544600	-2.124974
H	0.111023	-1.845150	-0.994503
C	-0.971758	0.137771	1.106791
H	-0.961187	1.106861	1.622726
H	-0.651854	-0.563815	1.882650
C	-1.741442	-0.962679	-1.523798
H	-2.111129	-0.031302	-1.962926
H	-1.850493	-1.720163	-2.312157
C	-2.425074	-0.306446	0.812636
H	-2.833457	-0.725832	1.742470
C	-2.578859	-1.356036	-0.304360
Cl	-4.294432	-1.568667	-0.848487
C	-2.164845	-2.742636	0.227982
H	-1.154685	-2.746228	0.641449
H	-2.196374	-3.500191	-0.563991
H	-2.833547	-3.074548	1.031498
Br	-3.592283	1.265549	0.619964

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2462078**

SCF Energy (B3LYP/6-31G) = -6264.28497702**

1i_C009

MMFF Geometry

C	-1.442787	-0.537962	-0.261582
C	-3.093973	1.461941	-0.167538
C	-0.183615	0.495836	-0.078060
C	-2.677487	0.113965	0.443432
H	-3.703363	2.015220	0.556730
H	-2.433764	0.276567	1.499326
C	-1.919171	2.294787	-0.582087
H	-2.173662	3.288270	-0.947649
C	-0.626831	1.901729	-0.593471
O	-3.882705	1.289304	-1.344551
H	-4.188568	2.166435	-1.627781
Br	-4.249916	-1.063389	0.604065
C	-1.140185	-1.929893	0.353662
H	-1.901810	-2.666788	0.074264
H	-1.108881	-1.907053	1.446354
H	-0.193805	-2.338307	-0.009591
C	-1.741748	-0.795742	-1.769609
H	-2.718617	-1.269276	-1.911649
H	-1.014328	-1.480168	-2.218389
H	-1.729664	0.118498	-2.368998
C	0.386739	2.878864	-1.143781
H	-0.028999	3.888052	-1.245680
H	0.712766	2.569191	-2.141740
H	1.260035	2.972638	-0.500268
C	0.154027	0.673584	1.450455
H	-0.577094	1.333331	1.935063
H	0.077128	-0.281810	1.977727
C	1.093135	-0.043772	-0.819152
H	1.575440	0.729955	-1.422232
H	0.822813	-0.806585	-1.553361
C	1.547700	1.230656	1.761645
H	1.578794	2.282963	1.463355
H	1.657701	1.259695	2.854170
C	2.145727	-0.626537	0.132936
H	1.711661	-1.464773	0.688428
C	2.703983	0.412639	1.131104
Cl	3.819661	1.595257	0.330145
C	3.508190	-0.276900	2.246940
H	2.885779	-1.000345	2.785957
H	3.876273	0.449805	2.981062
H	4.380425	-0.813268	1.859243
Br	3.537885	-1.515903	-0.937201

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2497497**

SCF Energy (B3LYP/6-31G) = -6264.28430699**

1i_C010

MMFF Geometry

C	1.707084	1.432624	0.387259
C	3.040848	-0.619516	1.220626
C	0.280706	0.662736	0.675989
C	2.884456	0.434709	0.116061
H	3.670238	-0.177986	2.004104
H	3.828858	0.991582	0.050155
C	1.772628	-1.015186	1.899508
H	1.913903	-1.773219	2.670229
C	0.556936	-0.450709	1.736601
O	3.722830	-1.797490	0.812806
H	3.297337	-2.094098	-0.012401
Br	2.855561	-0.406716	-1.668166
C	2.120245	2.266378	1.650763
H	3.130690	2.676725	1.533533
H	2.115428	1.676923	2.571837
H	1.454461	3.121621	1.809121
C	1.646886	2.489771	-0.753056
H	2.629127	2.960865	-0.886510
H	0.946262	3.299842	-0.531574
H	1.367085	2.081752	-1.725365
C	-0.507398	-0.871019	2.725094
H	-1.401755	-1.248068	2.240756
H	-0.783111	-0.035294	3.375081
H	-0.163805	-1.673543	3.388627
C	-0.751245	1.712401	1.211438
H	-0.556154	1.931815	2.268944
H	-0.608855	2.670197	0.703668
C	-0.264019	-0.017471	-0.637738
H	0.223355	-0.989724	-0.776496
H	0.049814	0.585601	-1.491833
C	-2.237626	1.369710	1.064571
H	-2.516174	0.571592	1.757835
H	-2.817654	2.244904	1.388639
C	-1.777425	-0.192003	-0.861878
H	-1.941133	-0.316694	-1.940968
C	-2.625275	0.990916	-0.367526
Cl	-4.398871	0.632933	-0.400159
C	-2.439846	2.192948	-1.317169
H	-1.392108	2.490220	-1.416341
H	-2.995007	3.069738	-0.963420
H	-2.798526	1.958496	-2.326698
Br	-2.344013	-1.956738	-0.214518

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.2489265**

SCF Energy (B3LYP/6-31G) = -6264.28691829**

1i_C011

MMFF Geometry

C	1.578078	0.305286	-0.619716
C	2.807556	-1.292835	1.019553
C	0.133533	-0.048826	0.085231
C	2.703547	0.127989	0.454016
H	3.365800	-1.272330	1.963073
H	2.523562	0.812993	1.289132
C	1.466234	-1.897827	1.257181
H	1.498539	-2.851630	1.782158
C	0.278277	-1.391376	0.866842
O	3.488872	-2.193804	0.149526
H	4.309800	-1.748481	-0.127081
Br	4.497094	0.698155	-0.146167
C	1.594445	1.763839	-1.156097
H	2.463543	1.947835	-1.797262
H	1.631358	2.498167	-0.345424
H	0.719209	1.992113	-1.769959
C	1.835485	-0.625912	-1.842357
H	2.865809	-0.550659	-2.203339
H	1.203141	-0.361782	-2.696436
H	1.640924	-1.677970	-1.615650
C	-0.957815	-2.182274	1.222410
H	-0.732246	-3.023455	1.888286
H	-1.418037	-2.609107	0.328678
H	-1.682156	-1.563609	1.749397
C	-0.243206	1.042968	1.140578
H	-0.582232	0.576275	2.073795
H	0.633505	1.617545	1.452399
C	-0.966716	-0.177940	-1.032993
H	-0.992197	-1.206850	-1.414626
H	-0.618157	0.391909	-1.901417
C	-1.301518	2.050836	0.689574
H	-1.452580	2.783025	1.494172
H	-0.925910	2.623945	-0.166353
C	-2.390990	0.376464	-0.819676
H	-2.616119	0.907453	-1.756560
C	-2.633153	1.381344	0.325976
Cl	-3.322548	0.648713	1.828549
C	-3.636398	2.463076	-0.114691
H	-3.272393	3.004755	-0.995455
H	-3.799375	3.205467	0.675584
H	-4.609717	2.029949	-0.371120
Br	-3.730977	-1.051644	-0.958762

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2458515**

SCF Energy (B3LYP/6-31G) = -6264.28484945**

1i_C012

MMFF Geometry

C	-1.534440	0.398518	1.335945
C	-3.451986	0.955124	-0.286204
C	-0.405538	0.980657	0.300515
C	-2.826432	-0.119267	0.612782
H	-3.947558	1.699459	0.348406
H	-3.576563	-0.423042	1.354860
C	-2.441414	1.688619	-1.106317
H	-2.847247	2.267214	-1.933921
C	-1.112355	1.730419	-0.874583
O	-4.485001	0.431033	-1.113451
H	-4.739438	1.112305	-1.756104
Br	-2.590168	-1.807193	-0.377142
C	-2.030266	1.539331	2.293687
H	-2.918431	1.223019	2.854276
H	-2.290294	2.454478	1.752948
H	-1.278458	1.806240	3.043896
C	-0.986532	-0.696013	2.287070
H	-1.775076	-1.052010	2.961409
H	-0.179704	-0.314100	2.920655
H	-0.600756	-1.572457	1.761682
C	-0.286508	2.570438	-1.825196
H	-0.855286	2.868051	-2.713965
H	0.587866	2.030125	-2.193564
H	0.034295	3.494156	-1.334996
C	0.536480	1.967757	1.090618
H	0.051504	2.946997	1.195716
H	0.689015	1.596691	2.110933
C	0.490400	-0.152628	-0.317029
H	0.695402	0.034476	-1.377704
H	-0.035326	-1.104359	-0.323389
C	1.945074	2.191128	0.522881
H	1.874975	2.779204	-0.395161
H	2.482655	2.849955	1.218371
C	1.825057	-0.341390	0.411327
H	1.636078	-0.556138	1.468103
C	2.750701	0.887794	0.295535
Cl	3.511978	1.022003	-1.345154
C	3.897167	0.805611	1.317565
H	3.505153	0.746858	2.339411
H	4.543489	1.689875	1.265207
H	4.533892	-0.070300	1.155369
Br	2.657875	-2.014681	-0.202824

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2496697**

SCF Energy (B3LYP/6-31G) = -6264.28237928**

1j_C001

MMFF Geometry

C	-1.439536	-0.349983	-0.461804
C	-3.041528	1.397212	0.599846
C	-0.156329	0.384113	0.255562
C	-2.696786	-0.086282	0.426723
H	-3.682789	1.525812	1.479726
H	-2.525157	-0.519661	1.419269
C	-1.827819	2.251934	0.745019
H	-2.053615	3.297479	0.951665
C	-0.544938	1.861230	0.590026
O	-3.747877	1.938093	-0.515926
H	-4.448563	1.299339	-0.740459
Br	-4.322341	-1.043118	-0.159665
C	-1.235244	-1.887536	-0.603438
H	-1.945395	-2.320713	-1.317454
H	-1.386841	-2.411333	0.346028
H	-0.242525	-2.153602	-0.972085
C	-1.632312	0.198792	-1.904004
H	-2.568841	-0.149426	-2.350903
H	-0.831422	-0.143601	-2.568900
H	-1.635867	1.291500	-1.943792
C	0.505936	2.938309	0.709153
H	0.073179	3.914164	0.959748
H	1.032421	3.074382	-0.239728
H	1.223005	2.715827	1.499915
C	0.171946	-0.331466	1.608929
H	-0.552258	-0.038253	2.380165
H	0.054102	-1.412752	1.507035
C	1.080996	0.314271	-0.706397
H	0.963845	1.060327	-1.504682
H	1.088226	-0.647182	-1.227993
C	1.572695	-0.102008	2.182938
H	1.647250	0.922516	2.562144
H	1.691187	-0.742598	3.067795
C	2.466323	0.493394	-0.066765
H	2.633096	1.541925	0.190144
C	2.708227	-0.376518	1.179191
Cl	2.700118	-2.139954	0.778473
C	4.049044	-0.061339	1.860828
H	4.907554	-0.325266	1.234879
H	4.154641	-0.614393	2.801774
H	4.126537	1.005629	2.099058
Br	3.821633	0.209964	-1.475615

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2642846**

SCF Energy (B3LYP/6-31G) = -6264.30169961**

1j_C002

MMFF Geometry

C	-1.441464	-0.342646	-0.476013
C	-3.053740	1.397013	0.578092
C	-0.163198	0.378880	0.263386
C	-2.705753	-0.085852	0.404843
H	-3.730577	1.512636	1.433046
H	-2.530013	-0.513425	1.399398
C	-1.837577	2.243021	0.779621
H	-2.051714	3.280487	1.031142
C	-0.554119	1.848893	0.634983
O	-3.716446	1.930760	-0.566817
H	-4.014963	2.827631	-0.344467
Br	-4.315151	-1.073761	-0.165413
C	-1.235977	-1.878047	-0.639297
H	-1.934088	-2.298738	-1.372496
H	-1.403600	-2.417404	0.298734
H	-0.236896	-2.138013	-0.995302
C	-1.621115	0.225340	-1.912183
H	-2.563994	-0.100566	-2.362888
H	-0.825551	-0.124351	-2.579795
H	-1.602250	1.318336	-1.939766
C	0.501887	2.913798	0.809944
H	0.071568	3.882569	1.090435
H	1.041985	3.081609	-0.126136
H	1.206676	2.658398	1.601385
C	0.162561	-0.369786	1.600507
H	-0.559955	-0.090361	2.378438
H	0.038555	-1.447699	1.474615
C	1.076615	0.335384	-0.696896
H	0.962040	1.104870	-1.473077
H	1.083474	-0.610540	-1.246511
C	1.564643	-0.165510	2.180848
H	1.644616	0.845636	2.592912
H	1.679637	-0.834013	3.045351
C	2.460667	0.493468	-0.049425
H	2.627531	1.533459	0.240165
C	2.699542	-0.414038	1.169856
Cl	2.686772	-2.164286	0.717128
C	4.040911	-0.123247	1.861402
H	4.899124	-0.371850	1.228803
H	4.143837	-0.703724	2.785994
H	4.121807	0.936091	2.130562
Br	3.818749	0.253067	-1.463306

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2605934**

SCF Energy (B3LYP/6-31G) = -6264.29368623**

1j_C003

MMFF Geometry

C	-1.605688	0.969793	1.063373
C	-3.353883	0.626594	-0.794095
C	-0.388921	1.082203	-0.034765
C	-2.811804	0.118620	0.547800
H	-4.012624	1.480485	-0.593309
H	-3.631170	0.148111	1.278169
C	-2.305327	1.119995	-1.734125
H	-2.687524	1.355885	-2.727285
C	-1.009468	1.361564	-1.442608
O	-4.165422	-0.319939	-1.478953
H	-3.685731	-1.168414	-1.452233
Br	-2.470022	-1.822556	0.469970
C	-2.182845	2.398543	1.360142
H	-3.104646	2.333503	1.951014
H	-2.417571	2.956675	0.449004
H	-1.485122	3.007822	1.944792
C	-1.155572	0.444999	2.456152
H	-1.997505	0.460157	3.159825
H	-0.368941	1.063714	2.897044
H	-0.787049	-0.582269	2.443121
C	-0.176993	1.969843	-2.546577
H	-0.734604	2.055559	-3.486894
H	0.701472	1.367886	-2.774628
H	0.131145	2.985272	-2.282362
C	0.564592	2.248357	0.407080
H	0.116681	3.216041	0.144978
H	0.649983	2.260752	1.497779
C	0.422438	-0.254980	-0.126429
H	-0.115366	-0.965061	-0.765467
H	0.478177	-0.723833	0.858220
C	2.002509	2.242756	-0.126380
H	2.011150	2.544628	-1.178347
H	2.564618	3.029132	0.396369
C	1.856688	-0.174472	-0.664446
H	1.841228	-0.005207	-1.743919
C	2.723685	0.893149	0.020554
Cl	2.945922	0.554599	1.782289
C	4.119693	1.013084	-0.610588
H	4.728268	0.117026	-0.451783
H	4.674896	1.857855	-0.185669
H	4.048579	1.179792	-1.691488
Br	2.645157	-1.983286	-0.550106

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2580378**

SCF Energy (B3LYP/6-31G) = -6264.29746189**

1j_C004

MMFF Geometry

C	-1.431363	-0.307890	-0.409031
C	-3.092154	1.402080	0.626501
C	-0.182013	0.405338	0.366822
C	-2.729227	-0.074412	0.431422
H	-3.795085	1.498950	1.462468
H	-2.605045	-0.530718	1.419564
C	-1.890733	2.241233	0.897946
H	-2.124356	3.266278	1.182512
C	-0.603768	1.850119	0.798746
O	-3.716886	1.983847	-0.515054
H	-4.408432	1.361444	-0.804063
Br	-4.324741	-1.020114	-0.249533
C	-1.202922	-1.830317	-0.585185
H	-1.929634	-2.272209	-1.275950
H	-1.299507	-2.364578	0.365275
H	-0.221204	-2.056509	-1.009077
C	-1.582712	0.284993	-1.841034
H	-2.511933	-0.037506	-2.320902
H	-0.773686	-0.045452	-2.501456
H	-1.570477	1.378566	-1.845900
C	0.455540	2.877448	1.134885
H	0.019813	3.838647	1.431571
H	1.096882	3.082689	0.273597
H	1.071100	2.546194	1.975377
C	0.214354	-0.332739	1.696769
H	0.608965	0.383477	2.429509
H	-0.666638	-0.762833	2.183416
C	1.067561	0.455132	-0.582836
H	1.022600	1.356617	-1.207952
H	1.051431	-0.376364	-1.294831
C	1.273201	-1.433973	1.558239
H	1.476129	-1.837542	2.559313
H	0.833419	-2.274152	1.014431
C	2.399171	0.379950	0.169180
H	2.461688	1.188203	0.901744
C	2.595398	-0.972162	0.891597
Cl	3.087296	-2.297854	-0.245206
C	3.700204	-0.858720	1.955183
H	4.666197	-0.586114	1.517264
H	3.840876	-1.805811	2.489462
H	3.446647	-0.097059	2.701398
Br	3.856687	0.843601	-1.065126

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2565690**

SCF Energy (B3LYP/6-31G) = -6264.29470353**

1j_C005

MMFF Geometry

C	-1.604911	0.934224	1.083075
C	-3.365410	0.614995	-0.766653
C	-0.395073	1.071116	-0.019039
C	-2.806495	0.079595	0.558833
H	-4.009672	1.472622	-0.534296
H	-3.620304	0.090291	1.296169
C	-2.322038	1.125449	-1.710597
H	-2.694804	1.384757	-2.699998
C	-1.025306	1.367884	-1.420202
O	-4.215614	-0.318198	-1.422542
H	-4.418965	0.018492	-2.309505
Br	-2.441101	-1.855015	0.461220
C	-2.190894	2.354360	1.404271
H	-3.111680	2.273491	1.994739
H	-2.429358	2.926884	0.503121
H	-1.496414	2.958153	1.998473
C	-1.143846	0.394116	2.466840
H	-1.983454	0.390010	3.173447
H	-0.362598	1.015199	2.914002
H	-0.763528	-0.628465	2.438514
C	-0.197046	1.993258	-2.518262
H	-0.755918	2.087538	-3.456984
H	0.683776	1.398236	-2.754869
H	0.106398	3.007002	-2.242467
C	0.551090	2.238842	0.435251
H	0.094594	3.206432	0.187996
H	0.640408	2.237216	1.525682
C	0.427261	-0.258063	-0.133660
H	-0.106143	-0.961945	-0.783174
H	0.488840	-0.741929	0.843290
C	1.987098	2.252169	-0.102890
H	1.990069	2.567840	-1.150796
H	2.544374	3.036310	0.428346
C	1.859874	-0.158883	-0.672529
H	1.841069	0.024356	-1.749661
C	2.719764	0.906846	0.024280
Cl	2.950869	0.547890	1.780729
C	4.112833	1.047177	-0.609440
H	4.729787	0.154592	-0.463979
H	4.661927	1.891276	-0.175331
H	4.036967	1.227156	-1.687889
Br	2.665483	-1.961630	-0.584149

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2547215**

SCF Energy (B3LYP/6-31G) = -6264.28849581**

1j_C006

MMFF Geometry

C	-1.435653	-0.309680	-0.420703
C	-3.099759	1.413596	0.582886
C	-0.189777	0.398983	0.365142
C	-2.738473	-0.066478	0.410160
H	-3.835597	1.513895	1.389778
H	-2.609663	-0.501348	1.407587
C	-1.896933	2.241903	0.898418
H	-2.119564	3.259203	1.215773
C	-0.611421	1.841621	0.813327
O	-3.678869	1.973661	-0.592606
H	-3.920190	2.893478	-0.395980
Br	-4.321726	-1.049766	-0.236583
C	-1.209324	-1.832568	-0.595793
H	-1.931167	-2.272485	-1.292963
H	-1.313560	-2.367655	0.353363
H	-0.224868	-2.059135	-1.013406
C	-1.574389	0.280441	-1.854674
H	-2.512229	-0.022690	-2.330784
H	-0.773994	-0.071470	-2.514678
H	-1.534812	1.373412	-1.863961
C	0.451335	2.853212	1.186754
H	0.018950	3.811886	1.496213
H	1.105924	3.070501	0.338392
H	1.052765	2.501207	2.028898
C	0.203159	-0.355323	1.688139
H	0.592924	0.351701	2.431954
H	-0.679135	-0.792955	2.165755
C	1.062641	0.459489	-0.579756
H	1.019348	1.368635	-1.193883
H	1.048364	-0.364110	-1.301018
C	1.264877	-1.453369	1.542208
H	1.466405	-1.864368	2.540579
H	0.828280	-2.290677	0.991567
C	2.392249	0.375612	0.174972
H	2.452614	1.174847	0.917453
C	2.587752	-0.984319	0.882225
Cl	3.082428	-2.296246	-0.268841
C	3.691046	-0.882633	1.948704
H	4.657698	-0.605067	1.515384
H	3.831024	-1.835645	2.472550
H	3.436289	-0.129404	2.703034
Br	3.852866	0.856115	-1.049203

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2529937**

SCF Energy (B3LYP/6-31G) = -6264.28680997**

1k_C001

MMFF Geometry

C	-1.278515	-0.369078	-0.397395
C	-3.224195	1.310826	-0.067690
C	-0.199033	0.721311	0.198186
C	-2.676961	-0.079683	0.251296
H	-3.653191	1.363968	-1.075365
H	-2.638534	-0.229468	1.336430
C	-2.179606	2.360593	0.054954
H	-2.566302	3.379006	0.042099
C	-0.854919	2.149719	0.178779
O	-4.257668	1.657356	0.854312
H	-4.948342	0.976099	0.765999
Br	-4.094192	-1.374549	-0.266983
C	-0.910396	-1.839530	-0.091403
H	-1.533836	-2.540613	-0.657850
H	-1.052633	-2.079583	0.966663
H	0.109023	-2.089114	-0.373538
C	-1.365050	-0.250563	-1.945486
H	-2.193023	-0.834083	-2.359427
H	-0.459763	-0.641715	-2.422943
H	-1.498987	0.782900	-2.278708
C	0.014199	3.382874	0.337082
H	-0.574730	4.271306	0.593162
H	0.537963	3.606166	-0.597851
H	0.748640	3.260575	1.137208
C	0.164487	0.433877	1.695710
H	0.492749	1.358674	2.185685
H	-0.727025	0.134482	2.257601
C	1.130773	0.794392	-0.638224
H	1.635636	1.746840	-0.446879
H	0.912931	0.839515	-1.710516
C	1.265661	-0.604064	1.954562
H	1.496310	-0.594021	3.028952
H	0.880399	-1.608954	1.763736
C	2.180528	-0.282595	-0.353345
H	1.850684	-1.248194	-0.738196
C	2.552875	-0.375731	1.139471
Cl	3.610660	-1.820834	1.418037
C	3.305255	0.847861	1.691593
H	3.467216	0.753743	2.772321
H	2.753948	1.778657	1.531885
H	4.293253	0.969044	1.235756
Br	3.745538	0.092802	-1.502899

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2619414**

SCF Energy (B3LYP/6-31G) = -6264.29891747**

1k_C002

MMFF Geometry

C	1.438407	0.328109	-0.676417
C	2.757433	-1.552549	0.496351
C	0.026224	-0.235169	-0.036383
C	2.590949	-0.044033	0.307721
H	3.347241	-1.999629	-0.313153
H	2.443371	0.445507	1.277848
C	1.454129	-2.272471	0.561759
H	1.546746	-3.327474	0.816912
C	0.234784	-1.744103	0.322837
O	3.441577	-1.825665	1.718531
H	4.305513	-1.380104	1.658686
Br	4.360927	0.671017	-0.228482
C	1.423394	1.872046	-0.876749
H	2.240246	2.197440	-1.531307
H	1.545742	2.413030	0.066646
H	0.508207	2.233317	-1.348607
C	1.679615	-0.299646	-2.082713
H	2.660278	-0.028272	-2.486221
H	0.945633	0.054364	-2.813952
H	1.624873	-1.391713	-2.074892
C	-0.935986	-2.680529	0.452278
H	-0.641169	-3.663809	0.838237
H	-1.388223	-2.862682	-0.525039
H	-1.675958	-2.296754	1.154041
C	-0.262834	0.492461	1.317280
H	0.278294	0.002135	2.138472
H	0.141412	1.506777	1.304854
C	-1.133246	-0.022341	-1.090476
H	-1.180415	-0.888966	-1.763007
H	-0.841565	0.793765	-1.757971
C	-1.727661	0.603233	1.738275
H	-2.106689	-0.380890	2.031019
H	-1.774398	1.213155	2.650893
C	-2.550571	0.387578	-0.633798
H	-3.003858	0.967443	-1.449925
C	-2.625304	1.214121	0.658701
Cl	-2.021812	2.891276	0.269894
C	-4.046208	1.417565	1.207789
H	-4.053952	2.142257	2.031317
H	-4.467711	0.491780	1.612772
H	-4.724775	1.791301	0.432467
Br	-3.756053	-1.167131	-0.636811

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2522965**

SCF Energy (B3LYP/6-31G) = -6264.29307080**

1k_C003

MMFF Geometry

C	-1.290030	-0.374462	-0.409284
C	-3.237426	1.308716	-0.061675
C	-0.207863	0.722689	0.167748
C	-2.687885	-0.086033	0.246417
H	-3.707181	1.346118	-1.051169
H	-2.640515	-0.240140	1.330444
C	-2.186304	2.360478	0.001507
H	-2.569836	3.379035	-0.058374
C	-0.860999	2.151340	0.114752
O	-4.237740	1.673995	0.890749
H	-3.806916	1.751650	1.758806
Br	-4.094076	-1.394933	-0.263448
C	-0.913417	-1.840896	-0.093277
H	-1.535197	-2.549752	-0.651766
H	-1.050139	-2.073272	0.967135
H	0.105602	-2.088055	-0.377659
C	-1.387422	-0.269051	-1.958154
H	-2.215642	-0.858868	-2.362346
H	-0.484420	-0.661414	-2.438755
H	-1.527553	0.760860	-2.299454
C	0.013502	3.386777	0.214445
H	-0.569986	4.286651	0.441398
H	0.528505	3.571523	-0.733634
H	0.754290	3.291976	1.012737
C	0.149061	0.470622	1.672449
H	0.479312	1.406890	2.139443
H	-0.745049	0.188702	2.238993
C	1.126701	0.770706	-0.665007
H	1.631409	1.727561	-0.497623
H	0.913839	0.786181	-1.739013
C	1.244977	-0.565018	1.959678
H	1.467516	-0.534830	3.035380
H	0.858506	-1.572283	1.784342
C	2.177851	-0.296471	-0.346997
H	1.855759	-1.271886	-0.712641
C	2.538864	-0.354965	1.150206
Cl	3.594398	-1.792500	1.470802
C	3.286559	0.881432	1.679762
H	3.436747	0.814179	2.764183
H	2.738195	1.808449	1.490654
H	4.279598	0.990351	1.231805
Br	3.751314	0.058526	-1.491921

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2594237**

SCF Energy (B3LYP/6-31G) = -6264.29375653**

1k_C004

MMFF Geometry

C	-1.28680	-0.37780	-0.40366
C	-3.23749	1.29594	-0.02856
C	-0.20554	0.71876	0.17262
C	-2.68052	-0.09797	0.26413
H	-3.72813	1.33376	-1.00865
H	-2.63110	-0.26591	1.34604
C	-2.18950	2.35174	0.02738
H	-2.56730	3.37208	-0.01183
C	-0.86179	2.14598	0.12354
O	-4.21090	1.63089	0.96133
H	-4.72893	2.37695	0.61582
Br	-4.08928	-1.40428	-0.26467
C	-0.90432	-1.84507	-0.09906
H	-1.52783	-2.55216	-0.65782
H	-1.03389	-2.08449	0.96065
H	0.11345	-2.08778	-0.39146
C	-1.39347	-0.26271	-1.95146
H	-2.22027	-0.85431	-2.35570
H	-0.49122	-0.64730	-2.43963
H	-1.54096	0.76860	-2.28531
C	0.01123	3.38224	0.22513
H	-0.57210	4.28070	0.45790
H	0.52197	3.57146	-0.72440
H	0.75555	3.28544	1.01985
C	0.15502	0.46421	1.67631
H	0.48436	1.40013	2.14460
H	-0.73717	0.17947	2.24437
C	1.12724	0.77091	-0.66267
H	1.62970	1.72901	-0.49574
H	0.91246	0.78648	-1.73626
C	1.25329	-0.57003	1.95921
H	1.47694	-0.54289	3.03475
H	0.86905	-1.57757	1.78057
C	2.18215	-0.29336	-0.34743
H	1.86317	-1.26924	-0.71444
C	2.54541	-0.35380	1.14904
Cl	3.60681	-1.78855	1.46442
C	3.28994	0.88382	1.68008
H	3.44129	0.81508	2.76424
H	2.73881	1.80958	1.49300
H	4.28224	0.99641	1.23137
Br	3.75306	0.06878	-1.49434

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2586026**

SCF Energy (B3LYP/6-31G) = -6264.29245023**

1k_C005

MMFF Geometry

C	-1.362023	-0.604427	-0.377798
C	-3.154675	1.259784	-0.386394
C	-0.199222	0.545419	-0.359281
C	-2.615244	0.009472	0.324209
H	-3.862442	0.989967	-1.180154
H	-2.397475	0.233531	1.374742
C	-2.091864	2.104219	-1.014209
H	-2.466546	3.002772	-1.502267
C	-0.775046	1.810550	-1.066144
O	-3.854362	2.090853	0.537287
H	-4.593547	1.560934	0.885238
Br	-4.128090	-1.253626	0.518591
C	-0.914232	-1.897044	0.350950
H	-1.655880	-2.696833	0.249061
H	-0.761175	-1.744461	1.422191
H	0.006561	-2.302998	-0.076466
C	-1.704837	-1.035727	-1.837927
H	-2.556945	-1.722583	-1.865792
H	-0.878248	-1.575353	-2.309618
H	-1.952592	-0.193655	-2.489197
C	0.119813	2.753986	-1.833863
H	-0.393682	3.686057	-2.096586
H	0.439311	2.292456	-2.773865
H	1.003835	3.039629	-1.262646
C	0.121152	0.975020	1.124300
H	-0.644958	1.663720	1.503233
H	0.098335	0.113559	1.798007
C	1.128002	0.035507	-1.029862
H	1.590528	0.801036	-1.658907
H	0.922092	-0.783913	-1.722895
C	1.481860	1.652106	1.301832
H	1.488267	2.579979	0.722579
H	1.580063	1.981839	2.344518
C	2.184927	-0.408329	-0.009613
H	1.771002	-1.213535	0.605643
C	2.671881	0.748478	0.894068
Cl	3.362572	0.019309	2.406743
C	3.763451	1.645394	0.287616
H	3.978406	2.498395	0.943113
H	3.450648	2.050061	-0.681008
H	4.711699	1.118114	0.141852
Br	3.638668	-1.317809	-0.969762

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2586734**

SCF Energy (B3LYP/6-31G) = -6264.29508213**

1k_C006

MMFF Geometry

C	1.450420	0.323168	-0.678173
C	2.756568	-1.552615	0.531507
C	0.035252	-0.236582	-0.042541
C	2.604227	-0.044515	0.309933
H	3.381630	-2.006307	-0.246406
H	2.460760	0.465668	1.270004
C	1.452763	-2.278741	0.554545
H	1.545009	-3.341220	0.779695
C	0.237192	-1.748499	0.305050
O	3.395526	-1.810767	1.782415
H	2.781676	-1.542394	2.487066
Br	4.370691	0.661753	-0.248183
C	1.435714	1.867736	-0.880695
H	2.255116	2.193085	-1.531971
H	1.553353	2.409333	0.062975
H	0.523293	2.230092	-1.356742
C	1.694529	-0.307915	-2.082453
H	2.667184	-0.020952	-2.494359
H	0.949913	0.028523	-2.811113
H	1.660954	-1.400715	-2.068143
C	-0.934668	-2.688440	0.396084
H	-0.644185	-3.680078	0.763525
H	-1.374940	-2.848832	-0.590439
H	-1.682636	-2.319973	1.097928
C	-0.250646	0.481720	1.315924
H	0.291315	-0.014387	2.133096
H	0.154258	1.495916	1.309544
C	-1.123918	-0.010395	-1.095537
H	-1.174528	-0.870814	-1.775614
H	-0.829415	0.808923	-1.757459
C	-1.715500	0.587955	1.738018
H	-2.094884	-0.400315	2.016682
H	-1.762239	1.185760	2.658573
C	-2.539960	0.401585	-0.635901
H	-2.990301	0.991823	-1.446166
C	-2.611874	1.214200	0.665616
Cl	-2.002550	2.893082	0.295542
C	-4.031780	1.416281	1.217658
H	-4.036754	2.132105	2.048931
H	-4.456017	0.487584	1.612998
H	-4.709549	1.800526	0.446792
Br	-3.751827	-1.148303	-0.654879

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2505502**

SCF Energy (B3LYP/6-31G) = -6264.28803081**

1k_C007

MMFF Geometry

C	1.445737	0.335885	-0.672589
C	2.757486	-1.533552	0.542312
C	0.033271	-0.231068	-0.040726
C	2.598368	-0.027415	0.318277
H	3.397343	-1.982195	-0.227363
H	2.456900	0.486121	1.276926
C	1.457616	-2.268374	0.556814
H	1.541991	-3.329258	0.786207
C	0.240677	-1.744049	0.298877
O	3.380799	-1.758085	1.807086
H	3.637563	-2.694495	1.841312
Br	4.366952	0.677118	-0.250541
C	1.425257	1.880860	-0.872243
H	2.245046	2.210841	-1.520665
H	1.538410	2.421119	0.072744
H	0.512684	2.240802	-1.349806
C	1.694630	-0.292036	-2.077519
H	2.663044	0.005920	-2.491506
H	0.945116	0.036285	-2.804831
H	1.673580	-1.385151	-2.063484
C	-0.928808	-2.687208	0.385349
H	-0.636743	-3.679419	0.749910
H	-1.366988	-2.845685	-0.602430
H	-1.678932	-2.322985	1.087043
C	-0.255543	0.480868	1.320561
H	0.289051	-0.015672	2.135668
H	0.144424	1.497069	1.317522
C	-1.126663	-0.004636	-1.092721
H	-1.173996	-0.862136	-1.776708
H	-0.835535	0.818654	-1.751145
C	-1.720380	0.578830	1.743891
H	-2.095177	-0.412225	2.018829
H	-1.769318	1.172769	2.666828
C	-2.544176	0.399455	-0.630935
H	-2.996193	0.992523	-1.438238
C	-2.620012	1.205144	0.674607
Cl	-2.020885	2.889420	0.311087
C	-4.040865	1.396835	1.228026
H	-4.049441	2.108552	2.062789
H	-4.459879	0.463884	1.618921
H	-4.720998	1.781169	0.459284
Br	-3.751319	-1.154237	-0.661027

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2496857**

SCF Energy (B3LYP/6-31G) = -6264.28692394**

1k_C008

MMFF Geometry

C	1.599483	0.722083	1.137623
C	2.480784	-1.483642	-0.022546
C	0.119526	0.081687	0.919514
C	2.676769	0.027671	0.228204
H	2.329350	-1.723950	-1.081204
H	3.669232	0.199792	0.665967
C	1.352843	-2.105014	0.732614
H	1.458720	-3.171390	0.925308
C	0.276187	-1.438772	1.198669
O	3.667770	-2.177665	0.375313
H	4.362919	-1.932063	-0.259802
Br	2.935274	0.892907	-1.539433
C	2.071563	0.485986	2.615964
H	3.064140	0.924310	2.779533
H	2.150551	-0.572677	2.878219
H	1.399134	0.958853	3.338762
C	1.646620	2.269626	0.987221
H	2.682842	2.629231	1.015670
H	1.133464	2.778492	1.809988
H	1.199213	2.632675	0.060033
C	-0.686202	-2.199871	2.076630
H	-0.345116	-3.225170	2.263533
H	-1.672889	-2.286955	1.623871
H	-0.780125	-1.729341	3.059136
C	-0.905800	0.775454	1.874389
H	-0.738857	0.469743	2.913449
H	-0.738773	1.855887	1.873193
C	-0.347887	0.294189	-0.567870
H	0.206771	-0.366976	-1.243680
H	-0.071597	1.306986	-0.874797
C	-2.392652	0.572273	1.551527
H	-2.694444	-0.451649	1.783921
H	-2.978907	1.198653	2.238201
C	-1.845595	0.172350	-0.890636
H	-2.008110	0.575783	-1.899030
C	-2.763647	0.904593	0.100917
Cl	-2.519367	2.697849	-0.148087
C	-4.261272	0.660883	-0.135868
H	-4.875082	1.316925	0.493319
H	-4.554879	-0.364643	0.110329
H	-4.535966	0.850131	-1.179858
Br	-2.315240	-1.714386	-1.163916

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2559863**

SCF Energy (B3LYP/6-31G) = -6264.29286899**

1k_C009

MMFF Geometry

C	-1.619311	-0.734639	1.119465
C	-2.584496	1.447361	-0.003007
C	-0.148160	-0.067949	0.910770
C	-2.699793	-0.080011	0.186950
H	-2.547024	1.730997	-1.060731
H	-3.695520	-0.324058	0.581449
C	-1.428435	2.094843	0.691980
H	-1.529408	3.164675	0.864338
C	-0.331761	1.456485	1.150718
O	-3.773561	2.044651	0.528920
H	-3.795884	2.965410	0.217751
Br	-2.839963	-0.914148	-1.609160
C	-2.113693	-0.490283	2.588593
H	-3.106444	-0.931999	2.741143
H	-2.199635	0.569534	2.843400
H	-1.449398	-0.955338	3.324030
C	-1.636705	-2.284672	0.983676
H	-2.667167	-2.661345	0.998892
H	-1.127541	-2.776889	1.818850
H	-1.170119	-2.649785	0.066973
C	0.635108	2.257139	1.989589
H	0.743116	1.822640	2.987236
H	0.288534	3.285942	2.144352
H	1.616381	2.336318	1.525209
C	0.870675	-0.721230	1.900982
H	0.683828	-0.385327	2.927473
H	0.714672	-1.802831	1.931214
C	0.350739	-0.297885	-0.563089
H	-0.193570	0.355658	-1.255112
H	0.084765	-1.315470	-0.862071
C	2.360611	-0.513117	1.596172
H	2.650501	0.518979	1.806553
H	2.940870	-1.116029	2.308519
C	1.853030	-0.179725	-0.864033
H	2.032854	-0.611483	-1.857752
C	2.758076	-0.880344	0.161299
Cl	2.528496	-2.680705	-0.045174
C	4.258128	-0.633482	-0.056111
H	4.864833	-1.269235	0.600217
H	4.541385	0.399880	0.168557
H	4.551929	-0.847856	-1.089994
Br	2.320763	1.699218	-1.189629

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2537305**

SCF Energy (B3LYP/6-31G) = -6264.29030984**

1k_C010

MMFF Geometry

C	1.635351	0.727439	1.091821
C	2.640090	-1.447588	0.000557
C	0.166181	0.047591	0.897647
C	2.714338	0.086211	0.147759
H	2.659997	-1.764517	-1.047325
H	3.709848	0.363783	0.520105
C	1.467268	-2.104209	0.655964
H	1.571673	-3.180800	0.788996
C	0.362576	-1.479860	1.113187
O	3.811347	-2.021081	0.597706
H	3.723848	-1.930389	1.561963
Br	2.799996	0.887745	-1.661419
C	2.141516	0.488733	2.557652
H	3.144073	0.912454	2.695429
H	2.206118	-0.569311	2.824621
H	1.493962	0.974663	3.294860
C	1.640737	2.277906	0.953528
H	2.668785	2.661315	0.968257
H	1.127559	2.768718	1.786832
H	1.173812	2.639408	0.035752
C	-0.613783	-2.307175	1.914824
H	-0.270320	-3.341301	2.037875
H	-1.591477	-2.368672	1.441619
H	-0.729399	-1.905781	2.925536
C	-0.838868	0.675245	1.917979
H	-0.638089	0.310655	2.932261
H	-0.680394	1.755175	1.977005
C	-0.358340	0.291183	-0.565155
H	0.168642	-0.363806	-1.269386
H	-0.088295	1.307672	-0.863033
C	-2.333203	0.477767	1.628841
H	-2.623057	-0.558430	1.818627
H	-2.901851	1.065020	2.363301
C	-1.866268	0.193993	-0.844648
H	-2.056726	0.649871	-1.825604
C	-2.749045	0.880488	0.208888
Cl	-2.504731	2.682717	0.038719
C	-4.254505	0.652472	0.009287
H	-4.561856	0.891958	-1.015099
H	-4.845007	1.279540	0.688354
H	-4.544302	-0.382810	0.216085
Br	-2.358630	-1.670977	-1.207886

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2545869**

SCF Energy (B3LYP/6-31G) = -6264.29198209**

1k_C011

MMFF Geometry

C	-1.369061	-0.619645	-0.363994
C	-3.144930	1.272627	-0.331922
C	-0.206925	0.527324	-0.377948
C	-2.613633	0.000509	0.351890
H	-3.922246	1.022699	-1.064489
H	-2.387594	0.201327	1.405628
C	-2.097946	2.077325	-1.041876
H	-2.472731	2.952350	-1.569681
C	-0.786550	1.767314	-1.122580
O	-3.739696	2.119918	0.650325
H	-4.175979	2.849739	0.180142
Br	-4.130855	-1.265691	0.528248
C	-0.906796	-1.901041	0.376720
H	-1.652959	-2.700144	0.310440
H	-0.724494	-1.727975	1.440296
H	0.001765	-2.318221	-0.066235
C	-1.733753	-1.070676	-1.813179
H	-2.543517	-1.807618	-1.814381
H	-0.893931	-1.559653	-2.314765
H	-2.055364	-0.245325	-2.453439
C	0.097734	2.661127	-1.958254
H	-0.416667	3.579372	-2.264172
H	0.399063	2.146116	-2.876175
H	0.991869	2.973818	-1.416593
C	0.114550	1.002486	1.091298
H	-0.653693	1.697840	1.453069
H	0.099352	0.161124	1.790485
C	1.122023	-0.003183	-1.031521
H	1.584808	0.741322	-1.684925
H	0.918014	-0.845758	-1.696796
C	1.471772	1.693674	1.237503
H	1.472603	2.594151	0.615703
H	1.571059	2.069310	2.264355
C	2.179390	-0.411651	0.003352
H	1.766087	-1.196865	0.644629
C	2.663841	0.776789	0.866841
Cl	3.350528	0.102974	2.406211
C	3.756319	1.652789	0.232056
H	3.968105	2.529035	0.857224
H	3.446169	2.022132	-0.751436
H	4.705646	1.121807	0.108357
Br	3.635342	-1.349312	-0.925841

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2561634**

SCF Energy (B3LYP/6-31G) = -6264.28942400**

1k_C012

MMFF Geometry

C	-1.372273	-0.613773	-0.368444
C	-3.154020	1.270174	-0.370987
C	-0.208321	0.533533	-0.379769
C	-2.622951	0.009849	0.334988
H	-3.904404	1.004389	-1.124952
H	-2.399414	0.229988	1.385251
C	-2.098803	2.080048	-1.060211
H	-2.480681	2.952264	-1.590091
C	-0.785068	1.777293	-1.121432
O	-3.797682	2.131799	0.567101
H	-3.107189	2.531202	1.122871
Br	-4.131913	-1.257506	0.532479
C	-0.915744	-1.892997	0.379346
H	-1.659903	-2.693437	0.306407
H	-0.744590	-1.718089	1.444442
H	-0.002644	-2.309927	-0.054201
C	-1.727107	-1.070644	-1.818234
H	-2.554691	-1.787430	-1.823955
H	-0.891906	-1.585324	-2.301860
H	-2.018153	-0.244304	-2.471670
C	0.102898	2.678108	-1.946344
H	-0.411584	3.597293	-2.249404
H	0.410777	2.169418	-2.865617
H	0.993244	2.989266	-1.397868
C	0.112403	1.005188	1.090404
H	-0.653567	1.703500	1.451209
H	0.092086	0.163263	1.788630
C	1.120618	0.003812	-1.034019
H	1.586382	0.751921	-1.681267
H	0.915457	-0.833429	-1.705609
C	1.472665	1.689736	1.240619
H	1.479661	2.591192	0.620547
H	1.571211	2.063518	2.268254
C	2.175518	-0.413692	-0.000070
H	1.759040	-1.201082	0.636218
C	2.661786	0.768033	0.871661
Cl	3.334262	0.083386	2.412342
C	3.762595	1.641206	0.247760
H	4.709908	1.105852	0.127500
H	3.975046	2.513480	0.878231
H	3.460213	2.016623	-0.735882
Br	3.629899	-1.350418	-0.931491

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2571214**

SCF Energy (B3LYP/6-31G) = -6264.29015652**

1k_C013

MMFF Geometry

C	-1.432373	-0.594076	-1.041005
C	-3.582269	-0.375273	0.429251
C	-0.516882	-0.963733	0.267449
C	-2.726992	0.229136	-0.683836
H	-4.238323	0.383842	0.870858
H	-3.346452	0.320154	-1.586523
C	-2.777679	-1.000556	1.514763
H	-3.350123	-1.249265	2.407281
C	-1.455009	-1.255570	1.493496
O	-4.449648	-1.372940	-0.110456
H	-4.906825	-1.799070	0.633818
Br	-2.405635	2.127220	-0.243327
C	-1.942618	-1.908585	-1.718947
H	-2.704702	-1.694885	-2.478316
H	-2.383691	-2.605114	-0.999738
H	-1.134442	-2.434064	-2.239811
C	-0.701017	0.157041	-2.180753
H	-1.385326	0.345500	-3.018364
H	0.129484	-0.413741	-2.597007
H	-0.321168	1.133135	-1.874397
C	-0.873813	-1.881500	2.750141
H	-1.539024	-1.761386	3.613300
H	0.078789	-1.430523	3.036160
H	-0.726422	-2.956994	2.608624
C	0.357162	-2.255877	0.053454
H	0.719221	-2.630571	1.016405
H	-0.240930	-3.087834	-0.331426
C	0.466655	0.185741	0.687827
H	0.756909	0.053086	1.736559
H	-0.046000	1.148301	0.686649
C	1.610237	-2.090638	-0.804295
H	2.132832	-3.056427	-0.840558
H	1.326717	-1.882104	-1.838751
C	1.769434	0.310432	-0.123748
H	1.565702	0.715481	-1.115513
C	2.558614	-1.005160	-0.257522
Cl	3.882882	-0.809415	-1.478805
C	3.216953	-1.483140	1.049291
H	3.644187	-2.486069	0.930134
H	2.503850	-1.530642	1.877589
H	4.036709	-0.828800	1.364327
Br	2.839773	1.760840	0.687574

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2545603**

SCF Energy (B3LYP/6-31G) = -6264.28960484**

1k_C014

MMFF Geometry

C	1.495736	-0.477606	1.126462
C	3.492774	-0.541763	-0.544996
C	0.458780	-0.996152	-0.021544
C	2.768554	0.240062	0.554421
H	4.068611	0.130526	-1.191305
H	3.472072	0.411652	1.380640
C	2.590821	-1.367657	-1.399886
H	3.084417	-1.816177	-2.260845
C	1.274067	-1.588397	-1.213732
O	4.449022	-1.421558	0.051852
H	4.859085	-1.938129	-0.661839
Br	2.487984	2.086029	-0.073373
C	2.041296	-1.708100	1.934568
H	2.869916	-1.414206	2.590220
H	2.403672	-2.507994	1.282084
H	1.279192	-2.143326	2.589551
C	0.830323	0.426685	2.194671
H	1.564730	0.745071	2.944829
H	0.037154	-0.096541	2.737692
H	0.394404	1.334768	1.771681
C	0.580102	-2.459949	-2.237693
H	1.240981	-2.729890	-3.069739
H	-0.276049	-1.947573	-2.683770
H	0.252002	-3.400792	-1.786627
C	-0.488163	-2.092145	0.605314
H	0.012884	-3.068619	0.604130
H	-0.694296	-1.862354	1.656325
C	-0.453008	0.141836	-0.603510
H	-0.665245	-0.030443	-1.666451
H	0.068290	1.096254	-0.592220
C	-1.857234	-2.243932	-0.068740
H	-1.719218	-2.571506	-1.101671
H	-2.396678	-3.072165	0.409727
C	-1.795814	0.286156	0.123305
H	-1.609498	0.469270	1.184724
C	-2.706708	-0.950236	-0.045467
Cl	-3.811419	-1.030745	1.392506
C	-3.599402	-0.953265	-1.297866
H	-4.125632	-1.910281	-1.401833
H	-3.004783	-0.808267	-2.206686
H	-4.370440	-0.176473	-1.269863
Br	-2.640451	1.968516	-0.440284

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2525066**

SCF Energy (B3LYP/6-31G) = -6264.28815474**

1k_C015

MMFF Geometry

C	-1.439652	-0.607297	-1.028741
C	-3.561583	-0.364007	0.484899
C	-0.506984	-0.991692	0.262410
C	-2.721091	0.224852	-0.648424
H	-4.170695	0.406370	0.972646
H	-3.357057	0.312899	-1.539885
C	-2.751669	-1.041239	1.530192
H	-3.328503	-1.331826	2.407473
C	-1.433283	-1.313230	1.486972
O	-4.481051	-1.335639	-0.013768
H	-5.163247	-0.856645	-0.514191
Br	-2.388491	2.126281	-0.238388
C	-1.975758	-1.915393	-1.700387
H	-2.749013	-1.692260	-2.445648
H	-2.412064	-2.608608	-0.975030
H	-1.182444	-2.447498	-2.237156
C	-0.720257	0.139130	-2.178729
H	-1.416632	0.334931	-3.004688
H	0.098034	-0.437269	-2.610146
H	-0.327378	1.111352	-1.877477
C	-0.850272	-1.992528	2.713694
H	-1.507753	-1.899101	3.586016
H	0.108495	-1.559197	3.007673
H	-0.713596	-3.063101	2.530344
C	0.378129	-2.270646	0.014082
H	0.747592	-2.664653	0.966414
H	-0.213845	-3.098601	-0.388265
C	0.466077	0.157219	0.702436
H	0.765108	0.001357	1.746045
H	-0.057370	1.113570	0.729016
C	1.628356	-2.076133	-0.841769
H	2.162039	-3.035125	-0.894653
H	1.341866	-1.854929	-1.872461
C	1.760407	0.313602	-0.115981
H	1.543490	0.732316	-1.099180
C	2.565353	-0.989204	-0.278484
Cl	3.881123	-0.753227	-1.502120
C	3.235827	-1.483813	1.015827
H	3.678305	-2.477192	0.874336
H	2.526526	-1.560114	1.845209
H	4.046296	-0.823303	1.341755
Br	2.817335	1.763687	0.712389

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2572687**

SCF Energy (B3LYP/6-31G) = -6264.29141608**

1k_C016

MMFF Geometry

C	1.494945	-0.504177	1.111252
C	3.460435	-0.547026	-0.605893
C	0.443430	-1.022116	-0.022515
C	2.760161	0.213493	0.524467
H	3.980064	0.133719	-1.290369
H	3.480612	0.363526	1.340209
C	2.556320	-1.408660	-1.416389
H	3.055940	-1.888998	-2.257019
C	1.244918	-1.638589	-1.208352
O	4.466304	-1.412363	-0.073865
H	5.188560	-0.848009	0.250719
Br	2.489780	2.077500	-0.050269
C	2.053387	-1.736563	1.907853
H	2.879564	-1.440106	2.565491
H	2.425243	-2.526277	1.248391
H	1.295831	-2.185228	2.558934
C	0.843234	0.397115	2.190501
H	1.587763	0.715574	2.930613
H	0.058354	-0.126613	2.744682
H	0.400216	1.304901	1.774395
C	0.549037	-2.546525	-2.197775
H	0.219282	-3.470175	-1.713793
H	1.208010	-2.846904	-3.020848
H	-0.306651	-2.047033	-2.659585
C	-0.514461	-2.096436	0.624822
H	-0.027457	-3.079927	0.633775
H	-0.710469	-1.851884	1.674233
C	-0.453414	0.118411	-0.618883
H	-0.676520	-0.072700	-1.676775
H	0.084494	1.063790	-0.630756
C	-1.889395	-2.236199	-0.039935
H	-1.761374	-2.578049	-1.069634
H	-2.438698	-3.050280	0.451393
C	-1.788345	0.295491	0.114455
H	-1.591796	0.491755	1.171624
C	-2.719190	-0.929498	-0.028251
Cl	-3.811659	-0.971977	1.420844
C	-3.623228	-0.937214	-1.272363
H	-4.382028	-0.148310	-1.248916
H	-4.164850	-1.887478	-1.357440
H	-3.034810	-0.814695	-2.188501
Br	-2.610023	1.982011	-0.468937

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2544413**

SCF Energy (B3LYP/6-31G) = -6264.28991794**

1k_C017

MMFF Geometry

C	1.500329	-0.482374	1.117817
C	3.489562	-0.536252	-0.567506
C	0.459587	-0.999912	-0.027893
C	2.772395	0.236868	0.543644
H	4.044016	0.144791	-1.222667
H	3.480963	0.401462	1.366866
C	2.585110	-1.365298	-1.417193
H	3.082346	-1.804602	-2.282088
C	1.271592	-1.594108	-1.221611
O	4.480589	-1.395490	0.005124
H	4.175160	-2.314949	-0.072173
Br	2.487928	2.089051	-0.065609
C	2.045888	-1.714094	1.923430
H	2.885420	-1.425829	2.567425
H	2.390876	-2.520300	1.270177
H	1.287790	-2.140176	2.589203
C	0.837502	0.420064	2.189621
H	1.574004	0.737170	2.938282
H	0.045781	-0.103949	2.734012
H	0.399858	1.328644	1.769581
C	0.575470	-2.466918	-2.243241
H	1.235590	-2.739751	-3.074954
H	-0.280359	-1.954232	-2.689590
H	0.246380	-3.406303	-1.789863
C	-0.487892	-2.094026	0.601079
H	0.010620	-3.071770	0.597592
H	-0.690326	-1.864964	1.652914
C	-0.451312	0.139155	-0.609266
H	-0.668172	-0.035659	-1.670906
H	0.073135	1.091945	-0.602910
C	-1.858972	-2.241287	-0.069937
H	-1.724161	-2.565333	-1.104431
H	-2.398867	-3.070034	0.407131
C	-1.791361	0.288774	0.121797
H	-1.600691	0.474037	1.182003
C	-2.705939	-0.945995	-0.040138
Cl	-3.798801	-1.025064	1.406864
C	-3.608531	-0.947733	-1.285310
H	-4.136894	-1.904009	-1.385152
H	-3.020872	-0.803552	-2.198789
H	-4.378226	-0.169851	-1.251065
Br	-2.633614	1.971693	-0.442392

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2550608**

SCF Energy (B3LYP/6-31G) = -6264.29009730**

1k_C018

MMFF Geometry

C	-1.556930	0.683580	1.051316
C	-3.244180	-0.000651	-0.844763
C	-0.542875	1.217147	-0.102317
C	-2.598262	-0.355119	0.505667
H	-3.278909	-0.857300	-1.527428
H	-3.393283	-0.473461	1.254834
C	-2.610508	1.133386	-1.580256
H	-3.188955	1.494744	-2.429589
C	-1.434700	1.720142	-1.280623
O	-4.604826	0.388118	-0.626216
H	-5.096268	-0.417177	-0.388791
Br	-1.938742	-2.216861	0.438238
C	-2.423012	1.884888	1.589846
H	-3.196931	1.527558	2.281031
H	-2.936981	2.437357	0.799009
H	-1.823056	2.603645	2.156505
C	-0.896305	0.131684	2.335705
H	-1.654238	-0.300329	3.002483
H	-0.414959	0.919403	2.920541
H	-0.165354	-0.651623	2.151163
C	-0.962032	2.853402	-2.160938
H	-0.940107	3.792540	-1.599130
H	-1.621995	3.012792	-3.021154
H	0.034787	2.648145	-2.562861
C	0.400796	2.359119	0.418042
H	0.780424	2.948946	-0.422577
H	-0.147125	3.084533	1.025352
C	0.371161	0.139087	-0.777088
H	0.717662	0.533813	-1.744098
H	-0.210654	-0.738223	-1.067171
C	1.652064	1.910265	1.184476
H	2.247767	2.803231	1.419195
H	1.371671	1.496242	2.154648
C	1.619707	-0.289708	-0.001715
H	1.340132	-0.879070	0.872021
C	2.514367	0.895093	0.408578
Cl	3.804610	0.326720	1.546994
C	3.223821	1.597336	-0.763162
H	3.756624	2.492222	-0.419367
H	2.522759	1.919436	-1.538670
H	3.968764	0.954118	-1.243074
Br	2.579021	-1.619957	-1.102771

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2550313**

SCF Energy (B3LYP/6-31G) = -6264.28986588**

1k_C019

MMFF Geometry

C	1.530343	0.387230	-0.649815
C	2.911257	-1.447883	0.535216
C	0.142877	-0.190567	0.021117
C	2.719951	0.052745	0.309057
H	3.466738	-1.916264	-0.286262
H	2.608766	0.563698	1.271148
C	1.618283	-2.171971	0.688730
H	1.725363	-3.210737	0.999083
C	0.389171	-1.664525	0.464425
O	3.653846	-1.675237	1.732563
H	4.513701	-1.233263	1.614602
Br	4.464966	0.775002	-0.299736
C	1.461542	1.923638	-0.863049
H	2.302347	2.287311	-1.463574
H	1.486839	2.466862	0.086882
H	0.562304	2.232804	-1.401535
C	1.765908	-0.258289	-2.049496
H	2.735655	0.022990	-2.471361
H	1.020525	0.069467	-2.781007
H	1.729484	-1.351028	-2.018643
C	-0.782533	-2.587540	0.685504
H	-0.488198	-3.518096	1.184775
H	-1.230070	-2.873579	-0.269233
H	-1.534094	-2.124932	1.323915
C	-0.219622	0.606410	1.315357
H	-0.563087	-0.071046	2.106683
H	0.663317	1.084617	1.748694
C	-1.021931	-0.104403	-1.036317
H	-1.030618	-1.010197	-1.656613
H	-0.757759	0.682769	-1.750825
C	-1.277962	1.689670	1.120171
H	-1.385339	2.246392	2.060725
H	-0.932163	2.420411	0.380701
C	-2.455018	0.292335	-0.611460
H	-2.818499	0.910396	-1.444959
C	-2.629184	1.098413	0.695615
Cl	-3.724318	2.518123	0.355857
C	-3.277775	0.364820	1.882319
H	-3.271140	0.991693	2.782771
H	-2.756091	-0.558931	2.137771
H	-4.326708	0.112254	1.690789
Br	-3.690408	-1.219868	-0.808803

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2495174**

SCF Energy (B3LYP/6-31G) = -6264.28670115**

1k_C020

MMFF Geometry

C	1.347507	-0.386113	0.575197
C	2.827804	1.591431	-0.170490
C	-0.023211	0.428379	0.160690
C	2.515407	0.105458	-0.340104
H	3.469214	1.776924	0.699649
H	2.313273	-0.125341	-1.391379
C	1.599338	2.417217	-0.017641
H	1.787112	3.490117	-0.040110
C	0.339325	1.960036	0.140913
O	3.517926	2.085533	-1.317778
H	4.337923	1.565570	-1.393605
Br	4.224565	-0.869616	-0.064920
C	1.202830	-1.915722	0.418216
H	2.040597	-2.452882	0.876898
H	1.176132	-2.215956	-0.632009
H	0.316669	-2.296739	0.921862
C	1.691197	-0.126374	2.076896
H	2.665786	-0.543588	2.349206
H	0.969098	-0.599427	2.749591
H	1.714190	0.937397	2.328984
C	-0.738794	3.013160	0.238137
H	-0.326573	4.029582	0.235516
H	-1.302440	2.926608	1.169201
H	-1.408932	2.960806	-0.622154
C	-0.519518	0.113613	-1.287063
H	-1.132951	0.948415	-1.651124
H	0.319495	0.082280	-1.990042
C	-1.182074	0.100294	1.180798
H	-1.292484	0.906026	1.915701
H	-0.885891	-0.757760	1.791055
C	-1.363688	-1.146183	-1.501327
H	-1.771046	-1.077695	-2.519959
H	-0.708801	-2.020631	-1.547643
C	-2.563273	-0.299415	0.616764
H	-3.159199	-0.686705	1.454414
C	-2.517831	-1.361897	-0.500232
Cl	-2.247076	-2.978097	0.320645
C	-3.846502	-1.552975	-1.255002
H	-3.809101	-2.431902	-1.910740
H	-4.076849	-0.699286	-1.901047
H	-4.685132	-1.693151	-0.563152
Br	-3.627545	1.277481	0.143424

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2464502**

SCF Energy (B3LYP/6-31G) = -6264.28748728**

1l_C001

MMFF Geometry

C	-1.311326	-0.288428	-0.321134
C	-3.238460	1.300378	0.434349
C	-0.202187	0.655232	0.450323
C	-2.688677	-0.127455	0.415685
H	-4.032430	1.378894	1.186753
H	-2.578799	-0.468579	1.451749
C	-2.174706	2.289799	0.745768
H	-2.548814	3.291798	0.951667
C	-0.848721	2.052132	0.774094
O	-3.797640	1.707191	-0.811058
H	-4.407092	0.999583	-1.088369
Br	-4.127501	-1.312659	-0.251360
C	-0.950546	-1.793482	-0.321310
H	-1.598337	-2.365698	-0.995223
H	-1.063143	-2.236418	0.673047
H	0.057401	-1.988147	-0.678874
C	-1.429936	0.126973	-1.812891
H	-2.293385	-0.334416	-2.302075
H	-0.552729	-0.198743	-2.383668
H	-1.520187	1.209747	-1.939384
C	0.038122	3.223863	1.151244
H	-0.530504	4.036026	1.619041
H	0.520343	3.642775	0.262276
H	0.807345	2.934030	1.871588
C	0.229339	0.052679	1.832219
H	0.587490	0.851357	2.493256
H	-0.637130	-0.362706	2.358456
C	1.089393	0.912645	-0.409841
H	1.613185	1.798246	-0.035781
H	0.823856	1.194787	-1.434267
C	1.334263	-1.013327	1.810860
H	1.618608	-1.228302	2.850405
H	0.931817	-1.957380	1.434951
C	2.136759	-0.203077	-0.419600
H	1.774010	-1.061475	-0.986312
C	2.581273	-0.616501	0.997504
Cl	3.634181	-2.088852	0.905211
C	3.374829	0.458570	1.761225
H	4.338947	0.676781	1.290682
H	3.592079	0.131914	2.785533
H	2.825842	1.401265	1.837513
Br	3.648505	0.407734	-1.538756

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2583628**

SCF Energy (B3LYP/6-31G) = -6264.29682098**

1l_C002

MMFF Geometry

C	1.459702	0.283004	-0.575810
C	2.751622	-1.459024	0.847817
C	0.027610	-0.216940	0.077460
C	2.584207	0.017877	0.476006
H	3.284265	-1.539739	1.802699
H	2.356326	0.582362	1.388230
C	1.443185	-2.165214	0.952662
H	1.529047	-3.190505	1.310787
C	0.230830	-1.671483	0.620145
O	3.503773	-2.196420	-0.114460
H	4.290542	-1.661491	-0.324126
Br	4.353805	0.741019	-0.021612
C	1.446638	1.799132	-0.932312
H	2.276944	2.058464	-1.599525
H	1.547093	2.434060	-0.046579
H	0.540556	2.105883	-1.457596
C	1.737755	-0.476727	-1.906549
H	2.755587	-0.301154	-2.269054
H	1.069651	-0.143025	-2.707741
H	1.604243	-1.557855	-1.812879
C	-0.939327	-2.599576	0.805158
H	-0.655785	-3.530682	1.310531
H	-1.349479	-2.893976	-0.163295
H	-1.709681	-2.147585	1.429276
C	-0.318696	0.659086	1.325892
H	0.194259	0.273770	2.218040
H	0.076834	1.670267	1.210922
C	-1.092612	-0.136745	-1.036698
H	-1.106697	-1.073018	-1.609995
H	-0.781128	0.604724	-1.778452
C	-1.799583	0.798678	1.677320
H	-2.181401	-0.150329	2.066423
H	-1.885842	1.507751	2.512108
C	-2.529692	0.305266	-0.683685
H	-2.955031	0.783849	-1.576890
C	-2.660881	1.271799	0.502976
Cl	-2.057616	2.902327	-0.049496
C	-4.103305	1.517731	0.973059
H	-4.755226	1.792707	0.136014
H	-4.148504	2.330706	1.708236
H	-4.531844	0.638388	1.464855
Br	-3.723524	-1.253103	-0.555403

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2490217**

SCF Energy (B3LYP/6-31G) = -6264.29126528**

1l_C003

MMFF Geometry

C	-1.322518	-0.782635	-1.114672
C	-3.552726	-0.835579	0.185842
C	-0.449618	-1.010813	0.261157
C	-2.709206	-0.091323	-0.851089
H	-3.944007	-1.759874	-0.253076
H	-3.287351	-0.023412	-1.781958
C	-2.767612	-1.207406	1.392529
H	-3.373441	-1.461825	2.261784
C	-1.423801	-1.286021	1.467654
O	-4.699121	-0.096810	0.595360
H	-4.382434	0.791025	0.845536
Br	-2.579060	1.819328	-0.349989
C	-1.668213	-2.158431	-1.773534
H	-2.390934	-2.035125	-2.589588
H	-2.102994	-2.865525	-1.060353
H	-0.784206	-2.629415	-2.216639
C	-0.608435	0.008856	-2.236316
H	-1.262001	0.111159	-3.112391
H	0.293227	-0.492268	-2.592156
H	-0.339870	1.024127	-1.937609
C	-0.856863	-1.712850	2.811700
H	-0.568559	-2.768487	2.788802
H	-1.591312	-1.601593	3.618237
H	0.009579	-1.119663	3.109217
C	0.501586	-2.260243	0.173491
H	0.848458	-2.541313	1.173356
H	-0.035644	-3.151005	-0.167660
C	0.454753	0.220691	0.633703
H	0.710642	0.179889	1.697753
H	-0.106124	1.151458	0.542252
C	1.768893	-2.079548	-0.660054
H	2.342028	-3.016107	-0.624805
H	1.503606	-1.944051	-1.712060
C	1.782252	0.363739	-0.135067
H	1.597824	0.696127	-1.157307
C	2.641962	-0.913386	-0.155517
Cl	3.995690	-0.726444	-1.345103
C	3.277166	-1.270276	1.200294
H	4.054295	-0.556958	1.494775
H	3.754539	-2.256823	1.163042
H	2.539317	-1.296653	2.007726
Br	2.744085	1.917291	0.618739

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2597052**

SCF Energy (B3LYP/6-31G) = -6264.29580157**

1l_C004

MMFF Geometry

C	-1.312277	-0.294674	-0.329282
C	-3.243752	1.300935	0.395121
C	-0.210582	0.641227	0.462729
C	-2.698472	-0.129270	0.390360
H	-4.072915	1.370579	1.109573
H	-2.592808	-0.456637	1.431660
C	-2.184188	2.278814	0.768315
H	-2.551977	3.272696	1.017976
C	-0.859999	2.032565	0.815136
O	-3.742026	1.702424	-0.877215
H	-4.092152	2.603877	-0.787676
Br	-4.122270	-1.338903	-0.255695
C	-0.954320	-1.800809	-0.333100
H	-1.594498	-2.368215	-1.018308
H	-1.078867	-2.248982	0.657538
H	0.057622	-1.994879	-0.680384
C	-1.409703	0.125309	-1.820693
H	-2.273394	-0.326272	-2.318951
H	-0.529172	-0.207571	-2.382351
H	-1.485770	1.209359	-1.945605
C	0.026393	3.186125	1.248328
H	-0.545978	3.982144	1.738754
H	0.520889	3.636212	0.381588
H	0.786566	2.869093	1.966388
C	0.219814	0.009423	1.833149
H	0.570790	0.793406	2.514734
H	-0.646834	-0.422328	2.346010
C	1.081242	0.921100	-0.388783
H	1.602417	1.799483	0.005513
H	0.816543	1.225689	-1.407051
C	1.331327	-1.049746	1.793764
H	1.617390	-1.279771	2.829654
H	0.934280	-1.990472	1.404137
C	2.128925	-0.193650	-0.422199
H	1.765237	-1.041023	-1.005029
C	2.575856	-0.633434	0.986383
Cl	3.634334	-2.099589	0.864951
C	3.366456	0.429274	1.770471
H	4.328337	0.661862	1.302277
H	3.587891	0.082336	2.787203
H	2.813240	1.367475	1.868093
Br	3.638710	0.441658	-1.530602

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2544965**

SCF Energy (B3LYP/6-31G) = -6264.28880081**

1l_C005

MMFF Geometry

C	-1.38550	-0.44209	-0.37512
C	-3.14886	1.39822	0.12936
C	-0.19315	0.64753	-0.10335
C	-2.61232	0.00166	0.48797
H	-3.70499	1.80910	0.97990
H	-2.32170	0.00141	1.54454
C	-2.07119	2.35549	-0.26896
H	-2.43452	3.35345	-0.51164
C	-0.76097	2.06591	-0.42160
O	-4.04351	1.37343	-0.98374
H	-4.66129	0.63551	-0.83153
Br	-4.11528	-1.27721	0.49905
C	-0.95384	-1.88312	0.00118
H	-1.70744	-2.62066	-0.29653
H	-0.79629	-2.00855	1.07536
H	-0.04092	-2.18101	-0.52081
C	-1.76157	-0.49690	-1.88723
H	-2.68841	-1.05573	-2.05220
H	-0.99684	-1.01171	-2.47785
H	-1.89454	0.49223	-2.33285
C	0.13328	3.16588	-0.94408
H	-0.36120	4.14391	-0.92157
H	0.40394	2.97116	-1.98694
H	1.04601	3.26991	-0.35673
C	0.19981	0.66377	1.42374
H	-0.53134	1.23891	2.00631
H	0.18286	-0.34483	1.84634
C	1.09124	0.31368	-0.94709
H	1.54500	1.21107	-1.37642
H	0.83441	-0.29205	-1.81976
C	1.58400	1.24956	1.71192
H	1.58988	2.29956	1.40594
H	1.73360	1.28381	2.79918
C	2.18037	-0.39586	-0.13158
H	1.77516	-1.32998	0.26967
C	2.73342	0.47483	1.02060
Cl	3.47426	-0.63581	2.25156
C	3.81700	1.48923	0.61978
H	4.74547	1.00980	0.29341
H	4.08056	2.13576	1.46596
H	3.47060	2.13928	-0.19091
Br	3.56978	-1.03639	-1.36507

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2553988**

SCF Energy (B3LYP/6-31G) = -6264.29326878**

1l_C006

MMFF Geometry

C	1.577416	1.315666	0.655768
C	3.019716	-0.785174	1.078392
C	0.192066	0.440861	0.818477
C	2.789274	0.441677	0.185522
H	3.635528	-0.460914	1.927117
H	3.706645	1.045295	0.202749
C	1.783897	-1.369705	1.675929
H	1.973976	-2.256834	2.280214
C	0.539775	-0.846890	1.633683
O	3.758723	-1.828748	0.457636
H	3.351340	-1.975582	-0.415677
Br	2.747694	-0.071538	-1.718998
C	1.985769	1.918397	2.046037
H	2.978775	2.381354	1.993882
H	2.018880	1.169472	2.842287
H	1.294134	2.704323	2.368104
C	1.443919	2.561773	-0.267013
H	2.395816	3.106420	-0.309294
H	0.698768	3.272866	0.100405
H	1.180006	2.326765	-1.299182
C	-0.490613	-1.512378	2.516794
H	-0.104571	-2.421473	2.993035
H	-1.375063	-1.816407	1.967217
H	-0.791718	-0.845286	3.329986
C	-0.860988	1.317662	1.575548
H	-0.646781	1.322544	2.652136
H	-0.760070	2.364120	1.275618
C	-0.363171	0.007581	-0.590130
H	0.148303	-0.903984	-0.921217
H	-0.084440	0.771746	-1.317989
C	-2.339086	0.957479	1.389738
H	-2.574645	0.030884	1.920325
H	-2.941452	1.729145	1.888890
C	-1.873955	-0.167846	-0.820446
H	-2.057760	-0.073244	-1.899691
C	-2.762774	0.837402	-0.077152
Cl	-2.534383	2.463289	-0.876319
C	-4.266833	0.542944	-0.174505
H	-4.579112	0.399717	-1.215257
H	-4.860722	1.366988	0.239462
H	-4.547665	-0.352010	0.390174
Br	-2.384550	-2.045277	-0.556339

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2507400**

SCF Energy (B3LYP/6-31G) = -6264.29273655**

1l_C007

MMFF Geometry

C	-1.317452	-0.289339	-0.330232
C	-3.247815	1.303334	0.423823
C	-0.211223	0.645634	0.456141
C	-2.702448	-0.127684	0.394404
H	-4.046493	1.364175	1.172615
H	-2.591389	-0.467031	1.431364
C	-2.181831	2.283112	0.776239
H	-2.555699	3.274786	1.030308
C	-0.856960	2.040135	0.801501
O	-3.819732	1.716386	-0.814859
H	-3.194141	2.300571	-1.273555
Br	-4.124963	-1.333596	-0.259409
C	-0.958258	-1.795632	-0.335044
H	-1.598981	-2.363379	-1.019450
H	-1.080664	-2.244136	0.655700
H	0.053183	-1.989023	-0.683764
C	-1.419259	0.129838	-1.821196
H	-2.295334	-0.304125	-2.312933
H	-0.549088	-0.220630	-2.388570
H	-1.472107	1.214219	-1.948235
C	0.032919	3.196966	1.219192
H	-0.535755	3.998391	1.705073
H	0.522956	3.638344	0.345469
H	0.796505	2.885147	1.935996
C	0.217480	0.021090	1.830344
H	0.570458	0.808755	2.506803
H	-0.650146	-0.405169	2.346021
C	1.081563	0.915382	-0.397706
H	1.603334	1.797098	-0.011824
H	0.817776	1.209718	-1.419178
C	1.326039	-1.041275	1.797676
H	1.609421	-1.267808	2.835056
H	0.927126	-1.982312	1.410605
C	2.129489	-0.199918	-0.420726
H	1.767340	-1.050967	-0.999062
C	2.573222	-0.631342	0.991222
Cl	3.629752	-2.099383	0.880314
C	3.363441	0.435266	1.770106
H	4.327202	0.662581	1.303155
H	3.581026	0.095167	2.789962
H	2.811854	1.375275	1.859078
Br	3.640970	0.428321	-1.530636

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2562556**

SCF Energy (B3LYP/6-31G) = -6264.29068035**

1l_C008

MMFF Geometry

C	1.403119	-0.607364	1.260184
C	3.494521	-0.943935	-0.201738
C	0.400669	-1.038402	0.037796
C	2.763843	-0.006873	0.766240
H	3.953531	-1.759590	0.368746
H	3.425132	0.185749	1.621265
C	2.590064	-1.568782	-1.207018
H	3.111642	-2.038833	-2.040479
C	1.244592	-1.636939	-1.136820
O	4.570913	-0.313251	-0.887199
H	4.220581	0.523997	-1.243796
Br	2.638540	1.801783	-0.010949
C	1.797639	-1.871990	2.102342
H	2.613901	-1.641702	2.797953
H	2.126050	-2.705443	1.473775
H	0.968602	-2.234647	2.718916
C	0.751266	0.356016	2.281983
H	1.460236	0.613848	3.078373
H	-0.116222	-0.098975	2.770560
H	0.423141	1.296982	1.834229
C	0.549476	-2.362358	-2.268963
H	0.136256	-3.312596	-1.918369
H	1.235983	-2.605150	-3.088642
H	-0.246280	-1.758067	-2.710715
C	-0.625169	-2.109007	0.576206
H	-0.167272	-3.106416	0.567792
H	-0.877722	-1.899069	1.621661
C	-0.432512	0.165707	-0.535932
H	-0.589933	0.059303	-1.615980
H	0.120432	1.097452	-0.443740
C	-1.960932	-2.179280	-0.173669
H	-1.781847	-2.476163	-1.209382
H	-2.558233	-3.000005	0.245294
C	-1.806858	0.335181	0.124426
H	-1.669343	0.465829	1.201194
C	-2.756703	-0.852278	-0.145856
Cl	-3.944122	-0.939939	1.224165
C	-3.574758	-0.767668	-1.445291
H	-4.313078	0.040586	-1.428702
H	-4.133426	-1.695932	-1.617918
H	-2.923044	-0.613707	-2.312524
Br	-2.551850	2.074655	-0.405796

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2564030**

SCF Energy (B3LYP/6-31G) = -6264.29341090**

1l_C009

MMFF Geometry

C	1.464279	0.283892	-0.582677
C	2.764948	-1.481772	0.799753
C	0.034324	-0.218323	0.074595
C	2.593475	0.002713	0.460392
H	3.332778	-1.576766	1.732982
H	2.355885	0.541012	1.386101
C	1.449811	-2.177435	0.938565
H	1.520714	-3.195518	1.318113
C	0.237035	-1.673880	0.621396
O	3.483909	-2.188030	-0.209538
H	3.612693	-3.098957	0.101163
Br	4.349204	0.773891	-0.001923
C	1.450875	1.802604	-0.927812
H	2.274827	2.065041	-1.601770
H	1.561047	2.431408	-0.038900
H	0.539946	2.113431	-1.442312
C	1.733665	-0.463046	-1.922169
H	2.757614	-0.303605	-2.275243
H	1.077677	-0.104412	-2.722713
H	1.574880	-1.542089	-1.844072
C	-0.940083	-2.587869	0.833858
H	-0.659654	-3.514148	1.349720
H	-1.362296	-2.892600	-0.126151
H	-1.700305	-2.120984	1.458936
C	-0.310649	0.659930	1.322994
H	0.199692	0.272397	2.215693
H	0.089388	1.669309	1.208915
C	-1.087984	-0.139878	-1.037330
H	-1.104629	-1.078466	-1.606851
H	-0.776472	0.599022	-1.781810
C	-1.790836	0.809023	1.674299
H	-2.177325	-0.134791	2.070826
H	-1.872799	1.523887	2.504639
C	-2.523642	0.306129	-0.683802
H	-2.950188	0.780721	-1.578550
C	-2.651887	1.278431	0.498501
Cl	-2.047095	2.905330	-0.060675
C	-4.093672	1.528629	0.968679
H	-4.745820	1.800963	0.130940
H	-4.137082	2.344834	1.700387
H	-4.523271	0.652148	1.464637
Br	-3.718802	-1.250836	-0.545287

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2452207**

SCF Energy (B3LYP/6-31G) = -6264.28335022**

1l_C010

MMFF Geometry

C	1.463821	0.283405	-0.581067
C	2.752522	-1.448787	0.884165
C	0.033121	-0.216265	0.072035
C	2.597034	0.019025	0.465547
H	3.234452	-1.484017	1.868320
H	2.368427	0.600769	1.367404
C	1.443262	-2.162029	0.962641
H	1.524465	-3.180345	1.343216
C	0.235624	-1.674480	0.606614
O	3.577848	-2.215890	0.010227
H	3.074419	-2.416870	-0.794120
Br	4.355598	0.753596	-0.040772
C	1.449399	1.802401	-0.931907
H	2.273810	2.062917	-1.605989
H	1.557928	2.433904	-0.044599
H	0.539080	2.113112	-1.447404
C	1.728898	-0.467799	-1.917790
H	2.763810	-0.351984	-2.253871
H	1.100980	-0.078444	-2.726979
H	1.518636	-1.538128	-1.849656
C	-0.935449	-2.604635	0.778888
H	-0.653786	-3.540507	1.276422
H	-1.341566	-2.890627	-0.193795
H	-1.708061	-2.158062	1.404115
C	-0.309314	0.654224	1.325215
H	0.207723	0.266312	2.213839
H	0.084201	1.666485	1.212551
C	-1.089973	-0.128104	-1.039481
H	-1.106495	-1.060930	-1.618250
H	-0.779403	0.616412	-1.778489
C	-1.789241	0.789627	1.682353
H	-2.168698	-0.162739	2.065610
H	-1.873625	1.492586	2.522475
C	-2.526140	0.313097	-0.680281
H	-2.952644	0.798734	-1.569114
C	-2.654747	1.270487	0.514092
Cl	-2.054680	2.904978	-0.029151
C	-4.095883	1.511569	0.990393
H	-4.750663	1.792174	0.157458
H	-4.139536	2.318997	1.731747
H	-4.522034	0.628127	1.476899
Br	-3.720234	-1.246047	-0.563015

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2478580**

SCF Energy (B3LYP/6-31G) = -6264.28640854**

1l_C011

MMFF Geometry

C	-1.390770	-0.437094	-0.394220
C	-3.167699	1.380715	0.135898
C	-0.201521	0.644052	-0.075489
C	-2.626468	-0.019852	0.470039
H	-3.762714	1.749900	0.979566
H	-2.335305	-0.031647	1.526470
C	-2.081642	2.361276	-0.188565
H	-2.428709	3.376251	-0.374806
C	-0.768752	2.077615	-0.332167
O	-4.017822	1.359733	-1.010883
H	-4.450307	2.227029	-1.073430
Br	-4.105894	-1.322072	0.479294
C	-0.961113	-1.890029	-0.063113
H	-1.706458	-2.617923	-0.402808
H	-0.823639	-2.055308	1.008436
H	-0.038061	-2.166300	-0.578775
C	-1.752499	-0.443083	-1.910317
H	-2.691127	-0.974796	-2.097697
H	-0.994136	-0.960692	-2.507028
H	-1.855197	0.560932	-2.330228
C	0.135632	3.203054	-0.779368
H	-0.354994	4.180301	-0.702996
H	0.414929	3.069543	-1.829584
H	1.043690	3.268750	-0.180167
C	0.190181	0.593555	1.451581
H	-0.542208	1.142383	2.057492
H	0.172658	-0.432554	1.829314
C	1.083631	0.348782	-0.932049
H	1.533267	1.264348	-1.325844
H	0.828345	-0.221987	-1.828443
C	1.573659	1.164097	1.772188
H	1.578053	2.229878	1.527711
H	1.721332	1.137548	2.859979
C	2.176021	-0.390186	-0.147563
H	1.776220	-1.342794	0.213314
C	2.726211	0.432044	1.040750
Cl	3.483982	-0.725806	2.216783
C	3.799066	1.473240	0.681234
H	4.730033	1.017389	0.329184
H	4.061392	2.083076	1.554615
H	3.443268	2.156255	-0.097588
Br	3.568491	-0.969010	-1.408665

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2516880**

SCF Energy (B3LYP/6-31G) = -6264.28531024**

1l_C012

MMFF Geometry

C	-1.323654	-0.753099	-1.119273
C	-3.558782	-0.815555	0.167919
C	-0.456755	-0.993700	0.257869
C	-2.708375	-0.055347	-0.852668
H	-3.920080	-1.746589	-0.283347
H	-3.280952	0.025291	-1.786075
C	-2.780644	-1.178909	1.385886
H	-3.375256	-1.421840	2.264261
C	-1.436328	-1.262165	1.463246
O	-4.733496	-0.094719	0.524499
H	-5.188796	-0.585161	1.227721
Br	-2.557665	1.848575	-0.338035
C	-1.672467	-2.122548	-1.790146
H	-2.394141	-1.990158	-2.605685
H	-2.109018	-2.835350	-1.083886
H	-0.789356	-2.592367	-2.236242
C	-0.601933	0.041877	-2.234047
H	-1.253462	0.155533	-3.110235
H	0.296440	-0.463750	-2.592260
H	-0.325565	1.052777	-1.927776
C	-0.871379	-1.680647	2.811349
H	-1.608259	-1.568482	3.615546
H	-0.008008	-1.083883	3.109925
H	-0.580013	-2.735516	2.794470
C	0.480721	-2.253234	0.169628
H	0.823802	-2.539042	1.169436
H	-0.065897	-3.137770	-0.172798
C	0.462038	0.227494	0.632887
H	0.717294	0.182552	1.696629
H	-0.087657	1.164969	0.542695
C	1.749807	-2.084999	-0.663843
H	2.311964	-3.028279	-0.631414
H	1.485960	-1.942949	-1.715401
C	1.792080	0.356905	-0.134101
H	1.613294	0.694442	-1.155632
C	2.636376	-0.930464	-0.156380
Cl	3.993600	-0.758354	-1.344415
C	3.266130	-1.297903	1.199256
H	4.052469	-0.595410	1.495315
H	3.730511	-2.290584	1.160638
H	2.527601	-1.315859	2.006306
Br	2.773176	1.896024	0.625217

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2556922**

SCF Energy (B3LYP/6-31G) = -6264.28729609**

1l_C013

MMFF Geometry

C	1.405029	-0.571125	1.263984
C	3.504234	-0.918372	-0.181529
C	0.408728	-1.022041	0.044281
C	2.762480	0.034984	0.763084
H	3.938361	-1.732465	0.411180
H	3.418197	0.245867	1.618260
C	2.606014	-1.547991	-1.194949
H	3.116111	-2.019163	-2.032946
C	1.259919	-1.621676	-1.126096
O	4.612358	-0.294095	-0.820257
H	4.991162	-0.922082	-1.456051
Br	2.613238	1.832558	-0.031287
C	1.806194	-1.823296	2.121916
H	2.624080	-1.581215	2.811563
H	2.134063	-2.664759	1.503866
H	0.980245	-2.179927	2.746196
C	0.744020	0.397760	2.275142
H	1.450260	0.669998	3.069165
H	-0.119750	-0.059822	2.767968
H	0.407482	1.331132	1.817957
C	0.568036	-2.350596	-2.258575
H	0.163616	-3.304727	-1.908220
H	1.254584	-2.586844	-3.080114
H	-0.233607	-1.753082	-2.698606
C	-0.605413	-2.100389	0.589723
H	-0.136305	-3.092607	0.588550
H	-0.861031	-1.885633	1.633471
C	-0.438790	0.169266	-0.537106
H	-0.594236	0.055564	-1.616515
H	0.102294	1.108315	-0.449987
C	-1.939919	-2.191472	-0.159955
H	-1.757398	-2.494019	-1.193367
H	-2.527766	-3.015988	0.264921
C	-1.815355	0.326615	0.121707
H	-1.680023	0.465340	1.197732
C	-2.750904	-0.873616	-0.141881
Cl	-3.939446	-0.966934	1.227039
C	-3.568138	-0.807236	-1.442972
H	-4.316213	-0.007903	-1.432611
H	-4.115354	-1.743256	-1.610348
H	-2.917128	-0.651025	-2.310328
Br	-2.582573	2.053272	-0.418998

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2524267**

SCF Energy (B3LYP/6-31G) = -6264.28481075**

1l_C014

MMFF Geometry

C	1.553333	0.343053	-0.558563
C	2.907181	-1.339536	0.888818
C	0.145642	-0.160734	0.134050
C	2.715464	0.120960	0.467264
H	3.486656	-1.380580	1.818748
H	2.524110	0.712486	1.368604
C	1.606190	-2.037306	1.090536
H	1.704020	-3.036877	1.512468
C	0.383758	-1.564195	0.771702
O	3.611797	-2.114580	-0.078428
H	4.396766	-1.597399	-0.334125
Br	4.463595	0.837733	-0.111346
C	1.487744	1.846719	-0.942973
H	2.342074	2.143553	-1.561107
H	1.488708	2.493445	-0.059945
H	0.601050	2.088806	-1.534328
C	1.823821	-0.444925	-1.874866
H	2.835024	-0.270310	-2.255049
H	1.147027	-0.137643	-2.679049
H	1.699725	-1.524274	-1.749819
C	-0.791334	-2.464771	1.058533
H	-0.512608	-3.323910	1.679881
H	-1.199131	-2.870249	0.129633
H	-1.569684	-1.934705	1.605848
C	-0.270735	0.788889	1.303575
H	-0.638656	0.212208	2.161045
H	0.591449	1.328539	1.705232
C	-0.980100	-0.219097	-0.967555
H	-0.958714	-1.193924	-1.471987
H	-0.694703	0.478711	-1.762418
C	-1.329201	1.826559	0.936341
H	-1.475760	2.494562	1.795676
H	-0.961426	2.464131	0.124908
C	-2.430995	0.210245	-0.648310
H	-2.767460	0.714950	-1.565324
C	-2.659440	1.171419	0.540131
Cl	-3.750698	2.525185	-0.013474
C	-3.346792	0.584709	1.785391
H	-4.386029	0.297878	1.589316
H	-3.378327	1.319505	2.599596
H	-2.828459	-0.293465	2.173742
Br	-3.648320	-1.328272	-0.698354

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2460585**

SCF Energy (B3LYP/6-31G) = -6264.28493952**

1l_C015

MMFF Geometry

C	1.368932	-0.329754	0.468409
C	2.820980	1.592178	-0.500121
C	-0.021048	0.441739	0.027793
C	2.509459	0.093854	-0.516420
H	3.359383	1.865989	-1.415179
H	2.230139	-0.193646	-1.535465
C	1.585090	2.413618	-0.392585
H	1.764011	3.482372	-0.504880
C	0.333026	1.965086	-0.160667
O	3.638298	1.986275	0.600120
H	4.374163	1.349390	0.644062
Br	4.210707	-0.889137	-0.283281
C	1.228177	-1.867784	0.433953
H	2.077165	-2.364397	0.917263
H	1.180656	-2.249174	-0.589123
H	0.353082	-2.209288	0.983126
C	1.746007	0.041646	1.936303
H	2.763066	-0.275502	2.187555
H	1.093417	-0.453245	2.662946
H	1.678874	1.115634	2.130637
C	-0.747581	3.019827	-0.124570
H	-0.343279	4.032473	-0.243595
H	-1.273782	3.023721	0.832017
H	-1.449746	2.881376	-0.949024
C	-0.576913	-0.017750	-1.358699
H	-1.206700	0.777009	-1.779882
H	0.231758	-0.122987	-2.089332
C	-1.136195	0.216164	1.122845
H	-1.215677	1.088795	1.781416
H	-0.812970	-0.581437	1.798026
C	-1.427045	-1.291312	-1.408565
H	-1.874289	-1.327121	-2.412030
H	-0.773108	-2.167515	-1.390407
C	-2.539934	-0.232622	0.660637
H	-3.099081	-0.532909	1.557274
C	-2.540657	-1.401123	-0.345896
Cl	-2.239548	-2.929565	0.619719
C	-3.898377	-1.659877	-1.025224
H	-4.709189	-1.726404	-0.290535
H	-3.887795	-2.599933	-1.591009
H	-4.153151	-0.873775	-1.743809
Br	-3.626836	1.291126	0.077584

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2431448**

SCF Energy (B3LYP/6-31G) = -6264.28565196**

1m_C001

MMFF Geometry

C	1.492214	0.724255	0.497886
C	2.452904	-1.636593	-0.034565
C	-0.018638	0.074639	0.606570
C	2.320500	-0.174387	-0.478645
H	2.671417	-2.269830	-0.902139
H	1.841103	-0.158060	-1.464381
C	1.235155	-2.145901	0.660666
H	1.320251	-3.183648	0.981760
C	0.142368	-1.429255	1.001000
O	3.513441	-1.829700	0.903528
H	4.285628	-1.347081	0.557109
Br	4.118251	0.528198	-0.901636
C	2.146293	0.800353	1.906681
H	3.196089	1.105713	1.850544
H	2.112913	-0.150377	2.445146
H	1.643497	1.543361	2.535736
C	1.478365	2.183436	-0.049929
H	2.432835	2.688603	0.139493
H	0.716318	2.809357	0.417392
H	1.318476	2.219017	-1.132164
C	-0.858258	-2.123515	1.896643
H	-0.906043	-1.639722	2.876489
H	-0.587706	-3.169037	2.086898
H	-1.855331	-2.147955	1.466234
C	-0.846113	0.858510	1.676253
H	-0.548394	0.552246	2.687099
H	-0.602774	1.922910	1.642419
C	-0.715406	0.155156	-0.806090
H	-0.335693	-0.643727	-1.456883
H	-0.396326	1.078135	-1.297415
C	-2.373699	0.759821	1.575514
H	-2.712751	-0.227344	1.899681
H	-2.807207	1.456963	2.306086
C	-2.248472	0.194099	-0.892157
H	-2.516493	0.579789	-1.885349
C	-2.926754	1.062711	0.178040
Cl	-2.548558	2.805488	-0.216330
C	-4.459646	0.968431	0.181233
H	-4.902449	1.714450	0.852377
H	-4.810051	-0.007774	0.531790
H	-4.872084	1.137023	-0.820102
Br	-2.958027	-1.629605	-1.023594

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2564372**

SCF Energy (B3LYP/6-31G) = -6264.29816142**

1m_C002

MMFF Geometry

C	-1.388911	0.125332	0.750817
C	-3.006018	0.835194	-1.156595
C	-0.163082	0.955770	0.046449
C	-2.385720	-0.323549	-0.368469
H	-3.424653	0.456580	-2.096691
H	-1.863497	-0.977987	-1.074897
C	-2.009217	1.900229	-1.459097
H	-2.377076	2.665837	-2.140944
C	-0.760025	1.992891	-0.959128
O	-4.064714	1.486857	-0.458964
H	-4.653353	0.785676	-0.125730
Br	-3.848167	-1.494740	0.259314
C	-2.102280	1.018891	1.806997
H	-3.025433	0.560014	2.174328
H	-2.356880	2.008188	1.416525
H	-1.472554	1.177217	2.689397
C	-0.875989	-1.125764	1.510902
H	-1.667290	-1.590627	2.108991
H	-0.083276	-0.882797	2.223058
H	-0.499965	-1.891346	0.824968
C	0.077267	3.162245	-1.423713
H	-0.442469	3.774300	-2.170099
H	1.000860	2.819584	-1.898017
H	0.315456	3.828302	-0.589700
C	0.689667	1.665276	1.160415
H	0.216861	2.612455	1.449936
H	0.715308	1.061901	2.073326
C	0.780528	0.024367	-0.797020
H	1.144856	0.546736	-1.691837
H	0.218931	-0.827842	-1.192999
C	2.151365	1.937014	0.786195
H	2.184690	2.643698	-0.046303
H	2.633041	2.473130	1.614797
C	2.002849	-0.473666	-0.018086
H	1.664515	-1.030299	0.858968
C	2.953665	0.664927	0.415785
Cl	3.840696	0.111801	1.900112
C	4.018714	1.068788	-0.617985
H	4.577645	1.950696	-0.281132
H	3.558534	1.322440	-1.579486
H	4.758649	0.281175	-0.793536
Br	2.882627	-1.880408	-1.072112

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2589863**

SCF Energy (B3LYP/6-31G) = -6264.29682376**

1m_C003

MMFF Geometry

C	-1.355834	0.046347	0.728689
C	-3.079630	0.866708	-1.049801
C	-0.194888	1.022941	0.085612
C	-2.368261	-0.328504	-0.411718
H	-3.537353	0.559179	-1.997724
H	-1.831902	-0.871446	-1.198604
C	-2.139281	1.988493	-1.305529
H	-2.557035	2.784462	-1.920574
C	-0.878544	2.093600	-0.841700
O	-4.117886	1.405900	-0.236764
H	-4.674101	0.655379	0.039704
Br	-3.755296	-1.640478	0.112029
C	-2.082180	0.767240	1.897182
H	-2.987334	0.237375	2.209681
H	-2.371968	1.790577	1.641530
H	-1.443599	0.818883	2.786465
C	-0.797762	-1.271439	1.317397
H	-1.554973	-1.808093	1.900348
H	0.021740	-1.110095	2.013583
H	-0.463715	-1.955883	0.531528
C	-0.103453	3.325974	-1.268089
H	-0.574059	3.834158	-2.117821
H	0.912346	3.076103	-1.584778
H	-0.054462	4.051308	-0.449711
C	0.631766	1.793490	1.177333
H	1.120491	2.667668	0.736476
H	-0.021649	2.226633	1.940751
C	0.803386	0.233231	-0.833569
H	1.243244	0.919342	-1.568708
H	0.255419	-0.492614	-1.445988
C	1.764368	1.026741	1.858674
H	2.298627	1.722795	2.520483
H	1.350931	0.269985	2.529296
C	1.965540	-0.484483	-0.126173
H	1.602962	-1.373211	0.393287
C	2.753912	0.403722	0.853950
Cl	3.901955	-0.612538	1.819872
C	3.586404	1.506090	0.175900
H	4.025353	2.181211	0.920319
H	2.984956	2.118828	-0.501619
H	4.418678	1.098095	-0.407268
Br	3.109981	-1.278824	-1.528123

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2595556**

SCF Energy (B3LYP/6-31G) = -6264.29710058**

1m_C004

MMFF Geometry

C	1.49817	0.71709	0.51149
C	2.48416	-1.63149	-0.01855
C	-0.00965	0.05880	0.61124
C	2.33344	-0.17271	-0.46745
H	2.74295	-2.25425	-0.88298
H	1.83960	-0.17010	-1.44630
C	1.25245	-2.16252	0.64263
H	1.31911	-3.20902	0.93586
C	0.15302	-1.45369	0.97932
O	3.52751	-1.78140	0.94539
H	3.68063	-2.73261	1.06726
Br	4.10317	0.56521	-0.93412
C	2.14844	0.78710	1.92203
H	3.20262	1.07765	1.86725
H	2.09873	-0.16182	2.46255
H	1.65353	1.53773	2.54844
C	1.47625	2.18104	-0.02372
H	2.42337	2.69389	0.18170
H	0.70209	2.79466	0.44015
H	1.32826	2.22495	-1.10739
C	-0.86287	-2.16672	1.84286
H	-0.92292	-1.70653	2.83341
H	-0.59829	-3.21743	2.01158
H	-1.85369	-2.17735	1.39865
C	-0.83722	0.82153	1.69605
H	-0.54070	0.49311	2.70037
H	-0.59152	1.88602	1.68513
C	-0.70847	0.16100	-0.79983
H	-0.33367	-0.63197	-1.46065
H	-0.38440	1.08751	-1.28080
C	-2.36484	0.72800	1.59217
H	-2.70619	-0.26501	1.89548
H	-2.79734	1.41064	2.33691
C	-2.24119	0.21212	-0.88635
H	-2.50531	0.62116	-1.87126
C	-2.91667	1.06109	0.20114
Cl	-2.53366	2.80996	-0.15800
C	-4.44994	0.97164	0.20288
H	-4.89024	1.70555	0.88887
H	-4.80337	-0.01019	0.53417
H	-4.86211	1.16146	-0.79476
Br	-2.96259	-1.60377	-1.06177

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2530983**

SCF Energy (B3LYP/6-31G) = -6264.29061327**

1m_C005

MMFF Geometry

C	1.165276	-0.114641	-1.095166
C	3.225388	-1.491346	-0.368067
C	0.395778	-0.409280	0.328879
C	2.730652	-0.173200	-0.966807
H	3.118488	-2.294261	-1.105552
H	3.201918	-0.041595	-1.949625
C	2.457109	-1.885423	0.842386
H	2.949888	-2.632513	1.463976
C	1.234275	-1.432003	1.184071
O	4.610987	-1.460515	-0.040721
H	4.752029	-0.657227	0.493876
Br	3.517976	1.343288	0.033938
C	0.800697	1.219743	-1.789048
H	1.358268	1.330995	-2.728131
H	1.045513	2.095671	-1.185022
H	-0.254937	1.276142	-2.059116
C	0.797754	-1.210387	-2.148989
H	1.429060	-1.126671	-3.042245
H	-0.236585	-1.109951	-2.494885
H	0.923544	-2.224768	-1.758086
C	0.645994	-2.005320	2.462818
H	1.413766	-2.470740	3.092270
H	-0.089240	-2.782750	2.232507
H	0.168747	-1.244326	3.082690
C	0.175537	0.883671	1.192356
H	0.004199	0.612632	2.238923
H	1.077745	1.494141	1.226800
C	-1.020724	-1.065026	0.126223
H	-1.370578	-1.491187	1.073178
H	-0.954520	-1.940269	-0.529714
C	-0.999317	1.797211	0.803779
H	-1.098830	2.570387	1.578469
H	-0.756459	2.351640	-0.105375
C	-2.125191	-0.117407	-0.345778
H	-1.911740	0.239203	-1.355475
C	-2.340761	1.062549	0.622118
Cl	-3.497239	2.251742	-0.107690
C	-2.905164	0.672298	2.000069
H	-2.976553	1.548280	2.656434
H	-2.274359	-0.058179	2.514791
H	-3.912191	0.248416	1.932054
Br	-3.759857	-1.191208	-0.611347

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2586267**

SCF Energy (B3LYP/6-31G) = -6264.29563596**

1m_C006

MMFF Geometry

C	-1.394553	0.112874	0.760560
C	-3.035487	0.857059	-1.110962
C	-0.174172	0.951141	0.055717
C	-2.400990	-0.317622	-0.357772
H	-3.493832	0.487566	-2.036196
H	-1.874659	-0.942055	-1.088300
C	-2.028227	1.910064	-1.438062
H	-2.380221	2.669783	-2.133912
C	-0.773495	1.991209	-0.949098
O	-4.058983	1.499803	-0.355729
H	-4.456681	2.184062	-0.918511
Br	-3.825144	-1.543671	0.243025
C	-2.098796	0.991316	1.834856
H	-3.029695	0.535887	2.187112
H	-2.336651	1.993440	1.467007
H	-1.470001	1.120600	2.722746
C	-0.874582	-1.146354	1.502582
H	-1.659984	-1.616711	2.104232
H	-0.075609	-0.909615	2.209949
H	-0.504685	-1.905196	0.805991
C	0.074648	3.147394	-1.428367
H	-0.440065	3.755451	-2.181460
H	0.995574	2.792870	-1.898832
H	0.317779	3.820617	-0.601477
C	0.678528	1.659566	1.170067
H	0.202986	2.604382	1.462926
H	0.707342	1.052695	2.080692
C	0.770578	0.022559	-0.791111
H	1.129007	0.544360	-1.688374
H	0.210794	-0.832258	-1.184229
C	2.138998	1.937708	0.796005
H	2.169601	2.651388	-0.030520
H	2.619739	2.469095	1.628220
C	1.998361	-0.470864	-0.017609
H	1.667026	-1.031775	0.859284
C	2.945371	0.671333	0.414894
Cl	3.846263	0.117560	1.890524
C	4.001146	1.085422	-0.624568
H	4.557389	1.969134	-0.287965
H	3.533041	1.340289	-1.581903
H	4.744418	0.302850	-0.808344
Br	2.881967	-1.869775	-1.079711

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2552726**

SCF Energy (B3LYP/6-31G) = -6264.28868662**

1m_C007

MMFF Geometry

C	-1.359012	0.027728	0.733095
C	-3.111569	0.882220	-0.998751
C	-0.206509	1.014304	0.089279
C	-2.386593	-0.326072	-0.400784
H	-3.613498	0.581272	-1.926282
H	-1.851963	-0.837029	-1.210416
C	-2.161099	1.992451	-1.286002
H	-2.564526	2.782527	-1.917203
C	-0.893551	2.086569	-0.837772
O	-4.106075	1.411810	-0.127408
H	-4.549024	2.140344	-0.592477
Br	-3.735474	-1.684459	0.092044
C	-2.069553	0.726843	1.923533
H	-2.974308	0.193744	2.232337
H	-2.355603	1.757187	1.692997
H	-1.421404	0.757298	2.806984
C	-0.791510	-1.298322	1.294661
H	-1.540466	-1.845240	1.878785
H	0.035555	-1.145480	1.984154
H	-0.464771	-1.969797	0.494592
C	-0.107711	3.305897	-1.284286
H	-0.048499	4.041058	-0.475373
H	-0.577828	3.807484	-2.138195
H	0.904632	3.044936	-1.602133
C	0.617095	1.787440	1.180752
H	1.102723	2.663670	0.740527
H	-0.037980	2.218114	1.944231
C	0.794858	0.228054	-0.831528
H	1.229019	0.913822	-1.569821
H	0.248909	-0.502035	-1.440916
C	1.750141	1.021768	1.862184
H	2.279680	1.716553	2.529054
H	1.336843	0.259880	2.527291
C	1.963963	-0.482404	-0.127383
H	1.610444	-1.377713	0.386908
C	2.744928	0.407809	0.856962
Cl	3.898529	-0.603710	1.821081
C	3.571495	1.517583	0.183509
H	4.002168	2.195250	0.930441
H	2.968000	2.126179	-0.495880
H	4.409371	1.116939	-0.396758
Br	3.115870	-1.259015	-1.533951

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2558367**

SCF Energy (B3LYP/6-31G) = -6264.28908719**

1m_C008

MMFF Geometry

C	-1.445460	0.121704	1.304867
C	-3.003297	-1.642423	0.274306
C	-0.199758	-0.287877	0.300445
C	-2.852610	-0.175158	0.689649
H	-3.219927	-2.236592	1.170255
H	-3.639447	0.053914	1.420429
C	-1.773166	-2.223360	-0.334805
H	-1.929021	-3.206651	-0.778709
C	-0.535106	-1.683561	-0.328636
O	-4.098487	-1.873898	-0.604102
H	-4.033295	-1.204301	-1.309790
Br	-3.372150	1.022542	-0.788939
C	-1.400550	1.594237	1.800650
H	-2.220199	1.783952	2.505257
H	-1.505406	2.332290	1.003710
H	-0.474083	1.823932	2.333920
C	-1.371092	-0.734396	2.621311
H	-2.294902	-0.635233	3.204426
H	-0.560236	-0.411615	3.282336
H	-1.221163	-1.799774	2.423179
C	0.542482	-2.504014	-0.987634
H	0.132649	-3.345900	-1.558742
H	1.197928	-2.939727	-0.230781
H	1.117549	-1.917520	-1.702408
C	-0.074762	0.712862	-0.894630
H	-0.709884	0.388246	-1.728788
H	-0.458376	1.694663	-0.614934
C	1.129536	-0.324349	1.164209
H	1.245390	-1.318624	1.615755
H	0.983119	0.339810	2.021690
C	1.315575	0.958059	-1.485398
H	1.630754	0.090470	-2.072782
H	1.234786	1.777997	-2.212584
C	2.475569	0.166859	0.592524
H	3.086488	0.512590	1.438120
C	2.377080	1.296745	-0.439098
Cl	1.875551	2.809627	0.445471
C	3.705438	1.651425	-1.125020
H	3.608784	2.560023	-1.732020
H	4.041027	0.863291	-1.806833
H	4.499679	1.827066	-0.390463
Br	3.573636	-1.347265	-0.009257

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2445028**

SCF Energy (B3LYP/6-31G) = -6264.28759237**

1m_C009

MMFF Geometry

C	1.196271	-0.568185	-1.083506
C	3.351580	-1.379565	0.066846
C	0.382316	-0.527532	0.345236
C	2.736033	-0.354525	-0.892254
H	3.488970	-2.324798	-0.471693
H	3.255461	-0.438581	-1.855950
C	2.497263	-1.680019	1.250522
H	3.004469	-2.256988	2.023554
C	1.200091	-1.343005	1.410265
O	4.648553	-1.013346	0.523600
H	4.585614	-0.088522	0.825932
Br	3.232215	1.480409	-0.364827
C	0.687571	0.411818	-2.173208
H	1.356045	0.393454	-3.043859
H	0.633661	1.451822	-1.849627
H	-0.296035	0.126721	-2.554536
C	1.048773	-1.979472	-1.752853
H	1.775823	-2.107002	-2.564409
H	0.062196	-2.115339	-2.209270
H	1.199466	-2.800319	-1.045387
C	0.554055	-1.766931	2.712749
H	1.270418	-2.245871	3.391143
H	-0.238664	-2.500491	2.544660
H	0.154716	-0.911254	3.257671
C	0.227979	0.934803	0.904986
H	1.054716	1.172230	1.585866
H	0.272577	1.676976	0.107260
C	-1.067384	-1.131092	0.198508
H	-1.430092	-1.525025	1.153897
H	-1.067830	-2.007191	-0.454031
C	-1.077558	1.203999	1.665232
H	-1.119844	0.550726	2.541442
H	-1.049707	2.222590	2.074844
C	-2.105031	-0.098492	-0.255487
H	-1.777446	0.355546	-1.189933
C	-2.350751	0.996801	0.810032
Cl	-2.706387	2.549801	-0.057836
C	-3.519959	0.747983	1.777194
H	-3.548462	1.512729	2.563314
H	-3.421397	-0.223878	2.273819
H	-4.494023	0.779026	1.277814
Br	-3.729872	-1.044293	-0.820706

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2510379**

SCF Energy (B3LYP/6-31G) = -6264.28849797**

1m_C010

MMFF Geometry

C	1.167765	-0.098193	-1.088827
C	3.226727	-1.474183	-0.365485
C	0.399785	-0.390177	0.336215
C	2.734740	-0.150973	-0.956923
H	3.087871	-2.274298	-1.101336
H	3.205361	-0.016592	-1.939784
C	2.470771	-1.853744	0.861334
H	2.960514	-2.582213	1.504464
C	1.246371	-1.400247	1.200825
O	4.625128	-1.451263	-0.099345
H	4.865290	-2.289149	0.328186
Br	3.504287	1.374052	0.041356
C	0.798351	1.232574	-1.787862
H	1.357834	1.343617	-2.725825
H	1.036417	2.112003	-1.186250
H	-0.257022	1.282200	-2.060885
C	0.802740	-1.197204	-2.140467
H	1.436228	-1.115799	-3.032373
H	-0.230876	-1.098154	-2.488897
H	0.926603	-2.210714	-1.746934
C	0.665545	-1.953763	2.492247
H	1.436263	-2.412527	3.122994
H	-0.072763	-2.732897	2.278307
H	0.194595	-1.183982	3.105711
C	0.164695	0.908496	1.188495
H	-0.006538	0.645433	2.236836
H	1.060534	1.528340	1.219933
C	-1.009908	-1.060804	0.136841
H	-1.357350	-1.482257	1.086769
H	-0.934367	-1.940897	-0.511544
C	-1.018501	1.807467	0.790714
H	-1.127272	2.585394	1.559389
H	-0.779672	2.357628	-0.122069
C	-2.121871	-0.127255	-0.345681
H	-1.908695	0.224155	-1.357338
C	-2.351860	1.057810	0.612470
Cl	-3.519848	2.228656	-0.128757
C	-2.914924	0.672334	1.992328
H	-2.997487	1.552717	2.641457
H	-2.277224	-0.046903	2.514332
H	-3.917009	0.236702	1.925552
Br	-3.745070	-1.219529	-0.607767

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2546462**

SCF Energy (B3LYP/6-31G) = -6264.28729176**

1m_C011

MMFF Geometry

C	-1.448417	0.138284	1.294234
C	-3.015528	-1.621422	0.271095
C	-0.203352	-0.280074	0.293693
C	-2.856026	-0.150195	0.672503
H	-3.215330	-2.202567	1.180076
H	-3.642420	0.087827	1.401154
C	-1.786869	-2.210429	-0.343743
H	-1.928739	-3.194030	-0.788191
C	-0.546191	-1.674874	-0.335662
O	-4.146534	-1.841508	-0.563977
H	-4.111017	-2.752621	-0.896006
Br	-3.355669	1.058656	-0.801920
C	-1.394624	1.610833	1.790209
H	-2.216412	1.806772	2.490611
H	-1.489063	2.350198	0.993253
H	-0.469150	1.833215	2.328358
C	-1.382736	-0.716380	2.612353
H	-2.309610	-0.614981	3.190163
H	-0.575080	-0.393921	3.277518
H	-1.232494	-1.782168	2.416737
C	0.529900	-2.496657	-0.996257
H	0.118377	-3.333648	-1.573284
H	1.180904	-2.939355	-0.239645
H	1.109783	-1.909440	-1.706339
C	-0.066470	0.719970	-0.900867
H	-0.700054	0.399271	-1.737693
H	-0.444691	1.704201	-0.622493
C	1.123066	-0.326061	1.161732
H	1.230702	-1.321390	1.613007
H	0.978494	0.338549	2.019153
C	1.327432	0.957831	-1.486144
H	1.639450	0.089783	-2.074462
H	1.254185	1.779718	-2.211950
C	2.474290	0.156400	0.594998
H	3.084508	0.497287	1.443087
C	2.387544	1.287812	-0.435903
Cl	1.895218	2.803418	0.448854
C	3.720862	1.633062	-1.117105
H	3.633046	2.542831	-1.723699
H	4.052815	0.842954	-1.798419
H	4.513959	1.802166	-0.379779
Br	3.564644	-1.365093	-0.002956

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2404566**

SCF Energy (B3LYP/6-31G) = -6264.27903519**

1n_C001

MMFF Geometry

C	1.507736	0.630675	-0.740727
C	2.757028	0.216930	1.483696
C	0.124504	0.930452	0.089882
C	2.372825	-0.347243	0.114064
H	3.643170	0.860259	1.419099
H	1.861551	-1.309960	0.232264
C	1.667265	1.014313	2.116994
H	1.895555	1.343804	3.129898
C	0.500715	1.372044	1.540622
O	3.069167	-0.842643	2.386478
H	3.803305	-1.342443	1.986612
Br	4.054047	-0.907470	-0.775403
C	2.264046	1.962417	-1.017127
H	3.236323	1.789837	-1.489254
H	2.444823	2.543135	-0.108295
H	1.703036	2.601927	-1.707190
C	1.236961	-0.020309	-2.128614
H	2.121804	0.030003	-2.773628
H	0.437066	0.473835	-2.683332
H	0.974654	-1.079645	-2.041170
C	-0.416566	2.249912	2.357070
H	-0.011625	2.456547	3.354928
H	-1.387946	1.781758	2.517771
H	-0.551864	3.223271	1.877142
C	-0.699252	2.037899	-0.650442
H	-0.257875	3.024458	-0.457389
H	-0.621043	1.907328	-1.732788
C	-0.717886	-0.386010	0.196768
H	-0.261900	-1.059256	0.935574
H	-0.674212	-0.934136	-0.748378
C	-2.200602	2.123969	-0.339806
H	-2.351562	2.593684	0.636746
H	-2.658311	2.821304	-1.055448
C	-2.196780	-0.207309	0.553543
H	-2.293638	0.111180	1.594894
C	-2.939291	0.773632	-0.373116
Cl	-2.965058	0.193156	-2.086606
C	-4.395478	1.003456	0.061224
H	-5.010307	0.103969	-0.045391
H	-4.868684	1.789013	-0.539963
H	-4.446442	1.319125	1.109524
Br	-3.027321	-1.998830	0.586377

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2658995**

SCF Energy (B3LYP/6-31G) = -6264.30299546**

1n_C002

MMFF Geometry

C	1.526586	0.709790	-0.660697
C	2.729872	-0.004125	1.520796
C	0.135200	0.916578	0.183859
C	2.380306	-0.373641	0.074671
H	3.642350	0.602283	1.561224
H	1.868549	-1.342972	0.047260
C	1.651674	0.754087	2.223068
H	1.882979	0.984961	3.262882
C	0.499087	1.193198	1.677253
O	2.978091	-1.179151	2.292722
H	2.142101	-1.671028	2.360042
Br	4.073468	-0.805011	-0.862285
C	2.292296	2.060715	-0.764479
H	3.261710	1.945028	-1.259201
H	2.480899	2.516468	0.211481
H	1.734561	2.788439	-1.363695
C	1.266933	0.234194	-2.120800
H	2.161391	0.347760	-2.744028
H	0.483252	0.803316	-2.624002
H	0.988270	-0.823609	-2.164466
C	-0.407683	2.006706	2.569239
H	-0.006313	2.108054	3.584629
H	-1.388302	1.542270	2.678216
H	-0.522393	3.024232	2.185311
C	-0.684208	2.098933	-0.437384
H	-0.242943	3.058554	-0.138111
H	-0.601734	2.085580	-1.526891
C	-0.708199	-0.401546	0.138461
H	-0.254501	-1.155434	0.796396
H	-0.663929	-0.838444	-0.863093
C	-2.187464	2.153920	-0.127451
H	-2.342954	2.519640	0.891938
H	-2.640909	2.922856	-0.768591
C	-2.186701	-0.258216	0.513557
H	-2.280947	-0.048155	1.582530
C	-2.927457	0.815492	-0.305245
Cl	-2.949825	0.418643	-2.069798
C	-4.384214	0.999181	0.148315
H	-4.999348	0.116522	-0.054169
H	-4.855742	1.844419	-0.367125
H	-4.437002	1.201992	1.224074
Br	-3.018122	-2.042077	0.363234

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2641691**

SCF Energy (B3LYP/6-31G) = -6264.29794241**

1n_C003

MMFF Geometry

C	1.520348	0.702946	-0.671591
C	2.722761	-0.016295	1.509842
C	0.132457	0.914422	0.175294
C	2.370875	-0.382258	0.064229
H	3.647649	0.572101	1.551141
H	1.861660	-1.352924	0.033237
C	1.652680	0.754819	2.212045
H	1.874754	0.988334	3.251931
C	0.502635	1.200959	1.665422
O	2.937419	-1.211855	2.259340
H	3.358914	-0.958068	3.097125
Br	4.071725	-0.804904	-0.872001
C	2.289050	2.051939	-0.779544
H	3.254160	1.934755	-1.282196
H	2.486776	2.505893	0.195433
H	1.728800	2.781893	-1.373642
C	1.257344	0.224740	-2.130277
H	2.152177	0.331350	-2.754167
H	0.477012	0.797027	-2.635031
H	0.972753	-0.831564	-2.171111
C	-0.401132	2.019979	2.555049
H	0.002665	2.126932	3.568884
H	-1.381814	1.556827	2.669067
H	-0.515744	3.035546	2.165933
C	-0.689014	2.093580	-0.449246
H	-0.245956	3.054788	-0.157863
H	-0.611980	2.073661	-1.538990
C	-0.711605	-0.404117	0.138713
H	-0.255551	-1.155518	0.797763
H	-0.671673	-0.844646	-0.861453
C	-2.190562	2.151190	-0.132144
H	-2.341309	2.522556	0.885835
H	-2.646577	2.917119	-0.775096
C	-2.188135	-0.259348	0.519406
H	-2.277680	-0.046055	1.588198
C	-2.932094	0.812377	-0.299552
Cl	-2.965983	0.410011	-2.063084
C	-4.386130	0.999652	0.161768
H	-5.003750	0.117270	-0.034212
H	-4.859462	1.843821	-0.353785
H	-4.432435	1.206188	1.237119
Br	-3.024522	-2.041958	0.376490

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2631188**

SCF Energy (B3LYP/6-31G) = -6264.29662416**

1n_C004

MMFF Geometry

C	-1.453466	0.387721	-1.080604
C	-3.261309	1.224242	0.612970
C	-0.339021	0.431058	0.108879
C	-2.915975	0.266789	-0.537189
H	-3.915639	0.757087	1.357809
H	-3.610327	0.447841	-1.369016
C	-2.090238	1.801657	1.336064
H	-2.362934	2.559668	2.069730
C	-0.789072	1.501447	1.145490
O	-3.989218	2.344353	0.097052
H	-4.865983	2.017696	-0.168589
Br	-3.461252	-1.560266	-0.025932
C	-1.195898	-0.712229	-2.151291
H	-2.016743	-0.736427	-2.879277
H	-1.110600	-1.718011	-1.736688
H	-0.285821	-0.526326	-2.729396
C	-1.405647	1.727211	-1.895727
H	-2.214496	1.763141	-2.635808
H	-0.470412	1.829388	-2.456459
H	-1.506759	2.614270	-1.264400
C	0.215865	2.273287	1.963995
H	-0.263195	2.999502	2.631337
H	0.884637	2.849635	1.318550
H	0.800715	1.612582	2.605633
C	-0.257495	-0.934768	0.861623
H	-1.104168	-1.039465	1.550270
H	-0.343623	-1.764445	0.156975
C	1.061087	0.761356	-0.521534
H	1.097647	1.823769	-0.797634
H	1.168222	0.218831	-1.465485
C	1.007471	-1.190886	1.687446
H	0.998942	-0.544007	2.571650
H	0.960217	-2.215492	2.081400
C	2.302441	0.435641	0.322578
H	2.409377	1.156841	1.135897
C	2.315072	-0.988659	0.901873
Cl	2.400845	-2.242887	-0.398118
C	3.499310	-1.223008	1.852524
H	4.463301	-1.185014	1.335008
H	3.431264	-2.205206	2.335261
H	3.518959	-0.469227	2.647895
Br	3.897768	0.833479	-0.772515

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2595733**

SCF Energy (B3LYP/6-31G) = -6264.29475605**

1n_C005

MMFF Geometry

C	-1.449270	0.367384	-1.087341
C	-3.284380	1.263801	0.530491
C	-0.352611	0.392324	0.122624
C	-2.923191	0.260773	-0.572295
H	-4.038508	0.854268	1.211886
H	-3.601915	0.412210	-1.422827
C	-2.128269	1.759171	1.339297
H	-2.401352	2.477970	2.110369
C	-0.829644	1.423621	1.191155
O	-3.888516	2.409823	-0.080371
H	-4.157081	3.014110	0.631627
Br	-3.469631	-1.545347	0.004739
C	-1.190433	-0.733209	-2.157277
H	-1.972761	-0.708027	-2.926530
H	-1.181846	-1.747241	-1.754397
H	-0.241838	-0.589897	-2.682558
C	-1.367269	1.709008	-1.896484
H	-2.183681	1.777408	-2.625723
H	-0.436446	1.782872	-2.469244
H	-1.426406	2.594516	-1.257526
C	0.158614	2.116749	2.097633
H	-0.332063	2.798257	2.802637
H	0.853743	2.729889	1.517148
H	0.715727	1.403950	2.706256
C	-0.253637	-0.997910	0.829575
H	-1.089790	-1.127130	1.526582
H	-0.347622	-1.804303	0.099818
C	1.047469	0.776121	-0.478848
H	1.069349	1.853256	-0.694114
H	1.167118	0.290918	-1.452195
C	1.021081	-1.289099	1.628409
H	1.015056	-0.696079	2.549165
H	0.984877	-2.334838	1.964044
C	2.289871	0.422075	0.351357
H	2.381962	1.096739	1.205643
C	2.321215	-1.032224	0.847895
Cl	2.409988	-2.209247	-0.521296
C	3.513082	-1.309268	1.777435
H	4.473633	-1.236114	1.257314
H	3.455080	-2.316930	2.205993
H	3.532302	-0.600046	2.612796
Br	3.882918	0.904689	-0.711965

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2578012**

SCF Energy (B3LYP/6-31G) = -6264.29321928**

1n_C006

MMFF Geometry

C	-1.457625	0.381847	-1.079795
C	-3.273044	1.234019	0.599762
C	-0.347756	0.420205	0.115601
C	-2.926191	0.269078	-0.544131
H	-3.947736	0.768183	1.325920
H	-3.617662	0.447007	-1.378901
C	-2.103887	1.789391	1.346638
H	-2.380216	2.521008	2.106152
C	-0.803638	1.482872	1.160950
O	-4.001593	2.349947	0.073507
H	-3.361265	2.977560	-0.301322
Br	-3.467417	-1.557822	-0.020730
C	-1.202707	-0.721855	-2.148264
H	-2.012051	-0.728915	-2.889410
H	-1.143667	-1.730171	-1.735425
H	-0.279328	-0.553822	-2.710369
C	-1.388460	1.718142	-1.897877
H	-2.218394	1.785086	-2.611609
H	-0.467724	1.785613	-2.487823
H	-1.429093	2.608015	-1.264627
C	0.199230	2.225422	2.009654
H	-0.281160	2.938856	2.689718
H	0.878528	2.812397	1.385070
H	0.772806	1.545119	2.640480
C	-0.263260	-0.952440	0.856402
H	-1.106059	-1.061246	1.549140
H	-0.355371	-1.775698	0.145212
C	1.052713	0.764094	-0.507160
H	1.086576	1.831276	-0.765257
H	1.162002	0.238702	-1.460545
C	1.005609	-1.223239	1.671586
H	1.001195	-0.592994	2.567583
H	0.959634	-2.254698	2.047511
C	2.294362	0.426850	0.332129
H	2.398226	1.133115	1.158909
C	2.310259	-1.007668	0.884910
Cl	2.391014	-2.236663	-0.438632
C	3.497931	-1.259432	1.826702
H	4.459996	-1.212793	1.306316
H	3.431156	-2.250054	2.292094
H	3.521024	-0.519947	2.635289
Br	3.888356	0.850062	-0.754643

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2600461**

SCF Energy (B3LYP/6-31G) = -6264.29544814**

1o_C001

MMFF Geometry

C	-1.360390	0.163287	0.874598
C	-2.978874	1.008699	-0.963119
C	-0.110036	0.988516	0.194424
C	-2.378055	-0.207818	-0.259520
H	-3.771966	1.477919	-0.368903
H	-1.914457	-0.876943	-0.993306
C	-1.950327	2.036793	-1.270177
H	-2.287008	2.818447	-1.950162
C	-0.690629	2.063901	-0.793225
O	-3.554338	0.622722	-2.211157
H	-4.232056	-0.047252	-2.010121
Br	-3.908019	-1.317138	0.358411
C	-2.056545	1.034094	1.959576
H	-2.997487	0.593436	2.302783
H	-2.282808	2.043676	1.603836
H	-1.430815	1.126750	2.854165
C	-0.927870	-1.144351	1.576688
H	-1.737411	-1.567650	2.182085
H	-0.108381	-0.995846	2.275846
H	-0.641883	-1.914966	0.854390
C	0.199881	3.188053	-1.288744
H	-0.210954	3.674153	-2.181259
H	1.193975	2.827171	-1.565212
H	0.302408	3.962112	-0.521494
C	0.777395	1.737244	1.252504
H	1.324453	2.555764	0.775391
H	0.162585	2.250458	1.997778
C	0.809799	0.059128	-0.674107
H	1.309239	0.656461	-1.447654
H	0.196350	-0.647972	-1.244774
C	1.854609	0.920229	1.968073
H	2.455490	1.607854	2.579983
H	1.392683	0.243531	2.690830
C	1.899577	-0.719794	0.079249
H	1.455537	-1.530650	0.659257
C	2.776178	0.139755	1.008940
Cl	3.767169	1.333569	0.077567
C	3.744742	-0.709421	1.847416
H	3.204180	-1.477455	2.412310
H	4.286784	-0.091375	2.573095
H	4.495228	-1.216211	1.232237
Br	2.952945	-1.724969	-1.256009

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2629238**

SCF Energy (B3LYP/6-31G) = -6264.30096716**

1o_C002

MMFF Geometry

C	-1.448847	0.123999	0.915388
C	-2.901450	1.102083	-0.982989
C	-0.129491	0.904500	0.336342
C	-2.411128	-0.166598	-0.281360
H	-3.723270	1.579826	-0.436272
H	-1.942876	-0.839421	-1.008104
C	-1.816198	2.107151	-1.162014
H	-2.081507	2.938463	-1.814027
C	-0.590466	2.060183	-0.602462
O	-3.387464	0.787770	-2.287548
H	-4.105504	0.140478	-2.169487
Br	-4.023109	-1.206603	0.224174
C	-2.161374	0.998284	1.990060
H	-3.103659	0.551850	2.322286
H	-2.387270	2.005671	1.628578
H	-1.548857	1.106190	2.891519
C	-1.068686	-1.211801	1.607772
H	-1.924662	-1.660284	2.123374
H	-0.305174	-1.078903	2.378184
H	-0.702648	-1.952842	0.890414
C	0.370706	3.172009	-0.952511
H	1.300777	2.773367	-1.365312
H	0.589960	3.784895	-0.073654
H	-0.037842	3.849404	-1.711377
C	0.714194	1.457833	1.540713
H	0.279339	2.398508	1.903305
H	0.660443	0.770176	2.390944
C	0.765945	-0.047713	-0.531439
H	1.152305	0.475382	-1.416052
H	0.165858	-0.862019	-0.949883
C	2.211476	1.682772	1.284811
H	2.337215	2.562665	0.648635
H	2.668634	1.980709	2.238273
C	1.952864	-0.625635	0.243718
H	1.590236	-1.171549	1.119621
C	2.956940	0.455880	0.698002
Cl	3.968905	1.066647	-0.678307
C	3.925900	-0.107988	1.751207
H	3.378680	-0.476244	2.626558
H	4.626105	0.659630	2.101758
H	4.524615	-0.937474	1.360796
Br	2.765826	-2.063780	-0.823599

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2599294**

SCF Energy (B3LYP/6-31G) = -6264.29667529**

1o_C003

MMFF Geometry

C	-1.37565	0.17814	0.87993
C	-2.96150	0.97883	-1.01401
C	-0.11774	0.99382	0.20360
C	-2.38011	-0.21970	-0.25979
H	-3.79273	1.43443	-0.46388
H	-1.90634	-0.91296	-0.96382
C	-1.94295	2.03022	-1.28512
H	-2.28416	2.82394	-1.94961
C	-0.69240	2.06911	-0.78717
O	-3.47425	0.56767	-2.28250
H	-2.72037	0.29231	-2.83167
Br	-3.91200	-1.31513	0.37593
C	-2.08822	1.06791	1.93933
H	-3.03213	0.63165	2.27968
H	-2.31321	2.06975	1.56186
H	-1.47494	1.17934	2.84025
C	-0.94680	-1.11421	1.61247
H	-1.76066	-1.52713	2.21919
H	-0.13445	-0.94999	2.31591
H	-0.65246	-1.89853	0.90867
C	0.19117	3.21108	-1.25302
H	-0.21455	3.70765	-2.14212
H	1.19116	2.86243	-1.52483
H	0.27715	3.97356	-0.47233
C	0.77167	1.73692	1.26559
H	1.31762	2.55839	0.79267
H	0.15788	2.24518	2.01487
C	0.79909	0.06231	-0.66399
H	1.30186	0.66060	-1.43520
H	0.18472	-0.64114	-1.23783
C	1.85370	0.92017	1.97543
H	2.45907	1.60894	2.58170
H	1.39756	0.24559	2.70358
C	1.88414	-0.72210	0.09018
H	1.43547	-1.52724	0.67468
C	2.76859	0.13626	1.01316
Cl	3.75595	1.32640	0.07321
C	3.74015	-0.71334	1.84750
H	3.20138	-1.47985	2.41615
H	4.28696	-0.09521	2.56951
H	4.48665	-1.22201	1.22903
Br	2.92664	-1.73694	-1.24609

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2609895**

SCF Energy (B3LYP/6-31G) = -6264.29627805**

1o_C004

MMFF Geometry

C	-1.36920	0.15450	0.88137
C	-2.95724	0.97550	-1.00234
C	-0.11566	0.98574	0.21847
C	-2.37118	-0.22988	-0.26488
H	-3.79803	1.41263	-0.45047
H	-1.89951	-0.91630	-0.97711
C	-1.94403	2.03719	-1.25595
H	-2.27374	2.83775	-1.91590
C	-0.69558	2.07684	-0.75143
O	-3.44532	0.55397	-2.27649
H	-3.97675	1.28209	-2.63914
Br	-3.90894	-1.32925	0.36506
C	-2.08443	1.02515	1.95503
H	-3.02516	0.57950	2.29174
H	-2.31554	2.03109	1.59247
H	-1.46994	1.12662	2.85628
C	-0.93609	-1.14825	1.59273
H	-1.74854	-1.57372	2.19261
H	-0.12426	-0.99335	2.29875
H	-0.63951	-1.92010	0.87623
C	0.18598	3.22732	-1.20001
H	0.27019	3.97780	-0.40755
H	-0.22022	3.73712	-2.08133
H	1.18685	2.88533	-1.47685
C	0.77283	1.71294	1.29214
H	1.31696	2.54318	0.83258
H	0.15862	2.20770	2.05005
C	0.80369	0.07319	-0.66712
H	1.30444	0.68707	-1.42724
H	0.19112	-0.62134	-1.25361
C	1.85662	0.88645	1.98753
H	2.46059	1.56600	2.60552
H	1.40249	0.19852	2.70425
C	1.89130	-0.72165	0.07176
H	1.44511	-1.53928	0.64063
C	2.77299	0.12160	1.01150
Cl	3.75992	1.33134	0.09581
C	3.74529	-0.74150	1.83122
H	3.20733	-1.51956	2.38477
H	4.28988	-0.13585	2.56540
H	4.49370	-1.23703	1.20446
Br	2.93969	-1.70764	-1.28174

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2598279**

SCF Energy (B3LYP/6-31G) = -6264.29443057**

1o_C005

MMFF Geometry

C	-1.463889	0.126216	0.915014
C	-2.883882	1.083491	-1.027192
C	-0.137747	0.901575	0.345254
C	-2.418537	-0.176031	-0.287863
H	-3.736347	1.551002	-0.521148
H	-1.947914	-0.870249	-0.992485
C	-1.806547	2.106204	-1.168045
H	-2.074954	2.952537	-1.800134
C	-0.589694	2.061905	-0.591044
O	-3.313516	0.753853	-2.348959
H	-2.531380	0.469379	-2.852118
Br	-4.036969	-1.198765	0.231340
C	-2.185256	1.008754	1.976983
H	-3.122993	0.558306	2.316389
H	-2.421698	2.008220	1.600700
H	-1.574398	1.135330	2.877050
C	-1.088979	-1.205781	1.619314
H	-1.948546	-1.651350	2.131320
H	-0.331205	-1.069909	2.394625
H	-0.717442	-1.950825	0.908880
C	0.366880	3.187788	-0.907513
H	0.571680	3.786257	-0.015437
H	-0.037515	3.875896	-1.658938
H	1.303944	2.802032	-1.316870
C	0.702730	1.447269	1.555961
H	0.268947	2.387227	1.921671
H	0.642949	0.756857	2.403289
C	0.756844	-0.050420	-0.521602
H	1.144460	0.474342	-1.404901
H	0.156516	-0.863374	-0.942089
C	2.202427	1.669063	1.310401
H	2.335712	2.558745	0.689367
H	2.655128	1.950263	2.271101
C	1.941951	-0.631780	0.254198
H	1.578335	-1.179515	1.128709
C	2.946866	0.448380	0.709360
Cl	3.944860	1.071016	-0.672383
C	3.926314	-0.119468	1.750381
H	3.387373	-0.497528	2.626683
H	4.625415	0.648721	2.101890
H	4.526216	-0.942754	1.348888
Br	2.753435	-2.066112	-0.819795

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2582131**

SCF Energy (B3LYP/6-31G) = -6264.29215564**

1o_C006

MMFF Geometry

C	-1.456558	0.108232	0.914913
C	-2.882303	1.072435	-1.020139
C	-0.135904	0.895023	0.351046
C	-2.410149	-0.188673	-0.289824
H	-3.744476	1.525311	-0.515872
H	-1.942079	-0.880453	-0.998657
C	-1.811497	2.104259	-1.151529
H	-2.070105	2.953331	-1.781799
C	-0.595851	2.063974	-0.570482
O	-3.289689	0.722342	-2.343127
H	-3.749552	1.491223	-2.719068
Br	-4.032964	-1.211644	0.232960
C	-2.180552	0.978173	1.985736
H	-3.112899	0.518224	2.327063
H	-2.426927	1.977958	1.616733
H	-1.566978	1.104009	2.884026
C	-1.075006	-1.228584	1.606242
H	-1.932238	-1.683581	2.113801
H	-0.317878	-1.096673	2.382856
H	-0.700013	-1.964725	0.888358
C	0.357205	3.195137	-0.878771
H	-0.050390	3.889636	-1.622521
H	1.294502	2.816016	-1.293825
H	0.562297	3.785717	0.018507
C	0.704938	1.431252	1.565957
H	0.269028	2.366334	1.941501
H	0.649227	0.732506	2.406660
C	0.761983	-0.042683	-0.528954
H	1.149137	0.495357	-1.404397
H	0.163968	-0.851360	-0.960816
C	2.203035	1.660124	1.318903
H	2.331351	2.552688	0.701084
H	2.657042	1.939049	2.279629
C	1.948100	-0.631154	0.239314
H	1.584787	-1.190854	1.106290
C	2.950247	0.444858	0.710741
Cl	3.958683	1.081791	-0.656814
C	3.922318	-0.133951	1.752890
H	3.377307	-0.519124	2.622317
H	4.620372	0.629839	2.115881
H	4.523440	-0.954500	1.347610
Br	2.765848	-2.050518	-0.849553

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2570661**

SCF Energy (B3LYP/6-31G) = -6264.29030818**

1o_C007

MMFF Geometry

C	-1.599832	-0.933852	0.427832
C	-2.514989	1.494091	0.405853
C	-0.075291	-0.337392	0.609054
C	-2.438726	0.150129	-0.323828
H	-3.351588	1.512017	1.115616
H	-2.050800	0.296215	-1.338837
C	-1.283564	1.828825	1.177766
H	-1.340228	2.781462	1.702991
C	-0.201753	1.037494	1.338976
O	-2.729701	2.552762	-0.524222
H	-3.584365	2.377407	-0.956144
Br	-4.301044	-0.411714	-0.708306
C	-2.212280	-1.272831	1.817839
H	-3.245591	-1.624258	1.732331
H	-2.220378	-0.419625	2.501322
H	-1.657189	-2.079610	2.308453
C	-1.637988	-2.255890	-0.395028
H	-2.613957	-2.748338	-0.313554
H	-0.911924	-2.994646	-0.052118
H	-1.466204	-2.087489	-1.462327
C	0.828563	1.503916	2.342057
H	0.568775	2.475829	2.778484
H	1.813843	1.628640	1.901824
H	0.900040	0.805622	3.180894
C	0.792148	-1.344012	1.433139
H	0.543241	-1.278766	2.499646
H	0.543405	-2.373135	1.165532
C	0.556034	-0.100856	-0.819034
H	0.151385	0.819867	-1.260073
H	0.210364	-0.895121	-1.486039
C	2.314141	-1.220479	1.286064
H	2.675066	-0.325906	1.799651
H	2.773031	-2.060784	1.825358
C	2.085016	-0.111764	-0.979355
H	2.308550	-0.253215	-2.045288
C	2.784006	-1.221207	-0.173196
Cl	4.585998	-1.049486	-0.190358
C	2.505259	-2.591146	-0.826681
H	1.436610	-2.811251	-0.897639
H	2.966703	-3.406151	-0.256528
H	2.906258	-2.631929	-1.846587
Br	2.790077	1.696348	-0.694433

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2575983**

SCF Energy (B3LYP/6-31G) = -6264.29353361**

1o_C008

MMFF Geometry

C	-1.617950	-0.937861	0.413718
C	-2.462842	1.526190	0.353889
C	-0.085011	-0.367611	0.597392
C	-2.442102	0.158776	-0.342733
H	-3.334069	1.610211	1.014250
H	-2.069131	0.269375	-1.367917
C	-1.253363	1.811144	1.183089
H	-1.313813	2.744793	1.742245
C	-0.194543	0.992877	1.354962
O	-2.574579	2.570774	-0.612120
H	-1.689421	2.725682	-0.984534
Br	-4.321726	-0.375512	-0.683376
C	-2.237044	-1.268818	1.802761
H	-3.264966	-1.634964	1.714181
H	-2.262649	-0.407870	2.475941
H	-1.676529	-2.063483	2.306473
C	-1.675046	-2.259185	-0.410439
H	-2.665009	-2.725677	-0.349347
H	-0.977794	-3.018250	-0.052447
H	-1.476689	-2.096048	-1.473774
C	0.811879	1.405309	2.405728
H	0.549811	2.362009	2.873406
H	1.810415	1.537420	1.996958
H	0.852330	0.674224	3.218059
C	0.779239	-1.400833	1.392271
H	0.527976	-1.370776	2.459495
H	0.532135	-2.420318	1.089898
C	0.541717	-0.115054	-0.829070
H	0.129168	0.804794	-1.264110
H	0.205135	-0.909058	-1.501220
C	2.302265	-1.273605	1.252843
H	2.662538	-0.395769	1.794528
H	2.759641	-2.130075	1.767452
C	2.070817	-0.105296	-0.983361
H	2.301469	-0.212651	-2.051650
C	2.776473	-1.229995	-0.204530
Cl	4.576064	-1.039729	-0.212829
C	2.510958	-2.584669	-0.894616
H	1.444385	-2.815232	-0.967886
H	2.983364	-3.409653	-0.348255
H	2.909351	-2.593025	-1.916295
Br	2.747818	1.703378	-0.636962

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2560663**

SCF Energy (B3LYP/6-31G) = -6264.28941087**

1o_C009

MMFF Geometry

C	-1.615569	-0.945135	0.413347
C	-2.433847	1.530263	0.294331
C	-0.082923	-0.375855	0.592935
C	-2.433905	0.142145	-0.361645
H	-3.321703	1.661441	0.924821
H	-2.071886	0.217898	-1.394121
C	-1.240152	1.811902	1.149697
H	-1.294621	2.745386	1.707527
C	-0.194930	0.982549	1.351307
O	-2.487448	2.529011	-0.723709
H	-2.458702	3.397078	-0.288116
Br	-4.326641	-0.377983	-0.665719
C	-2.239495	-1.256283	1.804811
H	-3.259841	-1.643313	1.716943
H	-2.286662	-0.380889	2.457923
H	-1.669443	-2.029517	2.330449
C	-1.674175	-2.277181	-0.393192
H	-2.674228	-2.723891	-0.354944
H	-1.004274	-3.044567	-0.001905
H	-1.441122	-2.135070	-1.452212
C	0.795320	1.384127	2.420735
H	0.529897	2.339706	2.888748
H	1.801421	1.513024	2.029339
H	0.818133	0.648925	3.229987
C	0.784959	-1.410481	1.382189
H	0.535070	-1.387419	2.449736
H	0.541105	-2.428807	1.074018
C	0.542145	-0.116414	-0.833570
H	0.126594	0.802856	-1.266964
H	0.208653	-0.910210	-1.507611
C	2.307428	-1.279930	1.241511
H	2.666692	-0.404574	1.787888
H	2.767043	-2.138621	1.750394
C	2.071264	-0.097263	-0.985741
H	2.304618	-0.191842	-2.054583
C	2.778845	-1.227421	-0.216595
Cl	4.578928	-1.036807	-0.226483
C	2.512961	-2.577785	-0.914962
H	1.446575	-2.810212	-0.985768
H	2.988855	-3.405609	-0.375953
H	2.907646	-2.578336	-1.938103
Br	2.744653	1.708176	-0.613097

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2547966**

SCF Energy (B3LYP/6-31G) = -6264.28831877**

1o_C010

MMFF Geometry

C	-1.279809	0.356616	-0.972081
C	-3.302582	1.354114	0.349643
C	-0.376557	0.256534	0.392101
C	-2.830683	0.343175	-0.694842
H	-4.282360	1.069759	0.750650
H	-3.358102	0.546284	-1.636887
C	-2.351790	1.512204	1.484037
H	-2.757843	2.056089	2.335759
C	-1.092063	1.039712	1.550570
O	-3.488422	2.632206	-0.259435
H	-3.646409	3.277069	0.450396
Br	-3.570003	-1.423558	-0.211754
C	-0.988733	-0.718494	-2.048470
H	-1.628840	-0.565929	-2.927311
H	-1.185937	-1.734379	-1.702132
H	0.036650	-0.681055	-2.416832
C	-0.993004	1.711129	-1.700232
H	-1.710748	1.886866	-2.510797
H	-0.001342	1.717101	-2.166166
H	-1.047960	2.568695	-1.023133
C	-0.338667	1.317835	2.841113
H	-1.015945	1.585371	3.660681
H	0.349355	2.158972	2.708245
H	0.228565	0.450985	3.186737
C	-0.154274	-1.215680	0.882884
H	0.105317	-1.219913	1.947157
H	-1.081248	-1.787610	0.842609
C	1.050081	0.904750	0.227206
H	1.495711	1.074117	1.213810
H	0.974619	1.916665	-0.185807
C	0.940502	-2.034025	0.177386
H	1.063282	-2.980150	0.723293
H	0.602741	-2.336711	-0.816246
C	2.069809	0.076992	-0.556416
H	1.770801	-0.004013	-1.602466
C	2.300846	-1.322221	0.049544
Cl	3.033397	-1.233381	1.703865
C	3.228678	-2.186591	-0.818585
H	2.855730	-2.250105	-1.847212
H	3.293894	-3.210208	-0.430853
H	4.249023	-1.791913	-0.859339
Br	3.734007	1.131774	-0.690176

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2544729**

SCF Energy (B3LYP/6-31G) = -6264.29144462**

1o_C011

MMFF Geometry

C	1.283906	-0.368735	-0.955758
C	3.313751	-1.327264	0.392671
C	0.366569	-0.283172	0.399184
C	2.831400	-0.334825	-0.665485
H	4.262893	-1.006131	0.838169
H	3.366296	-0.542733	-1.602294
C	2.337401	-1.537570	1.491943
H	2.732782	-2.122420	2.321569
C	1.069094	-1.088040	1.547577
O	3.563771	-2.607970	-0.186206
H	4.370879	-2.529527	-0.722315
Br	3.555080	1.444228	-0.210136
C	0.986620	0.700314	-2.036031
H	1.637509	0.556201	-2.908420
H	1.165424	1.719272	-1.689596
H	-0.033692	0.647491	-2.415214
C	1.025135	-1.729470	-1.683871
H	1.752904	-1.895622	-2.487514
H	0.038187	-1.751376	-2.159315
H	1.088329	-2.584848	-1.004632
C	0.295220	-1.420987	2.811770
H	0.959617	-1.709344	3.634801
H	-0.380570	-2.264220	2.636328
H	-0.287418	-0.571050	3.174565
C	0.150006	1.178747	0.917829
H	-0.121075	1.160491	1.979609
H	1.081654	1.744128	0.900339
C	-1.062990	-0.919264	0.208073
H	-1.517631	-1.107889	1.186962
H	-0.990179	-1.921880	-0.227283
C	-0.931341	2.018276	0.217435
H	-1.049944	2.956563	0.777539
H	-0.583352	2.332881	-0.768865
C	-2.074152	-0.069034	-0.562346
H	-1.772287	0.028893	-1.605765
C	-2.296988	1.320569	0.068258
Cl	-3.041195	1.207938	1.715602
C	-3.211787	2.208658	-0.789807
H	-2.831254	2.288328	-1.814527
H	-3.271393	3.225364	-0.383437
H	-4.234971	1.823161	-0.844862
Br	-3.746041	-1.108117	-0.723009

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2565078**

SCF Energy (B3LYP/6-31G) = -6264.29305907**

1o_C012

MMFF Geometry

C	1.434414	-0.133222	1.128453
C	3.341586	1.174513	-0.108893
C	0.374758	0.570190	0.123395
C	2.888001	-0.146590	0.543002
H	3.849510	1.013687	-1.066621
H	3.585601	-0.402975	1.351907
C	2.263486	2.184912	-0.338213
H	2.628653	3.177814	-0.597910
C	0.935744	1.974774	-0.225649
O	4.298846	1.811799	0.744462
H	5.115374	1.285044	0.700544
Br	3.268055	-1.633554	-0.700290
C	0.998599	-1.552772	1.575895
H	1.771231	-2.016005	2.201718
H	0.807745	-2.232163	0.742822
H	0.085510	-1.522919	2.179892
C	1.543586	0.675522	2.472650
H	2.334286	0.259735	3.109943
H	0.627520	0.630993	3.068001
H	1.781939	1.731534	2.320250
C	0.014497	3.149244	-0.451454
H	0.545019	4.015350	-0.863444
H	-0.430746	3.471439	0.495337
H	-0.782848	2.910482	-1.157280
C	0.264549	-0.212717	-1.234767
H	1.115708	0.017563	-1.886853
H	0.294624	-1.293203	-1.067289
C	-1.058266	0.631309	0.776247
H	-1.545663	1.595992	0.612321
H	-0.998580	0.554146	1.863886
C	-1.010444	0.071807	-2.035790
H	-0.996341	1.122121	-2.343705
H	-0.960637	-0.493201	-2.975926
C	-1.999555	-0.454923	0.243667
H	-1.553534	-1.439749	0.420363
C	-2.305696	-0.285018	-1.263104
Cl	-3.487003	1.051612	-1.582628
C	-2.913644	-1.574375	-1.839502
H	-2.230950	-2.421359	-1.706210
H	-3.110189	-1.478582	-2.913957
H	-3.862465	-1.833680	-1.358284
Br	-3.605546	-0.522439	1.375258

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2501776**

SCF Energy (B3LYP/6-31G) = -6264.28565808**

1o_C013

MMFF Geometry

C	1.433213	-0.015439	1.136043
C	3.383376	1.148345	-0.155493
C	0.390111	0.550864	0.027263
C	2.896181	-0.110911	0.583427
H	4.015866	0.893485	-1.013020
H	3.573481	-0.312227	1.424746
C	2.306941	2.081473	-0.619310
H	2.667252	3.017668	-1.042471
C	0.975756	1.877689	-0.533087
O	4.216530	1.891986	0.742619
H	4.580549	2.645113	0.247776
Br	3.262741	-1.699771	-0.528401
C	0.992419	-1.364926	1.760097
H	1.750772	-1.731646	2.462780
H	0.829471	-2.154532	1.024216
H	0.063705	-1.260425	2.330882
C	1.519437	0.963616	2.363696
H	2.341405	0.676841	3.031557
H	0.617046	0.944093	2.981700
H	1.690872	2.003135	2.071905
C	0.065505	2.988130	-1.004027
H	0.610915	3.760033	-1.559097
H	-0.402237	3.484685	-0.147764
H	-0.715535	2.623177	-1.671751
C	0.260826	-0.425855	-1.197521
H	1.104870	-0.296220	-1.885529
H	0.291003	-1.468715	-0.870046
C	-1.040816	0.741065	0.658527
H	-1.513006	1.672192	0.333972
H	-0.981575	0.848270	1.743362
C	-1.019782	-0.271719	-2.025533
H	-0.999193	0.706396	-2.515306
H	-0.981046	-0.992575	-2.853067
C	-1.998500	-0.405000	0.313966
H	-1.564242	-1.354820	0.643770
C	-2.313855	-0.476114	-1.198215
Cl	-3.475664	0.812764	-1.722905
C	-2.948404	-1.830306	-1.555734
H	-2.279393	-2.656904	-1.290411
H	-3.151339	-1.905723	-2.630632
H	-3.897956	-1.991227	-1.034680
Br	-3.597372	-0.266184	1.449572

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2482882**

SCF Energy (B3LYP/6-31G) = -6264.28394480**

1o_C014

MMFF Geometry

C	1.440973	-0.045009	1.129115
C	3.369549	1.161301	-0.168694
C	0.387717	0.559174	0.051570
C	2.901766	-0.112361	0.561380
H	3.947421	0.921636	-1.067499
H	3.590463	-0.317858	1.392098
C	2.287961	2.120501	-0.557533
H	2.653865	3.069287	-0.949887
C	0.959186	1.915605	-0.449172
O	4.272194	1.879118	0.682454
H	3.742039	2.377190	1.327521
Br	3.270926	-1.683771	-0.576319
C	1.007764	-1.419271	1.703848
H	1.772733	-1.811459	2.385250
H	0.838254	-2.179256	0.938775
H	0.083395	-1.340031	2.285763
C	1.527057	0.885749	2.393404
H	2.363218	0.589070	3.038694
H	0.633045	0.824615	3.021176
H	1.671805	1.939332	2.141694
C	0.040093	3.045595	-0.850179
H	0.576959	3.848526	-1.368309
H	-0.420306	3.493410	0.036392
H	-0.746455	2.712595	-1.528396
C	0.265405	-0.363785	-1.214640
H	1.111414	-0.203447	-1.893769
H	0.297522	-1.419880	-0.932548
C	-1.042327	0.705956	0.695629
H	-1.521566	1.650030	0.423100
H	-0.980076	0.755123	1.784686
C	-1.014363	-0.174412	-2.036595
H	-0.996568	0.826765	-2.477849
H	-0.972092	-0.854386	-2.897815
C	-1.993592	-0.426771	0.293090
H	-1.553707	-1.389383	0.575340
C	-2.308481	-0.423246	-1.221025
Cl	-3.473515	0.887429	-1.679653
C	-2.939390	-1.759391	-1.646182
H	-2.268435	-2.596528	-1.422012
H	-3.141489	-1.781442	-2.723653
H	-3.888854	-1.948567	-1.134554
Br	-3.592534	-0.353440	1.434496

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2503364**

SCF Energy (B3LYP/6-31G) = -6264.28607247**

1p_C001

MMFF Geometry

C	1.496886	0.843259	0.508628
C	2.461037	-1.555808	0.309294
C	-0.013476	0.205521	0.661509
C	2.348270	-0.167167	-0.325626
H	3.300517	-1.601560	1.014350
H	1.951179	-0.251970	-1.344069
C	1.240492	-1.974259	1.057481
H	1.318781	-2.963285	1.506998
C	0.142946	-1.220575	1.280345
O	2.698865	-2.543014	-0.691621
H	3.537142	-2.304471	-1.125584
Br	4.194262	0.459396	-0.689012
C	2.117730	1.094663	1.913371
H	3.145585	1.464976	1.843837
H	2.142621	0.196554	2.536305
H	1.557017	1.858344	2.463019
C	1.499008	2.220255	-0.220502
H	2.457468	2.736938	-0.093271
H	0.743004	2.908772	0.160242
H	1.344329	2.119634	-1.299164
C	-0.878546	-1.786525	2.239342
H	-0.957476	-1.165388	3.136206
H	-0.606084	-2.789924	2.587839
H	-1.862790	-1.883646	1.789798
C	-0.884010	1.128227	1.574195
H	-0.624413	0.975258	2.629299
H	-0.645152	2.178723	1.395337
C	-0.657129	0.068428	-0.771872
H	-0.248327	-0.813080	-1.283665
H	-0.324614	0.912545	-1.381975
C	-2.406201	1.000527	1.432161
H	-2.752638	0.067968	1.884902
H	-2.870614	1.792794	2.035726
C	-2.185926	0.076832	-0.917402
H	-2.420055	0.304867	-1.966245
C	-2.906135	1.089946	-0.014603
Cl	-2.516355	2.758495	-0.647230
C	-4.437907	0.985840	-0.055101
H	-4.907374	1.819982	0.480499
H	-4.800028	0.070054	0.423253
H	-4.811867	1.000821	-1.085210
Br	-2.882872	-1.751973	-0.790984

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2596815**

SCF Energy (B3LYP/6-31G) = -6264.29938274**

1p_C002

MMFF Geometry

C	-1.36559	0.18875	0.87790
C	-3.02216	0.96946	-0.94409
C	-0.14473	1.00028	0.14737
C	-2.40454	-0.22472	-0.21375
H	-3.82894	1.43148	-0.36247
H	-1.95959	-0.91758	-0.93623
C	-2.01878	2.02347	-1.26260
H	-2.38912	2.80218	-1.92825
C	-0.75148	2.07878	-0.80580
O	-3.58288	0.55030	-2.18787
H	-4.25406	-0.12357	-1.97761
Br	-3.91004	-1.31255	0.48435
C	-2.03518	1.09073	1.95756
H	-2.91837	0.61654	2.39667
H	-2.34985	2.05954	1.55903
H	-1.35614	1.28882	2.79364
C	-0.86147	-1.08139	1.61003
H	-1.64615	-1.53550	2.22474
H	-0.04316	-0.86606	2.30162
H	-0.52429	-1.84762	0.90484
C	0.10042	3.23123	-1.28542
H	-0.43267	3.87362	-1.99602
H	0.99154	2.87082	-1.80637
H	0.39542	3.87287	-0.45040
C	0.77192	1.66052	1.24002
H	0.34126	2.61630	1.56502
H	0.81404	1.03987	2.14046
C	0.73527	0.06111	-0.75402
H	1.08195	0.59360	-1.64982
H	0.13118	-0.76299	-1.14716
C	2.22532	1.89418	0.81144
H	2.24720	2.61335	-0.01075
H	2.75645	2.40100	1.62817
C	1.96915	-0.49339	-0.03377
H	1.64557	-1.05800	0.84379
C	2.97178	0.60456	0.38845
Cl	3.88972	-0.00669	1.83081
C	4.01372	0.99484	-0.67356
H	4.72096	0.18751	-0.88965
H	4.61242	1.85131	-0.33944
H	3.52964	1.28262	-1.61348
Br	2.76348	-1.90372	-1.14806

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2620850**

SCF Energy (B3LYP/6-31G) = -6264.29854987**

1p_C003

MMFF Geometry

C	1.516125	0.849161	0.500415
C	2.410761	-1.583263	0.249503
C	-0.003651	0.236552	0.654783
C	2.353015	-0.169580	-0.344624
H	3.285333	-1.693276	0.901598
H	1.969611	-0.212702	-1.371002
C	1.210663	-1.959904	1.055272
H	1.292230	-2.935238	1.534721
C	0.135987	-1.180594	1.295695
O	2.545182	-2.553368	-0.788752
H	1.674562	-2.656199	-1.209927
Br	4.217259	0.427885	-0.664443
C	2.143550	1.085381	1.904873
H	3.166052	1.470228	1.835428
H	2.185240	0.177522	2.512478
H	1.577908	1.833598	2.470247
C	1.538337	2.229692	-0.222860
H	2.514043	2.718463	-0.119851
H	0.815562	2.939288	0.182678
H	1.351106	2.139499	-1.297059
C	-0.860668	-1.700337	2.306574
H	-0.584454	-2.691824	2.685095
H	-1.858380	-1.808191	1.888690
H	-0.908835	-1.045968	3.181528
C	-0.872519	1.184517	1.543618
H	-0.609244	1.064972	2.601805
H	-0.638446	2.229287	1.330417
C	-0.643158	0.090208	-0.778596
H	-0.223601	-0.785952	-1.290440
H	-0.323467	0.939931	-1.388054
C	-2.395626	1.049469	1.410753
H	-2.738839	0.129915	1.891068
H	-2.859712	1.857263	1.993698
C	-2.172297	0.072320	-0.918249
H	-2.414866	0.270203	-1.971186
C	-2.902008	1.096893	-0.035929
Cl	-2.534921	2.754435	-0.708990
C	-4.432186	0.971633	-0.068789
H	-4.911017	1.810945	0.450145
H	-4.780325	0.061550	0.430364
H	-4.809558	0.959005	-1.097682
Br	-2.834306	-1.765132	-0.738315

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2581472**

SCF Energy (B3LYP/6-31G) = -6264.29493005**

1p_C004

MMFF Geometry

C	1.512997	0.858083	0.500398
C	2.384624	-1.580763	0.196308
C	-0.006354	0.246301	0.651228
C	2.344014	-0.151215	-0.360894
H	3.275932	-1.729100	0.818183
H	1.969818	-0.163023	-1.391687
C	1.198899	-1.956060	1.026283
H	1.274029	-2.930798	1.505336
C	0.136066	-1.168818	1.293828
O	2.466383	-2.505694	-0.887633
H	2.502618	-3.399883	-0.509579
Br	4.221184	0.432355	-0.648812
C	2.145045	1.076547	1.905653
H	3.160549	1.479924	1.838228
H	2.206090	0.157432	2.494409
H	1.571213	1.804171	2.489178
C	1.536872	2.247129	-0.206249
H	2.522724	2.719189	-0.125259
H	0.839281	2.963450	0.230514
H	1.317514	2.174921	-1.275448
C	-0.846263	-1.679941	2.322326
H	-0.881120	-1.019653	3.193406
H	-0.565339	-2.668895	2.703937
H	-1.850038	-1.789749	1.919223
C	-0.879544	1.195723	1.534367
H	-0.616708	1.084313	2.593389
H	-0.650497	2.239929	1.314077
C	-0.643896	0.094359	-0.782785
H	-0.219780	-0.779828	-1.294214
H	-0.328952	0.945719	-1.392545
C	-2.402043	1.054721	1.401199
H	-2.742348	0.136702	1.886437
H	-2.869442	1.864138	1.979232
C	-2.172726	0.064897	-0.921448
H	-2.417932	0.251690	-1.975728
C	-2.907029	1.092657	-0.046400
Cl	-2.546620	2.748557	-0.727617
C	-4.436866	0.961645	-0.079907
H	-4.919228	1.802582	0.433113
H	-4.782542	0.053724	0.424830
H	-4.813085	0.941030	-1.109094
Br	-2.827015	-1.773768	-0.719269

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2568859**

SCF Energy (B3LYP/6-31G) = -6264.29375116**

1p_C005

MMFF Geometry

C	-1.332205	0.044094	0.874327
C	-3.097550	1.029106	-0.746810
C	-0.175018	1.044634	0.267444
C	-2.385582	-0.230352	-0.254973
H	-3.886206	1.352495	-0.057094
H	-1.921628	-0.754616	-1.098290
C	-2.153609	2.159797	-0.945200
H	-2.577046	3.004996	-1.486695
C	-0.874105	2.207102	-0.526426
O	-3.711746	0.786616	-2.012381
H	-4.333887	0.048310	-1.882942
Br	-3.810242	-1.517372	0.261809
C	-2.018896	0.699443	2.106302
H	-1.348379	0.711405	2.972716
H	-2.906733	0.146509	2.427834
H	-2.331978	1.729546	1.911709
C	-0.784173	-1.319893	1.353877
H	-1.533340	-1.881110	1.923816
H	0.060345	-1.221984	2.031305
H	-0.490931	-1.955435	0.512733
C	-0.089043	3.453359	-0.888754
H	0.017991	4.106582	-0.016918
H	-0.586803	4.041006	-1.668892
H	0.903626	3.208746	-1.275153
C	0.720249	1.698758	1.380315
H	1.206133	2.600104	0.994247
H	0.114191	2.073704	2.210520
C	0.756663	0.314636	-0.763547
H	1.179765	1.050806	-1.458983
H	0.160855	-0.343289	-1.407189
C	1.868838	0.856362	1.933840
H	2.453245	1.484841	2.620488
H	1.474073	0.054942	2.562294
C	1.930019	-0.487583	-0.176199
H	1.566750	-1.405492	0.289357
C	2.789890	0.298711	0.830508
Cl	3.959009	-0.818178	1.648991
C	3.614626	1.436062	0.202796
H	4.110622	2.034962	0.976067
H	2.994814	2.118112	-0.386089
H	4.403283	1.060887	-0.457844
Br	2.982854	-1.193352	-1.691975

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2624456**

SCF Energy (B3LYP/6-31G) = -6264.29872807**

1p_C006

MMFF Geometry

C	-1.376915	0.190218	0.877949
C	-3.013514	0.946638	-0.980793
C	-0.153150	1.001742	0.152643
C	-2.410960	-0.236921	-0.216289
H	-3.849758	1.392749	-0.430227
H	-1.960566	-0.946669	-0.918640
C	-2.019417	2.021460	-1.267183
H	-2.396779	2.814278	-1.912912
C	-0.757891	2.083435	-0.797468
O	-3.527600	0.516656	-2.242147
H	-2.775719	0.224152	-2.784763
Br	-3.916179	-1.313257	0.499099
C	-2.055616	1.096782	1.948237
H	-2.931077	0.616987	2.396497
H	-2.384858	2.055896	1.538310
H	-1.377365	1.314105	2.780079
C	-0.871757	-1.074578	1.619953
H	-1.656677	-1.526854	2.235619
H	-0.055525	-0.854869	2.312377
H	-0.531409	-1.844045	0.919757
C	0.086205	3.253456	-1.248251
H	-0.449006	3.905222	-1.948663
H	0.982142	2.909756	-1.772397
H	0.372507	3.881163	-0.399865
C	0.762464	1.657297	1.249765
H	0.333252	2.612953	1.576864
H	0.801460	1.035333	2.149200
C	0.728217	0.067677	-0.751219
H	1.079799	0.607466	-1.641013
H	0.123772	-0.751756	-1.153380
C	2.217315	1.888517	0.824901
H	2.242249	2.607425	0.002512
H	2.747659	2.394099	1.642899
C	1.958537	-0.495072	-0.030701
H	1.630775	-1.066697	0.840709
C	2.962283	0.597497	0.403557
Cl	3.866122	-0.022743	1.850327
C	4.014221	0.988264	-0.648396
H	4.613065	1.841410	-0.306106
H	3.538792	1.281381	-1.591100
H	4.720491	0.179327	-0.861702
Br	2.752161	-1.896683	-1.156603

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2602386**

SCF Energy (B3LYP/6-31G) = -6264.29365075**

1p_C007

MMFF Geometry

C	-1.370522	0.170863	0.879962
C	-3.007625	0.937935	-0.974515
C	-0.151008	0.995457	0.164895
C	-2.400807	-0.248772	-0.220369
H	-3.856330	1.365353	-0.426843
H	-1.951825	-0.955088	-0.927179
C	-2.020422	2.023977	-1.244485
H	-2.387363	2.821389	-1.888389
C	-0.761098	2.089030	-0.767915
O	-3.489067	0.491440	-2.242428
H	-4.074479	1.184603	-2.590281
Br	-3.912221	-1.326722	0.492708
C	-2.053040	1.062711	1.960328
H	-2.922705	0.572185	2.408137
H	-2.391835	2.022423	1.559700
H	-1.373776	1.278508	2.791714
C	-0.861071	-1.100739	1.607303
H	-1.644833	-1.563650	2.216478
H	-0.046374	-0.886393	2.303181
H	-0.517111	-1.860430	0.898247
C	0.080394	3.265956	-1.205082
H	-0.456392	3.925652	-1.896787
H	0.976646	2.930720	-1.734111
H	0.365920	3.883760	-0.349183
C	0.764374	1.638931	1.269462
H	0.332877	2.588809	1.610140
H	0.806746	1.005135	2.160419
C	0.731995	0.076110	-0.753212
H	1.080685	0.628937	-1.636056
H	0.129790	-0.739819	-1.165575
C	2.217769	1.880442	0.845552
H	2.239452	2.611238	0.033653
H	2.747916	2.375864	1.669875
C	1.964531	-0.492395	-0.041496
H	1.639466	-1.074825	0.823758
C	2.965666	0.597745	0.404580
Cl	3.876409	-0.037924	1.840824
C	4.013168	1.006271	-0.645138
H	4.609851	1.857055	-0.293320
H	3.533972	1.310006	-1.582553
H	4.721841	0.202907	-0.871116
Br	2.763011	-1.878772	-1.182643

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2592252**

SCF Energy (B3LYP/6-31G) = -6264.29209561**

1p_C008

MMFF Geometry

C	-1.346302	0.043182	0.882411
C	-3.086360	1.015805	-0.782406
C	-0.183589	1.044055	0.287920
C	-2.388542	-0.241293	-0.257788
H	-3.908970	1.321939	-0.126051
H	-1.912888	-0.780152	-1.085041
C	-2.152017	2.164609	-0.933334
H	-2.581562	3.024564	-1.447244
C	-0.879898	2.215361	-0.494879
O	-3.648690	0.774651	-2.073256
H	-2.916164	0.605549	-2.689874
Br	-3.811516	-1.526670	0.264767
C	-2.048852	0.702152	2.104053
H	-2.938289	0.148228	2.419091
H	-2.363475	1.730186	1.901644
H	-1.388523	0.719871	2.978049
C	-0.798498	-1.316951	1.373900
H	-1.550334	-1.877141	1.941278
H	0.040024	-1.213637	2.057368
H	-0.496911	-1.956206	0.538657
C	-0.103068	3.478683	-0.812847
H	-0.010781	4.108170	0.077885
H	-0.598048	4.083651	-1.581436
H	0.895042	3.251584	-1.196524
C	0.714233	1.681215	1.409959
H	1.198896	2.588562	1.036981
H	0.109735	2.042752	2.247060
C	0.746136	0.325781	-0.751442
H	1.171344	1.071661	-1.435727
H	0.149546	-0.321290	-1.405080
C	1.867330	0.834545	1.948994
H	2.455152	1.457696	2.637661
H	1.478276	0.027564	2.573563
C	1.916775	-0.487383	-0.174224
H	1.550259	-1.407556	0.284386
C	2.782859	0.286861	0.836361
Cl	3.953901	-0.840164	1.637102
C	3.606389	1.429633	0.216961
H	4.109460	2.017522	0.994120
H	2.984510	2.120877	-0.358839
H	4.389311	1.060503	-0.453809
Br	2.960888	-1.181811	-1.701185

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2603597**

SCF Energy (B3LYP/6-31G) = -6264.29372422**

1p_C009

MMFF Geometry

C	-1.340162	0.020154	0.881111
C	-3.078956	1.011525	-0.774290
C	-0.181168	1.034940	0.306497
C	-2.377598	-0.249320	-0.266803
H	-3.914419	1.294923	-0.122828
H	-1.902770	-0.779490	-1.100206
C	-2.151197	2.169309	-0.899381
H	-2.569556	3.036282	-1.407981
C	-0.881897	2.219840	-0.451258
O	-3.605902	0.763769	-2.078116
H	-4.247634	1.467843	-2.269633
Br	-3.807622	-1.539100	0.244810
C	-2.047105	0.656335	2.112529
H	-2.933529	0.093138	2.419215
H	-2.367240	1.685658	1.925994
H	-1.387448	0.663810	2.987155
C	-0.789033	-1.346465	1.350328
H	-1.540199	-1.918692	1.906439
H	0.047818	-1.252457	2.037093
H	-0.484052	-1.970527	0.504916
C	-0.107053	3.489898	-0.746268
H	-0.602159	4.108108	-1.504130
H	0.891885	3.271855	-1.132965
H	-0.016812	4.103392	0.155784
C	0.715833	1.652262	1.440225
H	1.197636	2.568207	1.084981
H	0.111231	1.995546	2.284873
C	0.749927	0.339869	-0.748050
H	1.172982	1.100296	-1.417432
H	0.154765	-0.295405	-1.414360
C	1.871815	0.798549	1.961295
H	2.458818	1.409986	2.661092
H	1.486051	-0.021319	2.570863
C	1.922567	-0.481873	-0.187725
H	1.558433	-1.411515	0.253326
C	2.787346	0.274901	0.837253
Cl	3.962554	-0.863774	1.616044
C	3.607446	1.431819	0.239732
H	4.109415	2.005840	1.027898
H	2.983359	2.132486	-0.322097
H	4.390996	1.078015	-0.438512
Br	2.969955	-1.144398	-1.726766

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2592986**

SCF Energy (B3LYP/6-31G) = -6264.29209230**

1p_C010

MMFF Geometry

C	1.256150	-0.181776	-0.982875
C	3.381954	-1.318066	0.027314
C	0.427954	-0.374833	0.418588
C	2.818599	-0.151962	-0.784126
H	4.372836	-1.070934	0.425773
H	3.299490	-0.152145	-1.771829
C	2.501865	-1.725177	1.157068
H	2.973800	-2.400987	1.868911
C	1.232718	-1.328471	1.373438
O	3.574683	-2.452322	-0.818013
H	3.822763	-3.202947	-0.252722
Br	3.522498	1.523598	-0.010310
C	0.869645	1.059147	-1.825131
H	1.462585	1.097219	-2.748374
H	1.054606	2.001690	-1.307185
H	-0.173597	1.046545	-2.141527
C	0.974585	-1.389963	-1.936005
H	1.652044	-1.382540	-2.798595
H	-0.040517	-1.352129	-2.346757
H	1.094878	-2.354545	-1.434006
C	0.564604	-1.876364	2.623379
H	1.295455	-2.268865	3.340173
H	-0.106419	-2.702675	2.367662
H	-0.004874	-1.113176	3.158007
C	0.183827	0.969210	1.188607
H	-0.024896	0.763435	2.244211
H	1.088590	1.576197	1.217490
C	-0.984169	-1.041092	0.204712
H	-1.368007	-1.410662	1.162005
H	-0.899262	-1.953692	-0.395429
C	-0.971535	1.857260	0.698084
H	-1.090944	2.684177	1.412006
H	-0.697451	2.343165	-0.240723
C	-2.074835	-0.126248	-0.355163
H	-1.840850	0.158716	-1.382176
C	-2.310881	1.116139	0.526227
Cl	-3.440751	2.258181	-0.312863
C	-2.916482	0.819918	1.910273
H	-2.995849	1.736625	2.507426
H	-2.308176	0.117573	2.487316
H	-3.926066	0.402180	1.841825
Br	-3.707322	-1.214428	-0.584463

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2537213**

SCF Energy (B3LYP/6-31G) = -6264.28961815**

1p_C011

MMFF Geometry

C	1.261380	-0.201494	-0.968721
C	3.392877	-1.301568	0.079736
C	0.418220	-0.401528	0.422088
C	2.820379	-0.153973	-0.752489
H	4.355662	-1.028107	0.527718
H	3.309726	-0.163144	-1.736012
C	2.487266	-1.747037	1.169881
H	2.948769	-2.454988	1.857342
C	1.209772	-1.369859	1.369268
O	3.648505	-2.445864	-0.734243
H	4.408608	-2.232724	-1.301671
Br	3.506818	1.540280	-0.007941
C	0.869654	1.030699	-1.820810
H	1.473421	1.071964	-2.736925
H	1.036977	1.977558	-1.305282
H	-0.168768	1.004679	-2.150603
C	1.007974	-1.418278	-1.919614
H	1.696201	-1.406197	-2.773606
H	-0.002064	-1.395235	-2.343797
H	1.135475	-2.378793	-1.411513
C	0.521227	-1.960744	2.587151
H	1.240134	-2.369523	3.306905
H	-0.138762	-2.783198	2.293160
H	-0.063607	-1.215645	3.131369
C	0.180414	0.931354	1.210348
H	-0.039490	0.709079	2.260826
H	1.090830	1.528635	1.257404
C	-0.997961	-1.053280	0.186900
H	-1.391009	-1.436520	1.134963
H	-0.916160	-1.955599	-0.428869
C	-0.962201	1.836555	0.722933
H	-1.077454	2.656890	1.445034
H	-0.677675	2.328845	-0.209362
C	-2.080141	-0.121789	-0.361755
H	-1.842915	0.174765	-1.384389
C	-2.307925	1.110674	0.535512
Cl	-3.422479	2.275204	-0.293466
C	-2.922863	0.801524	1.912506
H	-2.993272	1.710132	2.522986
H	-2.325860	0.082830	2.481162
H	-3.937310	0.397565	1.833796
Br	-3.721555	-1.192348	-0.610499

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2558681**

SCF Energy (B3LYP/6-31G) = -6264.29145051**

1p_C012

MMFF Geometry

C	-1.516483	-0.046946	1.160985
C	-3.034488	-1.540307	-0.331432
C	-0.221824	-0.320431	0.187787
C	-2.889525	-0.218104	0.427639
H	-3.712278	-1.436166	-1.186187
H	-3.694395	-0.150349	1.172319
C	-1.745908	-2.122926	-0.812089
H	-1.863525	-3.038371	-1.390215
C	-0.503089	-1.638031	-0.605310
O	-3.642928	-2.504752	0.534006
H	-3.707673	-3.340629	0.042764
Br	-3.381091	1.263256	-0.777214
C	-1.487990	1.333195	1.880828
H	-2.377326	1.450803	2.512995
H	-1.476306	2.185880	1.200172
H	-0.625521	1.443078	2.543902
C	-1.522060	-1.093224	2.333222
H	-2.459897	-1.041409	2.899622
H	-0.720352	-0.909549	3.055925
H	-1.407895	-2.122690	1.982421
C	0.628472	-2.428468	-1.206533
H	0.272786	-3.235227	-1.858713
H	1.213118	-2.910914	-0.420357
H	1.264205	-1.802864	-1.832019
C	-0.069050	0.805123	-0.883490
H	-0.686789	0.580337	-1.762753
H	-0.456535	1.751498	-0.504561
C	1.068939	-0.429322	1.103066
H	1.181070	-1.462173	1.458330
H	0.876039	0.139209	2.017560
C	1.339109	1.099108	-1.403053
H	1.676549	0.282534	-2.048831
H	1.282062	1.978404	-2.059493
C	2.430174	0.132617	0.641677
H	2.993684	0.411557	1.543079
C	2.359615	1.348051	-0.291039
Cl	1.814670	2.773674	0.707508
C	3.708101	1.770705	-0.894211
H	3.624648	2.729558	-1.420523
H	4.074177	1.048939	-1.631601
H	4.474449	1.884572	-0.118978
Br	3.589257	-1.304876	-0.032581

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2424572**

SCF Energy (B3LYP/6-31G) = -6264.28282751**

1p_C013

MMFF Geometry

C	-1.511718	-0.090596	1.155354
C	-3.003816	-1.540473	-0.416271
C	-0.209428	-0.340074	0.188402
C	-2.877187	-0.254227	0.407211
H	-3.617564	-1.395021	-1.312722
H	-3.684872	-0.232474	1.151540
C	-1.706593	-2.137489	-0.842705
H	-1.822435	-3.067368	-1.398785
C	-0.467180	-1.660980	-0.601823
O	-3.667056	-2.547098	0.355017
H	-4.597341	-2.276768	0.438912
Br	-3.398487	1.274373	-0.723879
C	-1.494076	1.275366	1.902957
H	-2.405818	1.392901	2.502393
H	-1.442366	2.139939	1.239408
H	-0.658574	1.361633	2.603140
C	-1.523763	-1.159972	2.305917
H	-2.452625	-1.098997	2.886124
H	-0.707332	-1.008116	3.019396
H	-1.439884	-2.184846	1.934059
C	0.676165	-2.468556	-1.154056
H	0.334289	-3.294805	-1.789003
H	1.245983	-2.926959	-0.342919
H	1.322885	-1.859314	-1.785010
C	-0.077043	0.785195	-0.884005
H	-0.703861	0.557315	-1.756124
H	-0.465638	1.729436	-0.500722
C	1.080836	-0.421941	1.106590
H	1.206756	-1.448966	1.473588
H	0.879049	0.152552	2.015181
C	1.325683	1.080874	-1.416175
H	1.665186	0.255563	-2.050007
H	1.259303	1.949753	-2.085350
C	2.434758	0.153169	0.638993
H	2.991834	0.453752	1.537463
C	2.348973	1.354036	-0.311647
Cl	1.794505	2.788461	0.670648
C	3.690385	1.781826	-0.926693
H	3.594901	2.732432	-1.465766
H	4.060173	1.053567	-1.655823
H	4.459037	1.914195	-0.156703
Br	3.618282	-1.276184	-0.009141

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2442034**

SCF Energy (B3LYP/6-31G) = -6264.28435788**

1p_C014

MMFF Geometry

C	-1.519472	-0.076372	1.154358
C	-3.019345	-1.546533	-0.391155
C	-0.218980	-0.332570	0.184762
C	-2.889743	-0.247857	0.412580
H	-3.656898	-1.406300	-1.270778
H	-3.697461	-0.212078	1.156210
C	-1.723176	-2.131738	-0.845398
H	-1.842561	-3.043161	-1.431668
C	-0.483919	-1.652086	-0.610612
O	-3.687813	-2.534539	0.401658
H	-3.013880	-3.068233	0.854973
Br	-3.396273	1.267538	-0.746017
C	-1.501818	1.296705	1.889478
H	-2.401804	1.408359	2.507514
H	-1.475400	2.156626	1.218482
H	-0.651395	1.399232	2.569198
C	-1.518992	-1.132569	2.316700
H	-2.466710	-1.110675	2.868043
H	-0.733090	-0.934516	3.053237
H	-1.368679	-2.154809	1.960403
C	0.657038	-2.442659	-1.193396
H	0.311325	-3.257214	-1.841242
H	1.236500	-2.915341	-0.397460
H	1.295359	-1.818952	-1.818331
C	-0.078690	0.795947	-0.884286
H	-0.699445	0.569871	-1.761152
H	-0.470163	1.738991	-0.501179
C	1.071122	-0.426443	1.102465
H	1.193011	-1.457155	1.460590
H	0.871219	0.141609	2.015626
C	1.326359	1.097626	-1.407554
H	1.668505	0.280268	-2.049965
H	1.262199	1.973840	-2.067393
C	2.427491	0.147710	0.640598
H	2.986439	0.436188	1.541853
C	2.346283	1.358610	-0.297331
Cl	1.790444	2.782743	0.697818
C	3.690513	1.790291	-0.903327
H	3.598479	2.746418	-1.433145
H	4.061816	1.068735	-1.638317
H	4.456639	1.913546	-0.129316
Br	3.602357	-1.281080	-0.023973

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2446890**

SCF Energy (B3LYP/6-31G) = -6264.28521885**

1p_C015

MMFF Geometry

C	1.378257	-0.491185	-1.024076
C	3.408463	-0.861340	0.595255
C	0.396322	-0.664447	0.254074
C	2.831630	-0.082200	-0.602653
H	3.912481	-0.206861	1.315444
H	3.494503	-0.217009	-1.468184
C	2.426866	-1.693296	1.356374
H	2.883001	-2.394485	2.054165
C	1.084568	-1.662903	1.226415
O	4.407145	-1.772716	0.122840
H	5.171418	-1.238659	-0.154672
Br	3.092532	1.849412	-0.286720
C	0.820636	0.473256	-2.101875
H	1.550519	0.617685	-2.907943
H	0.569639	1.462152	-1.713069
H	-0.083546	0.071529	-2.571581
C	1.541116	-1.857055	-1.785714
H	2.288782	-1.767293	-2.583943
H	0.618013	-2.177076	-2.277051
H	1.866380	-2.675088	-1.137564
C	0.277625	-2.636303	2.050898
H	0.894919	-3.165165	2.786197
H	-0.170597	-3.400351	1.407566
H	-0.511771	-2.134878	2.613832
C	0.229767	0.685232	1.042375
H	1.084225	0.855128	1.708656
H	0.199650	1.539020	0.360054
C	-1.037116	-1.149474	-0.188511
H	-1.463330	-1.865325	0.520191
H	-0.990390	-1.704560	-1.127910
C	-1.040486	0.753736	1.894154
H	-1.013990	-0.058779	2.626901
H	-1.021101	1.672322	2.495105
C	-2.044875	0.000460	-0.312541
H	-1.660963	0.735251	-1.026964
C	-2.336301	0.676641	1.048659
Cl	-2.895260	2.371280	0.720029
C	-3.418656	0.003376	1.908144
H	-3.484502	0.476121	2.895913
H	-3.193418	-1.056567	2.069391
H	-4.416258	0.072838	1.462552
Br	-3.654484	-0.664755	-1.220028

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2519115**

SCF Energy (B3LYP/6-31G) = -6264.28481178**

1p_C016

MMFF Geometry

C	1.368030	-0.504306	-1.009992
C	3.455431	-0.879398	0.515652
C	0.412702	-0.609800	0.300260
C	2.833417	-0.084814	-0.645244
H	4.099465	-0.247966	1.137690
H	3.463311	-0.209522	-1.536755
C	2.480844	-1.588592	1.404205
H	2.937793	-2.228699	2.157071
C	1.134734	-1.527432	1.331551
O	4.309087	-1.885439	-0.043695
H	4.777204	-2.313036	0.692905
Br	3.088642	1.843919	-0.317386
C	0.802443	0.415406	-2.122171
H	1.519584	0.510399	-2.946958
H	0.573385	1.426270	-1.779780
H	-0.113984	0.003071	-2.557166
C	1.498956	-1.906144	-1.709557
H	2.275380	-1.882502	-2.484457
H	0.579369	-2.205620	-2.221245
H	1.761590	-2.709414	-1.016132
C	0.347103	-2.392077	2.288214
H	0.985601	-2.848718	3.053310
H	-0.134804	-3.214340	1.749550
H	-0.413426	-1.822782	2.823834
C	0.223978	0.785899	0.999347
H	1.068703	1.001982	1.664683
H	0.196352	1.594179	0.264276
C	-1.016293	-1.156007	-0.080507
H	-1.426128	-1.801886	0.701689
H	-0.967815	-1.804686	-0.957552
C	-1.056338	0.910670	1.830393
H	-1.030435	0.163472	2.628642
H	-1.050272	1.875625	2.354258
C	-2.041858	-0.038096	-0.307882
H	-1.670490	0.637182	-1.083963
C	-2.345716	0.752490	0.986940
Cl	-2.912849	2.408264	0.508818
C	-3.429660	0.150600	1.896280
H	-3.503495	0.707151	2.838801
H	-3.199888	-0.890033	2.150407
H	-4.425128	0.175726	1.441255
Br	-3.639008	-0.808011	-1.152318

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2499748**

SCF Energy (B3LYP/6-31G) = -6264.28481178**

1p_C017

MMFF Geometry

C	1.379251	-0.500440	-1.008217
C	3.440836	-0.862494	0.567365
C	0.410238	-0.629704	0.288238
C	2.841473	-0.084107	-0.618865
H	4.016690	-0.208338	1.230460
H	3.488896	-0.220834	-1.495672
C	2.460165	-1.621072	1.405361
H	2.921391	-2.269131	2.150552
C	1.116052	-1.579035	1.301107
O	4.383126	-1.820348	0.068277
H	3.882958	-2.575497	-0.284582
Br	3.092331	1.850083	-0.311894
C	0.819918	0.435744	-2.110457
H	1.543336	0.545824	-2.927795
H	0.583555	1.439737	-1.752909
H	-0.092663	0.028991	-2.558874
C	1.515772	-1.890245	-1.729875
H	2.307075	-1.858595	-2.489085
H	0.603762	-2.174803	-2.263519
H	1.757003	-2.708044	-1.046299
C	0.317371	-2.481468	2.211950
H	0.945625	-2.962374	2.970591
H	-0.150680	-3.285784	1.635274
H	-0.455671	-1.934837	2.753874
C	0.229733	0.750796	1.018406
H	1.077623	0.950337	1.684895
H	0.202546	1.575118	0.301108
C	-1.019542	-1.153166	-0.119456
H	-1.437364	-1.826039	0.635133
H	-0.969494	-1.767913	-1.020786
C	-1.048177	0.857575	1.855305
H	-1.023471	0.087484	2.631877
H	-1.037527	1.807415	2.405936
C	-2.037661	-0.021674	-0.311047
H	-1.659864	0.675681	-1.064592
C	-2.338926	0.728204	1.008569
Cl	-2.903288	2.398907	0.582680
C	-3.423225	0.099578	1.899016
H	-3.495977	0.626475	2.858502
H	-3.194748	-0.948788	2.120344
H	-4.418796	0.140086	1.445348
Br	-3.637560	-0.754247	-1.182847

SCF Energy (SMD/wB97XD/6-31+G) = -6264.2521069**

SCF Energy (B3LYP/6-31G) = -6264.28693015**

2a_C001

MMFF Geometry

C	-0.380364	1.420165	-1.148891
C	1.523633	0.151071	-0.034127
C	-0.812670	-0.124589	0.888936
C	0.544617	-0.857928	0.621824
C	-1.366782	0.604199	-0.330257
C	0.980668	0.750740	-1.331483
H	-1.525184	-0.881413	1.232074
H	1.698170	1.470879	-1.747887
H	-0.787910	1.609922	-2.148796
H	1.772966	0.953657	0.669509
H	0.887780	-0.031271	-2.096552
Cl	-0.186163	3.046667	-0.428607
Br	3.277716	-0.645171	-0.443676
C	0.244909	-2.079049	-0.289835
H	-0.195262	-1.792319	-1.249295
H	-0.466745	-2.756999	0.197118
H	1.144483	-2.665947	-0.500028
C	1.120480	-1.419380	1.944645
H	1.935079	-2.129429	1.765423
H	0.350643	-1.957502	2.509950
H	1.519143	-0.627246	2.587056
Cl	-0.739491	1.039612	2.255943
C	-2.653150	0.503571	-0.738541
H	-2.959901	1.033747	-1.640508
C	-3.774181	-0.225909	-0.064388
H	-3.633737	-0.322021	1.015118
H	-4.718180	0.302987	-0.227575
Cl	-3.915779	-1.848832	-0.765232

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7383593**

SCF Energy (B3LYP/6-31G) = -4341.80544998**

2a_C002

MMFF Geometry

C	-0.436009	1.482327	-0.697433
C	1.646444	0.235781	0.067328
C	-0.613682	-0.823193	0.472641
C	0.886005	-1.115244	0.126520
C	-1.255739	0.229916	-0.423300
C	1.047057	1.211924	-0.945153
H	-1.150906	-1.771908	0.382673
H	1.605338	2.158035	-0.938511
H	-0.824826	2.000183	-1.582062
H	1.676765	0.701109	1.059248
H	1.167616	0.818982	-1.963251

Cl	-0.640715	2.657656	0.635365
Br	3.551141	0.017811	-0.384053
C	0.913592	-1.876643	-1.227041
H	0.470442	-1.301047	-2.044855
H	0.346989	-2.812971	-1.153128
H	1.930912	-2.148006	-1.525858
C	1.506623	-2.061714	1.183058
H	2.467487	-2.469243	0.850608
H	0.849853	-2.917971	1.376082
H	1.685344	-1.551860	2.135538
Cl	-0.871117	-0.349644	2.184977
C	-2.469234	0.090698	-1.007399
H	-2.823205	0.895913	-1.653664
C	-3.453746	-1.030704	-0.859817
H	-3.549500	-1.570676	-1.805977
H	-3.196879	-1.742115	-0.074170
Cl	-5.051299	-0.365113	-0.453121

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7372877**
SCF Energy (B3LYP/6-31G) = -4341.80458500**

2b_C001

MMFF Geometry

C	0.955683	-0.119002	1.136914
C	-1.460549	-0.047976	0.321356
C	0.315572	1.069193	-1.077606
C	-1.018624	0.255688	-1.134503
C	1.393523	0.424765	-0.211106
C	-0.405143	-0.816507	1.116399
H	0.687852	1.177502	-2.104103
H	-0.752800	-0.986960	2.144489
H	1.676119	-0.853621	1.509126
H	-1.715596	0.880071	0.845792
H	-0.275967	-1.820992	0.691879
Cl	0.973143	1.189080	2.356080
Br	-3.132972	-1.084445	0.408188
C	-0.749724	-1.031588	-1.959875
H	0.026560	-1.663067	-1.518020
H	-0.414170	-0.775795	-2.972357
H	-1.650288	-1.643457	-2.071948
C	-2.103082	1.056241	-1.895715
H	-2.964282	0.430854	-2.154783
H	-1.707108	1.454971	-2.836992
H	-2.481901	1.897415	-1.305792
Cl	0.090803	2.766539	-0.527015
C	2.655045	0.307191	-0.686678
H	2.880829	0.698468	-1.678910
C	3.848176	-0.266100	0.014375
H	3.758120	-0.244696	1.103143
H	4.747439	0.296862	-0.253626
Cl	4.068639	-1.948761	-0.501173

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7379085**
SCF Energy (B3LYP/6-31G) = -4341.80587360**

2b_C002

MMFF Geometry

C	0.746510	-1.233325	-0.013364
C	-1.609808	-0.268101	0.165076
C	0.344315	1.324367	0.103475
C	-1.139228	1.118910	-0.346502
C	1.268487	0.167850	-0.274121
C	-0.736695	-1.416567	-0.340240
H	0.710083	2.250513	-0.357449
H	-1.093325	-2.372693	0.066715
H	1.287342	-1.964199	-0.621409
H	-1.642883	-0.282384	1.260513
H	-0.844035	-1.515820	-1.428642
Cl	1.080329	-1.712183	1.674811
Br	-3.468209	-0.675559	-0.344841
C	-1.181872	1.233747	-1.894223
H	-0.560852	0.483011	-2.391467
H	-0.814636	2.215655	-2.216938
H	-2.199038	1.134047	-2.285899
C	-2.031439	2.254993	0.210256
H	-3.015788	2.272244	-0.270015
H	-1.574645	3.235283	0.030962
H	-2.200699	2.153537	1.287352
Cl	0.513070	1.632788	1.866756
C	2.465600	0.431624	-0.848863
H	2.736860	1.474803	-1.019182
C	3.531812	-0.538951	-1.261510
H	3.628627	-0.547340	-2.350758
H	3.354736	-1.558430	-0.916106
Cl	5.093041	-0.025366	-0.583812

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7371911**
SCF Energy (B3LYP/6-31G) = -4341.80468667**

2c_C001

MMFF Geometry

C	-0.115621	1.451665	-1.013794
C	1.335033	-0.697747	-1.034350

C	-0.650679	-0.491033	0.609887
C	0.232739	-1.449540	-0.245180
C	-1.136224	0.732966	-0.151792
C	0.826522	0.529588	-1.794926
H	-1.510455	-1.080320	0.944943
H	1.659868	1.105608	-2.218275
H	-0.637232	2.063860	-1.759645
H	1.775911	-1.385043	-1.768341
H	0.269092	0.164801	-2.668816
Cl	0.776654	2.649594	-0.034509
Br	2.912945	-0.213385	0.020149
C	-0.704514	-2.131561	-1.291658
H	-1.209391	-1.409398	-1.940446
H	-1.486333	-2.719117	-0.795658
H	-0.141270	-2.815877	-1.936922
C	0.799579	-2.615556	0.599558
H	1.373786	-3.308349	-0.026769
H	-0.010396	-3.188859	1.066079
H	1.458271	-2.285466	1.407060
Cl	0.092781	0.047947	2.146256
C	-2.422059	1.156355	-0.142043
H	-2.691653	2.027359	-0.739824
C	-3.563391	0.602760	0.654251
H	-3.243367	0.105699	1.573337
H	-4.249454	1.407134	0.936692
Cl	-4.452891	-0.564655	-0.342239

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7316210**
SCF Energy (B3LYP/6-31G) = -4341.79550996**

2c_C002

MMFF Geometry

C	-0.265464	-1.163714	1.196360
C	1.763861	0.429984	0.940967
C	-0.451229	0.940942	-0.294805
C	0.828392	1.529253	0.375703
C	-1.151420	-0.113522	0.548606
C	1.042540	-0.623929	1.784688
H	-1.126653	1.786697	-0.457252
H	1.715595	-1.452292	2.042239
H	-0.806536	-1.632870	2.027184
H	2.521884	0.904154	1.578219
H	0.794513	-0.157994	2.748450
Cl	0.018677	-2.513283	0.062253
Br	2.894789	-0.450449	-0.393102
C	0.358324	2.403666	1.581329
H	-0.220964	1.834978	2.315065
H	-0.276364	3.231485	1.243131
H	1.214848	2.842120	2.106738
C	1.568986	2.512469	-0.562287
H	2.434599	2.956921	-0.057160
H	0.908837	3.333539	-0.866290
H	1.933626	2.044296	-1.480298
Cl	-0.204904	0.295129	-1.943803
C	-2.485762	-0.134122	0.779932
H	-2.882773	-0.919804	1.425059
C	-3.541035	0.772169	0.219404
H	-3.930889	1.423612	1.006445
H	-3.193704	1.388942	-0.610545
Cl	-4.896526	-0.201685	-0.393848

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7304104**
SCF Energy (B3LYP/6-31G) = -4341.79412978**

2c_C003

MMFF Geometry

C	-0.246153	1.549708	-1.077402
C	1.774656	0.189632	-0.386013
C	-0.344633	-0.927007	-1.115886
C	0.918768	-1.105751	-0.202289
C	-1.122674	0.340317	-0.743799
C	1.008250	1.505848	-0.198963
H	0.011893	-0.782922	-2.144626
H	0.736573	1.642769	0.856733
H	0.040980	1.497576	-2.134088
H	2.206828	0.189550	-1.395475
H	1.665788	2.347357	-0.456689
Cl	-1.023417	3.144870	-0.902800
Br	3.356319	0.251147	0.778573
C	1.739612	-2.332993	-0.669686
H	2.013095	-2.244487	-1.727051
H	1.184079	-3.268226	-0.544331
H	2.664660	-2.449788	-0.096399
C	0.498859	-1.339207	1.267266
H	1.358915	-1.574228	1.902842
H	-0.188426	-2.187475	1.355674
H	0.001087	-0.466380	1.700352
Cl	-1.344428	-2.395016	-1.290379
C	-2.341772	0.446405	-0.160512
H	-2.747291	1.443845	0.005999
C	-3.249296	-0.620515	0.380198
H	-3.962991	-0.947550	-0.379865
H	-2.704109	-1.470527	0.789917
Cl	-4.194857	0.029070	1.749617

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7295224**
SCF Energy (B3LYP/6-31G) = -4341.79903479**

2c_C004

MMFF Geometry

C	-0.376391	1.062303	-1.465104
C	1.302118	-0.532438	-0.366718
C	-0.749271	0.094670	0.911222
C	0.814320	-0.059605	1.025645
C	-1.310671	0.414942	-0.468542
C	1.052385	0.503433	-1.466300
H	-1.173457	-0.878123	1.190889
H	1.790699	1.314204	-1.412697
H	-0.769526	0.935853	-2.481016
H	0.801845	-1.472646	-0.633890
H	1.234355	0.024428	-2.438942
Cl	-0.395375	2.834772	-1.219404
Br	3.204958	-1.018879	-0.420990
C	1.097928	-1.129637	2.110929
H	0.727622	-2.114308	1.803709
H	0.607864	-0.871520	3.056783
H	2.167213	-1.227211	2.325024
C	1.534198	1.234388	1.477828
H	2.622661	1.117512	1.468482
H	1.273712	1.501064	2.508343
H	1.296937	2.092963	0.849155
Cl	-1.448954	1.234450	2.107748
C	-2.552261	0.049373	-0.869620
H	-2.863932	0.285039	-1.888033
C	-3.620532	-0.633878	-0.070206
H	-3.430469	-0.641509	1.004225
H	-4.585554	-0.146548	-0.238041
Cl	-3.745345	-2.320971	-0.611529

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7271592**
SCF Energy (B3LYP/6-31G) = -4341.79558252**

2c_C005

MMFF Geometry

C	-0.192719	1.670184	-0.731008
C	1.780457	0.108020	-0.468925
C	-0.540551	-0.784566	-0.787620
C	0.853984	-1.106082	-0.139191
C	-1.107782	0.537532	-0.254443
C	1.196553	1.480914	-0.115345
H	-0.376918	-0.640731	-1.864042
H	1.148145	1.606529	0.975024
H	-0.121234	1.629786	-1.824195
H	2.008136	0.101197	-1.543071
H	1.870770	2.266455	-0.483291
Cl	-0.756013	3.326568	-0.379156
Br	3.554982	-0.014436	0.367854
C	1.449818	-2.388887	-0.771155
H	1.519220	-2.295303	-1.860686
H	0.845260	-3.274198	-0.548315
H	2.453683	-2.604633	-0.392131
C	0.702216	-1.344279	1.381341
H	1.640957	-1.677676	1.835747
H	-0.034997	-2.126694	1.591396
H	0.383577	-0.442519	1.912795
Cl	-1.675045	-2.158236	-0.778817
C	-2.184680	0.750062	0.540584
H	-2.436164	1.775495	0.810766
C	-3.126234	-0.192174	1.226495
H	-2.721224	-1.189797	1.395143
H	-3.370814	0.206016	2.217204
Cl	-4.640654	-0.298508	0.311994

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7282039**
SCF Energy (B3LYP/6-31G) = -4341.79711465**

2d_C001

MMFF Geometry

C	-0.036514	1.611448	0.095047
C	1.429671	-0.108122	-1.092315
C	-0.447104	-0.858876	0.533615
C	0.453727	-1.244089	-0.683393
C	-1.069334	0.529066	0.403581
C	0.774598	1.274736	-1.160004
H	-1.224130	-1.625108	0.608664
H	1.537468	2.046475	-1.329933
H	0.633208	1.710510	0.955054
H	1.864544	-0.334054	-2.074090
H	0.118151	1.311593	-2.039663
Cl	-0.727175	3.252222	-0.118445
Br	3.033858	0.025500	0.036318
C	-0.491854	-1.493162	-1.899719
H	-1.090416	-0.613671	-2.155269
H	-1.191132	-2.312059	-1.693431
H	0.080839	-1.770416	-2.792562
C	1.174615	-2.593703	-0.456079
H	1.765026	-2.874382	-1.336156

H	0.450292	-3.397100	-0.276402
H	1.852778	-2.583312	0.401154
Cl	0.369720	-0.938916	2.129311
C	-2.400915	0.741464	0.532821
H	-2.803887	1.744742	0.407783
C	-3.464032	-0.253411	0.889269
H	-3.096290	-1.059127	1.529621
H	-4.276600	0.244371	1.427659
Cl	-4.133251	-0.961134	-0.592072

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7363747**
SCF Energy (B3LYP/6-31G) = -4341.80383709**

2d_C002

MMFF Geometry

C	0.269041	1.854887	-0.139343
C	-1.718371	0.267031	0.066118
C	0.472416	-0.324339	1.132504
C	-0.799021	-0.938340	0.444779
C	1.177786	0.687704	0.224606
C	-1.029742	1.350977	-0.769683
H	0.133656	0.217805	2.022677
H	-0.805011	0.961016	-1.771754
H	0.751575	2.528721	-0.856049
H	-2.116287	0.721289	0.982152
H	-1.713228	2.195653	-0.930367
Cl	-0.053416	2.864835	1.299829
Br	-3.344773	-0.271885	-0.904261
C	-1.545097	-1.858035	1.443841
H	-1.812504	-1.313030	2.356051
H	-0.940270	-2.722745	1.735750
H	-2.467316	-2.264868	1.017446
C	-0.393179	-1.788450	-0.782285
H	-1.256163	-2.287857	-1.234292
H	0.308377	-2.582382	-0.504261
H	0.085802	-1.189749	-1.562723
Cl	1.558693	-1.549838	1.852020
C	2.416408	0.660783	-0.324073
H	2.710694	1.524902	-0.923397
C	3.470801	-0.405332	-0.278607
H	4.086457	-0.311157	0.619093
H	3.051309	-1.408464	-0.362188
Cl	4.560824	-0.232319	-1.683974

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7326329**
SCF Energy (B3LYP/6-31G) = -4341.80316049**

2d_C003

MMFF Geometry

C	0.105208	1.560032	-0.137664
C	-1.756877	0.143871	0.897247
C	0.470709	-0.937611	0.130129
C	-0.772502	-1.045907	1.068519
C	1.110421	0.447978	0.160943
C	-1.072376	1.513756	0.843176
H	1.184332	-1.704250	0.442458
H	-1.802898	2.292749	0.586387
H	-0.257084	1.449357	-1.164245
H	-2.472792	0.147868	1.728876
H	-0.716148	1.766345	1.851090
Cl	0.795558	3.214237	-0.081470
Br	-2.951347	-0.007200	-0.656241
C	-0.248871	-1.000650	2.537956
H	0.286561	-0.074252	2.766813
H	0.441091	-1.829703	2.735371
H	-1.075957	-1.085652	3.252585
C	-1.470363	-2.419816	0.935115
H	-2.314542	-2.498367	1.630143
H	-0.774880	-3.234536	1.169445
H	-1.855806	-2.613987	-0.069178
Cl	0.150192	-1.360353	-1.584315
C	2.426214	0.641361	0.418989
H	2.835984	1.649743	0.399453
C	3.471744	-0.379719	0.752370
H	4.222788	0.062172	1.414886
H	3.068709	-1.256044	1.264939
Cl	4.286481	-0.910308	-0.727231

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7352096**
SCF Energy (B3LYP/6-31G) = -4341.80161006**

2d_C004

MMFF Geometry

C	0.224285	0.224285	0.224285
C	-1.730732	-1.730732	-1.730732
C	0.617225	0.617225	0.617225
C	-0.798738	-0.798738	-0.798738
C	1.150481	1.150481	1.150481
C	-1.196238	-1.196238	-1.196238
H	0.500678	0.500678	0.500678
H	-1.204915	-1.204915	-1.204915
H	0.565689	0.565689	0.565689
H	-1.904913	-1.904913	-1.904913
H	-1.865341	-1.865341	-1.865341

Cl	0.251213	0.251213	0.251213
Br	-3.547500	-3.547500	-3.547500
C	-1.350231	-1.350231	-1.350231
H	-1.390506	-1.390506	-1.390506
H	-0.735073	-0.735073	-0.735073
H	-2.359390	-2.359390	-2.359390
C	-0.700641	-0.700641	-0.700641
H	-1.660626	-1.660626	-1.660626
H	0.009035	0.009035	0.009035
H	-0.373429	-0.373429	-0.373429
Cl	1.769143	1.769143	1.769143
C	2.247360	2.247360	2.247360
H	2.424461	2.424461	2.424461
C	3.301345	3.301345	3.301345
H	2.983240	2.983240	2.983240
H	3.592577	3.592577	3.592577
Cl	4.744134	4.744134	4.744134

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7310354**
SCF Energy (B3LYP/6-31G) = -4341.80068211**

2e_C001

MMFF Geometry

C	-0.410991	1.712447	0.504914
C	1.571747	0.161761	0.272770
C	-0.692038	-0.789765	0.882016
C	0.656858	-1.083756	0.141778
C	-1.352495	0.510563	0.426862
C	0.914165	1.453762	-0.215142
H	-1.352225	-1.646797	0.722215
H	1.594089	2.298214	-0.036206
H	-0.204645	1.921733	1.560298
H	1.882581	0.292906	1.316292
H	0.758027	1.419971	-1.301564
Cl	-1.099775	3.238828	-0.128720
Br	3.282067	-0.036654	-0.676647
C	0.322645	-1.422102	-1.335376
H	-0.147454	-0.586979	-1.862759
H	-0.370304	-2.270357	-1.388551
H	1.213057	-1.710684	-1.902875
C	1.332343	-2.336982	0.748865
H	2.158993	-2.695762	0.126215
H	0.617635	-3.163638	0.835542
H	1.741588	-2.140440	1.745259
Cl	-0.515885	-0.701086	2.673429
C	-2.633931	0.559000	-0.009032
H	-3.055564	1.504854	-0.344464
C	-3.636041	-0.554604	-0.061596
H	-3.478661	-1.306581	0.715624
H	-4.645921	-0.154844	0.073735
Cl	-3.561817	-1.346016	-1.645442

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7394351**
SCF Energy (B3LYP/6-31G) = -4341.80826546**

2e_C002

MMFF Geometry

C	-0.376160	1.548728	0.603015
C	1.630766	0.016095	0.369876
C	-0.702473	-0.942168	0.210143
C	0.772547	-1.097031	-0.289031
C	-1.252276	0.463726	-0.023736
C	1.081047	1.427029	0.146432
H	-1.314522	-1.698527	-0.287877
H	1.695707	2.148657	0.702211
H	-0.419431	1.453986	1.693154
H	1.719500	-0.163678	1.447999
H	1.171906	1.708849	-0.911252
Cl	-0.917826	3.223294	0.270546
Br	3.501465	-0.000590	-0.237403
C	0.760933	-1.003117	-1.838060
H	0.431956	-0.024035	-2.198430
H	0.080081	-1.750005	-2.264099
H	1.748412	-1.197252	-2.268822
C	1.309973	-2.502153	0.074080
H	2.254466	-2.720874	-0.435651
H	0.599453	-3.281877	-0.223987
H	1.492584	-2.606917	1.148573
Cl	-0.897750	-1.323003	1.961446
C	-2.398896	0.693605	-0.707057
H	-2.764455	1.712886	-0.819218
C	-3.293682	-0.301612	-1.382126
H	-3.798843	0.168932	-2.231571
H	-2.751363	-1.167315	-1.769974
Cl	-4.530741	-0.863868	-0.246884

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7384930**
SCF Energy (B3LYP/6-31G) = -4341.80695235**

2e_C003

MMFF Geometry

C	0.039362	-1.683345	0.379538
C	-1.577574	0.226050	1.102308

C	0.221899	0.620407	-0.647028
C	-0.599818	1.283542	0.502246
C	0.982432	-0.608499	-0.143594
C	-0.935166	-1.129992	1.430604
H	-0.476669	0.282394	-1.419394
H	-0.363749	-0.998517	2.360276
H	0.602304	-2.489837	0.863725
H	-2.027648	0.625515	2.020037
H	-1.698127	-1.881956	1.670309
Cl	-0.783963	-2.487020	-0.984321
Br	-3.168404	-0.083834	-0.019322
C	-1.363116	2.539527	0.012074
H	-1.891719	2.359288	-0.929539
H	-0.686650	3.384349	-0.160736
H	-2.094692	2.870600	0.758359
C	0.337855	1.772792	1.640569
H	-0.242094	2.240123	2.445357
H	1.053150	2.520487	1.281073
H	0.914679	0.959824	2.091396
Cl	1.227789	1.790723	-1.551447
C	2.314571	-0.838896	-0.047486
H	2.620795	-1.821537	0.317536
C	3.477162	0.064349	-0.334119
H	3.761584	0.016823	-1.387968
H	3.292302	1.093331	-0.024862
Cl	4.894116	-0.462661	0.619299

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7293553**
SCF Energy (B3LYP/6-31G) = -4341.79722294**

2f_C001

MMFF Geometry

C	0.813975	-0.958007	-0.547471
C	-1.296763	0.427322	-1.155658
C	0.098192	1.043454	0.928755
C	-0.821013	1.564414	-0.215455
C	1.204804	0.113678	0.450285
C	-0.173283	-0.498773	-1.627438
H	0.552505	1.922569	1.403545
H	-0.575962	-1.364997	-2.168824
H	1.700251	-1.305696	-1.087721
H	-1.756262	0.874451	-2.046970
H	0.407862	0.052146	-2.380144
Cl	0.240252	-2.412914	0.313081
Br	-2.784075	-0.643354	-0.464418
C	0.025023	2.555999	-1.074707
H	0.920648	2.090785	-1.497659
H	0.360019	3.409897	-0.473806
H	-0.563871	2.954300	-1.909260
C	-1.994808	2.412039	0.330100
H	-2.600888	2.813548	-0.490525
H	-1.623132	3.264213	0.911485
H	-2.666373	1.851536	0.985635
Cl	-0.765320	0.255252	2.285507
C	2.476018	0.310244	0.872179
H	2.677583	1.122608	1.570744
C	3.688026	-0.504297	0.539003
H	3.449508	-1.527683	0.239454
H	4.352957	-0.560486	1.406249
Cl	4.565466	0.282588	-0.787124

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7314777**
SCF Energy (B3LYP/6-31G) = -4341.79578246**

2f_C002

MMFF Geometry

C	0.640319	-0.812105	-1.002370
C	-1.724014	0.264633	-1.020928
C	0.121144	1.217855	0.513891
C	-1.153390	1.527479	-0.326272
C	1.158391	0.383656	-0.229184
C	-0.671450	-0.565919	-1.758936
H	0.569037	2.181761	0.787570
H	-1.093151	-1.517047	-2.109922
H	1.367223	-1.101708	-1.767570
H	-2.477672	0.576028	-1.756165
H	-0.414283	-0.021708	-2.678481
Cl	0.543362	-2.240584	0.060423
Br	-2.789525	-0.902209	0.135398
C	-0.737105	2.529282	-1.448810
H	0.050058	2.133564	-2.097772
H	-0.359664	3.465374	-1.020186
H	-1.592150	2.782866	-2.086406
C	-2.220757	2.280628	0.502995
H	-3.087950	2.536440	-0.117097
H	-1.814540	3.217581	0.902323
H	-2.590313	1.707355	1.357202
Cl	-0.198328	0.456727	2.102887
C	2.459528	0.758801	-0.204305
H	2.726795	1.653772	0.359882
C	3.635874	0.065969	-0.825323
H	4.018471	0.656515	-1.662394
H	3.414261	-0.942939	-1.176468
Cl	4.941202	-0.078038	0.373279

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7305053**
SCF Energy (B3LYP/6-31G) = -4341.79420759**

2f_C003

MMFF Geometry

C	0.483475	-1.189988	-1.151098
C	-1.752373	-0.309384	-0.400567
C	0.127660	1.258417	-0.982120
C	-1.161642	1.104287	-0.092233
C	1.124729	0.116570	-0.700946
C	-0.750187	-1.466614	-0.291703
H	-0.169660	1.179077	-2.035886
H	-0.458347	-1.631479	0.754187
H	0.168227	-1.068778	-2.194555
H	-2.161423	-0.308149	-1.419637
H	-1.232873	-2.395131	-0.625829
Cl	1.525172	-2.624449	-1.200220
Br	-3.310400	-0.767733	0.705631
C	-2.196664	2.188813	-0.480835
H	-2.437296	2.138125	-1.548620
H	-1.831363	3.198748	-0.267897
H	-3.132774	2.080330	0.075871
C	-0.816322	1.281818	1.406045
H	-1.714243	1.280152	2.032575
H	-0.317296	2.238478	1.593244
H	-0.157523	0.490530	1.776189
Cl	0.853273	2.896983	-0.903426
C	2.323803	0.310286	-0.098515
H	2.613478	1.330939	0.148332
C	3.342323	-0.692820	0.360019
H	3.978563	-1.012828	-0.468587
H	2.881721	-1.549009	0.854681
Cl	4.414848	0.038721	1.587209

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7280242**
SCF Energy (B3LYP/6-31G) = -4341.79813792**

2f_C004

MMFF Geometry

C	0.826401	-0.712838	-1.310339
C	-1.547196	-0.346252	-0.535007
C	0.053491	1.575559	-0.742555
C	-1.207267	1.063014	0.044669
C	1.228909	0.584105	-0.617448
C	-0.368827	-1.326647	-0.576645
H	-0.207137	1.634369	-1.807431
H	-0.079020	-1.627435	0.439211
H	0.524737	-0.466349	-2.335540
H	-1.927433	-0.227257	-1.558277
H	-0.683898	-2.245756	-1.089555
Cl	2.076384	-1.947992	-1.529070
Br	-3.032638	-1.238450	0.391776
C	-2.400478	2.020082	-0.198155
H	-2.609355	2.124746	-1.268701
H	-2.212014	3.020326	0.205290
H	-3.315936	1.665074	0.285464
C	-0.923885	1.021615	1.565289
H	-1.820947	0.765236	2.138353
H	-0.592231	1.996188	1.938852
H	-0.151200	0.291427	1.823635
Cl	0.491224	3.274358	-0.358918
C	2.354227	0.870073	0.082181
H	2.431294	1.846576	0.559745
C	3.575591	0.061656	0.394567
H	4.386694	0.735022	0.692327
H	3.957246	-0.513136	-0.449155
Cl	3.249788	-1.003747	1.774710

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7268102**
SCF Energy (B3LYP/6-31G) = -4341.79611724**

2g_C001

MMFF Geometry

C	-0.881135	-1.047498	0.924189
C	1.486211	-0.305041	0.346961
C	-0.331899	1.409412	0.556695
C	0.991998	1.062916	-0.216160
C	-1.387191	0.299629	0.439344
C	0.445484	-1.423602	0.266158
H	-0.086322	1.517048	1.619863
H	0.256412	-1.683629	-0.784063
H	-1.588151	-1.853616	0.714242
H	1.799745	-0.177772	1.390547
H	0.837877	-2.339881	0.727760
Cl	-0.731615	-1.018425	2.707913
Br	3.121838	-0.965180	-0.528150
C	2.058319	2.151545	0.064210
H	2.251819	2.244835	1.138704
H	1.749327	3.134533	-0.305647
H	3.010653	1.930065	-0.427524
C	0.736997	1.017914	-1.742187
H	1.654501	0.811821	-2.302386

H	0.363112	1.977314	-2.115424
H	0.003760	0.254491	-2.018764
Cl	-0.974844	3.036985	0.133594
C	-2.627189	0.454625	-0.083226
H	-2.940330	1.425670	-0.461786
C	-3.709200	-0.575610	-0.205015
H	-4.690658	-0.091323	-0.205292
H	-3.700970	-1.295900	0.617337
Cl	-3.521744	-1.450211	-1.736102

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7379534**
SCF Energy (B3LYP/6-31G) = -4341.80804344**

2g_C002

MMFF Geometry

C	-0.851870	-1.229433	0.085201
C	1.564756	-0.452862	0.266459
C	-0.299876	1.197384	0.605628
C	1.170113	1.043170	0.065908
C	-1.272767	0.220916	-0.075019
C	0.589455	-1.445256	-0.371655
H	-0.296120	0.970085	1.677987
H	0.630094	-1.361190	-1.465938
H	-1.487782	-1.910643	-0.483956
H	1.650021	-0.666831	1.338984
H	0.896344	-2.475469	-0.145556
Cl	-1.062267	-1.732988	1.791064
Br	3.361855	-0.884820	-0.413739
C	2.123970	1.941893	0.892529
H	2.075178	1.691090	1.958081
H	1.881065	3.004291	0.788562
H	3.165698	1.837672	0.573535
C	1.255932	1.482471	-1.416338
H	2.278268	1.418115	-1.802009
H	0.950210	2.526177	-1.545262
H	0.619493	0.875182	-2.066785
Cl	-0.869690	2.904979	0.561253
C	-2.387386	0.579863	-0.756441
H	-2.658292	1.631080	-0.835193
C	-3.362945	-0.302620	-1.475743
H	-2.896283	-1.192100	-1.905690
H	-3.824681	0.249038	-2.300794
Cl	-4.645950	-0.809694	-0.365746

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7365611**
SCF Energy (B3LYP/6-31G) = -4341.80593190**

2g_C003

MMFF Geometry

C	-0.376593	1.209902	0.121398
C	1.617495	0.142432	-1.068317
C	0.016670	-1.275923	0.396893
C	1.048880	-1.273487	-0.775283
C	-1.027342	-0.161789	0.261658
C	0.554624	1.247811	-1.096139
H	-0.477187	-2.255471	0.399534
H	1.036937	2.231886	-1.169737
H	0.199584	1.415577	1.028475
H	2.136250	0.136296	-2.035212
H	-0.041265	1.142467	-2.012737
Cl	-1.493913	2.593705	0.012523
Br	3.053373	0.704210	0.152502
C	0.294028	-1.736237	-2.060623
H	-0.535086	-1.072928	-2.324947
H	-0.124250	-2.741485	-1.931045
H	0.971079	-1.772127	-2.922246
C	2.157526	-2.330362	-0.561163
H	2.851108	-2.346726	-1.410014
H	1.726238	-3.334366	-0.469795
H	2.750383	-2.159232	0.341124
Cl	0.737242	-1.173015	2.036110
C	-2.334979	-0.518152	0.261000
H	-2.556350	-1.578061	0.400214
C	-3.562457	0.327768	0.095796
H	-3.515397	0.935868	-0.809381
H	-3.739344	0.946121	0.978931
Cl	-5.000849	-0.714040	-0.098755

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7299126**
SCF Energy (B3LYP/6-31G) = -4341.79848703**

2g_C004

MMFF Geometry

C	0.584824	-1.035136	0.312475
C	-1.377707	-0.218268	-1.115176
C	-0.187536	1.366003	0.549342
C	-1.048314	1.252690	-0.747164
C	1.011311	0.409013	0.559011
C	-0.178020	-1.165282	-1.013056
H	0.160174	2.404013	0.621204
H	-0.507386	-2.203572	-1.155586
H	-0.060663	-1.350373	1.137955
H	-1.767413	-0.261512	-2.140025
H	0.506327	-0.957556	-1.846825

Cl	1.885458	-2.250212	0.300024
Br	-2.863546	-0.996370	-0.088872
C	-0.201956	1.839720	-1.919707
H	0.738913	1.302180	-2.071725
H	0.052338	2.890047	-1.734116
H	-0.757812	1.799520	-2.863872
C	-2.308102	2.147032	-0.676696
H	-2.880903	2.089383	-1.609678
H	-2.032335	3.197386	-0.524769
H	-2.984917	1.878242	0.138513
Cl	-1.094161	1.133681	2.080836
C	2.238337	0.954294	0.741674
H	2.287742	2.036366	0.881815
C	3.608535	0.356818	0.810918
H	3.648662	-0.630345	1.269559
H	4.250777	1.000187	1.421998
Cl	4.310019	0.306982	-0.817544

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7290073**
SCF Energy (B3LYP/6-31G) = -4341.79684924**

2h_C001

MMFF Geometry

C	0.643189	-1.308575	0.001997
C	-1.367996	-0.105534	1.129649
C	-0.027000	1.043303	-0.698060
C	-0.835987	1.265383	0.618547
C	1.119268	0.043168	-0.498814
C	-0.305490	-1.208038	1.204898
H	-0.695110	0.635692	-1.464333
H	0.315620	-0.999186	2.087227
H	1.481921	-1.929164	0.328459
H	-1.803749	0.021371	2.128867
H	-0.764008	-2.184854	1.406903
Cl	-0.064142	-2.218825	-1.363244
Br	-2.910746	-0.771783	0.102561
C	-1.995818	2.272057	0.412666
H	-2.574569	2.054293	-0.490746
H	-1.629991	3.300384	0.314335
H	-2.680421	2.262669	1.268810
C	0.066014	1.872845	1.729569
H	-0.499341	1.998743	2.660683
H	0.446131	2.860986	1.448905
H	0.932085	1.245356	1.960069
Cl	0.514813	2.599542	-1.424482
C	2.432773	0.315062	-0.690089
H	2.741856	1.308080	-1.010218
C	3.595913	-0.618985	-0.543141
H	4.409709	-0.313104	-1.207921
H	3.343263	-1.653335	-0.790679
Cl	4.190712	-0.558342	1.126941

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7349228**
SCF Energy (B3LYP/6-31G) = -4341.80265948**

2h_C002

MMFF Geometry

C	0.597679	-0.945754	0.968367
C	-1.719254	-0.150981	0.301422
C	0.225090	1.455935	0.227051
C	-1.143263	1.086518	-0.434088
C	1.201269	0.273205	0.275094
C	-0.751740	-1.335251	0.353286
H	0.661794	2.292903	-0.331243
H	-1.201601	-2.142017	0.948762
H	0.443564	-0.700941	2.024719
H	-2.006684	0.117680	1.325050
H	-0.603293	-1.752746	-0.651735
Cl	1.616347	-2.407503	0.998591
Br	-3.407286	-0.789586	-0.479349
C	-0.885498	0.818371	-1.940736
H	-0.233739	-0.043767	-2.109948
H	-0.403394	1.684927	-2.409299
H	-1.814920	0.641128	-2.491318
C	-2.115040	2.287720	-0.348801
H	-3.000003	2.140637	-0.977262
H	-1.629919	3.208639	-0.692620
H	-2.470578	2.456479	0.672965
Cl	0.055833	2.094003	1.904333
C	2.424119	0.446536	-0.283309
H	2.628654	1.421922	-0.728809
C	3.582694	-0.502344	-0.372264
H	3.345611	-1.359886	-1.005876
H	3.916151	-0.821726	0.617449
Cl	4.982351	0.306943	-1.131733

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7331267**
SCF Energy (B3LYP/6-31G) = -4341.80352507**

2h_C003

MMFF Geometry

C	-0.820239	-0.274246	-1.238067
C	1.567788	-0.147493	-0.382695

C	-0.074282	1.669689	0.215920
C	1.179198	0.877949	0.712020
C	-1.239212	0.756820	-0.192324
C	0.415713	-1.066067	-0.792087
H	-0.383937	2.354229	1.015004
H	0.747834	-1.713109	-1.616126
H	-0.577691	0.257448	-2.164452
H	1.940434	0.373027	-1.273100
H	0.154104	-1.743122	0.032315
Cl	-2.058136	-1.456429	-1.722235
Br	3.088096	-1.282274	0.134230
C	0.811049	0.201802	2.059486
H	0.012975	-0.539125	1.955364
H	0.465234	0.949294	2.783754
H	1.670018	-0.301696	2.514490
C	2.344138	1.854932	0.999907
H	3.161532	1.365559	1.540406
H	2.007786	2.692490	1.622010
H	2.769364	2.269273	0.079900
Cl	0.275699	2.762691	-1.174792
C	-2.429817	0.965251	0.419991
H	-2.476576	1.765808	1.161680
C	-3.769834	0.315480	0.271468
H	-3.985640	-0.052815	-0.730586
H	-4.551267	1.048696	0.498586
Cl	-3.920184	-0.998678	1.452380

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7323331**
SCF Energy (B3LYP/6-31G) = -4341.80180178**

2h_C004

MMFF Geometry

C	0.672159	-1.084007	0.652431
C	-1.714978	-0.111437	0.992014
C	-0.028534	1.065603	-0.507196
C	-1.225213	1.273488	0.476111
C	1.114718	0.279890	0.154010
C	-0.597928	-1.024045	1.512608
H	-0.372699	0.493827	-1.375595
H	-0.300606	-0.642852	2.499552
H	1.440790	-1.554065	1.269302
H	-2.441149	0.037388	1.801383
H	-0.973720	-2.038011	1.702059
Cl	0.507046	-2.193972	-0.738367
Br	-2.790888	-1.098348	-0.328482
C	-2.380972	2.061494	-0.190839
H	-2.622174	1.674443	-1.186116
H	-2.133193	3.121771	-0.314716
H	-3.288868	2.021059	0.422237
C	-0.791005	2.114200	1.710206
H	-1.625883	2.231186	2.411488
H	-0.470052	3.121414	1.423627
H	0.033813	1.655585	2.263672
Cl	0.511552	2.622874	-1.233716
C	2.385983	0.728838	0.292986
H	2.656164	1.709410	-0.095041
C	3.557696	0.050429	0.937157
H	3.275474	-0.684661	1.693062
H	4.188542	0.794995	1.433084
Cl	4.532171	-0.759845	-0.300155

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7333603**
SCF Energy (B3LYP/6-31G) = -4341.80016246**

2h_C005

MMFF Geometry

C	-0.795388	-0.797904	-0.697823
C	1.641018	-0.168585	-0.387012
C	-0.167920	1.525059	0.101227
C	1.269863	1.050462	0.497074
C	-1.201432	0.391367	0.168424
C	0.608549	-1.297607	-0.338491
H	-0.453502	2.345260	0.771086
H	0.905459	-2.086283	-1.043913
H	-0.790290	-0.473757	-1.743906
H	1.771706	0.147568	-1.428996
H	0.600267	-1.769821	0.653067
Cl	-1.891499	-2.196808	-0.690302
Br	3.393070	-0.938262	0.065901
C	1.256494	0.706176	2.010440
H	0.598793	-0.135855	2.245206
H	0.906623	1.563819	2.597726
H	2.254964	0.457407	2.384059
C	2.281684	2.205507	0.305803
H	3.250627	1.977633	0.762941
H	1.917044	3.126740	0.774841
H	2.467336	2.417681	-0.752216
Cl	-0.249246	2.260464	-1.540738
C	-2.291016	0.590340	0.948945
H	-2.370473	1.553487	1.458038
C	-3.468243	-0.273070	1.280312
H	-3.846545	0.003568	2.270444
H	-3.245507	-1.337944	1.332974
Cl	-4.772527	0.022180	0.118023

SCF Energy (SMD/wB97XD/6-31+G) = -4341.7317756**
SCF Energy (B3LYP/6-31G) = -4341.80107468**

3a_C001

MMFF Geometry

C	-2.299675	-0.228626	0.153306
C	-2.735913	0.900962	1.154484
H	-2.972196	0.468653	2.134118
C	-1.687012	1.966155	1.334931
H	-2.104279	2.949166	1.513388
C	-0.328619	1.814259	0.664275
C	-0.102513	0.507664	-0.167340
C	-0.111201	-0.717366	0.809868
H	0.139844	-0.447189	1.839413
O	-1.465540	-1.199311	0.835280
Br	-3.921123	-1.191203	-0.421032
C	-1.409119	0.255410	-1.023856
O	-3.911097	1.588625	0.696609
H	-4.604324	0.909981	0.590367
O	-0.519610	1.624283	2.078288
C	1.232476	0.542423	-0.953219
H	1.386106	1.518360	-1.424603
H	1.235416	-0.169170	-1.783916
C	2.395205	0.160726	-0.026744
H	2.357280	0.802380	0.861596
C	2.338107	-1.337967	0.385254
C	0.868015	-1.832666	0.443682
H	0.587420	-2.264594	-0.521310
H	0.754132	-2.668781	1.146978
C	3.112349	-2.308183	-0.522855
H	2.799633	-2.205055	-1.567976
H	2.929719	-3.349626	-0.230205
H	4.195830	-2.157203	-0.475070
Cl	3.051538	-1.486126	2.044263
Br	4.078289	0.695957	-0.872127
C	0.404983	3.079410	0.327434
H	0.077823	3.913753	0.958263
H	0.224634	3.369813	-0.711882
H	1.481580	2.967419	0.482453
C	-1.239410	-0.838496	-2.115268
H	-0.469969	-0.572185	-2.845776
H	-2.158722	-0.957134	-2.701445
H	-1.008234	-1.823983	-1.710137
C	-1.920178	1.495498	-1.784774
H	-1.184418	1.814987	-2.532032
H	-2.126377	2.362420	-1.155314
H	-2.852858	1.271726	-2.315273

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4318534**
SCF Energy (B3LYP/6-31G) = -6413.49942284**

3a_C002

MMFF Geometry

C	1.984707	-0.177660	-0.390349
C	2.870574	1.110502	-0.280881
H	3.171417	1.451597	-1.278730
C	2.174500	2.237642	0.425865
H	2.854441	2.869164	0.983738
C	0.723815	2.078906	0.867928
C	-0.008338	0.721812	0.494923
C	-0.109330	0.618547	-1.062076
H	-0.094012	1.603199	-1.536269
O	1.086734	-0.046904	-1.514352
Br	3.175937	-1.693642	-0.806742
C	1.040833	-0.429684	0.819177
O	4.073973	0.865968	0.465385
H	4.537409	0.138343	0.009217
O	1.110943	2.896779	-0.253373
C	-1.396426	0.637016	1.213903
H	-1.695807	1.656187	1.478815
H	-1.282729	0.136271	2.182899
C	-2.642087	0.123768	0.458926
H	-3.523502	0.607301	0.902537
C	-2.643515	0.378735	-1.055481
C	-1.321599	-0.085251	-1.666130
H	-1.221888	-1.172286	-1.587798
H	-1.318097	0.097759	-2.750411
C	-3.826843	-0.256164	-1.801563
H	-3.754366	-1.347949	-1.837367
H	-3.866597	0.082808	-2.844034
H	-4.781711	0.005373	-1.331414
Cl	-2.820894	2.174698	-1.305909
Br	-3.007863	-1.748622	0.927314
C	0.311706	2.874398	2.074669
H	1.082054	3.598188	2.363518
H	0.143095	2.223833	2.938127
H	-0.598846	3.447092	1.872490
C	0.423021	-1.845700	0.800690
H	-0.297262	-1.963080	1.612856
H	1.178259	-2.617863	0.987637
H	-0.053488	-2.101714	-0.144536
C	1.712659	-0.321233	2.206951
H	0.969535	-0.429597	3.005317

H	2.233158	0.619504	2.391197
H	2.456310	-1.115298	2.342021

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4243456**
SCF Energy (B3LYP/6-31G) = -6413.49640925**

3b_C001

MMFF Geometry

C	-2.340084	-0.127696	0.025523
C	-2.763329	0.994671	1.032094
H	-3.627600	1.535453	0.627498
C	-1.696859	2.025906	1.272378
H	-2.102025	3.010669	1.464481
C	-0.328418	1.853670	0.625517
C	-0.116161	0.555126	-0.223251
C	-0.183890	-0.688987	0.729751
H	0.051411	-0.444764	1.769472
O	-1.553089	-1.132754	0.718759
Br	-3.980003	-0.990826	-0.620759
C	-1.406521	0.357156	-1.116547
O	-3.171212	0.452828	2.290827
H	-2.535997	-0.262208	2.490895
O	-0.550882	1.641342	2.030069
C	1.239461	0.566358	-0.973726
H	1.432998	1.546262	-1.421574
H	1.244178	-0.129143	-1.817940
C	2.366429	0.133438	-0.025715
H	2.323054	0.758700	0.874047
C	2.256630	-1.371008	0.354068
C	0.772007	-1.824724	0.365241
H	0.504100	-2.229355	-0.614986
H	0.616680	-2.670816	1.048376
C	3.026889	-2.344942	-0.553301
H	2.744480	-2.212704	-1.603756
H	2.807753	-3.386264	-0.286432
H	4.112537	-2.225675	-0.474879
Cl	2.921530	-1.571290	2.027490
Br	4.084894	0.637227	-0.817131
C	0.445140	3.104707	0.328693
H	0.123812	3.936245	0.966172
H	0.297430	3.417244	-0.709332
H	1.514458	2.961978	0.507318
C	-1.873138	1.628111	-1.855972
H	-1.097350	1.973461	-2.549053
H	-2.116888	2.468080	-1.203172
H	-2.775836	1.429584	-2.445244
C	-1.236225	-0.714709	-2.228911
H	-0.443970	-0.448959	-2.934844
H	-2.143269	-0.799660	-2.839407
H	-1.037299	-1.714019	-1.841081

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4350803**
SCF Energy (B3LYP/6-31G) = -6413.49823274**

3b_C002

MMFF Geometry

C	2.023236	-0.233464	-0.240125
C	2.923695	1.011838	0.041494
H	3.784627	0.707303	0.649095
C	2.225547	2.093262	0.808767
H	2.898779	2.646976	1.449967
C	0.752234	1.929503	1.168397
C	0.008957	0.635771	0.627828
C	-0.013367	0.682151	-0.936475
H	0.044174	1.707151	-1.311640
O	1.193198	0.036298	-1.394352
Br	3.214704	-1.725637	-0.699196
C	1.013312	-0.568528	0.892685
O	3.450644	1.571603	-1.164632
H	2.711220	1.558945	-1.803645
O	1.206537	2.841234	0.151568
C	-1.417164	0.524046	1.263872
H	-1.706898	1.523534	1.604264
H	-1.366463	-0.064366	2.187922
C	-2.632259	0.114355	0.402749
H	-3.525052	0.578586	0.844236
C	-2.548866	0.506275	-1.079865
C	-1.206265	0.067569	-1.663923
H	-1.132759	-1.024143	-1.682899
H	-1.142200	0.349947	-2.724741
C	-3.704134	-0.027486	-1.940241
H	-3.652332	-1.112919	-2.073235
H	-3.682048	0.406278	-2.947506
H	-4.676803	0.214099	-1.496664
Cl	-2.675592	2.321573	-1.170959
Br	-3.062478	-1.782228	0.677936
C	0.298665	2.614426	2.426792
H	1.071108	3.283298	2.822621
H	0.070632	1.887540	3.212143
H	-0.586323	3.230488	2.239192
C	1.625949	-0.604649	2.311945
H	0.841437	-0.720066	3.068405
H	2.200881	0.282280	2.582980
H	2.310939	-1.453893	2.419304

C	0.362860	-1.958189	0.715479
H	-0.396989	-2.128062	1.481039
H	1.088250	-2.766662	0.862486
H	-0.074473	-2.112120	-0.269857

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4275830**
SCF Energy (B3LYP/6-31G) = -6413.49520893**

H	-0.437904	-2.258310	-0.541653
C	-1.635684	0.359516	-2.421536
H	-0.796948	0.402299	-3.125690
H	-2.051710	1.366672	-2.365441
H	-2.412791	-0.266071	-2.876038

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4398102**
SCF Energy (B3LYP/6-31G) = -6413.50324715**

3c_C001

MMFF Geometry

C	-2.264262	-0.204936	0.049141
C	-3.008448	1.161140	0.189625
H	-3.805029	1.223029	-0.561657
C	-2.113801	2.344569	-0.028709
H	-2.640864	3.196847	-0.436650
C	-0.631941	2.124747	-0.315828
C	-0.100826	0.637713	-0.298657
C	-0.210871	0.074197	1.155883
H	-0.121122	0.869371	1.902375
O	-1.545368	-0.467148	1.280185
Br	-3.623333	-1.604650	-0.161057
C	-1.179870	-0.229226	-1.065510
O	-3.635409	1.294433	1.468156
H	-2.971861	0.985423	2.116162
O	-1.113969	2.613590	0.950124
C	1.348839	0.576787	-0.843628
H	1.869666	1.499559	-0.563463
H	1.328254	0.586547	-1.941063
C	2.229420	-0.580857	-0.351734
H	1.928445	-1.518553	-0.826123
C	2.225356	-0.759708	1.177533
C	0.773289	-1.008588	1.607182
H	0.444933	-1.993938	1.260153
H	0.708509	-1.093779	2.701987
C	3.080315	-1.951027	1.637576
H	2.787007	-2.869242	1.116000
H	2.959633	-2.132943	2.712224
H	4.148644	-1.793054	1.458092
Cl	2.831970	0.712552	2.027603
Br	4.038983	-0.302861	-1.086203
C	0.059818	3.176685	-1.135150
H	-0.553950	4.079270	-1.231875
H	0.263853	2.815574	-2.147513
H	1.000956	3.481683	-0.667686
C	-0.689016	-1.656600	-1.413083
H	0.177882	-1.625499	-2.080171
H	-1.452785	-2.218865	-1.963488

3c_C002

MMFF Geometry

C	2.131867	-0.087453	-0.211954
C	2.530967	1.343024	-0.686717
H	3.464735	1.643432	-0.196015
C	1.511883	2.383529	-0.345914
H	1.954046	3.358937	-0.189876
C	0.226197	1.978688	0.366314
C	-0.000553	0.435997	0.639915
C	-0.147435	-0.314832	-0.727699
H	-0.568869	0.336739	-1.499111
O	1.191602	-0.642004	-1.164202
Br	3.754865	-1.193356	-0.257878
C	1.387932	-0.135351	1.155319
O	2.773131	1.387421	-2.095601
H	2.045106	0.875700	-2.500657
O	0.258073	2.350503	-1.023148
C	-1.233914	0.191636	1.555421
H	-1.480470	1.067987	2.160015
H	-1.002941	-0.559241	2.312277
C	-2.504693	-0.284781	0.829139
H	-3.298765	-0.427639	1.572762
C	-2.280133	-1.598875	0.050240
C	-0.990468	-1.594794	-0.793057
H	-0.371547	-2.468074	-0.559130
H	-1.223774	-1.758456	-1.855359
C	-2.221305	-2.777567	1.048600
H	-1.378076	-2.691293	1.738312
H	-2.111957	-3.737467	0.529068
H	-3.132956	-2.833104	1.655415
Cl	-3.694665	-1.996025	-1.015872
Br	-3.219352	1.179112	-0.271614
C	-0.355403	3.029250	1.269664
H	0.012138	4.029433	1.012416
H	-0.076094	2.844816	2.311516
H	-1.443942	3.072366	1.196495
C	1.300644	-1.579356	1.723175
H	0.659562	-1.639139	2.606489

H	2.280424	-1.929635	2.069162
H	0.954142	-2.312023	0.996621
C	2.038727	0.692926	2.283060
H	1.390864	0.710917	3.167033
H	2.248954	1.730784	2.019051
H	2.997425	0.256324	2.586153

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4279868**
SCF Energy (B3LYP/6-31G) = -6413.49059957**

3d_C001

MMFF Geometry

C	-2.346336	-0.123058	0.058722
C	-2.841412	1.218368	0.696430
H	-3.690016	1.603303	0.117857
C	-1.803738	2.305083	0.699081
H	-2.232842	3.293549	0.600484
C	-0.402808	2.004292	0.183419
C	-0.124791	0.530358	-0.272911
C	-0.217730	-0.410264	0.980199
H	-0.024901	0.115335	1.920078
O	-1.580660	-0.867720	1.044508
Br	-3.934691	-1.183034	-0.392783
C	-1.364522	0.058073	-1.131082
O	-3.308695	1.028011	2.034808
H	-2.703321	0.374729	2.436657
O	-0.691099	2.169732	1.582661
C	1.268514	0.386426	-0.935605
H	1.474058	1.222408	-1.611192
H	1.329427	-0.501828	-1.570393
C	2.337977	0.246430	0.153907
H	2.208862	1.054207	0.884596
C	2.241890	-1.125536	0.878935
C	0.762522	-1.584723	0.988732
H	0.506830	-2.270589	0.176627
H	0.603036	-2.183463	1.895659
C	2.870887	-1.028842	2.276994
H	3.928883	-0.749397	2.227530
H	2.807402	-1.983108	2.812855
H	2.357398	-0.277493	2.887424
Cl	3.107732	-2.449712	-0.006658
Br	4.098041	0.648117	-0.601337
C	0.364966	3.152021	-0.404304
H	-0.002581	4.114429	-0.030433
H	0.266692	3.169655	-1.493817
H	1.425488	3.093962	-0.143801
C	-1.121201	-1.270518	-1.898958
H	-0.296651	-1.185569	-2.612665
H	-1.993944	-1.543178	-2.504534
H	-0.929578	-2.120886	-1.244660
C	-1.814433	1.065068	-2.209703
H	-1.011740	1.229049	-2.937920
H	-2.101236	2.044568	-1.823069
H	-2.685042	0.688270	-2.758857

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4331146**
SCF Energy (B3LYP/6-31G) = -6413.49643845**

3d_C002

MMFF Geometry

C	2.0465810	-0.3021550	-0.2562290
C	3.0256220	0.9129000	-0.1709440
H	3.8975450	0.6346230	0.4335890
C	2.4267350	2.1214020	0.4829270
H	3.1612230	2.7059250	1.0215670
C	0.9679700	2.0897430	0.9243840
C	0.1273820	0.7911480	0.5735170
C	0.0404420	0.6481810	-0.9847990
H	0.1408740	1.6147010	-1.4857840
O	1.1833410	-0.1231130	-1.4038910
Br	3.1315020	-1.9075400	-0.5700880
C	1.0703890	-0.4334330	0.9463070
O	3.5223210	1.2877210	-1.4589870
H	2.7729210	1.1692850	-2.0751910
O	1.4159070	2.8476240	-0.2131710
C	-1.2752160	0.8537230	1.2695970
H	-1.4835170	1.9029100	1.5031310
H	-1.2240000	0.3699470	2.2524390
C	-2.5514900	0.4406220	0.5021700
H	-3.3930680	1.0114220	0.9176300
C	-2.4879500	0.6792370	-1.0165490
C	-1.2226030	0.0385000	-1.5853690
H	-1.2344700	-1.0480790	-1.4571630
H	-1.1803910	0.1751410	-2.6756020
C	-2.5322850	2.1928540	-1.3095290
H	-3.4818280	2.6313650	-0.9796250
H	-2.4285010	2.3928320	-2.3824830
H	-1.7378590	2.7437850	-0.7968420
Cl	-3.9193780	-0.0132390	-1.8800690
Br	-3.0735330	-1.3868000	1.0039320
C	0.6217020	2.9397900	2.1147370
H	1.4533880	3.5942400	2.3988180
H	0.3870860	2.3223160	2.9869650
H	-0.2308330	3.5902220	1.8954150

C	0.3320320	-1.7898650	0.9642940
H	-0.4043410	-1.8171430	1.7701980
H	1.0140990	-2.6192020	1.1844030
H	-0.1539370	-2.0332250	0.0204790
C	1.7440000	-0.3374830	2.3344530
H	0.9893600	-0.3065550	3.1285180
H	2.3852480	0.5350540	2.4697060
H	2.3790860	-1.2114310	2.5210620

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4256051**
SCF Energy (B3LYP/6-31G) = -6413.48986967**

H	0.987739	3.543810	-0.002346
C	-0.731433	-1.407442	-1.562911
H	0.106755	-1.259614	-2.250644
H	-1.520363	-1.869194	-2.168702
H	-0.445446	-2.148808	-0.819162
C	-1.709250	0.745740	-2.173269
H	-0.910175	0.870774	-2.913128
H	-2.072690	1.747229	-1.939011
H	-2.535911	0.224217	-2.669571

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4362366**
SCF Energy (B3LYP/6-31G) = -6413.50393842**

3e_C001

MMFF Geometry

C	-2.234927	-0.238988	0.195546
C	-2.981881	1.072443	0.612882
H	-3.380965	0.977524	1.629935
C	-2.093733	2.282361	0.555117
H	-2.631730	3.192804	0.323829
C	-0.625266	2.130113	0.172624
C	-0.091152	0.669085	-0.099207
C	-0.131442	-0.140310	1.236380
H	-0.012113	0.512374	2.106626
O	-1.455241	-0.711838	1.318829
Br	-3.592823	-1.620475	-0.165507
C	-1.203444	-0.062494	-0.955931
O	-4.090714	1.352402	-0.255885
H	-4.685861	0.581220	-0.199741
O	-1.056015	2.383810	1.524690
C	1.330610	0.719820	-0.714171
H	1.862313	1.585453	-0.302958
H	1.257062	0.919499	-1.791001
C	2.236592	-0.495696	-0.472752
H	1.915540	-1.340182	-1.088103
C	2.306196	-0.936858	1.000706
C	0.877191	-1.273003	1.447365
H	0.536610	-2.187368	0.950241
H	0.864761	-1.547113	2.512616
C	3.185539	-2.180477	1.206363
H	2.870503	-2.997352	0.547073
H	3.116524	-2.547638	2.237365
H	4.243696	-1.981882	1.007954
Cl	2.948909	0.371789	2.064969
Br	4.008633	-0.075590	-1.231176
C	0.027695	3.317443	-0.476056
H	-0.591168	4.217109	-0.384796
H	0.188077	3.143593	-1.544231

3e_C002

MMFF Geometry

C	-2.239946	-0.249709	0.184922
C	-2.995153	1.059886	0.594611
H	-3.405920	0.948214	1.605886
C	-2.108240	2.273488	0.549600
H	-2.641381	3.184742	0.311594
C	-0.637242	2.126753	0.174236
C	-0.096351	0.668410	-0.101035
C	-0.134722	-0.139940	1.232867
H	-0.011220	0.513194	2.102291
O	-1.458508	-0.706366	1.318663
Br	-3.570008	-1.658607	-0.165782
C	-1.202767	-0.067854	-0.961713
O	-4.087631	1.335877	-0.294574
H	-4.766352	1.799191	0.227095
O	-1.078427	2.374577	1.525490
C	1.326884	0.725477	-0.712226
H	1.855221	1.590875	-0.296257
H	1.255561	0.929024	-1.788472
C	2.235523	-0.488731	-0.472938
H	1.919161	-1.331837	-1.092432
C	2.302470	-0.935440	0.999032
C	0.872964	-1.273472	1.442852
H	0.533112	-2.186950	0.943891
H	0.859196	-1.549622	2.507572
C	3.182158	-2.179281	1.201529
H	2.868151	-2.994121	0.539239
H	3.112244	-2.549844	2.231249
H	4.240406	-1.979548	1.004774
Cl	2.943357	0.370054	2.069073
Br	4.008776	-0.060333	-1.224670
C	0.017438	3.318474	-0.464822
H	-0.603256	4.216746	-0.372340

H	0.183756	3.150304	-1.533003
H	0.974478	3.543904	0.015359
C	-0.723168	-1.409457	-1.570174
H	0.116358	-1.256729	-2.255171
H	-1.508186	-1.872683	-2.179998
H	-0.436569	-2.151558	-0.827536
C	-1.705917	0.739947	-2.180684
H	-0.906205	0.862016	-2.920404
H	-2.065931	1.743119	-1.948345
H	-2.533635	0.219549	-2.676418

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4332766**
SCF Energy (B3LYP/6-31G) = -6413.49652088**

H	0.083218	4.071197	0.680192
H	0.005412	2.974725	2.055101
H	-1.386392	3.160454	0.962480
C	1.273271	-1.520555	1.702689
H	0.651296	-1.519212	2.601506
H	2.254906	-1.868616	2.045968
H	0.897130	-2.286204	1.026509
C	2.065115	0.760855	2.120821
H	1.457448	0.802346	3.032323
H	2.245679	1.792944	1.816905
H	3.041519	0.344320	2.393920

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4246934**
SCF Energy (B3LYP/6-31G) = -6413.49165348**

3e_C003

MMFF Geometry

C	2.078942	-0.160343	-0.335563
C	2.505068	1.228226	-0.912724
H	2.630749	1.168720	-2.000556
C	1.514747	2.308804	-0.601672
H	1.973802	3.285554	-0.513364
C	0.238073	1.978541	0.162870
C	-0.015089	0.462300	0.541548
C	-0.219009	-0.365944	-0.770902
H	-0.646040	0.247247	-1.570205
O	1.098888	-0.752876	-1.218193
Br	3.661438	-1.337552	-0.385564
C	1.374335	-0.112118	1.053027
O	3.756745	1.669337	-0.362347
H	4.413862	0.985651	-0.592568
O	0.246958	2.262166	-1.249120
C	-1.225504	0.306172	1.505316
H	-1.434527	1.224586	2.059487
H	-0.987864	-0.400426	2.301869
C	-2.527593	-0.184665	0.847551
H	-3.301535	-0.262521	1.621429
C	-2.355006	-1.549260	0.146569
C	-1.093822	-1.625912	-0.735167
H	-0.488727	-2.500194	-0.470685
H	-1.365687	-1.843607	-1.778445
C	-2.288168	-2.664719	1.214610
H	-1.421676	-2.555087	1.871165
H	-2.215480	-3.657258	0.753232
H	-3.180701	-2.661885	1.851641
Cl	-3.811441	-1.981148	-0.847957
Br	-3.244867	1.223051	-0.322831
C	-0.297466	3.097837	1.010771

3f_C001

MMFF Geometry

C	-2.308960	-0.199625	0.199126
C	-2.818603	1.092586	0.932011
H	-3.105830	0.854913	1.963259
C	-1.795538	2.196640	0.957367
H	-2.235740	3.185386	0.925976
C	-0.403851	1.953503	0.390836
C	-0.112387	0.517037	-0.164992
C	-0.144765	-0.496143	1.030803
H	0.066668	-0.023659	1.994562
O	-1.493734	-0.986349	1.105549
Br	-3.880481	-1.303763	-0.242756
C	-1.370207	0.067501	-1.010333
O	-3.973928	1.648728	0.285014
H	-4.647172	0.942399	0.265514
O	-0.661614	2.028862	1.805634
C	1.260370	0.443763	-0.880230
H	1.425720	1.322739	-1.510810
H	1.317778	-0.403700	-1.568818
C	2.368755	0.263686	0.163447
H	2.248961	1.024838	0.944022
C	2.324030	-1.149263	0.810394
C	0.858956	-1.646996	0.937967
H	0.591707	-2.288289	0.093753
H	0.740919	-2.302577	1.811303
C	2.994496	-1.118304	2.192142
H	4.044354	-0.812606	2.126899
H	2.967799	-2.102777	2.673704
H	2.484961	-0.414828	2.860207
Cl	3.189148	-2.401483	-0.175303
Br	4.094491	0.745776	-0.623592

C	0.326106	3.150425	-0.145200
H	-0.046149	4.080475	0.299268
H	0.194788	3.234545	-1.228129
H	1.394822	3.096613	0.080144
C	-1.129477	-1.213425	-1.856964
H	-0.326080	-1.077784	-2.586708
H	-2.015500	-1.464298	-2.452765
H	-0.908378	-2.095994	-1.256690
C	-1.863638	1.121560	-2.022040
H	-1.099655	1.303656	-2.786914
H	-2.108617	2.091031	-1.585637
H	-2.768710	0.777061	-2.535396

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4299064**
SCF Energy (B3LYP/6-31G) = -6413.49788311**

3f_C002

MMFF Geometry

C	2.007119	-0.277178	-0.397782
C	2.975100	0.951533	-0.499344
H	3.261302	1.125341	-1.543579
C	2.377443	2.213461	0.053936
H	3.117128	2.870804	0.493802
C	0.939911	2.214617	0.559855
C	0.108962	0.872762	0.403409
C	-0.052321	0.556820	-1.121268
H	0.007319	1.461786	-1.731737
O	1.080257	-0.243565	-1.505405
Br	3.084912	-1.912485	-0.623616
C	1.092427	-0.291098	0.860135
O	4.186122	0.736795	0.243111
H	4.584343	-0.081637	-0.109361
O	1.328048	2.840894	-0.677781
C	-1.257315	0.991288	1.161815
H	-1.473685	2.056224	1.294029
H	-1.147343	0.615924	2.186311
C	-2.562617	0.481554	0.510304
H	-3.392611	1.083555	0.904476
C	-2.578868	0.554416	-1.026459
C	-1.332774	-0.130133	-1.586236
H	-1.319576	-1.196107	-1.339669
H	-1.347195	-0.113676	-2.685588
C	-2.663479	2.026496	-1.478775
H	-3.602753	2.487343	-1.149924
H	-2.616664	2.109598	-2.570971
H	-1.854040	2.639145	-1.070195
Cl	-4.039738	-0.244353	-1.735687
Br	-3.026561	-1.287286	1.231849
C	0.631786	3.193391	1.658415
H	1.460815	3.890881	1.822527
H	0.452768	2.679153	2.607480
H	-0.244435	3.799174	1.406889
C	0.383876	-1.649607	1.058610
H	-0.316257	-1.601494	1.895159
H	1.093379	-2.437656	1.336457
H	-0.138016	-2.002989	0.170306
C	1.819485	-0.035696	2.199681
H	1.099987	0.022872	3.024450
H	2.407822	0.882300	2.232673
H	2.513166	-0.853334	2.427836

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4224483**
SCF Energy (B3LYP/6-31G) = -6413.49143855**

3g_C001

MMFF Geometry

C	-2.270350	-0.245045	-0.005529
C	-3.094133	0.982082	0.500323
H	-3.895289	1.205218	-0.214633
C	-2.272586	2.229727	0.634006
H	-2.852516	3.129139	0.474130
C	-0.783115	2.186000	0.311126
C	-0.163025	0.786611	-0.075770
C	-0.236372	-0.165056	1.164081
H	-0.186700	0.395230	2.102977
O	-1.535752	-0.792530	1.118104
Br	-3.543057	-1.607665	-0.613552
C	-1.188725	0.104492	-1.067644
O	-3.723798	0.716557	1.756846
H	-3.059490	0.230341	2.284064
O	-1.281736	2.275938	1.658415
C	1.287785	0.968170	-0.590945
H	1.747452	1.808458	-0.058026
H	1.267072	1.277573	-1.643886
C	2.244146	-0.219782	-0.416870
H	2.009989	-1.007069	-1.138715
C	2.242158	-0.797456	1.009781
C	0.813800	-1.269078	1.309430
H	0.553181	-2.129204	0.684113
H	0.749690	-1.668732	2.332129
C	2.723407	0.178337	2.095271
H	2.630244	-0.268451	3.092521
H	2.141794	1.105250	2.105882
H	3.775366	0.453016	1.966000

Cl	3.302296	-2.263289	1.091166
Br	4.032408	0.381512	-0.996636
C	-0.165171	3.462894	-0.183684
H	-0.835801	4.317222	-0.038448
H	0.055422	3.404461	-1.253645
H	0.757446	3.688191	0.359749
C	-0.612093	-1.138515	-1.789618
H	0.255620	-0.874089	-2.401613
H	-1.338685	-1.565184	-2.491462
H	-0.331472	-1.946106	-1.116356
C	-1.683411	1.018241	-2.213615
H	-0.850509	1.305842	-2.865300
H	-2.161649	1.942705	-1.886003
H	-2.421068	0.497980	-2.835724

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4392561**
SCF Energy (B3LYP/6-31G) = -6413.50138883**

H	4.418014	1.982194	-0.788185
Cl	2.126307	3.026923	0.648724
Br	3.307707	-1.218341	-0.372710
C	0.512148	-2.873855	1.599521
H	0.131237	-3.899134	1.526269
H	0.308985	-2.530392	2.618501
H	1.592584	-2.934406	1.450639
C	-1.135047	1.776392	1.405322
H	-0.427667	1.984816	2.211621
H	-2.088884	2.183578	1.761728
H	-0.855263	2.372212	0.537801
C	-1.834078	-0.366673	2.383289
H	-1.138822	-0.234263	3.220250
H	-2.047001	-1.434668	2.310687
H	-2.778976	0.114823	2.660386

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4298965**
SCF Energy (B3LYP/6-31G) = -6413.49572098**

3g_C002

MMFF Geometry

C	-2.077297	-0.008091	-0.196966
C	-2.506705	-1.492415	-0.402508
H	-3.405517	-1.699494	0.190914
C	-1.464947	-2.472554	0.034135
H	-1.892870	-3.408299	0.369451
C	-0.138337	-1.970291	0.590625
C	0.101711	-0.404084	0.606204
C	0.168595	0.119304	-0.867122
H	0.554125	-0.651495	-1.541639
O	-1.193870	0.366460	-1.283625
Br	-3.699501	1.091818	-0.334572
C	-1.253918	0.257411	1.097490
O	-2.840756	-1.764218	-1.766906
H	-2.150896	-1.316608	-2.295715
O	-0.257615	-2.553217	-0.720018
C	1.382080	-0.034267	1.406514
H	1.685012	-0.824986	2.096796
H	1.177065	0.796212	2.084112
C	2.599507	0.362055	0.553794
H	3.426013	0.625091	1.226328
C	2.309570	1.534881	-0.399881
C	1.001111	1.366137	-1.193501
H	0.379693	2.268046	-1.149733
H	1.234513	1.302211	-2.267059
C	3.478511	1.869576	-1.341468
H	3.297044	2.805936	-1.883267
H	3.627709	1.095909	-2.101619

3h_C001

MMFF Geometry

C	-2.240910	-0.302831	0.156975
C	-3.068709	0.876225	0.770811
H	-3.472247	0.590581	1.749711
C	-2.253601	2.127728	0.933340
H	-2.844305	3.031090	0.849001
C	-0.777696	2.126925	0.551496
C	-0.153810	0.764742	0.052908
C	-0.156676	-0.256219	1.236274
H	-0.076911	0.249436	2.203661
O	-1.444618	-0.904361	1.204820
Br	-3.509524	-1.681767	-0.449437
C	-1.212021	0.120807	-0.931512
O	-4.182592	1.234384	-0.061513
H	-4.728474	0.430584	-0.152651
O	-1.226585	2.127452	1.920867
C	1.268613	1.002418	-0.515898
H	1.738699	1.820518	0.041714
H	1.194600	1.368911	-1.547888
C	2.251165	-0.174872	-0.451349
H	1.997655	-0.925439	-1.205047
C	2.322845	-0.830207	0.939461
C	0.917735	-1.345812	1.273624
H	0.644975	-2.174847	0.612531
H	0.905871	-1.802920	2.273951
C	2.834889	0.093494	2.055986
H	2.794392	-0.409614	3.029664

H	2.238042	1.006485	2.144163
H	3.874973	0.396052	1.896430
Cl	3.410923	-2.277353	0.892884
Br	4.001861	0.490702	-1.074431
C	-0.198523	3.441937	0.112289
H	-0.874344	4.274842	0.336434
H	-0.020519	3.452843	-0.967124
H	0.742026	3.648626	0.631899
C	-0.653681	-1.075498	-1.742074
H	0.186404	-0.769880	-2.373043
H	-1.405332	-1.470437	-2.436196
H	-0.339043	-1.915467	-1.125825
C	-1.755836	1.087775	-2.008544
H	-0.959672	1.379613	-2.703172
H	-2.181293	2.013796	-1.619356
H	-2.545318	0.608007	-2.598630

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4358017**
SCF Energy (B3LYP/6-31G) = -6413.50236023**

H	-3.449456	-2.884189	-1.606161
H	-3.762744	-1.190831	-1.945752
H	-4.514453	-1.957502	-0.537799
Cl	-2.184850	-2.928831	0.888874
Br	-3.341341	1.244356	-0.418554
C	-0.448796	2.999078	1.302169
H	-0.056773	4.008530	1.131918
H	-0.215494	2.737236	2.338792
H	-1.532720	3.065370	1.185045
C	1.121059	-1.690590	1.416283
H	0.435272	-1.829825	2.255465
H	2.080670	-2.083531	1.773486
H	0.807800	-2.344347	0.603586
C	1.875836	0.503026	2.216889
H	1.224056	0.400307	3.092338
H	2.054613	1.571012	2.083229
H	2.843579	0.056001	2.471749

SCF Energy (SMD/wB97XD/6-31+G) = -6413.4264635**
SCF Energy (B3LYP/6-31G) = -6413.49664987**

3h_C002

MMFF Geometry

C	2.029236	-0.045482	-0.344923
C	2.484966	1.410162	-0.683508
H	2.680610	1.509500	-1.758047
C	1.470040	2.437014	-0.284055
H	1.915332	3.391798	-0.033934
C	0.153718	2.004831	0.350146
C	-0.111124	0.449618	0.502080
C	-0.241956	-0.184784	-0.920435
H	-0.638312	0.538260	-1.640072
O	1.099503	-0.491179	-1.360009
Br	3.616272	-1.209480	-0.485737
C	1.250502	-0.199642	0.995133
O	3.696276	1.762049	0.004037
H	4.365991	1.105836	-0.266435
O	0.243607	2.479308	-1.007551
C	-1.365525	0.169063	1.375914
H	-1.628935	1.017565	2.011649
H	-1.147422	-0.608937	2.109599
C	-2.620743	-0.270631	0.603235
H	-3.424435	-0.465350	1.324875
C	-2.385934	-1.519295	-0.265439
C	-1.107347	-1.436317	-1.118789
H	-0.500155	-2.344637	-1.030634
H	-1.382116	-1.448670	-2.184373
C	-3.595623	-1.905308	-1.133203

1a_C001

B3LYP/6-31G* Geometry

C	-1.388911	-0.489523	-0.462962
C	-3.045760	1.457615	-0.138361
C	-0.173464	0.439045	0.059907
C	-2.656674	0.036680	0.240616
H	-3.464007	1.450533	-1.158694
H	-2.562842	-0.033538	1.323750
C	-1.833718	2.339488	-0.133982
H	-2.061453	3.401124	-0.210078
C	-0.557231	1.930483	-0.110038
O	-4.001494	2.005201	0.762057
H	-4.788106	1.435200	0.700205
Br	-4.288519	-1.107843	-0.096734
C	-1.200490	-1.983314	-0.107889
H	-1.906100	-2.585193	-0.686360
H	-1.398692	-2.193260	0.947125
H	-0.193596	-2.340695	-0.338469
C	-1.533081	-0.383084	-1.999148
H	-2.489476	-0.818590	-2.305289
H	-0.740462	-0.940959	-2.506180
H	-1.498072	0.651339	-2.352715
C	0.512347	2.996605	-0.248869
H	0.048722	3.983495	-0.334841
H	1.123113	2.847721	-1.148138
H	1.197424	3.035665	0.605343

C	0.105550	0.142423	1.572799
H	-0.656716	0.630217	2.188526
H	0.015796	-0.931609	1.745693
C	1.097360	0.071327	-0.779794
H	1.035305	0.525487	-1.772160
H	1.122156	-1.007871	-0.938520
C	1.484335	0.560481	2.099143
H	1.582673	1.652883	2.125008
H	1.592133	0.219387	3.134832
C	2.449366	0.455432	-0.170836
H	2.609245	1.532222	-0.193649
C	2.669840	0.015530	1.279873
Cl	2.649339	-1.832892	1.393338
C	4.006258	0.482961	1.852119
H	4.841370	0.073737	1.280697
H	4.102468	0.173244	2.896390
H	4.060004	1.578281	1.809357
Br	3.882460	-0.196561	-1.397852

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57273596**

C	0.099449	0.182208	1.565311
H	-0.662977	0.684238	2.170070
H	0.006503	-0.887095	1.763688
C	1.093067	0.054587	-0.783068
H	1.032593	0.486052	-1.785574
H	1.116124	-1.027613	-0.918061
C	1.477963	0.611211	2.084032
H	1.578601	1.703927	2.083242
H	1.583924	0.295021	3.127819
C	2.445225	0.450332	-0.181625
H	2.607552	1.526042	-0.229186
C	2.663281	0.044190	1.279511
Cl	2.638453	-1.800072	1.437642
C	3.999831	0.522880	1.842227
H	4.834668	0.098234	1.281814
H	4.094261	0.238102	2.893733
H	4.056064	1.616721	1.772991
Br	3.878670	-0.233571	-1.390024

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57038236**

Number of imaginary frequencies = 0

1a_C002

B3LYP/6-31G* Geometry

C	-1.397390	-0.492808	-0.454632
C	-3.058911	1.459533	-0.147364
C	-0.179423	0.442517	0.045929
C	-2.678421	0.033413	0.239914
H	-3.540657	1.445985	-1.131955
H	-2.569933	-0.035756	1.323938
C	-1.837207	2.332153	-0.208913
H	-2.062668	3.390038	-0.339016
C	-0.558624	1.928089	-0.165052
O	-4.051803	2.016454	0.710706
H	-3.641525	2.148784	1.581155
Br	-4.277528	-1.129229	-0.087470
C	-1.200679	-1.980107	-0.074500
H	-1.905530	-2.595069	-0.638731
H	-1.395589	-2.172909	0.984577
H	-0.192577	-2.336626	-0.300924
C	-1.546762	-0.414581	-1.992080
H	-2.499782	-0.865073	-2.285757
H	-0.750413	-0.973147	-2.492582
H	-1.524132	0.613727	-2.364173
C	0.510514	2.989103	-0.338736
H	0.047692	3.972774	-0.459673
H	1.122630	2.808787	-1.231056
H	1.194476	3.056127	0.514649

1a_C003

B3LYP/6-31G* Geometry

C	-1.388988	-0.489625	-0.462901
C	-3.045761	1.457627	-0.138478
C	-0.173508	0.438918	0.059865
C	-2.656790	0.036722	0.240599
H	-3.463896	1.450521	-1.158835
H	-2.562955	-0.033334	1.323737
C	-1.833678	2.339442	-0.134004
H	-2.061346	3.401090	-0.210132
C	-0.557206	1.930375	-0.110050
O	-4.001615	2.005302	0.761791
H	-4.788175	1.435206	0.700012
Br	-4.288704	-1.107786	-0.096604
C	-1.200760	-1.983365	-0.107576
H	-1.906508	-2.585192	-0.685915
H	-1.398938	-2.193096	0.947495
H	-0.193935	-2.340885	-0.338190
C	-1.533018	-0.383447	-1.999130
H	-2.489270	-0.819211	-2.305336
H	-0.740211	-0.941236	-2.505969
H	-1.498162	0.650924	-2.352873
C	0.512339	2.996455	-0.249274
H	0.048722	3.983321	-0.335514
H	1.123027	2.847307	-1.148532

H	1.197471	3.035754	0.604898
C	0.105541	0.142258	1.572700
H	-0.656864	0.629849	2.188420
H	0.015975	-0.931821	1.745395
C	1.097344	0.071172	-0.779813
H	1.035180	0.525233	-1.772221
H	1.122224	-1.008040	-0.938409
C	1.484249	0.560540	2.099067
H	1.582464	1.652944	2.124929
H	1.592012	0.219477	3.134771
C	2.449345	0.455400	-0.170938
H	2.609212	1.532196	-0.193920
C	2.669936	0.015802	1.279869
Cl	2.650060	-1.832602	1.393643
C	4.006192	0.483695	1.852114
H	4.841456	0.074741	1.280699
H	4.102478	0.174054	2.896387
H	4.059572	1.579037	1.809337
Br	3.882445	-0.196752	-1.397933

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57273352**

Number of imaginary frequencies = 0

H	-0.735748	-1.756334	-2.607589
H	-0.006637	-3.208026	-1.924611
C	-0.383276	-2.180612	0.626049
H	0.126235	-3.135042	0.458669
H	-0.428993	-2.047729	1.709385
C	-0.447073	0.262298	-0.098356
H	0.035107	1.003554	-0.734687
H	-0.559719	0.721297	0.884629
C	-1.835288	-2.326319	0.141158
H	-1.874848	-2.715811	-0.881284
H	-2.343849	-3.066405	0.769268
C	-1.857645	0.013771	-0.630546
H	-1.847155	-0.304887	-1.674104
C	-2.664371	-1.030630	0.147739
Cl	-2.873520	-0.489040	1.907687
C	-4.064376	-1.266177	-0.414697
H	-4.662503	-0.354460	-0.370944
H	-4.572628	-2.054605	0.147598
H	-3.989836	-1.581613	-1.463297
Br	-2.796151	1.771544	-0.741336

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56184490**

Number of imaginary frequencies = 0

1a_C004

B3LYP/6-31G* Geometry

C	1.692087	-0.725844	1.023661
C	3.280989	-0.249016	-0.992592
C	0.467237	-1.011360	0.024739
C	2.777045	0.184928	0.396361
H	3.577076	0.646986	-1.553386
H	3.625620	0.232879	1.079905
C	2.253756	-1.003109	-1.774108
H	2.596038	-1.302648	-2.762820
C	1.033705	-1.380329	-1.365199
O	4.417870	-1.120782	-0.871375
H	5.186663	-0.569447	-0.653180
Br	2.287152	2.140627	0.283197
C	2.427347	-2.063154	1.345115
H	3.342206	-1.860748	1.911776
H	2.714251	-2.613709	0.448029
H	1.797894	-2.703461	1.969365
C	1.268824	-0.122696	2.381913
H	2.140760	-0.098356	3.046521
H	0.500830	-0.721765	2.878202
H	0.904864	0.901896	2.296775
C	0.220359	-2.216531	-2.334205
H	0.780310	-2.368945	-3.261232

1a_C005

B3LYP/6-31G* Geometry

C	1.695576	-0.715301	1.022216
C	3.291375	-0.235992	-0.980594
C	0.472440	-1.004871	0.021856
C	2.783351	0.196824	0.398454
H	3.612579	0.654325	-1.536473
H	3.637636	0.242240	1.073064
C	2.259884	-0.979476	-1.773497
H	2.581486	-1.252603	-2.780370
C	1.040896	-1.367341	-1.369339
O	4.447124	-1.062132	-0.732207
H	4.674810	-1.504994	-1.565409
Br	2.286703	2.143322	0.275444
C	2.426351	-2.052923	1.351137
H	3.350152	-1.849856	1.901562
H	2.699243	-2.614273	0.456458
H	1.799719	-2.682811	1.988794
C	1.268099	-0.109285	2.377963
H	2.136647	-0.091134	3.046932
H	0.492938	-0.703077	2.869532
H	0.912098	0.917929	2.290648
C	0.228377	-2.197344	-2.344045

H	0.784902	-2.340196	-3.275030
H	-0.729772	-1.737799	-2.610178
H	0.005206	-3.192752	-1.941890
C	-0.373940	-2.179101	0.619466
H	0.139544	-3.131339	0.451363
H	-0.420256	-2.048090	1.702944
C	-0.448251	0.264792	-0.100974
H	0.030432	1.009132	-0.736282
H	-0.560113	0.721751	0.882987
C	-1.825414	-2.329774	0.134313
H	-1.864292	-2.716049	-0.889517
H	-2.330236	-3.074349	0.760120
C	-1.859224	0.012230	-0.630458
H	-1.850727	-0.302930	-1.675111
C	-2.660235	-1.037800	0.146179
Cl	-2.869021	-0.502566	1.907528
C	-4.060009	-1.277727	-0.415061
H	-4.661883	-0.368668	-0.367664
H	-4.564194	-2.069916	0.145636
H	-3.985850	-1.589659	-1.464758
Br	-2.804685	1.766516	-0.733825

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56066983**

Number of imaginary frequencies = 0

C	0.246285	-2.169732	-2.360575
H	0.807380	-2.305399	-3.289602
H	-0.709081	-1.704705	-2.627374
H	0.017440	-3.168067	-1.968606
C	-0.366179	-2.179581	0.602541
H	0.150704	-3.129447	0.429559
H	-0.417289	-2.056150	1.686826
C	-0.448511	0.269358	-0.101051
H	0.027123	1.018372	-0.732843
H	-0.561639	0.721230	0.885211
C	-1.815466	-2.333302	0.112266
H	-1.849554	-2.709136	-0.915539
H	-2.317796	-3.086687	0.729439
C	-1.858895	0.014747	-0.631888
H	-1.849150	-0.291683	-1.679114
C	-2.655635	-1.045131	0.135635
Cl	-2.866094	-0.526386	1.901779
C	-4.054422	-1.285711	-0.427695
H	-4.659316	-0.379072	-0.373186
H	-4.555986	-2.084020	0.126606
H	-3.979020	-1.588956	-1.479810
Br	-2.810424	1.765777	-0.719417

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56223535**

Number of imaginary frequencies = 0

1a_C006

B3LYP/6-31G* Geometry

C	1.692999	-0.709609	1.024698
C	3.310840	-0.235614	-0.968464
C	0.477065	-0.997056	0.015250
C	2.785536	0.202457	0.408912
H	3.655837	0.651178	-1.506206
H	3.632183	0.259605	1.092350
C	2.278623	-0.960326	-1.775284
H	2.617541	-1.236623	-2.772928
C	1.055856	-1.347923	-1.376013
O	4.496465	-1.036000	-0.833497
H	4.217457	-1.943774	-0.638077
Br	2.276066	2.148005	0.274117
C	2.413370	-2.054033	1.356502
H	3.382930	-1.863793	1.828289
H	2.576199	-2.675871	0.471023
H	1.821502	-2.642220	2.063306
C	1.260581	-0.110069	2.381563
H	2.120695	-0.114914	3.061895
H	0.466200	-0.691486	2.857028
H	0.927769	0.924958	2.296572

1a_C007

B3LYP/6-31G* Geometry

C	-1.39755	-0.37083	-0.48722
C	-3.06815	1.49576	0.11453
C	-0.19964	0.43678	0.21195
C	-2.69056	0.02796	0.25716
H	-3.42369	1.67583	-0.91324
H	-2.63548	-0.22069	1.31700
C	-1.86096	2.34730	0.37015
H	-2.08570	3.39889	0.53771
C	-0.58998	1.92417	0.38004
O	-4.07703	1.87825	1.04097
H	-4.85614	1.33284	0.83439
Br	-4.30677	-1.03419	-0.32767
C	-1.20685	-1.89889	-0.39622
H	-1.97817	-2.40056	-0.98575
H	-1.29998	-2.26672	0.63068
H	-0.23602	-2.21185	-0.79070
C	-1.50637	0.01126	-1.98336
H	-2.45006	-0.36603	-2.38954
H	-0.69637	-0.43743	-2.56490

H	-1.47399	1.09329	-2.13984
C	0.49750	2.95197	0.62552
H	0.06135	3.95183	0.70208
H	1.24291	2.97854	-0.17781
H	1.04138	2.76852	1.56184
C	0.14937	-0.10745	1.64753
H	0.49377	0.73105	2.26374
H	-0.75657	-0.46670	2.14562
C	1.08413	0.31145	-0.68232
H	1.09716	1.09945	-1.43760
H	1.08735	-0.63631	-1.22617
C	1.20710	-1.22761	1.70636
H	1.39354	-1.47993	2.75673
H	0.81339	-2.12997	1.24230
C	2.36679	0.36424	0.14437
H	2.36769	1.22692	0.80830
C	2.57198	-0.87289	1.03539
Cl	3.07540	-2.32523	-0.00146
C	3.68231	-0.65130	2.06109
H	4.61893	-0.37403	1.57159
H	3.84300	-1.55488	2.65499
H	3.38980	0.15984	2.74092
Br	3.92225	0.75360	-1.02876

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56514360**

Number of imaginary frequencies = 0

H	-0.696146	-0.437357	-2.564875
H	-1.474239	1.093193	-2.140056
C	0.497284	2.952222	0.625714
H	0.061078	3.952043	0.702413
H	1.242898	2.979043	-0.177413
H	1.040930	2.768571	1.562137
C	0.149270	-0.106855	1.647601
H	0.493581	0.731844	2.263602
H	-0.756707	-0.465957	2.145736
C	1.084214	0.311636	-0.682304
H	1.097258	1.099656	-1.437560
H	1.087379	-0.636098	-1.226191
C	1.207023	-1.226944	1.707006
H	1.393739	-1.478367	2.757545
H	0.813244	-2.129746	1.243836
C	2.366804	0.364301	0.144431
H	2.367882	1.227050	0.808263
C	2.571884	-0.872831	1.035435
Cl	3.074448	-2.325287	-0.001374
C	3.682538	-0.651577	2.060879
H	4.619209	-0.374862	1.571162
H	3.842912	-1.555136	2.654908
H	3.390598	0.159829	2.740626
Br	3.922362	0.753316	-1.028819

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56514369**

Number of imaginary frequencies = 0

1a_C008

B3LYP/6-31G* Geometry

C	-1.397426	-0.370731	-0.487218
C	-3.068191	1.495794	0.114221
C	-0.199649	0.437060	0.211892
C	-2.690460	0.028037	0.257076
H	-3.423812	1.675735	-0.913534
H	-2.635368	-0.220502	1.316944
C	-1.861064	2.347460	0.369674
H	-2.085861	3.399033	0.537247
C	-0.590072	1.924413	0.379729
O	-4.077084	1.878269	1.040733
H	-4.856067	1.332676	0.834100
Br	-4.306509	-1.034405	-0.327590
C	-1.206465	-1.898759	-0.396085
H	-1.977524	-2.400621	-0.985800
H	-1.299788	-2.266591	0.630790
H	-0.235463	-2.211544	-0.790279
C	-1.506303	0.011178	-1.983419
H	-2.449856	-0.366445	-2.389590

1a_C009

B3LYP/6-31G* Geometry

C	-1.405942	-0.368106	-0.487115
C	-3.080657	1.498240	0.118107
C	-0.205341	0.439250	0.205071
C	-2.712053	0.023089	0.251639
H	-3.496179	1.677443	-0.879988
H	-2.640477	-0.236123	1.310212
C	-1.860888	2.351764	0.324014
H	-2.080399	3.411248	0.450840
C	-0.589116	1.928759	0.353639
O	-4.130269	1.884811	1.000811
H	-3.781464	1.836818	1.906218
Br	-4.296929	-1.051955	-0.333919
C	-1.208787	-1.895610	-0.392326
H	-1.979056	-2.401557	-0.978315
H	-1.300526	-2.260873	0.635842
H	-0.236501	-2.205771	-0.785509
C	-1.518126	0.008114	-1.984503

H	-2.456864	-0.383268	-2.388164
H	-0.702337	-0.431609	-2.564898
H	-1.500233	1.089983	-2.145007
C	0.498429	2.959500	0.585563
H	0.063826	3.961506	0.641953
H	1.247591	2.970319	-0.214388
H	1.038228	2.791013	1.527145
C	0.142664	-0.092307	1.645799
H	0.488730	0.750804	2.255461
H	-0.763818	-0.448909	2.145476
C	1.079701	0.303626	-0.686477
H	1.094025	1.083521	-1.450030
H	1.081541	-0.649360	-1.220763
C	1.198663	-1.213625	1.714463
H	1.382666	-1.459939	2.766711
H	0.803344	-2.117479	1.254892
C	2.361719	0.363446	0.140887
H	2.362590	1.231950	0.797285
C	2.565133	-0.865482	1.043616
Cl	3.070821	-2.327129	0.022441
C	3.673053	-0.634059	2.069873
H	4.610740	-0.361597	1.579712
H	3.832570	-1.531966	2.672630
H	3.379426	0.183655	2.741386
Br	3.918644	0.741764	-1.033515

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56270109**

Number of imaginary frequencies = 0

C	-1.683303	-1.352531	-1.521267
H	-2.663552	-1.837379	-1.566131
H	-0.926844	-2.123111	-1.696866
H	-1.622470	-0.626979	-2.337216
C	0.556791	2.294098	-1.742631
H	0.131972	3.116451	-2.325328
H	1.120869	1.662138	-2.440019
H	1.281235	2.731301	-1.047648
C	0.073303	0.809554	1.305842
H	-0.658352	1.572727	1.588653
H	-0.056784	-0.019029	2.006845
C	1.010549	-0.496309	-0.672391
H	0.947537	-0.619043	-1.756802
H	0.982911	-1.506159	-0.258492
C	1.476642	1.396381	1.528348
H	1.602783	2.327572	0.969667
H	1.596545	1.654191	2.586508
C	2.399457	0.081102	-0.349979
H	2.617046	0.966761	-0.939153
C	2.600213	0.417041	1.133348
Cl	4.192494	1.345106	1.304940
C	2.688777	-0.792516	2.062504
H	1.773573	-1.391759	2.007981
H	2.820768	-0.461671	3.096316
H	3.528996	-1.430571	1.783888
Br	3.752591	-1.222507	-1.027690

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57108247**

Number of imaginary frequencies = 0

1b_C001

B3LYP/6-31G* Geometry

C	-1.493869	-0.697545	-0.133140
C	-3.055547	1.246655	-0.789307
C	-0.226972	0.306420	-0.146719
C	-2.714409	0.172216	0.233774
H	-3.524888	0.764776	-1.663211
H	-2.586948	0.634962	1.211705
C	-1.808563	1.937350	-1.254293
H	-1.995892	2.822858	-1.858715
C	-0.550040	1.522124	-1.051617
O	-3.939752	2.224672	-0.255510
H	-4.759759	1.753352	-0.026200
Br	-4.404611	-0.900498	0.512450
C	-1.359517	-1.833703	0.906924
H	-2.144635	-2.574340	0.735966
H	-1.477715	-1.483201	1.936535
H	-0.401148	-2.354885	0.828822

1b_C002

B3LYP/6-31G* Geometry

C	-1.493590	-0.697184	-0.133813
C	-3.055946	1.246684	-0.788967
C	-0.226956	0.307047	-0.146973
C	-2.714353	0.172046	0.233700
H	-3.525145	0.764914	-1.662981
H	-2.586737	0.634591	1.211713
C	-1.809152	1.938019	-1.253628
H	-1.996718	2.823921	-1.857391
C	-0.550483	1.523166	-1.051109
O	-3.940526	2.224178	-0.254703
H	-4.760097	1.752348	-0.024845
Br	-4.404158	-0.901254	0.512516
C	-1.358697	-1.833944	0.905565
H	-2.143409	-2.574895	0.734125
H	-1.477102	-1.484169	1.935400

H	-0.400050	-2.354572	0.827161
C	-1.682971	-1.351446	-1.522299
H	-2.662975	-1.836784	-1.567213
H	-0.926161	-2.121548	-1.698473
H	-1.622668	-0.625415	-2.337866
C	0.556162	2.296337	-1.741054
H	0.131143	3.119044	-2.323099
H	1.120783	1.665335	-2.438868
H	1.280115	2.733238	-1.045365
C	0.073190	0.809429	1.305866
H	-0.658191	1.572858	1.588710
H	-0.057626	-0.019331	2.006518
C	1.010683	-0.495107	-0.673379
H	0.947739	-0.616469	-1.757946
H	0.982887	-1.505492	-0.260795
C	1.476709	1.395487	1.529190
H	1.603479	2.327114	0.971362
H	1.596343	1.652350	2.587615
C	2.399645	0.081652	-0.350016
H	2.617648	0.967842	-0.938240
C	2.600085	0.416130	1.133710
Cl	4.192507	1.343531	1.306769
C	2.687878	-0.794327	2.061786
H	1.772482	-1.393188	2.006364
H	2.819569	-0.464471	3.095945
H	3.528036	-1.432382	1.782934
Br	3.752587	-1.221667	-1.028621

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57108013**

Number of imaginary frequencies = 0

H	-1.473839	-1.473259	1.940219
H	-0.405459	-2.349565	0.828080
C	-1.697163	-1.353885	-1.516932
H	-2.674484	-1.844711	-1.552041
H	-0.936979	-2.120148	-1.695666
H	-1.647400	-0.631212	-2.336234
C	0.555478	2.269578	-1.775325
H	0.130736	3.081303	-2.372909
H	1.119585	1.625385	-2.461101
H	1.280261	2.718290	-1.087825
C	0.068841	0.819064	1.295729
H	-0.663920	1.582764	1.575745
H	-0.060489	-0.004047	2.003038
C	1.005303	-0.504146	-0.668623
H	0.942642	-0.638088	-1.751680
H	0.976094	-1.509629	-0.244997
C	1.471129	1.410461	1.512086
H	1.596830	2.334811	0.941683
H	1.591113	1.680803	2.567130
C	2.394977	0.074745	-0.351337
H	2.614660	0.953656	-0.949829
C	2.594973	0.427043	1.128371
Cl	4.186190	1.358348	1.290941
C	2.683298	-0.772025	2.071050
H	1.769137	-1.373279	2.021710
H	2.813625	-0.429830	3.101377
H	3.524656	-1.411982	1.800470
Br	3.746893	-1.237693	-1.012428

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56883166**

Number of imaginary frequencies = 0

1b_C003

B3LYP/6-31G* Geometry

C	-1.503218	-0.693285	-0.131945
C	-3.066249	1.259223	-0.780264
C	-0.232992	0.304255	-0.152093
C	-2.736631	0.169213	0.237277
H	-3.596918	0.806904	-1.626229
H	-2.596870	0.618400	1.222075
C	-1.811591	1.914440	-1.285230
H	-1.996965	2.779547	-1.920776
C	-0.550626	1.508793	-1.071305
O	-3.989401	2.219843	-0.273450
H	-3.524063	2.743905	0.399086
Br	-4.397121	-0.918403	0.514089
C	-1.362727	-1.827082	0.910750
H	-2.150778	-2.565671	0.748883

1b_C004

B3LYP/6-31G* Geometry

C	-1.473117	-0.379676	-0.565170
C	-3.034228	1.487438	0.275032
C	-0.207859	0.320795	0.137850
C	-2.710162	0.000327	0.278552
H	-3.431762	1.764547	-0.715135
H	-2.612609	-0.338103	1.309886
C	-1.781966	2.268940	0.534578
H	-1.956129	3.309847	0.799940
C	-0.529316	1.803116	0.440621
O	-3.980143	1.828135	1.280207
H	-4.790836	1.332601	1.069774
Br	-4.396699	-0.949459	-0.303903
C	-1.347281	-1.916252	-0.618820

H	-2.185396	-2.333386	-1.182245
H	-1.370291	-2.372955	0.375696
H	-0.429486	-2.229613	-1.124834
C	-1.640173	0.135084	-2.015240
H	-2.621605	-0.161106	-2.398696
H	-0.884795	-0.297770	-2.677106
H	-1.560530	1.223873	-2.081913
C	0.604945	2.772918	0.706975
H	0.206276	3.767632	0.924518
H	1.281896	2.872796	-0.150101
H	1.216178	2.475968	1.568851
C	0.184541	-0.360192	1.500505
H	0.583040	0.400405	2.181203
H	-0.706439	-0.751687	2.000501
C	1.024888	0.205572	-0.827680
H	1.012511	1.020596	-1.554233
H	0.967438	-0.718548	-1.410331
C	1.222964	-1.482265	1.372127
H	1.396953	-1.946428	2.347192
H	0.839764	-2.271902	0.720184
C	2.367458	0.218581	-0.088343
H	2.453209	1.099342	0.536405
C	2.587448	-1.035159	0.787203
Cl	3.686523	-0.516770	2.195840
C	3.272646	-2.213554	0.098522
H	2.709393	-2.492853	-0.800440
H	3.294951	-3.074246	0.773545
H	4.291783	-1.966484	-0.199573
Br	3.831614	0.517842	-1.409934

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56649738**

Number of imaginary frequencies = 0

C	2.497461	-2.079845	1.387279
H	3.460716	-1.894629	1.874063
H	2.690484	-2.683041	0.499203
H	1.890309	-2.661796	2.086506
C	1.513235	-0.040711	2.410198
H	2.446945	0.016420	2.982121
H	0.804339	-0.610430	3.018122
H	1.143880	0.980500	2.305528
C	0.017029	-2.341648	-2.085253
H	0.505454	-2.582180	-3.033824
H	-0.936245	-1.858442	-2.324754
H	-0.221601	-3.291101	-1.591632
C	-0.380032	-2.076321	0.900510
H	0.064277	-3.068007	0.767286
H	-0.337874	-1.876426	1.974888
C	-0.367166	0.310931	0.024979
H	0.110635	0.990551	-0.679814
H	-0.386592	0.836081	0.981720
C	-1.867361	-2.174060	0.505955
H	-1.980880	-2.618697	-0.483659
H	-2.373476	-2.849763	1.205101
C	-1.823409	0.114952	-0.415081
H	-1.895478	-0.249110	-1.438006
C	-2.605166	-0.821628	0.513095
Cl	-4.273152	-1.132896	-0.229745
C	-2.841955	-0.278167	1.921575
H	-1.889935	-0.104497	2.434726
H	-3.419600	-0.999019	2.506437
H	-3.385750	0.667603	1.885017
Br	-2.657767	1.924144	-0.542178

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56027172**

Number of imaginary frequencies = 0

1b_C005

B3LYP/6-31G* Geometry

C	1.798314	-0.726368	1.054578
C	3.237867	-0.416198	-1.101447
C	0.487623	-1.000267	0.166862
C	2.868631	0.102417	0.301422
H	3.513653	0.440217	-1.730382
H	3.772317	0.135100	0.910855
C	2.126981	-1.173124	-1.755520
H	2.381677	-1.544105	-2.746166
C	0.930109	-1.480133	-1.234786
O	4.352927	-1.320574	-1.027181
H	5.155879	-0.786679	-0.914193
Br	2.462169	2.073465	0.144114

1b_C006

B3LYP/6-31G* Geometry

C	1.802583	-0.714308	1.053308
C	3.249886	-0.405624	-1.090281
C	0.492962	-0.993090	0.165035
C	2.876194	0.114341	0.302007
H	3.554171	0.442721	-1.716933
H	3.784566	0.145306	0.902583
C	2.133127	-1.150748	-1.755658
H	2.365973	-1.496547	-2.764351
C	0.936769	-1.467985	-1.238330
O	4.392868	-1.262408	-0.891877
H	4.538668	-1.752072	-1.717260

Br	2.461911	2.075667	0.131858
C	2.497153	-2.067536	1.395283
H	3.468465	-1.882970	1.864575
H	2.675283	-2.681943	0.511866
H	1.894294	-2.637268	2.108281
C	1.513941	-0.023395	2.405572
H	2.444870	0.027869	2.982329
H	0.796955	-0.586321	3.010436
H	1.153241	1.000384	2.296135
C	0.024058	-2.324704	-2.093676
H	-0.209636	-3.278935	-1.606903
H	0.508161	-2.555517	-3.047222
H	-0.931700	-1.842905	-2.324594
C	-0.370540	-2.074013	0.896454
H	0.078202	-3.063725	0.763060
H	-0.328950	-1.874697	1.970884
C	-0.368483	0.314189	0.023408
H	0.106251	0.996931	-0.680403
H	-0.387884	0.837749	0.980928
C	-1.857451	-2.177829	0.502127
H	-1.970070	-2.621223	-0.488241
H	-2.360069	-2.857247	1.200184
C	-1.824896	0.113602	-0.414182
H	-1.898280	-0.247448	-1.438071
C	-2.601541	-0.828750	0.512520
Cl	-4.268373	-1.146301	-0.230092
C	-2.839692	-0.289552	1.922355
H	-1.888079	-0.111838	2.434843
H	-3.412911	-1.014628	2.506355
H	-3.388538	0.653375	1.888353
Br	-2.666426	1.919754	-0.534884

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55919170**

Number of imaginary frequencies = 0

H	4.138333	-2.135256	-0.755344
Br	2.452049	2.080781	0.127198
C	2.485465	-2.066176	1.405282
H	3.495776	-1.900599	1.793338
H	2.553284	-2.736979	0.543986
H	1.923971	-2.590891	2.183531
C	1.510146	-0.018826	2.409864
H	2.435223	0.014598	2.997699
H	0.775211	-0.570113	3.003932
H	1.169802	1.011412	2.297608
C	0.039707	-2.307040	-2.104469
H	0.527719	-2.533831	-3.056707
H	-0.914115	-1.822218	-2.337212
H	-0.198643	-3.262999	-1.623107
C	-0.363828	-2.073031	0.887428
H	0.088573	-3.061262	0.753602
H	-0.327210	-1.875697	1.962531
C	-0.368443	0.318444	0.024617
H	0.103772	1.005053	-0.676828
H	-0.389476	0.838662	0.984054
C	-1.848975	-2.182266	0.488732
H	-1.956787	-2.619843	-0.504676
H	-2.349762	-2.868394	1.181485
C	-1.824342	0.114410	-0.414216
H	-1.895431	-0.240928	-1.440249
C	-2.598653	-0.836413	0.505956
Cl	-4.262404	-1.156833	-0.240654
C	-2.841122	-0.306267	1.918538
H	-3.395151	0.633733	1.888868
H	-1.891158	-0.125550	2.433101
H	-3.411003	-1.037494	2.498135
Br	-2.671556	1.917842	-0.524102

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55919170**

Number of imaginary frequencies = 0

1b_C007

B3LYP/6-31G* Geometry

C	1.801958	-0.707087	1.057070
C	3.268130	-0.407341	-1.082290
C	0.497551	-0.986047	0.161517
C	2.879885	0.120094	0.309796
H	3.595559	0.437050	-1.694379
H	3.783236	0.164328	0.917187
C	2.149199	-1.136299	-1.758834
H	2.397809	-1.486882	-2.759512
C	0.950080	-1.453571	-1.242794
O	4.432940	-1.244633	-1.000682

1b_C008

B3LYP/6-31G* Geometry

C	-1.480937	-0.388517	-0.556237
C	-3.045505	1.495589	0.251376
C	-0.213364	0.327461	0.123628
C	-2.731091	0.002293	0.274609
H	-3.503478	1.751987	-0.710755
H	-2.618033	-0.327073	1.309538
C	-1.783151	2.287461	0.442345
H	-1.953352	3.344046	0.645528
C	-0.528765	1.819023	0.374177

O	-4.032694	1.863151	1.210362
H	-3.637350	1.754849	2.091174
Br	-4.388021	-0.970891	-0.291843
C	-1.348816	-1.925911	-0.573077
H	-2.186896	-2.359082	-1.122950
H	-1.369545	-2.357645	0.432717
H	-0.430037	-2.248212	-1.071749
C	-1.652419	0.089196	-2.018593
H	-2.628624	-0.231769	-2.394798
H	-0.889515	-0.347514	-2.669330
H	-1.590071	1.177230	-2.112309
C	0.605488	2.798119	0.603147
H	0.207802	3.801702	0.778122
H	1.284860	2.861593	-0.255275
H	1.214537	2.535006	1.477618
C	0.177226	-0.310378	1.507969
H	0.577365	0.470425	2.165106
H	-0.714762	-0.687342	2.017870
C	1.021080	0.179535	-0.835896
H	1.011237	0.971025	-1.587952
H	0.961802	-0.761856	-1.389524
C	1.213718	-1.437953	1.416340
H	1.385822	-1.871623	2.405670
H	0.828437	-2.246147	0.789178
C	2.362843	0.213336	-0.095592
H	2.449258	1.112581	0.502172
C	2.579306	-1.012523	0.819000
Cl	3.677749	-0.451363	2.212486
C	3.262757	-2.213446	0.168634
H	2.698930	-2.520152	-0.720955
H	3.283388	-3.052177	0.870810
H	4.282311	-1.977763	-0.137019
Br	3.829322	0.469067	-1.422986

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56424409**

Number of imaginary frequencies = 0

C	-0.529259	1.803059	0.440544
O	-3.980217	1.828392	1.279874
H	-4.790475	1.331835	1.070088
Br	-4.396754	-0.949426	-0.303742
C	-1.347623	-1.916306	-0.618795
H	-2.185744	-2.333313	-1.182314
H	-1.370814	-2.373023	0.375716
H	-0.429844	-2.229786	-1.124742
C	-1.640380	0.134905	-2.015326
H	-2.621942	-0.161145	-2.398573
H	-0.885204	-0.298232	-2.677237
H	-1.560503	1.223669	-2.082159
C	0.604936	2.772882	0.707056
H	0.206217	3.767585	0.924529
H	1.281968	2.872767	-0.149934
H	1.216062	2.475965	1.569037
C	0.184520	-0.360357	1.500334
H	0.582866	0.400257	2.181085
H	-0.706487	-0.751978	2.000203
C	1.024944	0.205524	-0.827778
H	1.012516	1.020480	-1.554409
H	0.967575	-0.718647	-1.410361
C	1.223030	-1.482335	1.371862
H	1.396880	-1.946721	2.346850
H	0.839972	-2.271857	0.719686
C	2.367559	0.218588	-0.088429
H	2.453322	1.099321	0.536345
C	2.587543	-1.035095	0.787164
Cl	3.686258	-0.516530	2.196157
C	3.273137	-2.213349	0.098710
H	2.710118	-2.492931	-0.800321
H	3.295601	-3.073957	0.773812
H	4.292244	-1.965963	-0.199252
Br	3.831755	0.517730	-1.409965

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56649475**

Number of imaginary frequencies = 0

1b_C009

B3LYP/6-31G* Geometry

C	-1.473226	-0.379702	-0.565208
C	-3.034169	1.487489	0.274789
C	-0.207849	0.320724	0.137735
C	-2.710210	0.000395	0.278557
H	-3.431654	1.764563	-0.715368
H	-2.612600	-0.337783	1.309969
C	-1.781910	2.268950	0.534413
H	-1.956017	3.309893	0.799665

1c_C001

B3LYP/6-31G* Geometry

C	-1.594844	0.322458	0.828035
C	-2.744900	0.523045	-1.503201
C	-0.197399	0.813552	0.179007
C	-2.376230	-0.367722	-0.309972
H	-2.943492	-0.141512	-2.360785
H	-1.817362	-1.231102	-0.671389
C	-1.599470	1.434574	-1.832881

H	-1.758231	2.030101	-2.729679
C	-0.492009	1.628701	-1.103466
O	-3.872283	1.365789	-1.291353
H	-4.611850	0.783425	-1.041003
Br	-4.076136	-1.250976	0.323927
C	-2.380108	1.524707	1.400608
H	-3.392681	1.201697	1.658777
H	-2.470036	2.345764	0.687844
H	-1.907142	1.895074	2.315540
C	-1.394956	-0.695349	1.977358
H	-2.336823	-0.821139	2.516686
H	-0.650448	-0.357587	2.704053
H	-1.100117	-1.688133	1.623637
C	0.476366	2.687913	-1.592562
H	0.621574	3.481520	-0.850226
H	0.087894	3.158848	-2.499886
H	1.468514	2.290295	-1.832552
C	0.570961	1.658893	1.243843
H	0.127417	2.657427	1.312690
H	0.419008	1.202723	2.225370
C	0.672348	-0.439522	-0.196068
H	0.282384	-0.906631	-1.103658
H	0.599941	-1.188517	0.595199
C	2.090815	1.825745	1.037726
H	2.301588	2.499695	0.206645
H	2.518856	2.296112	1.930325
C	2.163976	-0.167950	-0.424887
H	2.335912	0.436180	-1.313767
C	2.835357	0.499320	0.782980
Cl	4.566932	0.952449	0.313052
C	2.928725	-0.378795	2.030082
H	3.476933	-1.298191	1.816565
H	1.929780	-0.649965	2.388142
H	3.441208	0.163852	2.828880
Br	3.018016	-1.906032	-0.909586

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56649475**

Number of imaginary frequencies = 0

C	-1.599888	1.446607	-1.821586
H	-1.730608	2.035054	-2.731203
C	-0.493846	1.639680	-1.088264
O	-3.909790	1.346291	-1.155065
H	-4.077243	1.938968	-1.904760
Br	-4.060007	-1.281095	0.311197
C	-2.377788	1.503652	1.430294
H	-3.400837	1.188831	1.652754
H	-2.439897	2.353541	0.748460
H	-1.914836	1.831995	2.366383
C	-1.395665	-0.729798	1.952473
H	-2.331411	-0.857295	2.500916
H	-0.636937	-0.412263	2.673832
H	-1.117349	-1.718606	1.575457
C	0.477971	2.699336	-1.568596
H	0.097690	3.174304	-2.477694
H	1.471493	2.302034	-1.801945
H	0.618759	3.489845	-0.821940
C	0.563607	1.644685	1.261702
H	0.119237	2.641976	1.343297
H	0.410017	1.176320	2.237099
C	0.668168	-0.435121	-0.204492
H	0.279016	-0.891851	-1.117632
H	0.594010	-1.193174	0.577591
C	2.083826	1.814689	1.060586
H	2.296768	2.499629	0.238940
H	2.510141	2.273334	1.960101
C	2.160237	-0.160859	-0.427017
H	2.335423	0.453361	-1.308314
C	2.829217	0.491758	0.790165
Cl	4.561646	0.951924	0.328467
C	2.920994	-0.401748	2.026428
H	1.921568	-0.679164	2.378182
H	3.430376	0.131774	2.833327
H	3.471378	-1.317443	1.802864
Br	3.015824	-1.892834	-0.931334

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56215039**

Number of imaginary frequencies = 0

1c_C002

B3LYP/6-31G* Geometry

C	-1.600893	0.311661	0.825148
C	-2.763633	0.554248	-1.486704
C	-0.204084	0.811855	0.186547
C	-2.401014	-0.358652	-0.319690
H	-3.008734	-0.084184	-2.350074
H	-1.824560	-1.194457	-0.716215

1c_C003

B3LYP/6-31G* Geometry

C	1.463506	-0.806682	-1.006320
C	3.252749	-1.340493	0.756142
C	0.411020	-0.305369	0.104512
C	2.937658	-0.633893	-0.565413
H	3.326269	-2.410898	0.513020

H	3.600150	-0.994183	-1.353469
C	2.141462	-1.166709	1.751528
H	2.411955	-1.473272	2.760755
C	0.880374	-0.781319	1.500363
O	4.530033	-1.040436	1.288533
H	4.570655	-0.072939	1.391180
Br	3.549636	1.286332	-0.430924
C	1.288386	-0.141050	-2.389288
H	1.899013	-0.677289	-3.125276
H	1.616423	0.899980	-2.398080
H	0.253153	-0.185289	-2.741403
C	1.302377	-2.342837	-1.231672
H	2.152527	-2.734438	-1.801714
H	0.403502	-2.556543	-1.815536
H	1.235566	-2.899569	-0.293371
C	-0.099166	-0.838852	2.657083
H	0.419471	-1.136874	3.572809
H	-0.889937	-1.579319	2.481659
H	-0.592975	0.116207	2.859527
C	0.273065	1.259132	0.092906
H	1.117049	1.700763	0.623906
H	0.355220	1.610024	-0.938010
C	-0.982969	-0.928184	-0.270755
H	-1.015396	-1.981736	0.018344
H	-1.094448	-0.913030	-1.357738
C	-1.022254	1.849157	0.677611
H	-1.065391	1.716400	1.761499
H	-1.023709	2.931366	0.504618
C	-2.238065	-0.256607	0.310388
H	-2.339311	-0.434663	1.377056
C	-2.298457	1.252819	0.056341
Cl	-3.727472	1.946902	1.006617
C	-2.498971	1.653663	-1.403997
H	-1.673909	1.285097	-2.022918
H	-2.531353	2.742997	-1.491870
H	-3.430003	1.237582	-1.793366
Br	-3.819409	-1.223500	-0.437332

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56431906**

Number of imaginary frequencies = 0

1c_C004

B3LYP/6-31G* Geometry

C	1.469915	-0.783920	-1.015175
C	3.247004	-1.345087	0.727055
C	0.413326	-0.300434	0.099873
C	2.946475	-0.601697	-0.568196
H	3.291590	-2.414269	0.448464
H	3.604251	-0.962395	-1.360268
C	2.143909	-1.180528	1.732112
H	2.402344	-1.500602	2.742616
C	0.882125	-0.794991	1.489022
O	4.526133	-0.962968	1.218590
H	4.708907	-1.506315	2.001308
Br	3.542427	1.303176	-0.417153
C	1.294970	-0.095957	-2.386939
H	1.903675	-0.622536	-3.131626
H	1.628244	0.942970	-2.377578
H	0.259151	-0.132851	-2.738611
C	1.305575	-2.314557	-1.268470
H	2.160383	-2.697563	-1.837419
H	0.411860	-2.516641	-1.864599
H	1.227965	-2.889708	-0.341852
C	-0.095692	-0.868620	2.645983
H	0.422381	-1.179917	3.557892
H	-0.887957	-1.604933	2.460495
H	-0.587210	0.084381	2.862146
C	0.270056	1.263402	0.111050
H	1.114199	1.700447	0.645341
H	0.350534	1.627847	-0.915093
C	-0.978744	-0.921943	-0.284628
H	-1.008628	-1.980277	-0.013045
H	-1.089375	-0.889273	-1.371220
C	-1.027081	1.840471	0.704547
H	-1.069823	1.693325	1.786626
H	-1.032005	2.924956	0.546484
C	-2.236154	-0.263463	0.306203
H	-2.337964	-0.458061	1.369942
C	-2.301878	1.249317	0.075388
Cl	-3.733670	1.922923	1.037616
C	-2.505105	1.672466	-1.378214
H	-1.679238	1.316659	-2.003446
H	-2.540733	2.762966	-1.448440
H	-3.435329	1.260009	-1.773320
Br	-3.814602	-1.225202	-0.456294

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55911313**

Number of imaginary frequencies = 0

1c_C005

B3LYP/6-31G* Geometry

C	1.583896	0.610786	-0.714176
C	2.621163	-0.007433	1.596962
C	0.169997	0.849137	0.019729

C	2.309491	-0.442780	0.150806
H	2.726444	-0.925797	2.198951
H	1.733250	-1.367006	0.173257
C	1.505514	0.836762	2.150396
H	1.664718	1.144676	3.181825
C	0.446612	1.301583	1.474278
O	3.797507	0.781905	1.737573
H	4.527741	0.269953	1.346437
Br	4.030839	-1.100286	-0.669227
C	2.409490	1.916524	-0.795608
H	3.420495	1.677360	-1.138433
H	2.501195	2.420024	0.166956
H	1.975605	2.612189	-1.520797
C	1.415454	0.092232	-2.157957
H	2.398706	-0.037526	-2.616428
H	0.865379	0.812069	-2.770313
H	0.906608	-0.875469	-2.218084
C	-0.482780	2.268098	2.179333
H	-0.229105	2.328029	3.241528
H	-1.541564	1.996058	2.105700
H	-0.391938	3.280626	1.765073
C	-0.699903	1.884324	-0.771493
H	-1.241158	2.531794	-0.077783
H	-0.063865	2.552825	-1.356821
C	-0.650343	-0.498655	0.101625
H	-0.303626	-1.095775	0.946027
H	-0.504597	-1.104543	-0.797716
C	-1.737370	1.238553	-1.696880
H	-2.246600	2.005061	-2.288757
H	-1.246351	0.569910	-2.411783
C	-2.150130	-0.253099	0.285067
H	-2.324701	0.368336	1.157655
C	-2.804635	0.397415	-0.959288
Cl	-4.124734	1.553636	-0.337411
C	-3.480220	-0.559441	-1.939213
H	-2.767180	-1.330798	-2.253809
H	-3.807794	-0.006675	-2.824739
H	-4.341038	-1.054915	-1.489636
Br	-3.022485	-1.963756	0.834244

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56004783**

Number of imaginary frequencies = 0

1c_C006

B3LYP/6-31G* Geometry

C	-1.452764	-0.407927	1.207435
C	-3.200247	-1.571172	-0.276032
C	-0.383875	-0.326438	0.017862
C	-2.922023	-0.436810	0.715125
H	-3.239333	-2.491782	0.324255
H	-3.590429	-0.514000	1.573246
C	-2.087793	-1.702380	-1.276138
H	-2.344955	-2.311630	-2.141116
C	-0.841415	-1.220525	-1.158071
O	-4.482409	-1.519329	-0.874242
H	-4.550991	-0.654764	-1.317013
Br	-3.581409	1.294282	-0.093741
C	-1.309501	0.715907	2.252740
H	-2.039881	0.560307	3.055909
H	-1.496983	1.705877	1.832084
H	-0.319124	0.711888	2.718268
C	-1.289324	-1.758024	1.974739
H	-2.143058	-1.923726	2.641667
H	-0.395423	-1.744477	2.603184
H	-1.211454	-2.614265	1.299502
C	0.148946	-1.564037	-2.254737
H	-0.343671	-2.147173	-3.037836
H	0.986217	-2.166611	-1.880552
H	0.579140	-0.676718	-2.734620
C	-0.162718	1.128527	-0.543170
H	0.100728	1.062987	-1.604385
H	-1.095826	1.687671	-0.515763
C	1.007857	-0.817273	0.568033
H	1.074931	-1.906299	0.521525
H	1.109995	-0.550515	1.624469
C	0.937717	1.923981	0.169671
H	0.975042	2.943736	-0.224178
H	0.705680	2.017409	1.234634
C	2.202523	-0.214371	-0.179224
H	2.122695	-0.390974	-1.245122
C	2.353716	1.301584	0.065303
Cl	3.197522	2.003703	-1.437316
C	3.198114	1.699355	1.273899
H	2.796807	1.223596	2.177328
H	3.159381	2.784244	1.409686
H	4.237358	1.390741	1.157932
Br	3.845102	-1.248745	0.282616

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56060637**

Number of imaginary frequencies = 0

1d_C001

B3LYP/6-31G* Geometry

C	-1.523145	-0.574292	-0.197654

C	-3.049461	1.543583	-0.176157
C	-0.228893	0.370109	0.021466
C	-2.705833	0.182158	0.443569
H	-3.611238	2.116371	0.580946
H	-2.521546	0.315831	1.509511
C	-1.789995	2.279221	-0.530720
H	-1.963851	3.284738	-0.908826
C	-0.542703	1.789489	-0.510975
O	-3.813238	1.476697	-1.375234
H	-4.615703	0.965412	-1.166782
Br	-4.406568	-0.903150	0.483287
C	-1.382339	-1.949147	0.498833
H	-2.186227	-2.607894	0.162393
H	-1.462401	-1.886529	1.588462
H	-0.437488	-2.442205	0.253630
C	-1.767495	-0.833813	-1.701410
H	-2.739476	-1.318790	-1.830225
H	-1.005886	-1.507176	-2.106682
H	-1.778809	0.085777	-2.288396
C	0.559999	2.686221	-1.039666
H	0.137117	3.632769	-1.387836
H	1.078255	2.231677	-1.892726
H	1.322108	2.928839	-0.290957
C	0.128560	0.455132	1.543314
H	-0.575842	1.120753	2.052486
H	0.007672	-0.530238	2.001125
C	0.972265	-0.281137	-0.744012
H	0.873614	-0.103208	-1.817717
H	0.929370	-1.364586	-0.619654
C	1.549632	0.948642	1.859277
H	1.676034	1.990617	1.552637
H	1.709832	0.923902	2.942891
C	2.386046	0.162162	-0.328199
H	2.612358	1.167340	-0.670458
C	2.637956	0.091153	1.183283
Cl	4.255870	0.915499	1.540393
C	2.723817	-1.322490	1.757312
H	1.795351	-1.874316	1.574718
H	2.889928	-1.278897	2.837238
H	3.542684	-1.875435	1.294301
Br	3.682848	-0.943529	-1.369700

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56797283**

Number of imaginary frequencies = 0

1d_C002

B3LYP/6-31G* Geometry

C	-1.530028	-0.556800	-0.231672
C	-3.058330	1.545692	-0.108425
C	-0.234276	0.368600	0.042057
C	-2.728916	0.159791	0.439413
H	-3.658410	2.074075	0.649426
H	-2.529252	0.261795	1.505964
C	-1.791298	2.307864	-0.385862
H	-1.947221	3.349224	-0.673000
C	-0.543019	1.818408	-0.400884
O	-3.827976	1.428381	-1.310445
H	-3.947953	2.323625	-1.664788
Br	-4.400559	-0.937716	0.448299
C	-1.391505	-1.965588	0.394685
H	-2.186474	-2.608887	0.012103
H	-1.490843	-1.960118	1.484440
H	-0.439008	-2.438704	0.139142
C	-1.759828	-0.742060	-1.749019
H	-2.748095	-1.179300	-1.914863
H	-1.014950	-1.423094	-2.172936
H	-1.726330	0.202262	-2.295197
C	0.560744	2.745515	-0.870468
H	0.142382	3.715692	-1.154195
H	1.075759	2.345855	-1.752519
H	1.325446	2.934799	-0.109683
C	0.123521	0.362243	1.566854
H	-0.582202	0.993491	2.116224
H	0.001132	-0.650230	1.959079
C	0.967449	-0.237417	-0.758851
H	0.869931	0.000375	-1.821045
H	0.922961	-1.326097	-0.696394
C	1.544650	0.833173	1.915637
H	1.674261	1.892775	1.678150
H	1.702853	0.738056	2.995712
C	2.380979	0.179802	-0.316500
H	2.608386	1.203301	-0.598176
C	2.632873	0.018511	1.188263
Cl	4.251252	0.820873	1.593518
C	2.718433	-1.426862	1.676399
H	1.788207	-1.964585	1.463386
H	2.886995	-1.448150	2.756600
H	3.535180	-1.952509	1.179028
Br	3.678875	-0.860306	-1.422655

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56352233**

Number of imaginary frequencies = 0

1d_C003

B3LYP/6-31G* Geometry

C	1.690432	-0.912643	1.130360
C	3.402799	-0.787203	-0.776725
C	0.449404	-1.051351	0.113451
C	2.898819	-0.157245	0.524772
H	3.957059	-1.689372	-0.478664
H	3.704903	-0.108520	1.257893
C	2.262735	-1.210173	-1.658452
H	2.568487	-1.453673	-2.674765
C	0.982608	-1.393105	-1.298434
O	4.376724	-0.018100	-1.458347
H	3.981142	0.857327	-1.618515
Br	2.575439	1.808549	0.205702
C	2.248522	-2.330339	1.468701
H	3.218713	-2.246768	1.971557
H	2.377470	-2.953216	0.579678
H	1.580005	-2.855990	2.155100
C	1.329043	-0.250706	2.478613
H	2.163345	-0.381341	3.177981
H	0.449404	-0.708835	2.941821
H	1.154527	0.822878	2.385273
C	0.049164	-1.963917	-2.348586
H	-0.320535	-2.957258	-2.066197
H	0.577294	-2.074452	-3.299912
H	-0.829736	-1.339157	-2.534821
C	-0.491014	-2.178819	0.663432
H	-0.068776	-3.161627	0.428994
H	-0.502602	-2.114695	1.755682
C	-0.370462	0.294671	0.052195
H	0.145407	1.009029	-0.587867
H	-0.392146	0.745985	1.045104
C	-1.957285	-2.174825	0.189630
H	-2.031889	-2.464913	-0.859724
H	-2.512639	-2.929527	0.758190
C	-1.828018	0.203562	-0.422568
H	-1.903978	-0.017013	-1.484695
C	-2.658054	-0.815286	0.363692
Cl	-4.316954	-0.976884	-0.442069
C	-2.908457	-0.449662	1.825609
H	-3.440794	0.500389	1.898531
H	-1.961495	-0.352560	2.367448
H	-3.502786	-1.229498	2.309616
Br	-2.593650	2.046219	-0.322270

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56358287**

Number of imaginary frequencies = 0

1d_C004

B3LYP/6-31G* Geometry

C	-1.505011	-0.231656	-0.532663
C	-3.036455	1.229915	0.991650
C	-0.213986	0.230173	0.308485
C	-2.705016	-0.160899	0.437917
H	-3.649708	1.082487	1.896401
H	-2.549897	-0.841696	1.275447
C	-1.766750	1.931730	1.370805
H	-1.916120	2.861004	1.917091
C	-0.522250	1.542317	1.064033
O	-3.730785	2.084570	0.090732
H	-4.541146	1.612042	-0.171692
Br	-4.407848	-0.900175	-0.353745
C	-1.374324	-1.677202	-1.058143
H	-2.231429	-1.913010	-1.693030
H	-1.357465	-2.418457	-0.252365
H	-0.475974	-1.807478	-1.668412
C	-1.727340	0.696167	-1.750430
H	-2.695865	0.469217	-2.205316
H	-0.959124	0.531578	-2.512116
H	-1.734654	1.751683	-1.474902
C	0.621899	2.411854	1.546743
H	0.232397	3.298631	2.054289
H	1.261102	2.759363	0.726704
H	1.269182	1.889635	2.263364
C	0.234060	-0.832158	1.381116
H	0.661233	-0.310919	2.245567
H	-0.633990	-1.371759	1.772001
C	0.981559	0.432226	-0.688642
H	0.940021	1.429582	-1.130842
H	0.900581	-0.269572	-1.523562
C	1.266914	-1.847668	0.875057
H	1.479746	-2.586774	1.652836
H	0.858015	-2.403241	0.027060
C	2.351530	0.234243	-0.029938
H	2.459162	0.878910	0.833825
C	2.606635	-1.225130	0.405834
Cl	3.759566	-1.152404	1.865596
C	3.266408	-2.125182	-0.636677
H	2.672027	-2.118227	-1.558645
H	3.311724	-3.152295	-0.262555
H	4.274773	-1.788075	-0.877667
Br	3.764758	0.948155	-1.242980

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56299986**

Number of imaginary frequencies = 0

1d_C005

B3LYP/6-31G* Geometry

C	-1.511234	-0.221216	-0.535414
C	-3.043629	1.241404	0.972675
C	-0.219272	0.233244	0.305741
C	-2.725544	-0.145918	0.425978
H	-3.690904	1.112387	1.854617
H	-2.552334	-0.802961	1.278684
C	-1.768445	1.924125	1.382080
H	-1.904118	2.836965	1.964427
C	-0.522414	1.540564	1.070679
O	-3.746477	2.013770	-0.006530
H	-3.839908	2.911773	0.348694
Br	-4.400564	-0.921262	-0.346502
C	-1.383066	-1.668553	-1.057019
H	-2.236278	-1.900940	-1.697432
H	-1.378041	-2.408733	-0.250060
H	-0.479352	-1.803097	-1.658667
C	-1.720992	0.700998	-1.759807
H	-2.705996	0.507379	-2.192944
H	-0.970043	0.503204	-2.531151
H	-1.685682	1.759020	-1.495438
C	0.622702	2.402189	1.564224
H	0.236713	3.283437	2.084568
H	1.261389	2.758249	0.747413
H	1.270120	1.869373	2.272469
C	0.224591	-0.832997	1.376760
H	0.650815	-0.317087	2.244983
H	-0.646425	-1.371805	1.761782
C	0.978478	0.436130	-0.688333
H	0.940177	1.434642	-1.128466
H	0.896068	-0.262901	-1.525251
C	1.256287	-1.848847	0.869285
H	1.466337	-2.590591	1.645314
H	0.846864	-2.400836	0.019411
C	2.347353	0.232739	-0.029151
H	2.457153	0.874843	0.836174
C	2.598094	-1.228286	0.403541
Cl	3.749221	-1.161200	1.865663
C	3.257539	-2.127411	-0.639905
H	2.664627	-2.116785	-1.562755
H	3.299551	-3.155501	-0.268176
H	4.267171	-1.792228	-0.878350
Br	3.764120	0.946218	-1.239266

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55876756**

Number of imaginary frequencies = 0

1d_C006

B3LYP/6-31G* Geometry

C	-1.50780	-0.23330	-0.52501
C	-3.04914	1.23605	0.98773
C	-0.21828	0.23522	0.30856
C	-2.72468	-0.15866	0.43319
H	-3.67276	1.09756	1.87809
H	-2.55307	-0.82451	1.28005
C	-1.77513	1.93695	1.36491
H	-1.92345	2.86699	1.91176
C	-0.52787	1.55437	1.05160
O	-3.85104	2.06497	0.14979
H	-3.30160	2.36038	-0.59198
Br	-4.39394	-0.92123	-0.35819
C	-1.37522	-1.68039	-1.04603
H	-2.22623	-1.91710	-1.68794
H	-1.37284	-2.41614	-0.23549
H	-0.46842	-1.81637	-1.64266
C	-1.71873	0.68423	-1.75607
H	-2.73256	0.54959	-2.14529
H	-1.02168	0.43152	-2.56064
H	-1.56620	1.74342	-1.52267
C	0.61504	2.43326	1.52012
H	0.22503	3.32537	2.01799
H	1.25513	2.77082	0.69640
H	1.26282	1.92021	2.24280
C	0.22818	-0.81594	1.39229
H	0.65546	-0.28631	2.25153
H	-0.64153	-1.34947	1.78726
C	0.97809	0.42720	-0.68988
H	0.94093	1.42107	-1.14069
H	0.89666	-0.28143	-1.51894
C	1.25966	-1.83828	0.89672
H	1.47265	-2.56774	1.68344
H	0.84837	-2.40412	0.05677
C	2.34748	0.23290	-0.02933
H	2.45519	0.88403	0.82970
C	2.59986	-1.22337	0.41774
Cl	3.75828	-1.14078	1.87200
C	3.25329	-2.13331	-0.62025
H	2.65500	-2.13277	-1.53975
H	3.29784	-3.15743	-0.23809
H	4.26144	-1.80058	-0.86817
Br	3.76144	0.93594	-1.24763

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56048207**

Number of imaginary frequencies = 0

1e_C001

B3LYP/6-31G* Geometry

C	-1.294518	-0.517689	-0.266683
C	-3.125965	1.274142	-0.581150
C	-0.171713	0.618830	-0.046279
C	-2.633158	0.084104	0.227616
H	-3.457477	0.923185	-1.572179
H	-2.582265	0.367880	1.278473
C	-1.999896	2.246993	-0.748074
H	-2.314099	3.242152	-1.056737
C	-0.699246	1.982916	-0.569046
O	-4.195205	1.952171	0.066352
H	-4.920197	1.307587	0.144045
Br	-4.152777	-1.252816	0.246081
C	-1.023650	-1.814134	0.526215
H	-1.764738	-2.569715	0.254939
H	-1.100857	-1.665246	1.607525
H	-0.040909	-2.231550	0.299303
C	-1.413422	-0.900376	-1.761399
H	-2.350393	-1.441713	-1.925249
H	-0.599309	-1.564880	-2.065986
H	-1.401777	-0.026645	-2.419681
C	0.290839	3.102165	-0.834574
H	-0.231550	4.061941	-0.881981
H	0.811838	2.968864	-1.791180
H	1.064159	3.179310	-0.062465
C	0.177097	0.850903	1.467232
H	0.544816	1.875361	1.574516
H	-0.735285	0.805800	2.070663
C	1.157912	0.294236	-0.816137
H	1.703160	1.224310	-0.973361
H	0.941355	-0.095890	-1.811510
C	1.230122	-0.073246	2.100827
H	1.479744	0.305067	3.098490
H	0.835126	-1.084288	2.244601
C	2.145557	-0.645555	-0.123113
H	1.774696	-1.668455	-0.060363
C	2.535545	-0.223276	1.298846
Cl	3.380227	1.427037	1.261890
C	3.496376	-1.197536	1.976796
H	3.038328	-2.193901	2.019053
H	3.709960	-0.872266	2.998727
H	4.434348	-1.272063	1.423475
Br	3.730715	-0.859947	-1.317010

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56897174**

Number of imaginary frequencies = 0

1e_C002

B3LYP/6-31G* Geometry

C	-1.305710	-0.519581	-0.279589
C	-3.140418	1.279333	-0.563594
C	-0.177948	0.610634	-0.064521
C	-2.652248	0.069823	0.227545
H	-3.548401	0.943276	-1.523776
H	-2.577325	0.336377	1.283524
C	-1.999560	2.228198	-0.788725
H	-2.307514	3.213121	-1.138059
C	-0.697329	1.967859	-0.607777
O	-4.237355	1.937604	0.064065
H	-3.898934	2.358189	0.871791
Br	-4.142969	-1.271648	0.250440
C	-1.021876	-1.819780	0.502494
H	-1.765324	-2.574576	0.238075
H	-1.085900	-1.677246	1.585696
H	-0.040495	-2.232057	0.260187
C	-1.438943	-0.895285	-1.775027
H	-2.374900	-1.440977	-1.928609
H	-0.625487	-1.554183	-2.093203
H	-1.440557	-0.018477	-2.429392
C	0.294837	3.077222	-0.902984
H	-0.224045	4.037575	-0.973859
H	0.812624	2.917946	-1.857180
H	1.070911	3.169672	-0.135077
C	0.165256	0.862199	1.447726
H	0.532671	1.888233	1.543756
H	-0.749176	0.821942	2.048688
C	1.155283	0.271891	-0.823877
H	1.700673	1.198366	-0.999726
H	0.940808	-0.139829	-1.810991
C	1.215544	-0.052964	2.098187
H	1.457205	0.335503	3.093936
H	0.821128	-1.063365	2.247930
C	2.144938	-0.651612	-0.111330
H	1.779927	-1.675478	-0.034494
C	2.525995	-0.206807	1.305906
Cl	3.361277	1.448446	1.250206
C	3.488854	-1.165543	2.002638
H	3.035481	-2.163354	2.058248
H	3.696735	-0.823547	3.020263
H	4.429303	-1.243833	1.454103
Br	3.736617	-0.873244	-1.294733

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56660636**

Number of imaginary frequencies = 0

1e_C003

B3LYP/6-31G* Geometry

C	-1.294428	-0.517669	-0.266676
C	-3.126004	1.274012	-0.581380
C	-0.171739	0.618898	-0.046166
C	-2.633165	0.084120	0.227531
H	-3.457499	0.922915	-1.572324
H	-2.582300	0.368048	1.278346
C	-1.999943	2.246906	-0.748335
H	-2.314153	3.241985	-1.057225
C	-0.699298	1.982941	-0.569029
O	-4.195319	1.952079	0.066067
H	-4.920227	1.307484	0.144100
Br	-4.152803	-1.252868	0.246230
C	-1.023544	-1.814137	0.526173
H	-1.764292	-2.569877	0.254442
H	-1.101276	-1.665438	1.607464
H	-0.040580	-2.231228	0.299608
C	-1.413083	-0.900275	-1.761415
H	-2.349803	-1.442014	-1.925362
H	-0.598645	-1.564390	-2.066001
H	-1.401764	-0.026493	-2.419638
C	0.290693	3.102254	-0.834673
H	1.064022	3.179481	-0.062574
H	-0.231799	4.061960	-0.882106
H	0.811726	2.968981	-1.791259
C	0.177001	0.850863	1.467374
H	0.544528	1.875369	1.574703
H	-0.735392	0.805513	2.070780
C	1.157923	0.294335	-0.816032
H	1.703246	1.224380	-0.973137
H	0.941284	-0.095670	-1.811442
C	1.230191	-0.073159	2.100914
H	1.479786	0.305220	3.098560
H	0.835416	-1.084261	2.244684
C	2.145538	-0.645509	-0.123069
H	1.774596	-1.668366	-0.060083
C	2.535662	-0.223071	1.298894
Cl	3.380196	1.427254	1.261823
C	3.496585	-1.197241	1.976850
H	3.038656	-2.193661	2.019143
H	3.710113	-0.871918	2.998765
H	4.434560	-1.271641	1.423509
Br	3.730651	-0.860159	-1.317036

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56897160**

Number of imaginary frequencies = 0

1e_C004

B3LYP/6-31G* Geometry

C	-1.368571	-0.591606	-0.357962
C	-3.107989	1.309647	-0.439306
C	-0.203575	0.511065	-0.235801
C	-2.604720	0.064159	0.289340
H	-3.669297	0.985125	-1.331192
H	-2.420704	0.307795	1.333943
C	-1.967492	2.166544	-0.910605
H	-2.277942	3.119071	-1.336142
C	-0.674310	1.813508	-0.927468
O	-3.956564	2.094437	0.391797
H	-4.730682	1.539497	0.591160
Br	-4.189278	-1.179033	0.451989
C	-1.016618	-1.910006	0.362164
H	-1.819517	-2.635741	0.208413
H	-0.900269	-1.794072	1.444421
H	-0.099736	-2.349377	-0.043187
C	-1.659634	-0.943529	-1.836999
H	-2.599822	-1.500919	-1.897407
H	-0.877561	-1.583420	-2.255931
H	-1.745156	-0.057204	-2.470723
C	0.318010	2.731456	-1.609466
H	-0.149512	3.695766	-1.829587
H	0.657828	2.310266	-2.565217
H	1.219464	2.920114	-1.018228
C	0.077820	0.865001	1.273384
H	-0.676508	1.571249	1.629853
H	-0.021350	-0.031619	1.894391
C	1.124559	-0.048106	-0.860817
H	1.637307	0.714251	-1.449547
H	0.913611	-0.866265	-1.549906
C	1.459432	1.490945	1.526726
H	1.527474	2.445581	1.004238
H	1.557448	1.721330	2.593670
C	2.103774	-0.540692	0.203350
H	1.625577	-1.266391	0.861967
C	2.654103	0.578863	1.104583
Cl	3.854976	1.623583	0.154871
C	3.407291	0.019594	2.310448
H	2.713797	-0.558765	2.935306
H	3.818485	0.831535	2.916194
H	4.220566	-0.638109	1.995163
Br	3.531048	-1.630600	-0.645653

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56292509**

Number of imaginary frequencies = 0

1e_C005

B3LYP/6-31G* Geometry

C	-1.378927	-0.593653	-0.369290
C	-3.096309	1.341169	-0.349029
C	-0.211581	0.505828	-0.271486
C	-2.610775	0.050189	0.306734
H	-3.801450	1.082763	-1.153523
H	-2.412588	0.249985	1.358102
C	-1.971004	2.142607	-0.952188
H	-2.284805	3.072727	-1.428077
C	-0.680934	1.784189	-1.002838
O	-3.785256	2.073631	0.672319
H	-4.282020	2.787846	0.244425
Br	-4.180945	-1.195000	0.429335
C	-1.009015	-1.907162	0.351868
H	-1.822525	-2.627839	0.237689
H	-0.852909	-1.777431	1.427845
H	-0.109362	-2.357415	-0.079294
C	-1.693470	-0.953504	-1.841102
H	-2.607916	-1.553124	-1.878934
H	-0.892704	-1.552657	-2.284805
H	-1.839153	-0.069664	-2.467118
C	0.294175	2.655980	-1.763329
H	-0.180533	3.601956	-2.041207
H	0.622118	2.171493	-2.692670
H	1.203214	2.888574	-1.198657
C	0.059745	0.905269	1.227570
H	-0.701806	1.615669	1.559608
H	-0.034288	0.027710	1.876182
C	1.120692	-0.068877	-0.872154
H	1.641066	0.678435	-1.473445
H	0.914805	-0.902921	-1.543617
C	1.438026	1.546680	1.454289
H	1.507203	2.468272	0.874815
H	1.533494	1.839809	2.505936
C	2.088077	-0.534724	0.214006
H	1.600841	-1.240573	0.887173
C	2.631630	0.610200	1.088314
Cl	3.859725	1.614175	0.130136
C	3.353712	0.082710	2.326801
H	2.639463	-0.462432	2.958043
H	3.767205	0.908606	2.911691
H	4.161560	-0.598521	2.049410
Br	3.520761	-1.653077	-0.587319

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56037657**

Number of imaginary frequencies = 0

1e_C006

B3LYP/6-31G* Geometry

C	1.530399	-0.542933	1.091638
C	3.457885	-0.369038	-0.674934
C	0.489683	-1.029189	-0.027675
C	2.717662	0.272977	0.505858
H	3.944714	0.425059	-1.247326
H	3.439514	0.463985	1.299356
C	2.537489	-1.149673	-1.556255
H	2.990439	-1.499896	-2.482693
C	1.267434	-1.492137	-1.288556
O	4.548085	-1.183068	-0.210692
H	4.200777	-2.074028	-0.052184
Br	2.253602	2.162070	-0.037135
C	2.189379	-1.785582	1.766625
H	3.097294	-1.497733	2.305510
H	2.454054	-2.565440	1.046565
H	1.508673	-2.232873	2.497191
C	0.932358	0.295337	2.243133
H	1.728387	0.529116	2.960949
H	0.160039	-0.246307	2.793610
H	0.531464	1.249538	1.899082
C	0.549525	-2.350806	-2.315340
H	0.474852	-3.396098	-1.989708
H	1.096961	-2.343652	-3.262032
H	-0.471236	-2.010640	-2.518757
C	-0.401920	-2.222652	0.457201
H	-0.821058	-2.706993	-0.425339
H	0.200321	-2.987876	0.952860
C	-0.490713	0.092409	-0.541170
H	-0.882727	-0.212500	-1.514836
H	0.057861	1.017736	-0.707100
C	-1.605570	-1.876174	1.343763
H	-2.179881	-2.789272	1.536725
H	-1.297389	-1.496850	2.324679
C	-1.701462	0.387997	0.348164
H	-1.407328	0.862470	1.283382
C	-2.554031	-0.828756	0.727390
Cl	-3.310822	-1.573704	-0.793700
C	-3.703577	-0.489412	1.673243
H	-3.301315	-0.049420	2.594611
H	-4.260721	-1.392907	1.936492
H	-4.386026	0.230229	1.217370
Br	-2.775477	1.822721	-0.528250

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56109795**

Number of imaginary frequencies = 0

1e_C007

B3LYP/6-31G* Geometry

C	-1.377114	-0.585405	-0.351721
C	-3.120925	1.318649	-0.421694
C	-0.210471	0.514280	-0.239199
C	-2.625472	0.059129	0.299076
H	-3.738661	1.011229	-1.273615
H	-2.430549	0.288114	1.346955
C	-1.977545	2.151548	-0.938056
H	-2.290476	3.090015	-1.394404
C	-0.680365	1.808390	-0.943724
O	-4.011836	2.087330	0.384621
H	-3.478930	2.523607	1.069262
Br	-4.176590	-1.201821	0.448604
C	-1.015465	-1.901431	0.368961
H	-1.820047	-2.627017	0.228075
H	-0.887609	-1.781633	1.449797
H	-0.102332	-2.341132	-0.044547
C	-1.673106	-0.944053	-1.828582
H	-2.605900	-1.513968	-1.880163
H	-0.885371	-1.573997	-2.252068
H	-1.775902	-0.061014	-2.464322
C	0.308521	2.719403	-1.639401
H	-0.162075	3.678208	-1.876520
H	0.649831	2.283131	-2.587640
H	1.209475	2.920215	-1.051127
C	0.076459	0.878223	1.266509
H	-0.674801	1.588731	1.622273
H	-0.025003	-0.013113	1.894230
C	1.118013	-0.048733	-0.861216
H	1.633057	0.710554	-1.451931
H	0.904811	-0.868226	-1.547781
C	1.459597	1.503826	1.512477
H	1.530175	2.451371	0.977367
H	1.559769	1.746865	2.576472
C	2.096384	-0.539841	0.204424
H	1.616148	-1.260724	0.866800
C	2.650496	0.582958	1.099656
Cl	3.857439	1.617345	0.147317
C	3.397453	0.027138	2.310985
H	2.699213	-0.543063	2.938032
H	3.812894	0.840210	2.912295
H	4.206989	-0.637771	2.001254
Br	3.519869	-1.637282	-0.639205

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56092517**

Number of imaginary frequencies = 0

1e_C008

B3LYP/6-31G* Geometry

C	1.515531	-0.541546	1.091297
C	3.469872	-0.410580	-0.645297
C	0.483567	-1.016345	-0.042221
C	2.720435	0.253842	0.517424
H	3.977490	0.372020	-1.223876
H	3.420736	0.449770	1.330973
C	2.548296	-1.167186	-1.541995
H	3.011132	-1.527641	-2.458471
C	1.265005	-1.468433	-1.302727
O	4.453135	-1.340467	-0.158562
H	5.215332	-0.824627	0.150965
Br	2.293568	2.144099	-0.059230
C	2.153928	-1.783017	1.784018
H	2.993757	-1.473622	2.414824
H	2.536148	-2.513711	1.069610
H	1.424999	-2.269791	2.439197
C	0.910849	0.317152	2.224786
H	1.700085	0.552629	2.949637
H	0.129180	-0.212833	2.773535
H	0.519488	1.270572	1.867096
C	0.541301	-2.290037	-2.356199
H	0.452814	-3.342038	-2.057367
H	1.096410	-2.266801	-3.298162
H	-0.473532	-1.932569	-2.559269
C	-0.406009	-2.220209	0.417851
H	-0.831092	-2.680576	-0.474609
H	0.201093	-2.996689	0.888384
C	-0.499787	0.110436	-0.538234
H	-0.890372	-0.179822	-1.516795
H	0.044900	1.040874	-0.689793
C	-1.603209	-1.891140	1.318744
H	-2.174648	-2.807817	1.503209
H	-1.287746	-1.524818	2.302585
C	-1.712464	0.387579	0.355033
H	-1.421724	0.853794	1.295071
C	-2.558325	-0.837536	0.722601
Cl	-3.323567	-1.563102	-0.803860
C	-3.703032	-0.514058	1.679942
H	-3.295925	-0.087189	2.605384
H	-4.256940	-1.422411	1.933178
H	-4.389490	0.210911	1.238771
Br	-2.795920	1.828339	-0.502487

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56070642**

Number of imaginary frequencies = 0

1e_C009

B3LYP/6-31G* Geometry

C	1.515638	-0.541572	1.091216
C	3.469640	-0.410473	-0.645765
C	0.483569	-1.016506	-0.042059
C	2.720410	0.253827	0.517184
H	3.976626	0.372272	-1.224700
H	3.420926	0.449719	1.330552
C	2.548090	-1.167637	-1.541996
H	3.010933	-1.528430	-2.458338
C	1.264855	-1.468967	-1.302496
O	4.453472	-1.339818	-0.159297
H	5.215421	-0.823627	0.150257
Br	2.293368	2.144232	-0.059027
C	2.154267	-1.782930	1.783986
H	2.994024	-1.473447	2.414848
H	2.536612	-2.513558	1.069564
H	1.425457	-2.269923	2.439164
C	0.911011	0.317164	2.224713
H	1.700113	0.552110	2.949870
H	0.128926	-0.212611	2.773071
H	0.520209	1.270838	1.867095
C	0.541186	-2.291078	-2.355578
H	0.452899	-3.342978	-2.056323
H	1.096142	-2.268084	-3.297626
H	-0.473706	-1.933763	-2.558656
C	-0.406133	-2.220179	0.418427
H	-0.831263	-2.680834	-0.473876
H	0.200961	-2.996569	0.889132
C	-0.499778	0.110209	-0.538331
H	-0.890346	-0.180306	-1.516823
H	0.045004	1.040548	-0.690161
C	-1.603255	-1.890721	1.319246
H	-2.174709	-2.807321	1.504097
H	-1.287822	-1.524000	2.302930
C	-1.712410	0.387635	0.354876
H	-1.421619	0.854030	1.294810
C	-2.558377	-0.837327	0.722669
Cl	-3.323486	-1.563313	-0.803488
C	-3.703060	-0.513545	1.679953
H	-3.296003	-0.086334	2.605264
H	-4.256906	-1.421834	1.933524
H	-4.389605	0.211226	1.238550
Br	-2.795788	1.828350	-0.502939

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56070525**

Number of imaginary frequencies = 0

1e_C010

B3LYP/6-31G* Geometry

C	1.526912	-0.339815	0.708373
C	2.860558	1.486180	-0.514725
C	0.137738	0.211353	0.070193
C	2.626738	-0.004006	-0.320767
H	3.396307	1.878527	0.365402
H	2.420800	-0.467332	-1.285150
C	1.545914	2.195100	-0.631454
H	1.632374	3.224100	-0.974493
C	0.337979	1.698991	-0.325006
O	3.618686	1.755108	-1.688296
H	4.483458	1.328700	-1.555879
Br	4.431682	-0.799859	0.133850
C	1.530184	-1.863323	0.965233
H	2.451654	-2.137247	1.484222
H	1.501707	-2.454098	0.044834
H	0.700735	-2.178271	1.604461
C	1.819063	0.356490	2.059629
H	2.853367	0.155675	2.356938
H	1.170637	-0.030185	2.851537
H	1.679229	1.439279	2.009506
C	-0.843622	2.628955	-0.465640
H	-0.507216	3.601523	-0.836749
H	-1.358749	2.793083	0.485304
H	-1.601079	2.250006	-1.157854
C	-0.205528	-0.573712	-1.250194
H	0.291334	-0.082895	-2.092224
H	0.214099	-1.581557	-1.200225
C	-0.979338	-0.001712	1.165446
H	-1.042522	0.876577	1.811284
H	-0.646131	-0.809333	1.821244
C	-1.699450	-0.709894	-1.595899
H	-2.146324	0.259288	-1.835899
H	-1.799210	-1.335915	-2.488958
C	-2.429779	-0.415954	0.786195
H	-2.871513	-0.925738	1.642504
C	-2.492646	-1.336482	-0.448028
Cl	-4.232205	-1.573916	-1.016019
C	-2.011088	-2.746521	-0.070331
H	-0.994869	-2.736113	0.329460
H	-2.023260	-3.392958	-0.952763
H	-2.671899	-3.185405	0.682477
Br	-3.645304	1.163062	0.633909

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55442026**

Number of imaginary frequencies = 0

1e_C011

B3LYP/6-31G* Geometry

C	-1.592487	0.374004	1.159937
C	-3.403880	0.551909	-0.709193
C	-0.493728	1.034933	0.206112
C	-2.756232	-0.302200	0.386071
H	-3.809642	-0.113479	-1.482137
H	-3.532923	-0.580489	1.097359
C	-2.444929	1.515607	-1.337464
H	-2.845907	2.060096	-2.194105
C	-1.188412	1.778285	-0.950328
O	-4.504136	1.237568	-0.076424
H	-4.779969	1.955058	-0.669116
Br	-2.323536	-2.097361	-0.416796
C	-2.284573	1.481649	2.011686
H	-3.116378	1.053158	2.579569
H	-2.692686	2.285132	1.397050
H	-1.584739	1.909643	2.734558
C	-1.008053	-0.651500	2.155822
H	-1.818696	-1.059816	2.770374
H	-0.295547	-0.185367	2.844070
H	-0.523760	-1.497131	1.662781
C	-0.410923	2.815722	-1.733355
H	-0.131525	3.674280	-1.110758
H	-1.012732	3.196134	-2.563840
H	0.515522	2.411371	-2.157753
C	0.390211	2.014820	1.059930
H	-0.105565	2.986711	1.151682
H	0.458012	1.627430	2.081349
C	0.474084	-0.023238	-0.449917
H	0.787291	0.321713	-1.440225
H	-0.047604	-0.963505	-0.609946
C	1.825240	2.253636	0.550224
H	1.801441	2.774802	-0.404661
H	2.336282	2.925155	1.250163
C	1.731575	-0.248417	0.383767
H	1.474907	-0.451766	1.422658
C	2.683292	0.959234	0.393875
Cl	3.575965	1.083405	-1.227550
C	3.750270	0.831650	1.479433
H	3.266051	0.828343	2.465066
H	4.443904	1.675865	1.440810
H	4.312471	-0.098371	1.366445
Br	2.623957	-1.941781	-0.148668

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55436897**

Number of imaginary frequencies = 0

1e_C012

B3LYP/6-31G* Geometry

C	-1.664357	-0.657864	1.209611
C	-2.312784	1.513795	-0.178024
C	-0.174484	-0.117238	0.937314
C	-2.683524	0.079316	0.286265
H	-1.939135	1.460359	-1.210416
H	-3.639354	0.145277	0.804396
C	-1.251069	2.112616	0.692678
H	-1.346751	3.180912	0.871004
C	-0.227245	1.411957	1.199295
O	-3.456814	2.360856	-0.148691
H	-4.050035	2.053173	-0.853781
Br	-3.223496	-0.928344	-1.383352
C	-2.103215	-0.309286	2.661399
H	-3.097489	-0.727489	2.855215
H	-2.149411	0.766580	2.838817
H	-1.418722	-0.749529	3.393372
C	-1.817677	-2.191622	1.093193
H	-2.876341	-2.460070	1.163270
H	-1.303547	-2.698771	1.914706
H	-1.455244	-2.602007	0.148454
C	0.773975	2.123271	2.081599
H	1.757613	2.189507	1.607033
H	0.902375	1.630235	3.052246
H	0.435671	3.145697	2.275660
C	0.830637	-0.857366	1.867898
H	0.722157	-0.511195	2.899763
H	0.573292	-1.919549	1.885773
C	0.212567	-0.430122	-0.549595
H	-0.320208	0.226138	-1.237822
H	-0.118967	-1.444013	-0.794669
C	2.320307	-0.748393	1.481915
H	2.683607	0.274700	1.593692
H	2.912285	-1.372575	2.160358
C	1.701291	-0.375943	-0.925808
H	1.831580	-0.738056	-1.946354
C	2.571553	-1.198085	0.039846
Cl	4.361771	-0.956183	-0.339016
C	2.317869	-2.699708	-0.176073
H	2.965367	-3.282159	0.485198
H	1.280089	-2.970796	0.039245
H	2.540132	-2.984475	-1.208608
Br	2.299278	1.523327	-1.077015

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56070642**

Number of imaginary frequencies = 0

1e_C013

B3LYP/6-31G* Geometry

C	-1.592487	0.374004	1.159937
C	-3.403880	0.551909	-0.709193
C	-0.493728	1.034933	0.206112
C	-2.756232	-0.302200	0.386071
H	-3.809642	-0.113479	-1.482137
H	-3.532923	-0.580489	1.097359
C	-2.444929	1.515607	-1.337464
H	-2.845907	2.060096	-2.194105
C	-1.188412	1.778285	-0.950328
O	-4.504136	1.237568	-0.076424
H	-4.779969	1.955058	-0.669116
Br	-2.323536	-2.097361	-0.416796
C	-2.284573	1.481649	2.011686
H	-3.116378	1.053158	2.579569
H	-2.692686	2.285132	1.397050
H	-1.584739	1.909643	2.734558
C	-1.008053	-0.651500	2.155822
H	-1.818696	-1.059816	2.770374
H	-0.295547	-0.185367	2.844070
H	-0.523760	-1.497131	1.662781
C	-0.410923	2.815722	-1.733355
H	-0.131525	3.674280	-1.110758
H	-1.012732	3.196134	-2.563840
H	0.515522	2.411371	-2.157753
C	0.390211	2.014820	1.059930
H	-0.105565	2.986711	1.151682
H	0.458012	1.627430	2.081349
C	0.474084	-0.023238	-0.449917
H	0.787291	0.321713	-1.440225
H	-0.047604	-0.963505	-0.609946
C	1.825240	2.253636	0.550224
H	1.801441	2.774802	-0.404661
H	2.336282	2.925155	1.250163
C	1.731575	-0.248417	0.383767
H	1.474907	-0.451766	1.422658
C	2.683292	0.959234	0.393875
Cl	3.575965	1.083405	-1.227550
C	3.750270	0.831650	1.479433
H	3.266051	0.828343	2.465066
H	4.443904	1.675865	1.440810
H	4.312471	-0.098371	1.366445
Br	2.623957	-1.941781	-0.148668

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55236851**

Number of imaginary frequencies = 0

1e_C014

B3LYP/6-31G* Geometry

C	-1.536287	-0.329158	-0.709447
C	-2.85312	1.464836	0.586219
C	-0.142764	0.21681	-0.080235
C	-2.642524	-0.015964	0.326873
H	-3.48136	1.881787	-0.215557
H	-2.438058	-0.51289	1.274925
C	-1.540597	2.195981	0.617542
H	-1.618442	3.237432	0.93066
C	-0.334039	1.708598	0.294713
O	-3.538831	1.575492	1.83818
H	-3.939295	2.45668	1.883251
Br	-4.4311	-0.788242	-0.168398
C	-1.534728	-1.851645	-0.977219
H	-2.464526	-2.127978	-1.478629
H	-1.485845	-2.447374	-0.060713
H	-0.715465	-2.158435	-1.633172
C	-1.838323	0.375054	-2.053947
H	-2.864486	0.14895	-2.359899
H	-1.173204	0.017735	-2.846029
H	-1.730107	1.460694	-1.988566
C	0.84376	2.648364	0.389667
H	0.508848	3.629852	0.738871
H	1.344634	2.788519	-0.572849
H	1.613235	2.291412	1.080419
C	0.193108	-0.555002	1.249075
H	-0.307631	-0.0553	2.083541
H	-0.227623	-1.562683	1.207262
C	0.975408	-0.011642	-1.171189
H	1.04534	0.860981	-1.82382
H	0.63968	-0.821665	-1.822206
C	1.685579	-0.688457	1.599925
H	2.134291	0.283784	1.824899
H	1.783406	-1.300881	2.502532
C	2.422672	-0.42988	-0.783993
H	2.864159	-0.952281	-1.632785
C	2.477822	-1.334408	0.462093
Cl	4.21496	-1.574838	1.037057
C	1.98827	-2.746024	0.100574
H	0.975046	-2.733432	-0.306801
H	1.989301	-3.38025	0.99193
H	2.651119	-3.200039	-0.641367
Br	3.647325	1.144782	-0.648037

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55147048**

Number of imaginary frequencies = 0

1e_C015

B3LYP/6-31G* Geometry

C	-1.592487	0.374004	1.159937
C	-3.403880	0.551909	-0.709193
C	-0.493728	1.034933	0.206112
C	-2.756232	-0.302200	0.386071
H	-3.809642	-0.113479	-1.482137
H	-3.532923	-0.580489	1.097359
C	-2.444929	1.515607	-1.337464
H	-2.845907	2.060096	-2.194105
C	-1.188412	1.778285	-0.950328
O	-4.504136	1.237568	-0.076424
H	-4.779969	1.955058	-0.669116
Br	-2.323536	-2.097361	-0.416796
C	-2.284573	1.481649	2.011686
H	-3.116378	1.053158	2.579569
H	-2.692686	2.285132	1.397050
H	-1.584739	1.909643	2.734558
C	-1.008053	-0.651500	2.155822
H	-1.818696	-1.059816	2.770374
H	-0.295547	-0.185367	2.844070
H	-0.523760	-1.497131	1.662781
C	-0.410923	2.815722	-1.733355
H	-0.131525	3.674280	-1.110758
H	-1.012732	3.196134	-2.563840
H	0.515522	2.411371	-2.157753
C	0.390211	2.014820	1.059930
H	-0.105565	2.986711	1.151682
H	0.458012	1.627430	2.081349
C	0.474084	-0.023238	-0.449917
H	0.787291	0.321713	-1.440225
H	-0.047604	-0.963505	-0.609946
C	1.825240	2.253636	0.550224
H	1.801441	2.774802	-0.404661
H	2.336282	2.925155	1.250163
C	1.731575	-0.248417	0.383767
H	1.474907	-0.451766	1.422658
C	2.683292	0.959234	0.393875
Cl	3.575965	1.083405	-1.227550
C	3.750270	0.831650	1.479433
H	3.266051	0.828343	2.465066
H	4.443904	1.675865	1.440810
H	4.312471	-0.098371	1.366445
Br	2.623957	-1.941781	-0.148668

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55537662**

Number of imaginary frequencies = 0

1e_C016

B3LYP/6-31G* Geometry

C	-1.539668	-0.427539	-0.658248
C	-2.820316	1.553427	0.364449
C	-0.156056	0.089449	-0.007168
C	-2.665195	0.040982	0.289340
H	-3.249408	1.918140	-0.583019
H	-2.535552	-0.349658	1.297965
C	-1.471654	2.176449	0.572383
H	-1.507428	3.214553	0.896740
C	-0.287343	1.577285	0.385560
O	-3.657049	1.946712	1.445604
H	-4.529473	1.552051	1.271471
Br	-4.481074	-0.702604	-0.202428
C	-1.576448	-1.965280	-0.787423
H	-2.487458	-2.270276	-1.307829
H	-1.578625	-2.469882	0.183824
H	-0.728795	-2.344383	-1.367115
C	-1.761756	0.180740	-2.064958
H	-2.802662	0.028307	-2.367026
H	-1.132468	-0.303145	-2.816885
H	-1.549787	1.253237	-2.088506
C	0.971907	2.371169	0.647938
H	0.721049	3.405113	0.901846
H	1.650399	2.389556	-0.211130
H	1.549723	1.951598	1.477985
C	0.187711	-0.718745	1.295518
H	0.543184	-0.028525	2.064274
H	-0.718208	-1.168852	1.709930
C	0.964868	-0.110914	-1.092118
H	1.050430	0.789732	-1.701293
H	0.612718	-0.881242	-1.780826
C	1.244150	-1.817167	1.129891
H	1.381013	-2.345530	2.079900
H	0.915899	-2.567333	0.397842
C	2.395840	-0.593539	-0.713684
H	2.662539	-1.354726	-1.447402
C	2.604808	-1.284018	0.661429
Cl	3.237616	-0.142367	1.972753
C	3.656088	-2.390120	0.542797
H	3.302575	-3.164261	-0.149889
H	3.842686	-2.854765	1.514352
H	4.596496	-1.982490	0.160682
Br	3.787545	0.769354	-1.129908

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55550158**

Number of imaginary frequencies = 0

1e_C017

B3LYP/6-31G* Geometry

C	-1.592487	0.374004	1.159937
C	-3.403880	0.551909	-0.709193
C	-0.493728	1.034933	0.206112
C	-2.756232	-0.302200	0.386071
H	-3.809642	-0.113479	-1.482137
H	-3.532923	-0.580489	1.097359
C	-2.444929	1.515607	-1.337464
H	-2.845907	2.060096	-2.194105
C	-1.188412	1.778285	-0.950328
O	-4.504136	1.237568	-0.076424
H	-4.779969	1.955058	-0.669116
Br	-2.323536	-2.097361	-0.416796
C	-2.284573	1.481649	2.011686
H	-3.116378	1.053158	2.579569
H	-2.692686	2.285132	1.397050
H	-1.584739	1.909643	2.734558
C	-1.008053	-0.651500	2.155822
H	-1.818696	-1.059816	2.770374
H	-0.295547	-0.185367	2.844070
H	-0.523760	-1.497131	1.662781
C	-0.410923	2.815722	-1.733355
H	-0.131525	3.674280	-1.110758
H	-1.012732	3.196134	-2.563840
H	0.515522	2.411371	-2.157753
C	0.390211	2.014820	1.059930
H	-0.105565	2.986711	1.151682
H	0.458012	1.627430	2.081349
C	0.474084	-0.023238	-0.449917
H	0.787291	0.321713	-1.440225
H	-0.047604	-0.963505	-0.609946
C	1.825240	2.253636	0.550224
H	1.801441	2.774802	-0.404661
H	2.336282	2.925155	1.250163
C	1.731575	-0.248417	0.383767
H	1.474907	-0.451766	1.422658
C	2.683292	0.959234	0.393875
Cl	3.575965	1.083405	-1.227550
C	3.750270	0.831650	1.479433
H	3.266051	0.828343	2.465066
H	4.443904	1.675865	1.440810
H	4.312471	-0.098371	1.366445
Br	2.623957	-1.941781	-0.148668

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55730779**

Number of imaginary frequencies = 0

1e_C018

B3LYP/6-31G* Geometry

C	-1.737210	-0.707511	1.112076
C	-2.903559	1.375861	0.021940
C	-0.301729	-0.019752	0.868569
C	-2.823801	-0.161526	0.147883
H	-3.154929	1.631851	-1.010469
H	-3.800665	-0.512795	0.476695
C	-1.651083	2.073233	0.458267
H	-1.754191	3.157064	0.487626
C	-0.512030	1.517412	0.901585
O	-4.017408	1.874888	0.781042
H	-3.728770	1.953533	1.704253
Br	-2.775027	-0.946896	-1.713437
C	-2.237885	-0.361847	2.547291
H	-3.276813	-0.683792	2.677402
H	-2.177656	0.706361	2.769718
H	-1.641754	-0.888975	3.298050
C	-1.741087	-2.252277	1.036700
H	-2.751476	-2.614232	1.260181
H	-1.073147	-2.700740	1.777616
H	-1.485306	-2.641054	0.050246
C	0.525008	2.445871	1.500551
H	0.745698	2.187225	2.543367
H	0.152221	3.474363	1.492665
H	1.465767	2.431623	0.947571
C	0.672567	-0.487181	1.997438
H	0.460743	0.056117	2.923359
H	0.471339	-1.537253	2.225075
C	0.264351	-0.477833	-0.526397
H	-0.219029	0.081294	-1.326934
H	-0.022694	-1.520249	-0.684473
C	2.181836	-0.360166	1.704433
H	2.490882	0.685121	1.650274
H	2.741616	-0.813365	2.530104
C	1.781981	-0.452021	-0.776554
H	1.995577	-1.008949	-1.689359
C	2.576336	-1.050299	0.396555
Cl	4.389259	-0.814342	0.146852
C	2.372018	-2.574202	0.436212
H	2.721134	-3.033953	-0.492734
H	1.319307	-2.836980	0.574503
H	2.942973	-3.002656	1.264851
Br	2.383792	1.381998	-1.290954

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55375875**

Number of imaginary frequencies = 0

1f_C001

B3LYP/6-31G* Geometry

C	-1.592487	0.374004	1.159937
C	-3.403880	0.551909	-0.709193
C	-0.493728	1.034933	0.206112
C	-2.756232	-0.302200	0.386071
H	-3.809642	-0.113479	-1.482137
H	-3.532923	-0.580489	1.097359
C	-2.444929	1.515607	-1.337464
H	-2.845907	2.060096	-2.194105
C	-1.188412	1.778285	-0.950328
O	-4.504136	1.237568	-0.076424
H	-4.779969	1.955058	-0.669116
Br	-2.323536	-2.097361	-0.416796
C	-2.284573	1.481649	2.011686
H	-3.116378	1.053158	2.579569
H	-2.692686	2.285132	1.397050
H	-1.584739	1.909643	2.734558
C	-1.008053	-0.651500	2.155822
H	-1.818696	-1.059816	2.770374
H	-0.295547	-0.185367	2.844070
H	-0.523760	-1.497131	1.662781
C	-0.410923	2.815722	-1.733355
H	-0.131525	3.674280	-1.110758
H	-1.012732	3.196134	-2.563840
H	0.515522	2.411371	-2.157753
C	0.390211	2.014820	1.059930
H	-0.105565	2.986711	1.151682
H	0.458012	1.627430	2.081349
C	0.474084	-0.023238	-0.449917
H	0.787291	0.321713	-1.440225
H	-0.047604	-0.963505	-0.609946
C	1.825240	2.253636	0.550224
H	1.801441	2.774802	-0.404661
H	2.336282	2.925155	1.250163
C	1.731575	-0.248417	0.383767
H	1.474907	-0.451766	1.422658
C	2.683292	0.959234	0.393875
Cl	3.575965	1.083405	-1.227550
C	3.750270	0.831650	1.479433
H	3.266051	0.828343	2.465066
H	4.443904	1.675865	1.440810
H	4.312471	-0.098371	1.366445
Br	2.623957	-1.941781	-0.148668

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56935769**

Number of imaginary frequencies = 0

1f_C002

B3LYP/6-31G* Geometry

C	1.589682	0.566071	-0.815945
C	2.805789	0.464083	1.458930
C	0.194306	0.906050	-0.075916
C	2.436656	-0.272344	0.173891
H	3.643410	1.141014	1.254105
H	1.916455	-1.199992	0.419827
C	1.639257	1.265441	1.964450
H	1.802514	1.696219	2.951633
C	0.491978	1.515719	1.315199
O	3.311675	-0.409230	2.465107
H	2.573094	-0.961191	2.770888
Br	4.135774	-0.955146	-0.639876
C	2.328647	1.872972	-1.187722
H	3.356601	1.639158	-1.480802
H	2.362263	2.584119	-0.357530
H	1.847573	2.367180	-2.036951
C	1.396151	-0.252012	-2.115230
H	2.334431	-0.272885	-2.673745
H	0.636662	0.184254	-2.770517
H	1.125057	-1.294476	-1.922751
C	-0.509549	2.426318	1.996846
H	-0.705548	3.330676	1.408303
H	-0.122920	2.748812	2.967786
H	-1.478316	1.947385	2.175581
C	-0.619386	1.889756	-0.977201
H	-0.214518	2.902232	-0.876703
H	-0.462516	1.616176	-2.023417
C	-0.629730	-0.419021	0.109691
H	-0.212357	-1.003496	0.933127
H	-0.536058	-1.035880	-0.785695
C	-2.141509	1.960413	-0.737078
H	-2.366410	2.478399	0.196380
H	-2.597949	2.556156	-1.535704
C	-2.128374	-0.243406	0.382639
H	-2.317032	0.203989	1.356740
C	-2.832799	0.582860	-0.701670
Cl	-4.576635	0.887804	-0.164422
C	-2.899846	-0.086653	-2.073904
H	-3.419465	-1.044685	-2.012729
H	-1.893425	-0.267270	-2.466862
H	-3.430022	0.560409	-2.777837
Br	-2.914624	-2.066357	0.584427

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56738028**

Number of imaginary frequencies = 0

1f_C003

B3LYP/6-31G* Geometry

C	1.57700	0.54755	-0.83688
C	2.81669	0.53239	1.42084
C	0.18684	0.90345	-0.09197
C	2.41942	-0.25167	0.17872
H	3.60568	1.25262	1.14705
H	1.91146	-1.16777	0.47877
C	1.63954	1.30153	1.94169
H	1.79738	1.72983	2.92974
C	0.49310	1.53820	1.28788
O	3.28918	-0.31824	2.45757
H	4.07955	-0.76340	2.10485
Br	4.13402	-0.97711	-0.60738
C	2.30834	1.84595	-1.25102
H	3.33879	1.61090	-1.53548
H	2.33480	2.58332	-0.44384
H	1.82513	2.30880	-2.11649
C	1.38158	-0.31116	-2.10854
H	2.31542	-0.33779	-2.67553
H	0.61226	0.09758	-2.77027
H	1.12258	-1.34983	-1.88285
C	-0.51348	2.45036	1.96049
H	-0.12650	2.78669	2.92650
H	-1.47802	1.96674	2.14883
H	-0.71757	3.34649	1.36193
C	-0.62888	1.86831	-1.01062
H	-0.22329	2.88258	-0.93262
H	-0.47638	1.57210	-2.05166
C	-0.63515	-0.41849	0.12636
H	-0.21590	-0.98065	0.96410
H	-0.54249	-1.05649	-0.75434
C	-2.14959	1.94453	-0.76585
H	-2.36978	2.47937	0.15915
H	-2.60896	2.52613	-1.57319
C	-2.13460	-0.23881	0.39508
H	-2.32326	0.22414	1.36167
C	-2.84101	0.56824	-0.70260
Cl	-4.58357	0.88525	-0.16746
C	-2.91335	-0.12682	-2.06187
H	-1.90856	-0.32194	-2.45208
H	-3.44027	0.50968	-2.77788
H	-3.43857	-1.08026	-1.98138
Br	-2.91988	-2.05842	0.62626

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56935904**

Number of imaginary frequencies = 0

1f_C004

B3LYP/6-31G* Geometry

C	1.554806	-0.647010	-0.959146
C	3.315111	-1.037970	0.923564
C	0.429105	-0.309567	0.134553
C	2.990593	-0.396115	-0.430689
H	4.050965	-0.413456	1.446681
H	3.707350	-0.773626	-1.158920
C	2.105833	-1.229220	1.788156
H	2.319875	-1.669732	2.763744
C	0.827290	-0.972625	1.474142
O	3.928109	-2.305448	0.612305
H	3.956024	-2.827372	1.430277
Br	3.531493	1.542705	-0.337942
C	1.386963	0.111679	-2.295200
H	2.137568	-0.252831	-3.006175
H	1.539320	1.187603	-2.198769
H	0.407854	-0.066589	-2.749390
C	1.509743	-2.164749	-1.313243
H	2.361978	-2.427663	-1.947620
H	0.601815	-2.399187	-1.876218
H	1.553852	-2.803577	-0.430189
C	-0.225768	-1.368270	2.490416
H	0.247680	-1.814720	3.369883
H	-0.920323	-2.113714	2.084134
H	-0.828604	-0.524891	2.841935
C	0.279087	1.235584	0.339804
H	1.116832	1.610231	0.929814
H	0.355221	1.730247	-0.631581
C	-0.935268	-0.871353	-0.399479
H	-0.967414	-1.958189	-0.290930
H	-0.997810	-0.677877	-1.472570
C	-1.027578	1.700699	1.002009
H	-1.085126	1.363485	2.040859
H	-1.040146	2.795904	1.035489
C	-2.222442	-0.311188	0.229590
H	-2.376526	-0.678463	1.239790
C	-2.283371	1.219858	0.250097
Cl	-3.742625	1.729982	1.269668
C	-2.447428	1.876240	-1.119879
H	-1.618537	1.603643	-1.781881
H	-2.458171	2.964550	-1.014672
H	-3.378037	1.555427	-1.591138
Br	-3.760806	-1.125313	-0.753588

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56038155**

Number of imaginary frequencies = 0

1f_C005

B3LYP/6-31G* Geometry

C	1.550521	-0.649456	-0.961292
C	3.308635	-1.043097	0.930785
C	0.425983	-0.313183	0.133707
C	2.983862	-0.397453	-0.430592
H	4.027019	-0.403731	1.460227
H	3.695985	-0.765358	-1.169852
C	2.099047	-1.247108	1.786166
H	2.320171	-1.720648	2.740567
C	0.823379	-0.981753	1.470292
O	3.889687	-2.344177	0.742183
H	4.815357	-2.216882	0.478516
Br	3.529866	1.547362	-0.340408
C	1.380948	0.108641	-2.297371
H	2.134712	-0.250490	-3.007949
H	1.526124	1.185519	-2.199996
H	0.403783	-0.075377	-2.753335
C	1.512649	-2.168226	-1.313358
H	2.356065	-2.423361	-1.963553
H	0.598937	-2.410217	-1.863493
H	1.575075	-2.807364	-0.431509
C	-0.231102	-1.384147	2.482794
H	0.243144	-1.838384	3.357434
H	-0.926154	-2.126186	2.071135
H	-0.833103	-0.542901	2.841465
C	0.278157	1.231608	0.341242
H	1.116374	1.603885	0.932151
H	0.352676	1.729829	-0.628564
C	-0.938758	-0.872167	-0.402514
H	-0.971715	-1.959127	-0.295965
H	-1.001924	-0.675915	-1.475147
C	-1.027210	1.694908	1.007401
H	-1.083068	1.352348	2.044530
H	-1.039131	2.789962	1.045920
C	-2.225137	-0.312717	0.228763
H	-2.378993	-0.683842	1.237521
C	-2.284195	1.218262	0.254886
Cl	-3.742005	1.726773	1.277460
C	-2.448904	1.879801	-1.112559
H	-1.621426	1.607791	-1.776590
H	-2.457489	2.967774	-1.003618
H	-3.380701	1.562236	-1.583654
Br	-3.764791	-1.121212	-0.757324

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56139646**

Number of imaginary frequencies = 0

1f_C006

B3LYP/6-31G* Geometry

C	1.553991	-0.647494	-0.961376
C	3.321639	-1.052422	0.919245
C	0.433513	-0.298940	0.134010
C	2.992741	-0.403879	-0.437215
H	4.081093	-0.445690	1.419285
H	3.709197	-0.774005	-1.169696
C	2.118033	-1.209134	1.796144
H	2.339509	-1.651423	2.766494
C	0.838964	-0.947296	1.480108
O	3.966609	-2.321829	0.728578
H	3.273688	-2.985129	0.585895
Br	3.531283	1.538887	-0.338396
C	1.389024	0.101073	-2.303273
H	2.119841	-0.290994	-3.020566
H	1.574601	1.172339	-2.216400
H	0.398880	-0.051591	-2.742797
C	1.486841	-2.167869	-1.307987
H	2.384621	-2.479770	-1.851572
H	0.630318	-2.376322	-1.955309
H	1.385796	-2.798851	-0.420092
C	-0.211872	-1.325269	2.505997
H	0.264559	-1.761953	3.388458
H	-0.912955	-2.072352	2.113827
H	-0.808458	-0.474205	2.849576
C	0.280475	1.248116	0.320211
H	1.117460	1.631193	0.905460
H	0.355560	1.731241	-0.657241
C	-0.931207	-0.869583	-0.391113
H	-0.961604	-1.955718	-0.272671
H	-0.997376	-0.685895	-1.465805
C	-1.026855	1.718370	0.977772
H	-1.081273	1.395606	2.021228
H	-1.041600	2.813869	0.996168
C	-2.218457	-0.306385	0.234704
H	-2.367920	-0.661265	1.249991
C	-2.283563	1.224698	0.235700
Cl	-3.741079	1.742828	1.252603
C	-2.453629	1.863529	-1.141888
H	-1.624695	1.587847	-1.802651
H	-2.469797	2.952892	-1.049489
H	-3.383643	1.532538	-1.607279
Br	-3.755802	-1.138056	-0.734573

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56188819**

Number of imaginary frequencies = 0

1f_C007

B3LYP/6-31G* Geometry

C	-1.573768	-0.974776	-0.399813
C	-2.689931	0.400583	1.473325
C	-0.164645	-0.850273	0.370488
C	-2.353056	0.300113	-0.012811
H	-3.539350	-0.271298	1.681462
H	-1.822762	1.198380	-0.324514
C	-1.537056	-0.050592	2.323380
H	-1.682752	0.116965	3.388891
C	-0.442782	-0.690161	1.887474
O	-3.037276	1.729363	1.843946
H	-3.836683	1.953295	1.336026
Br	-4.102162	0.511398	-1.002543
C	-2.349877	-2.235564	0.052064
H	-3.386522	-2.164370	-0.292427
H	-2.356905	-2.358714	1.137725
H	-1.924395	-3.142495	-0.387549
C	-1.417809	-1.065930	-1.931086
H	-2.404462	-1.157648	-2.392461
H	-0.842002	-1.951120	-2.215014
H	-0.942955	-0.184485	-2.372765
C	0.533314	-1.222742	2.916242
H	0.273508	-0.848019	3.910480
H	1.574567	-0.945568	2.719455
H	0.508058	-2.319416	2.964068
C	0.748431	-2.083872	0.060020
H	1.309943	-2.373357	0.951516
H	0.142980	-2.956718	-0.198024
C	0.604648	0.449754	-0.093940
H	0.231565	1.315974	0.453991
H	0.434197	0.648554	-1.156451
C	1.765499	-1.830231	-1.058182
H	2.307851	-2.751001	-1.292939
H	1.253449	-1.529031	-1.978315
C	2.113762	0.354122	0.145498
H	2.315604	0.150261	1.192052
C	2.795235	-0.722512	-0.737004
Cl	4.156126	-1.479697	0.284216
C	3.437562	-0.221929	-2.028798
H	2.694310	0.322433	-2.623434
H	3.796551	-1.073356	-2.614760
H	4.271770	0.450614	-1.828474
Br	2.915058	2.170149	-0.067255

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56281532**

Number of imaginary frequencies = 0

1f_C008

B3LYP/6-31G* Geometry

C	-1.590967	-0.984200	-0.344556
C	-2.661533	0.536655	1.451292
C	-0.173569	-0.832969	0.400525
C	-2.369969	0.320095	-0.038422
H	-3.557944	-0.035797	1.717014
H	-1.835965	1.183267	-0.436736
C	-1.523964	0.066033	2.317524
H	-1.671455	0.263559	3.378623
C	-0.435565	-0.603623	1.909624
O	-3.021689	1.885646	1.741285
H	-2.214284	2.422169	1.681286
Br	-4.115160	0.444898	-1.016658
C	-2.375246	-2.208042	0.187584
H	-3.405998	-2.159293	-0.176612
H	-2.399705	-2.250505	1.279122
H	-1.945447	-3.145758	-0.177188
C	-1.442300	-1.172444	-1.868283
H	-2.430880	-1.285889	-2.319393
H	-0.870940	-2.076433	-2.097305
H	-0.964290	-0.322682	-2.365952
C	0.531217	-1.112879	2.958152
H	0.278762	-0.696701	3.937753
H	1.577672	-0.864140	2.750527
H	0.484408	-2.206191	3.046996
C	0.733018	-2.083861	0.137369
H	1.291285	-2.345479	1.039375
H	0.121060	-2.960509	-0.089888
C	0.597965	0.437844	-0.132434
H	0.227718	1.334133	0.366751
H	0.428915	0.580828	-1.204034
C	1.753463	-1.881073	-0.988535
H	2.292945	-2.812949	-1.182498
H	1.244077	-1.618304	-1.921887
C	2.105028	0.351501	0.118720
H	2.300324	0.192557	1.174316
C	2.786888	-0.764595	-0.712293
Cl	4.139851	-1.479441	0.348221
C	3.436487	-0.322612	-2.021662
H	2.697666	0.196529	-2.643748
H	3.796242	-1.199747	-2.567707
H	4.271605	0.355947	-1.846775
Br	2.911005	2.156295	-0.167333

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56100406**

Number of imaginary frequencies = 0

1f_C009

B3LYP/6-31G* Geometry

C	-1.603656	-1.006041	-0.301920
C	-2.583485	0.675745	1.405907
C	-0.176658	-0.832936	0.417695
C	-2.356868	0.323569	-0.062871
H	-3.525746	0.213345	1.737304
H	-1.836555	1.152509	-0.539433
C	-1.479252	0.173476	2.299817
H	-1.616150	0.403060	3.357482
C	-0.422337	-0.556938	1.920372
O	-2.706558	2.101956	1.458185
H	-3.014410	2.343804	2.345321
Br	-4.139819	0.393203	-0.982710
C	-2.395142	-2.192187	0.298355
H	-3.418423	-2.173805	-0.088441
H	-2.442193	-2.156573	1.389337
H	-1.954063	-3.151412	0.010664
C	-1.471751	-1.268617	-1.816346
H	-2.465734	-1.386699	-2.254799
H	-0.916001	-2.190908	-2.007598
H	-0.983203	-0.449936	-2.354288
C	0.520572	-1.080975	2.982073
H	0.273754	-0.645502	3.954943
H	1.574506	-0.861102	2.778020
H	0.445022	-2.171618	3.083599
C	0.726221	-2.090920	0.179290
H	1.286566	-2.335342	1.084779
H	0.113032	-2.971664	-0.029084
C	0.583150	0.425718	-0.158883
H	0.201012	1.334242	0.308310
H	0.417521	0.527933	-1.235977
C	1.743495	-1.911432	-0.952857
H	2.285309	-2.845792	-1.127696
H	1.230406	-1.670896	-1.890330
C	2.088743	0.348865	0.100727
H	2.278247	0.212825	1.160916
C	2.773587	-0.785921	-0.702556
Cl	4.127930	-1.473729	0.375607
C	3.423248	-0.374812	-2.021861
H	2.683936	0.129010	-2.655860
H	3.783645	-1.264396	-2.547075
H	4.257473	0.308673	-1.862991
Br	2.899834	2.144181	-0.222705

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56026742**

Number of imaginary frequencies = 0

1g_C001

B3LYP/6-31G* Geometry

C	-1.392465	0.155414	0.770462
C	-2.919447	0.825284	-1.244049
C	-0.155271	0.961361	0.118078
C	-2.294753	-0.292699	-0.404890
H	-3.246775	0.373614	-2.195251
H	-1.742018	-0.958224	-1.068306
C	-1.879043	1.864710	-1.528941
H	-2.170688	2.600982	-2.275392
C	-0.685466	1.974121	-0.931654
O	-4.023397	1.485686	-0.635902
H	-4.687692	0.798123	-0.449614
Br	-3.809791	-1.498132	0.172586
C	-2.181535	1.051951	1.752679
H	-3.140056	0.579259	1.984013
H	-2.394208	2.039736	1.340081
H	-1.637436	1.167464	2.695545
C	-0.956125	-1.108437	1.544948
H	-1.823902	-1.549175	2.041231
H	-0.226140	-0.875796	2.321898
H	-0.542294	-1.881393	0.889003
C	0.211438	3.120391	-1.363177
H	0.234494	3.922158	-0.614687
H	-0.158843	3.557722	-2.294641
H	1.249459	2.810231	-1.528412
C	0.678968	1.745425	1.185426
H	1.208206	2.548739	0.672990
H	0.015412	2.238373	1.900069
C	0.832786	0.031831	-0.685140
H	1.349710	0.640015	-1.431853
H	0.277029	-0.719884	-1.251637
C	1.759572	0.970027	1.952122
H	2.330395	1.675186	2.566894
H	1.328001	0.240785	2.647066
C	1.913517	-0.688534	0.126863
H	1.489021	-1.468533	0.756486
C	2.747719	0.204585	1.049790
Cl	3.692642	1.446148	0.047386
C	3.772127	-0.570074	1.875953
H	3.256635	-1.322738	2.485978
H	4.310408	0.106820	2.545220
H	4.490866	-1.080367	1.232139
Br	3.036378	-1.741446	-1.143957

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56550950**

Number of imaginary frequencies = 0

1g_C002

B3LYP/6-31G* Geometry

C	-1.438872	0.097591	0.801610
C	-2.884989	0.975192	-1.186263
C	-0.171428	0.918662	0.243442
C	-2.319335	-0.230992	-0.425000
H	-3.179006	0.618281	-2.187432
H	-1.767328	-0.857443	-1.126176
C	-1.819945	2.019982	-1.334333
H	-2.084299	2.836855	-2.002909
C	-0.639446	2.043714	-0.702112
O	-4.001988	1.604040	-0.568237
H	-4.680001	0.914181	-0.452896
Br	-3.881102	-1.430251	0.016400
C	-2.228170	0.936089	1.833068
H	-3.165291	0.424710	2.071917
H	-2.482760	1.927152	1.454859
H	-1.664055	1.042433	2.764442
C	-1.016289	-1.222793	1.483558
H	-1.899814	-1.728109	1.880571
H	-0.345206	-1.045067	2.329813
H	-0.528576	-1.920960	0.795051
C	0.294529	3.200718	-0.988592
H	-0.148927	3.870955	-1.730373
H	1.263397	2.868919	-1.381064
H	0.496972	3.796250	-0.090269
C	0.627187	1.492270	1.464170
H	0.167031	2.426401	1.801536
H	0.528180	0.800848	2.306148
C	0.799861	-0.000392	-0.591100
H	1.229842	0.564029	-1.423998
H	0.254561	-0.830208	-1.043292
C	2.131148	1.751904	1.239998
H	2.270707	2.586590	0.556072
H	2.569148	2.066065	2.194565
C	1.950605	-0.551208	0.246777
H	1.575327	-1.039330	1.145574
C	2.943855	0.526538	0.708845
Cl	3.954775	1.107039	-0.735616
C	3.925370	-0.009612	1.749425
H	3.369670	-0.316630	2.645347
H	4.639883	0.765937	2.038057
H	4.471684	-0.874510	1.366264
Br	2.823076	-2.062186	-0.705583

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56194954**

Number of imaginary frequencies = 0

1g_C003

B3LYP/6-31G* Geometry

C	1.188390	-0.469747	-1.057905
C	3.191239	-1.555040	0.147733
C	0.361240	-0.300224	0.312379
C	2.725408	-0.488153	-0.841599
H	3.078193	-2.519789	-0.367943
H	3.225651	-0.617541	-1.801929
C	2.325201	-1.548023	1.371907
H	2.764923	-2.052120	2.231114
C	1.084385	-1.048615	1.464742
O	4.575864	-1.503996	0.442068
H	4.753850	-0.615586	0.798916
Br	3.507718	1.284868	-0.261804
C	0.902325	0.593951	-2.141038
H	1.494702	0.360621	-3.034224
H	1.183971	1.599054	-1.823288
H	-0.145238	0.600387	-2.450526
C	0.881609	-1.850886	-1.711273
H	1.598203	-2.059721	-2.513876
H	-0.113294	-1.854486	-2.166202
H	0.926043	-2.674969	-0.993996
C	0.351900	-1.246685	2.782158
H	1.068231	-1.461344	3.580412
H	-0.341526	-2.095965	2.734085
H	-0.238229	-0.377814	3.089393
C	0.184551	1.190631	0.772941
H	-0.040870	1.182546	1.842346
H	1.130873	1.722314	0.673950
C	-1.081425	-0.915439	0.218749
H	-1.471077	-1.032472	1.230490
H	-1.055810	-1.917816	-0.208936
C	-0.927681	2.007571	0.094393
H	-1.032044	2.964419	0.618198
H	-0.666734	2.254328	-0.939500
C	-2.111959	-0.074554	-0.531390
H	-1.859869	0.045588	-1.585742
C	-2.311603	1.331321	0.049539
Cl	-2.946024	1.208695	1.788445
C	-3.318419	2.173397	-0.730532
H	-2.990224	2.262594	-1.773988
H	-3.385509	3.177904	-0.303501
H	-4.308718	1.714396	-0.718166
Br	-3.815459	-1.111080	-0.631397

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56527165**

Number of imaginary frequencies = 0

1g_C004

B3LYP/6-31G* Geometry

C	-1.40030	0.15274	0.76806
C	-2.93299	0.83199	-1.22886
C	-0.16246	0.95955	0.12145
C	-2.31948	-0.29081	-0.40353
H	-3.30260	0.39162	-2.16830
H	-1.75451	-0.92703	-1.08501
C	-1.87631	1.85413	-1.53527
H	-2.14335	2.57597	-2.30878
C	-0.68552	1.97124	-0.93199
O	-4.03606	1.41993	-0.53002
H	-4.30380	2.20730	-1.02963
Br	-3.79356	-1.52339	0.16309
C	-2.18006	1.03983	1.76614
H	-3.15049	0.58210	1.97433
H	-2.37019	2.04113	1.37504
H	-1.64006	1.12559	2.71494
C	-0.95956	-1.11797	1.52887
H	-1.82411	-1.56093	2.02757
H	-0.22190	-0.89122	2.30044
H	-0.55407	-1.88703	0.86311
C	0.21510	3.11294	-1.36677
H	-0.14644	3.54404	-2.30491
H	1.25400	2.80074	-1.52043
H	0.23363	3.91992	-0.62357
C	0.67002	1.74307	1.19075
H	1.19818	2.55013	0.68284
H	0.00423	2.23008	1.90737
C	0.82593	0.03097	-0.68365
H	1.34148	0.63712	-1.43294
H	0.26810	-0.72186	-1.24651
C	1.75147	0.96722	1.95573
H	2.32113	1.67132	2.57283
H	1.31978	0.23565	2.64801
C	1.90871	-0.68766	0.12700
H	1.48581	-1.47017	0.75443
C	2.74075	0.20533	1.05190
Cl	3.68352	1.45175	0.05160
C	3.76724	-0.56851	1.87614
H	3.25346	-1.32367	2.48446
H	4.30392	0.10818	2.54690
H	4.48702	-1.07575	1.23110
Br	3.03454	-1.73452	-1.14641

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56139312**

Number of imaginary frequencies = 0

1g_C005

B3LYP/6-31G* Geometry

C	-1.398204	0.161161	0.771992
C	-2.912311	0.798970	-1.267122
C	-0.159521	0.963471	0.127382
C	-2.304045	-0.309990	-0.399270
H	-3.236826	0.338237	-2.206839
H	-1.729965	-0.968231	-1.052246
C	-1.870097	1.842631	-1.544827
H	-2.155920	2.571698	-2.301666
C	-0.688996	1.976337	-0.923134
O	-4.104665	1.396124	-0.761138
H	-3.855138	1.982275	-0.030712
Br	-3.788021	-1.515355	0.188849
C	-2.193467	1.070526	1.741554
H	-3.188076	0.646785	1.909537
H	-2.302971	2.093503	1.365103
H	-1.698721	1.137052	2.715524
C	-0.965069	-1.087477	1.571976
H	-1.834439	-1.521436	2.070332
H	-0.235622	-0.840927	2.345213
H	-0.551153	-1.870511	0.928718
C	0.196454	3.137768	-1.335880
H	0.209929	3.931301	-0.578107
H	-0.172951	3.581758	-2.264548
H	1.238120	2.838670	-1.498992
C	0.675845	1.740395	1.200219
H	1.198137	2.553340	0.695920
H	0.014106	2.220634	1.926004
C	0.826525	0.036634	-0.681238
H	1.343063	0.648008	-1.425668
H	0.268168	-0.711019	-1.249942
C	1.764573	0.964460	1.956171
H	2.337987	1.669614	2.568489
H	1.340052	0.232524	2.652377
C	1.907616	-0.688404	0.125703
H	1.482557	-1.467659	0.756216
C	2.747322	0.202402	1.045957
Cl	3.684597	1.448340	0.041047
C	3.777444	-0.573575	1.863593
H	3.266479	-1.329585	2.473255
H	4.318457	0.101458	2.532514
H	4.493151	-1.080248	1.213659
Br	3.023059	-1.740642	-1.150886

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56308421**

Number of imaginary frequencies = 0

1g_C006

B3LYP/6-31G* Geometry

C	-1.449300	0.098687	0.801649
C	-2.893903	0.978397	-1.175750
C	-0.177905	0.914423	0.249329
C	-2.343048	-0.228839	-0.422794
H	-3.226568	0.628769	-2.165846
H	-1.775426	-0.827844	-1.135202
C	-1.810715	2.006734	-1.344804
H	-2.046640	2.811246	-2.043163
C	-0.634557	2.037359	-0.703192
O	-4.018039	1.529580	-0.480150
H	-4.279039	2.335708	-0.952696
Br	-3.866282	-1.452831	0.006686
C	-2.231430	0.934213	1.840987
H	-3.188855	0.447858	2.046518
H	-2.449488	1.941601	1.483037
H	-1.680037	1.003280	2.783804
C	-1.028275	-1.225040	1.478444
H	-1.911241	-1.725369	1.881461
H	-0.347561	-1.051336	2.317994
H	-0.552240	-1.925834	0.784443
C	0.306319	3.187411	-0.992762
H	-0.124190	3.851925	-1.747683
H	1.278556	2.847147	-1.368617
H	0.500382	3.791269	-0.098020
C	0.618501	1.486758	1.471662
H	0.157075	2.419848	1.810620
H	0.515971	0.793350	2.311296
C	0.792078	-0.008247	-0.583796
H	1.218661	0.549694	-1.422725
H	0.244499	-0.841354	-1.026852
C	2.123737	1.746798	1.256226
H	2.269035	2.591967	0.586353
H	2.558015	2.045208	2.217553
C	1.946848	-0.553142	0.251978
H	1.575540	-1.043161	1.151544
C	2.937586	0.528279	0.710450
Cl	3.931567	1.121220	-0.741893
C	3.933275	-0.006002	1.738467
H	3.388229	-0.324273	2.636967
H	4.643075	0.774256	2.026199
H	4.484107	-0.863131	1.344671
Br	2.824012	-2.059025	-0.704538

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55773159**

Number of imaginary frequencies = 0

1g_C007

B3LYP/6-31G* Geometry

C	-1.57720	-0.75167	0.53400
C	-2.51465	1.60701	-0.07467
C	-0.08139	-0.12325	0.59018
C	-2.35760	0.12934	-0.46515
H	-2.69808	2.17655	-1.00134
H	-1.89322	0.06971	-1.44879
C	-1.26797	2.10322	0.59934
H	-1.32566	3.14989	0.89060
C	-0.20628	1.37539	0.97264
O	-3.56760	1.86343	0.84991
H	-4.38267	1.50963	0.45131
Br	-4.20017	-0.58368	-0.88231
C	-2.22705	-0.73701	1.93555
H	-3.28730	-0.99109	1.84495
H	-2.16449	0.23957	2.41665
H	-1.75983	-1.48527	2.58403
C	-1.60637	-2.21607	0.03192
H	-2.60677	-2.62735	0.18489
H	-0.91066	-2.85544	0.58235
H	-1.39173	-2.31472	-1.03712
C	0.83253	2.05986	1.83857
H	0.95298	1.55259	2.80325
H	0.51852	3.08581	2.05106
H	1.81266	2.10590	1.36010
C	0.75055	-0.91081	1.65030
H	0.48531	-0.56704	2.65428
H	0.46238	-1.96427	1.62249
C	0.58046	-0.28314	-0.83202
H	0.22839	0.50786	-1.49796
H	0.23649	-1.22647	-1.26609
C	2.28549	-0.84397	1.50424
H	2.66153	0.15841	1.71648
H	2.74109	-1.51586	2.23999
C	2.11433	-0.33489	-0.95583
H	2.37699	-0.68764	-1.95377
C	2.75273	-1.24988	0.10379
Cl	4.59178	-1.11770	0.04978
C	2.44676	-2.71904	-0.23196
H	1.37102	-2.91416	-0.24518
H	2.90271	-3.37268	0.51697
H	2.85626	-2.98392	-1.21097
Br	2.87870	1.50976	-0.97796

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55893989**

Number of imaginary frequencies = 0

1g_C008

B3LYP/6-31G* Geometry

C	-1.441661	0.096638	0.797306
C	-2.885762	0.957628	-1.206098
C	-0.175408	0.917693	0.246329
C	-2.334056	-0.245737	-0.424609
H	-3.180080	0.595478	-2.197557
H	-1.765461	-0.864378	-1.119945
C	-1.818417	2.005306	-1.346012
H	-2.078605	2.818929	-2.021444
C	-0.644770	2.043863	-0.697446
O	-4.087968	1.528991	-0.695196
H	-3.869633	2.001953	0.122176
Br	-3.865100	-1.445811	0.032383
C	-2.227654	0.942017	1.828988
H	-3.214818	0.498875	1.991662
H	-2.353866	1.980841	1.505910
H	-1.714712	0.966892	2.794919
C	-1.021802	-1.218646	1.490757
H	-1.904781	-1.717918	1.895304
H	-0.341820	-1.038055	2.329312
H	-0.544472	-1.923077	0.801709
C	0.280420	3.211412	-0.968774
H	-0.164463	3.885022	-1.706732
H	1.252328	2.888684	-1.361327
H	0.478279	3.800101	-0.064773
C	0.622585	1.487695	1.469841
H	0.164442	2.421847	1.810948
H	0.522554	0.793931	2.309730
C	0.795835	0.002087	-0.591413
H	1.225602	0.569639	-1.422316
H	0.249031	-0.825195	-1.046080
C	2.126770	1.747610	1.248315
H	2.266981	2.585735	0.568594
H	2.564358	2.056800	2.204670
C	1.946631	-0.551940	0.244259
H	1.571252	-1.044818	1.140447
C	2.939274	0.524454	0.711276
Cl	3.949314	1.112781	-0.729951
C	3.920914	-0.016376	1.749409
H	3.365378	-0.328636	2.643620
H	4.635146	0.757879	2.042199
H	4.467627	-0.878989	1.361735
Br	2.820464	-2.056273	-0.715948

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55924364**

Number of imaginary frequencies = 0

1g_C009

B3LYP/6-31G* Geometry

C	1.194092	-0.454094	-1.058503
C	3.181700	-1.547197	0.128264
C	0.363505	-0.296467	0.311691
C	2.735253	-0.460478	-0.835896
H	3.026899	-2.502749	-0.405333
H	3.230285	-0.593540	-1.798707
C	2.330846	-1.540009	1.362576
H	2.765142	-2.040580	2.229001
C	1.088065	-1.048659	1.460228
O	4.572593	-1.409391	0.393348
H	4.826829	-2.134401	0.985572
Br	3.499048	1.298421	-0.251395
C	0.907826	0.620659	-2.130707
H	1.500564	0.395288	-3.025765
H	1.192336	1.621240	-1.802825
H	-0.139770	0.629070	-2.440370
C	0.881904	-1.825264	-1.728021
H	1.601642	-2.027706	-2.529510
H	-0.110991	-1.819268	-2.187885
H	0.917762	-2.659723	-1.022051
C	0.358601	-1.253863	2.777974
H	1.075929	-1.467405	3.575898
H	-0.332264	-2.105176	2.727748
H	-0.234107	-0.387985	3.087816
C	0.182795	1.190772	0.782613
H	-0.040993	1.176619	1.852292
H	1.128065	1.724057	0.682847
C	-1.076785	-0.916610	0.213844
H	-1.467288	-1.041936	1.224390
H	-1.047933	-1.915686	-0.221467
C	-0.932731	2.007469	0.109637
H	-1.040681	2.960440	0.639755
H	-0.671975	2.261939	-0.922369
C	-2.109123	-0.073785	-0.531379
H	-1.855589	0.054815	-1.584345
C	-2.314363	1.326938	0.059355
Cl	-2.949852	1.189046	1.797405
C	-3.324145	2.170896	-0.714756
H	-2.995584	2.269282	-1.757259
H	-3.395053	3.171891	-0.280189
H	-4.312772	1.708143	-0.706435
Br	-3.809287	-1.116054	-0.641891

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56014069**

Number of imaginary frequencies = 0

1g_C010

B3LYP/6-31G* Geometry

C	-1.583752	-0.737225	0.539160
C	-2.529459	1.606414	-0.079716
C	-0.088239	-0.114635	0.590980
C	-2.380808	0.135696	-0.463367
H	-2.754842	2.175565	-0.995615
H	-1.895857	0.090562	-1.437712
C	-1.265753	2.112892	0.560840
H	-1.290508	3.174783	0.812033
C	-0.206660	1.389271	0.952309
O	-3.618743	1.759706	0.839251
H	-3.592395	2.673207	1.165376
Br	-4.190899	-0.602047	-0.894532
C	-2.226368	-0.723505	1.944228
H	-3.293382	-0.945195	1.854825
H	-2.135499	0.245053	2.437752
H	-1.774034	-1.490049	2.582206
C	-1.612084	-2.203715	0.042179
H	-2.607044	-2.619878	0.212983
H	-0.901262	-2.835886	0.581896
H	-1.417780	-2.303622	-1.030569
C	0.835550	2.083938	1.805103
H	0.532088	3.117637	1.996169
H	1.816856	2.110679	1.328099
H	0.949127	1.594483	2.779833
C	0.742225	-0.890199	1.661171
H	0.476609	-0.534574	2.661086
H	0.451122	-1.943021	1.645579
C	0.576065	-0.290712	-0.828184
H	0.225531	0.492031	-1.504494
H	0.229991	-1.238275	-1.250702
C	2.277637	-0.829157	1.516464
H	2.657227	0.173956	1.719131
H	2.730304	-1.494883	2.259585
C	2.109783	-0.347864	-0.950178
H	2.372360	-0.713434	-1.943490
C	2.745890	-1.251003	0.121056
Cl	4.585539	-1.122244	0.068016
C	2.437903	-2.723383	-0.198457
H	1.361886	-2.916811	-0.210296
H	2.892294	-3.369265	0.558139
H	2.847719	-2.999819	-1.174111
Br	2.880147	1.495086	-0.996882

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55461365**

Number of imaginary frequencies = 0

1g_C011

B3LYP/6-31G* Geometry

C	-1.304983	-1.149300	-0.488845
C	-3.354842	0.133857	-1.360713
C	-0.400629	0.175670	-0.486373
C	-2.812084	-0.840975	-0.306243
H	-3.500257	-0.470467	-2.268870
H	-3.379293	-1.771730	-0.333158
C	-2.367459	1.217163	-1.694973
H	-2.786680	2.009549	-2.313368
C	-1.054506	1.227354	-1.416229
O	-4.655223	0.624528	-1.088450
H	-4.620244	1.042908	-0.209954
Br	-3.320449	-0.183043	1.534360
C	-0.880692	-2.214438	0.544130
H	-1.518030	-3.099630	0.430321
H	-0.986556	-1.878650	1.577804
H	0.149367	-2.544795	0.378519
C	-1.231398	-1.850572	-1.883869
H	-2.057414	-2.561983	-1.996301
H	-0.310085	-2.429948	-1.984796
H	-1.278246	-1.138630	-2.711738
C	-0.214500	2.330863	-2.030921
H	-0.861467	3.114006	-2.437005
H	0.393385	1.952402	-2.863254
H	0.481121	2.801839	-1.331409
C	-0.276284	0.816488	0.950830
H	-1.145505	1.445086	1.145955
H	-0.311704	0.027975	1.706997
C	1.060035	-0.171633	-0.960180
H	1.475944	0.640033	-1.560013
H	1.069761	-1.050527	-1.602132
C	0.989047	1.659773	1.195360
H	0.984753	2.540504	0.553663
H	0.957407	2.038944	2.223430
C	2.013624	-0.398718	0.211992
H	1.592525	-1.104614	0.927224
C	2.328187	0.884806	0.997650
Cl	3.468735	1.967584	0.016262
C	3.027246	0.584014	2.321955
H	2.353050	0.000504	2.962761
H	3.277953	1.511512	2.843534
H	3.940521	0.006179	2.161419
Br	3.641261	-1.358435	-0.403786

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55546329**

Number of imaginary frequencies = 0

1h_C001

B3LYP/6-31G* Geometry

C	-1.505557	0.220468	0.825132
C	-2.737068	0.641317	-1.437892
C	-0.153485	0.852473	0.201739
C	-2.294550	-0.363452	-0.365934
H	-2.929985	0.071540	-2.362546
H	-1.713159	-1.153349	-0.841530
C	-1.643941	1.639333	-1.685176
H	-1.857679	2.328971	-2.499450
C	-0.524399	1.797478	-0.965764
O	-3.894662	1.399642	-1.104643
H	-4.596579	0.756953	-0.896943
Br	-3.935069	-1.387197	0.207658
C	-2.320712	1.306991	1.562131
H	-3.307266	0.908977	1.816358
H	-2.473726	2.199873	0.953888
H	-1.828042	1.591012	2.497050
C	-1.214783	-0.920984	1.830443
H	-2.121415	-1.142788	2.398527
H	-0.434501	-0.653269	2.547019
H	-0.913510	-1.851796	1.339972
C	0.378792	2.954643	-1.347537
H	-0.059890	3.513651	-2.178817
H	1.379434	2.637657	-1.664043
H	0.513385	3.656992	-0.516449
C	0.608837	1.601868	1.340131
H	0.123578	2.563043	1.538531
H	0.513757	1.021332	2.260003
C	0.755928	-0.308124	-0.342919
H	0.358324	-0.681951	-1.289586
H	0.748804	-1.140379	0.362061
C	2.112142	1.853820	1.130220
H	2.281225	2.639547	0.386952
H	2.543037	2.222139	2.067932
C	2.220027	0.063323	-0.567349
H	2.332866	0.796149	-1.368090
C	2.927933	0.632387	0.667368
Cl	2.919464	-0.619541	2.033352
C	4.387225	1.005394	0.414754
H	4.972089	0.129805	0.127494
H	4.826448	1.449142	1.312562
H	4.442802	1.740990	-0.397807
Br	3.156442	-1.530825	-1.318487

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56856666**

Number of imaginary frequencies = 0

1h_C002

B3LYP/6-31G* Geometry

C	-1.512539	0.208298	0.821895
C	-2.757457	0.672263	-1.414829
C	-0.160497	0.849069	0.211937
C	-2.320384	-0.354363	-0.374440
H	-3.000700	0.129967	-2.342228
H	-1.722557	-1.110120	-0.883744
C	-1.644510	1.651759	-1.669578
H	-1.829689	2.338045	-2.497674
C	-0.526265	1.807155	-0.946080
O	-3.925718	1.367783	-0.963898
H	-4.144571	2.029448	-1.638823
Br	-3.917889	-1.418100	0.186232
C	-2.320031	1.279339	1.589512
H	-3.319166	0.891245	1.804987
H	-2.444963	2.199594	1.016081
H	-1.837797	1.517099	2.542916
C	-1.218488	-0.953637	1.802534
H	-2.120593	-1.180601	2.374856
H	-0.428078	-0.703094	2.514498
H	-0.930488	-1.877478	1.291552
C	0.380099	2.964845	-1.317747
H	0.509304	3.662637	-0.481848
H	-0.050834	3.528989	-2.150060
H	1.382768	2.648878	-1.627601
C	0.601163	1.584327	1.359896
H	0.114333	2.541814	1.572417
H	0.506023	0.990803	2.271396
C	0.751669	-0.302628	-0.347983
H	0.354421	-0.665979	-1.298824
H	0.743908	-1.143174	0.346897
C	2.104327	1.841389	1.154613
H	2.273718	2.638041	0.422973
H	2.534144	2.196918	2.097755
C	2.215804	0.072332	-0.566361
H	2.330246	0.814078	-1.358589
C	2.922442	0.627566	0.675627
Cl	2.917479	-0.640918	2.025571
C	4.380824	1.007230	0.427064
H	4.967366	0.136803	0.127782
H	4.819720	1.439960	1.330394
H	4.434285	1.753749	-0.375683
Br	3.154771	-1.512013	-1.335355

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56406678**

Number of imaginary frequencies = 0

1h_C003

B3LYP/6-31G* Geometry

C	1.3322660	-0.3326400	-1.2141210
C	3.1942760	-1.5776420	0.0383060
C	0.3543030	-0.3480510	0.0635180
C	2.8318740	-0.3713590	-0.8314380
H	3.2115640	-2.4427350	-0.6407440
H	3.4416270	-0.3582390	-1.7356770
C	2.1480770	-1.8284040	1.0870130
H	2.4661150	-2.5269470	1.8594790
C	0.8899390	-1.3610280	1.1030070
O	4.5099880	-1.5483760	0.5614830
H	4.5981580	-0.7107410	1.0504650
Br	3.5055110	1.3010700	0.0812660
C	1.0986010	0.8614990	-2.1663810
H	1.6194980	0.6739240	-3.1128850
H	1.4908390	1.7970320	-1.7631750
H	0.0394680	1.0045470	-2.3978660
C	1.1175370	-1.6255800	-2.0629120
H	1.9270400	-1.7384300	-2.7930640
H	0.1855440	-1.5651690	-2.6303770
H	1.0824960	-2.5306990	-1.4504170
C	-0.0186010	-1.8748140	2.2038600
H	0.5424420	-2.5248670	2.8814630
H	-0.8479040	-2.4709450	1.8023160
H	-0.4575830	-1.0764540	2.8109670
C	0.2513630	1.0784690	0.7140490
H	1.1259080	1.2518780	1.3422370
H	0.2916800	1.8265300	-0.0790690
C	-1.0689330	-0.7693490	-0.4574060
H	-1.1045660	-1.8496020	-0.6195360
H	-1.2411090	-0.3053700	-1.4306040
C	-1.0067670	1.3873710	1.5382830
H	-1.0132630	0.8320040	2.4840890
H	-0.9951510	2.4489110	1.8104280
C	-2.2693060	-0.3917060	0.4137870
H	-2.3023130	-0.9752780	1.3328580
C	-2.3380140	1.0780450	0.8322770
Cl	-2.4697610	2.1610800	-0.6651490
C	-3.5352100	1.4018430	1.7225400
H	-4.4751590	1.2015980	1.2051910
H	-3.5106220	2.4527210	2.0239520
H	-3.4983680	0.7815330	2.6271740
Br	-3.9214750	-1.0012560	-0.5289180

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56604176**

Number of imaginary frequencies = 0

1h_C004

B3LYP/6-31G* Geometry

C	1.339358	-0.314919	-1.211805
C	3.187575	-1.568367	0.019221
C	0.356918	-0.340211	0.062830
C	2.842002	-0.345342	-0.819430
H	3.173709	-2.421373	-0.683634
H	3.447010	-0.336873	-1.727137
C	2.151069	-1.823506	1.075374
H	2.458008	-2.527405	1.850376
C	0.893106	-1.357968	1.097007
O	4.506730	-1.444756	0.538573
H	4.717452	-2.277127	0.990183
Br	3.500871	1.310538	0.093053
C	1.107406	0.888731	-2.152143
H	1.625922	0.707584	-3.101357
H	1.506102	1.817214	-1.740028
H	0.048148	1.036579	-2.380618
C	1.120075	-1.596390	-2.075198
H	1.933600	-1.705506	-2.801480
H	0.191993	-1.524870	-2.648072
H	1.074956	-2.509482	-1.474848
C	-0.012156	-1.875630	2.198430
H	0.549490	-2.527454	2.874204
H	-0.842678	-2.470174	1.797254
H	-0.448750	-1.078345	2.808210
C	0.246536	1.082053	0.721044
H	1.121338	1.258715	1.347645
H	0.283266	1.832602	-0.069603
C	-1.064223	-0.763715	-0.462348
H	-1.096222	-1.842790	-0.633368
H	-1.236441	-0.292561	-1.432053
C	-1.013774	1.381303	1.545483
H	-1.019381	0.822553	2.489441
H	-1.006821	2.441725	1.822147
C	-2.267107	-0.397043	0.410123
H	-2.299004	-0.986222	1.325634
C	-2.343638	1.069715	0.837471
Cl	-2.481750	2.160692	-0.653311
C	-3.542631	1.381678	1.729613
H	-4.481616	1.180036	1.210996
H	-3.523215	2.430714	2.037712
H	-3.502647	0.755963	2.630427
Br	-3.916339	-1.009954	-0.537292

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56067155**

Number of imaginary frequencies = 0

1i_C001

B3LYP/6-31G* Geometry

C	-1.330344	-0.421858	-0.227753
C	-3.139822	1.459487	-0.071708
C	-0.176875	0.642359	0.148171
C	-2.633069	0.102653	0.424356
H	-3.854456	1.834150	0.680070
H	-2.516169	0.149934	1.507229
C	-1.985894	2.410087	-0.164485
H	-2.269454	3.449014	-0.321139
C	-0.688019	2.085017	-0.109269
O	-3.772898	1.433364	-1.345650
H	-4.510562	0.801265	-1.274284
Br	-4.181786	-1.185873	0.261629
C	-1.055798	-1.836969	0.327509
H	-1.823534	-2.525202	-0.033652
H	-1.084404	-1.872467	1.421172
H	-0.093482	-2.227456	-0.008949
C	-1.501284	-0.548947	-1.759308
H	-2.437618	-1.070852	-1.974972
H	-0.689598	-1.140752	-2.194452
H	-1.544116	0.420378	-2.259114
C	0.322440	3.209885	-0.244854
H	-0.170672	4.176988	-0.112543
H	0.790434	3.217965	-1.237123
H	1.134354	3.144598	0.487933
C	0.235424	0.603307	1.663861
H	0.627506	1.589497	1.929334
H	-0.651403	0.466150	2.291713
C	1.117919	0.435790	-0.717726
H	1.681941	1.367536	-0.728440
H	0.855882	0.232973	-1.756630
C	1.294167	-0.430220	2.085957
H	1.591183	-0.230990	3.121791
H	0.883124	-1.444727	2.072169
C	2.105142	-0.628432	-0.239333
H	1.709687	-1.639433	-0.333992
C	2.562891	-0.461050	1.214800
Cl	3.442071	1.158494	1.422344
C	3.527719	-1.551123	1.675484
H	3.050051	-2.533058	1.566238
H	3.788354	-1.409089	2.727982
H	4.440981	-1.543438	1.077858
Br	3.634139	-0.665390	-1.521545

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56540596**

Number of imaginary frequencies = 0

1i_C002

B3LYP/6-31G* Geometry

C	-1.337652	-0.416631	-0.237372
C	-3.144620	1.455800	-0.065520
C	-0.182305	0.636388	0.157565
C	-2.655171	0.094351	0.409487
H	-3.891777	1.813303	0.660704
H	-2.527863	0.151707	1.490608
C	-1.986989	2.411092	-0.105208
H	-2.260311	3.462929	-0.203446
C	-0.687746	2.085901	-0.065675
O	-3.768242	1.342305	-1.349374
H	-3.922012	2.243477	-1.674102
Br	-4.176450	-1.200167	0.253809
C	-1.065874	-1.837193	0.305660
H	-1.827607	-2.522529	-0.071680
H	-1.109308	-1.885261	1.398425
H	-0.097507	-2.219687	-0.022969
C	-1.494114	-0.532092	-1.771447
H	-2.443879	-1.022053	-2.000348
H	-0.691940	-1.141517	-2.200709
H	-1.503332	0.440790	-2.266767
C	0.323735	3.212556	-0.171445
H	-0.166024	4.177455	-0.011037
H	0.789950	3.246244	-1.164173
H	1.137654	3.124952	0.556506
C	0.226936	0.569203	1.673821
H	0.615194	1.550561	1.961866
H	-0.661779	0.415301	2.294931
C	1.113037	0.445600	-0.711286
H	1.677646	1.377126	-0.708492
H	0.850169	0.257268	-1.752693
C	1.287482	-0.469947	2.077296
H	1.583378	-0.289142	3.116841
H	0.877406	-1.484285	2.044517
C	2.100896	-0.625546	-0.250160
H	1.706280	-1.635003	-0.363164
C	2.556816	-0.482867	1.206939
Cl	3.432458	1.135684	1.443638
C	3.524120	-1.578024	1.649842
H	3.049358	-2.559146	1.522481
H	3.782520	-1.453890	2.705143
H	4.438353	-1.557204	1.054042
Br	3.631258	-0.638348	-1.531761

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56125328**

Number of imaginary frequencies = 0

1i_C003

B3LYP/6-31G* Geometry

C	1.392537	-0.687317	1.198236
C	3.496356	-0.840777	-0.282332
C	0.412842	-1.045309	-0.027680
C	2.719607	-0.019804	0.745034
H	3.906487	-1.704294	0.261186
H	3.341091	0.180317	1.618623
C	2.577005	-1.328936	-1.361607
H	3.085261	-1.643572	-2.271700
C	1.245778	-1.458462	-1.271770
O	4.652022	-0.192975	-0.783736
H	4.354240	0.646406	-1.177712
Br	2.500892	1.849094	0.010659
C	1.848590	-1.988284	1.923091
H	2.673172	-1.770959	2.611754
H	2.181605	-2.763829	1.227800
H	1.032954	-2.401462	2.523587
C	0.785986	0.223163	2.289913
H	1.531571	0.374052	3.080302
H	-0.089800	-0.224090	2.766346
H	0.522867	1.212364	1.910702
C	0.526086	-2.068794	-2.464257
H	1.155144	-1.999768	-3.356378
H	-0.429083	-1.586081	-2.694003
H	0.309177	-3.132589	-2.303678
C	-0.550324	-2.236648	0.293667
H	-0.954297	-2.598779	-0.652911
H	-0.001622	-3.079588	0.720238
C	-0.497615	0.157721	-0.482351
H	-0.848990	-0.040636	-1.496992
H	0.090063	1.072023	-0.540599
C	-1.764929	-1.917096	1.173515
H	-2.380947	-2.817125	1.279733
H	-1.465958	-1.627912	2.188680
C	-1.742742	0.424384	0.368907
H	-1.482669	0.817800	1.349687
C	-2.651967	-0.785078	0.615863
Cl	-3.381420	-1.370919	-0.985166
C	-3.821011	-0.477325	1.548718
H	-3.435177	-0.135543	2.517668
H	-4.423894	-1.374590	1.714118
H	-4.456532	0.307507	1.134190
Br	-2.723860	1.963224	-0.439077

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56645389**

Number of imaginary frequencies = 0

1i_C004

B3LYP/6-31G* Geometry

C	-1.337048	-0.418044	-0.242170
C	-3.151660	1.457809	-0.028847
C	-0.181512	0.634905	0.143039
C	-2.649649	0.081156	0.424304
H	-3.865232	1.809587	0.724703
H	-2.510288	0.115568	1.505322
C	-1.992913	2.407189	-0.116397
H	-2.276566	3.450269	-0.248847
C	-0.692055	2.080633	-0.100115
O	-3.911098	1.472808	-1.236116
H	-3.295427	1.353446	-1.975136
Br	-4.166874	-1.211702	0.251375
C	-1.053518	-1.846134	0.272356
H	-1.821495	-2.527263	-0.100222
H	-1.078908	-1.908112	1.364604
H	-0.090068	-2.221975	-0.077876
C	-1.512818	-0.513870	-1.777962
H	-2.487146	-0.955408	-2.007332
H	-0.750590	-1.159885	-2.224379
H	-1.440497	0.460589	-2.273406
C	0.317740	3.203743	-0.249658
H	-0.172211	4.171982	-0.113732
H	0.778420	3.209652	-1.245606
H	1.136020	3.137404	0.475990
C	0.225303	0.586930	1.660205
H	0.615660	1.571871	1.932856
H	-0.664274	0.445604	2.282541
C	1.115664	0.428275	-0.720544
H	1.676846	1.361605	-0.737094
H	0.858488	0.217139	-1.759524
C	1.283115	-0.447978	2.080050
H	1.571783	-0.257623	3.119868
H	0.874767	-1.463479	2.053369
C	2.108353	-0.630438	-0.239083
H	1.720671	-1.643896	-0.338327
C	2.557698	-0.465560	1.217342
Cl	3.423421	1.159810	1.435448
C	3.528213	-1.550413	1.678197
H	3.058052	-2.535299	1.563384
H	3.783183	-1.410348	2.732287
H	4.444094	-1.533978	1.084732
Br	3.642184	-0.652180	-1.515836

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56308093**

Number of imaginary frequencies = 0

1i_C005

B3LYP/6-31G* Geometry

C	-1.403578	-0.493584	-0.298282
C	-3.093365	1.474855	-0.049458
C	-0.202174	0.558333	-0.092467
C	-2.596055	0.111461	0.471466
H	-3.614920	1.972474	0.785856
H	-2.348142	0.202947	1.528012
C	-1.938035	2.324305	-0.505906
H	-2.235195	3.311732	-0.853626
C	-0.659742	1.938323	-0.618630
O	-3.971196	1.396012	-1.167401
H	-4.703616	0.808460	-0.908736
Br	-4.187662	-1.122908	0.570783
C	-1.053638	-1.889313	0.262624
H	-1.867634	-2.586034	0.047550
H	-0.908774	-1.898189	1.347954
H	-0.152768	-2.290465	-0.212285
C	-1.752846	-0.676617	-1.794030
H	-2.681318	-1.249468	-1.875882
H	-0.974523	-1.242933	-2.314740
H	-1.906773	0.271479	-2.309723
C	0.327542	2.892811	-1.256841
H	-0.120524	3.885096	-1.362864
H	0.608262	2.554929	-2.263341
H	1.261090	3.000553	-0.695419
C	0.145230	0.731739	1.433864
H	-0.581879	1.398781	1.904897
H	0.061043	-0.229194	1.952094
C	1.088720	0.040507	-0.825183
H	1.590706	0.847717	-1.360646
H	0.832434	-0.703800	-1.578899
C	1.544009	1.314271	1.696510
H	1.604476	2.318041	1.274221
H	1.687306	1.429986	2.776907
C	2.102937	-0.570624	0.140096
H	1.641068	-1.358288	0.735952
C	2.706490	0.438394	1.132568
Cl	3.889411	1.563540	0.255431
C	3.493352	-0.257308	2.242016
H	2.812165	-0.888140	2.828297
H	3.942486	0.479071	2.913740
H	4.281414	-0.889526	1.826663
Br	3.478236	-1.577630	-0.879903

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55994675**

Number of imaginary frequencies = 0

1h_C006

B3LYP/6-31G* Geometry

C	-1.493175	0.458587	1.318369
C	-3.478972	0.890148	-0.254175
C	-0.437376	1.053682	0.271779
C	-2.767769	-0.119569	0.651255
H	-3.979184	1.600449	0.420017
H	-3.449230	-0.479199	1.422871
C	-2.493693	1.645631	-1.099203
H	-2.946704	2.173679	-1.936770
C	-1.178354	1.779054	-0.872311
O	-4.550584	0.345647	-1.002559
H	-4.183147	-0.388640	-1.526174
Br	-2.482095	-1.823646	-0.394607
C	-2.036715	1.599748	2.234930
H	-2.906461	1.250610	2.802988
H	-2.333326	2.486655	1.668654
H	-1.283898	1.905253	2.965512
C	-0.900322	-0.616689	2.253917
H	-1.675724	-0.962607	2.947646
H	-0.086410	-0.215355	2.866287
H	-0.535021	-1.493279	1.714381
C	-0.389710	2.674893	-1.806697
H	-1.021771	3.005896	-2.635758
H	0.486634	2.178200	-2.237560
H	-0.028507	3.576247	-1.295427
C	0.523816	2.039072	1.034161
H	0.057907	3.026408	1.119604
H	0.652305	1.685167	2.062619
C	0.468118	-0.059845	-0.385443
H	0.730061	0.228317	-1.407715
H	-0.078893	-0.993927	-0.473203
C	1.926976	2.221509	0.423427
H	1.851109	2.693481	-0.553696
H	2.494553	2.915784	1.054144
C	1.767299	-0.279566	0.383363
H	1.567760	-0.429988	1.443512
C	2.746555	0.901417	0.282061
Cl	3.548449	0.926526	-1.389456
C	3.869428	0.797662	1.312328
H	3.441328	0.853299	2.322113
H	4.579180	1.620921	1.194977
H	4.402875	-0.150798	1.213701
Br	2.584065	-2.019700	-0.119624

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56006666**

Number of imaginary frequencies = 0

1i_C007

B3LYP/6-31G* Geometry

C	1.397829	-0.671111	1.198147
C	3.490226	-0.831608	-0.268936
C	0.417159	-1.040139	-0.024192
C	2.719913	0.010261	0.734696
H	3.867174	-1.703794	0.295773
H	3.341606	0.204078	1.609857
C	2.579510	-1.315096	-1.357134
H	3.077572	-1.629229	-2.275313
C	1.250150	-1.455170	-1.267187
O	4.610307	-0.096636	-0.747460
H	5.087032	-0.668257	-1.369541
Br	2.486698	1.859266	0.002976
C	1.850318	-1.965259	1.935699
H	2.675523	-1.741172	2.621519
H	2.182028	-2.750655	1.250612
H	1.034388	-2.371293	2.541045
C	0.788030	0.245927	2.282730
H	1.533142	0.402213	3.072594
H	-0.087388	-0.199783	2.761429
H	0.527529	1.232526	1.896213
C	0.533319	-2.071860	-2.457806
H	1.160889	-2.003205	-3.351227
H	-0.423180	-1.592655	-2.688329
H	0.319250	-3.135691	-2.293405
C	-0.540685	-2.233996	0.303181
H	-0.945215	-2.602218	-0.640940
H	0.011445	-3.072808	0.733604
C	-0.497724	0.157131	-0.485980
H	-0.849194	-0.046956	-1.499440
H	0.088881	1.071965	-0.546767
C	-1.754799	-1.914246	1.183551
H	-2.367344	-2.815886	1.296374
H	-1.454205	-1.617909	2.196088
C	-1.742934	0.422855	0.365077
H	-1.482647	0.823925	1.342680
C	-2.646834	-0.788651	0.621344
Cl	-3.377694	-1.387775	-0.975130
C	-3.815524	-0.480046	1.554273
H	-3.429118	-0.131046	2.520416
H	-4.414831	-1.378530	1.726044
H	-4.454390	0.300159	1.136193
Br	-2.733222	1.951521	-0.451072

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56110807**

Number of imaginary frequencies = 0

1i_C008

B3LYP/6-31G* Geometry

C	1.551641	-0.294129	0.616210
C	2.845772	1.353153	-0.927922
C	0.143942	0.189819	-0.038130
C	2.614626	-0.096551	-0.484944
H	3.314451	1.320743	-1.926043
H	2.360139	-0.699135	-1.357075
C	1.530588	2.066602	-1.020886
H	1.605381	3.069407	-1.436403
C	0.336888	1.621007	-0.602186
O	3.664300	2.121041	-0.052454
H	4.510565	1.645427	0.026328
Br	4.420821	-0.861569	-0.002848
C	1.547232	-1.782407	1.036566
H	2.476551	-2.008946	1.563752
H	1.491567	-2.472290	0.188616
H	0.729368	-2.016654	1.723410
C	1.888648	0.539163	1.875295
H	2.917019	0.328976	2.183064
H	1.233954	0.267136	2.709226
H	1.812453	1.612732	1.700479
C	-0.839402	2.552908	-0.770652
H	-0.508869	3.488827	-1.230597
H	-1.313294	2.797523	0.183906
H	-1.628639	2.131170	-1.400280
C	-0.252132	-0.740606	-1.243476
H	0.226944	-0.366611	-2.153630
H	0.148095	-1.744893	-1.083771
C	-0.937886	0.115203	1.109919
H	-0.967602	1.060092	1.656515
H	-0.589169	-0.618538	1.839818
C	-1.758152	-0.883680	-1.527159
H	-2.196753	0.063486	-1.855277
H	-1.898190	-1.599658	-2.344115
C	-2.405389	-0.320083	0.829940
H	-2.818647	-0.728428	1.752272
C	-2.520538	-1.369575	-0.293139
Cl	-4.280251	-1.642541	-0.778196
C	-2.044143	-2.736789	0.222586
H	-1.017154	-2.698149	0.591942
H	-2.088904	-3.475182	-0.583295
H	-2.688639	-3.080735	1.036396
Br	-3.617133	1.244265	0.550608

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55122201**

Number of imaginary frequencies = 0

1i_C009

B3LYP/6-31G* Geometry

C	-1.413803	-0.490335	-0.300950
C	-3.101784	1.469588	-0.060734
C	-0.207425	0.549940	-0.085105
C	-2.622114	0.110559	0.459582
H	-3.661561	1.961497	0.751071
H	-2.363320	0.224385	1.511218
C	-1.933027	2.327240	-0.476792
H	-2.204602	3.339124	-0.783233
C	-0.654669	1.939324	-0.593509
O	-3.980570	1.278863	-1.175716
H	-4.165432	2.154955	-1.549587
Br	-4.184713	-1.130898	0.577798
C	-1.074482	-1.888574	0.260891
H	-1.882022	-2.584321	0.022304
H	-0.958887	-1.903583	1.349590
H	-0.160416	-2.284210	-0.193392
C	-1.745648	-0.673957	-1.800889
H	-2.700519	-1.198795	-1.892260
H	-0.985489	-1.281289	-2.302410
H	-1.843427	0.274883	-2.329619
C	0.340742	2.901452	-1.206393
H	-0.097406	3.900709	-1.289714
H	0.620641	2.584277	-2.219953
H	1.274384	2.986837	-0.641882
C	0.138770	0.706485	1.443221
H	-0.590055	1.366003	1.921922
H	0.052726	-0.261458	1.947267
C	1.082526	0.035230	-0.822597
H	1.582093	0.842576	-1.360210
H	0.823702	-0.709337	-1.575039
C	1.536417	1.284850	1.720439
H	1.596833	2.299597	1.325136
H	1.677453	1.373042	2.803778
C	2.101777	-0.576612	0.136926
H	1.645444	-1.372478	0.726230
C	2.702547	0.425792	1.137242
Cl	3.869907	1.571628	0.264362
C	3.503711	-0.274755	2.233211
H	2.832821	-0.920466	2.815059
H	3.948059	0.458251	2.911826
H	4.296513	-0.892804	1.805839
Br	3.481781	-1.565769	-0.895216

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55548204**

Number of imaginary frequencies = 0

1i_C010

B3LYP/6-31G* Geometry

C	1.668690	1.461391	0.278614
C	3.153796	-0.411385	1.225485
C	0.309496	0.663682	0.630523
C	2.880600	0.524988	0.043575
H	3.672090	0.207644	1.973854
H	3.766227	1.124151	-0.171682
C	1.885146	-0.904033	1.858552
H	2.053689	-1.667915	2.616003
C	0.644465	-0.418047	1.692009
O	4.089700	-1.439461	0.956333
H	3.734871	-1.953805	0.209805
Br	2.781232	-0.571262	-1.651366
C	2.079858	2.343535	1.498377
H	3.099110	2.724217	1.366430
H	2.037968	1.796122	2.442974
H	1.423951	3.214111	1.582174
C	1.562431	2.423169	-0.926486
H	2.463942	3.045914	-0.965396
H	0.710824	3.104199	-0.838045
H	1.498281	1.902592	-1.884088
C	-0.425176	-0.923742	2.639314
H	-1.279076	-1.359325	2.118927
H	-0.803435	-0.118584	3.282251
H	-0.007028	-1.690956	3.297465
C	-0.720976	1.696154	1.202386
H	-0.498223	1.892136	2.255935
H	-0.583697	2.654641	0.693496
C	-0.278883	0.008707	-0.681861
H	0.203538	-0.950372	-0.862385
H	0.007572	0.640642	-1.525163
C	-2.214472	1.329479	1.090974
H	-2.465163	0.474046	1.721372
H	-2.811752	2.175048	1.449629
C	-1.799916	-0.190022	-0.862079
H	-2.000311	-0.342973	-1.922882
C	-2.621561	1.003056	-0.346803
Cl	-4.426966	0.622199	-0.359560
C	-2.460182	2.192551	-1.308110
H	-1.412969	2.489121	-1.411927
H	-3.024000	3.052001	-0.933979
H	-2.843288	1.938225	-2.300358
Br	-2.392152	-1.949009	-0.118331

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55385286**

Number of imaginary frequencies = 0

1i_C011

B3LYP/6-31G* Geometry

C	1.569112	0.301260	-0.618442
C	2.811178	-1.325568	0.995156
C	0.164342	-0.058794	0.092984
C	2.658222	0.103226	0.457851
H	3.345956	-1.254227	1.957201
H	2.485661	0.773920	1.299606
C	1.453812	-1.917628	1.233706
H	1.467633	-2.867294	1.764894
C	0.281502	-1.407268	0.832784
O	3.515793	-2.216111	0.136867
H	4.386903	-1.812316	-0.026808
Br	4.486399	0.710365	-0.147251
C	1.596702	1.766689	-1.107636
H	2.522559	1.955321	-1.656103
H	1.557275	2.488453	-0.285405
H	0.768217	1.982772	-1.789934
C	1.842408	-0.615789	-1.835358
H	2.874772	-0.473791	-2.167429
H	1.191785	-0.362414	-2.677648
H	1.717886	-1.672698	-1.595943
C	-0.986269	-2.150123	1.186183
H	-0.747729	-3.081767	1.707490
H	-1.586653	-2.400808	0.306264
H	-1.637951	-1.556529	1.835760
C	-0.231788	1.033188	1.153161
H	-0.616480	0.539788	2.049173
H	0.654132	1.581932	1.483342
C	-0.919164	-0.133368	-1.043488
H	-0.976865	-1.151917	-1.428938
H	-0.544207	0.459041	-1.879658
C	-1.286070	2.047827	0.694343
H	-1.457461	2.787288	1.484522
H	-0.936023	2.603527	-0.185950
C	-2.364825	0.406815	-0.839178
H	-2.606126	0.970776	-1.740626
C	-2.627004	1.399395	0.324441
Cl	-3.293856	0.591834	1.851582
C	-3.683378	2.428495	-0.083971
H	-3.314301	3.023315	-0.929069
H	-3.907153	3.106028	0.744023
H	-4.606650	1.926742	-0.387774
Br	-3.738932	-1.029438	-0.970122

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55214308**

Number of imaginary frequencies = 0

1i_C012

B3LYP/6-31G* Geometry

C	-1.500034	0.443012	1.315195
C	-3.472870	0.880788	-0.246086
C	-0.441043	1.046751	0.276516
C	-2.768615	-0.144390	0.633845
H	-3.948410	1.594309	0.451632
H	-3.452236	-0.495527	1.407773
C	-2.492845	1.636272	-1.096355
H	-2.933439	2.171592	-1.938564
C	-1.179825	1.776987	-0.865227
O	-4.502078	0.245855	-0.995111
H	-4.958653	0.935934	-1.501524
Br	-2.470021	-1.832425	-0.399785
C	-2.041181	1.575843	2.242173
H	-2.917039	1.224026	2.799099
H	-2.328732	2.473115	1.687244
H	-1.292355	1.867882	2.982574
C	-0.905789	-0.637660	2.243581
H	-1.681078	-0.986954	2.935813
H	-0.091539	-0.239102	2.857548
H	-0.544071	-1.511507	1.698234
C	-0.392024	2.679941	-1.793040
H	-1.021015	3.012412	-2.624162
H	0.487402	2.187714	-2.222173
H	-0.035772	3.580085	-1.276217
C	0.515291	2.029920	1.047578
H	0.046185	3.015201	1.140524
H	0.642500	1.667943	2.073246
C	0.468055	-0.060535	-0.387180
H	0.729135	0.232815	-1.408186
H	-0.078742	-0.994622	-0.478484
C	1.919238	2.222175	0.442041
H	1.844837	2.703924	-0.530465
H	2.483541	2.911575	1.081103
C	1.767411	-0.279497	0.380945
H	1.567267	-0.438692	1.439746
C	2.742658	0.905664	0.289420
Cl	3.544576	0.948353	-1.382149
C	3.866447	0.797418	1.318259
H	3.438411	0.842176	2.328614
H	4.572892	1.624560	1.208060
H	4.403464	-0.148050	1.210954
Br	2.593365	-2.012025	-0.133785

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55466514**

Number of imaginary frequencies = 0

1j_C001

B3LYP/6-31G* Geometry

C	-1.423671	-0.325370	-0.474715
C	-3.046828	1.394061	0.631333
C	-0.176768	0.386026	0.270243
C	-2.648931	-0.073936	0.429123
H	-3.650687	1.446427	1.553215
H	-2.487498	-0.533332	1.404302
C	-1.817037	2.239644	0.790194
H	-2.029391	3.282110	1.019661
C	-0.548907	1.853092	0.593784
O	-3.782614	1.966954	-0.443831
H	-4.556616	1.393081	-0.586836
Br	-4.297864	-1.059533	-0.189948
C	-1.227316	-1.853653	-0.627507
H	-1.968767	-2.244465	-1.328535
H	-1.364985	-2.396139	0.312814
H	-0.238898	-2.108126	-1.018229
C	-1.633193	0.267594	-1.885927
H	-2.585233	-0.089558	-2.289091
H	-0.841975	-0.063708	-2.565488
H	-1.667215	1.358252	-1.882552
C	0.520815	2.922568	0.702063
H	0.062517	3.890572	0.923628
H	1.078931	3.037280	-0.235036
H	1.252787	2.724066	1.493404
C	0.155623	-0.373457	1.598361
H	-0.583031	-0.117724	2.365086
H	0.073822	-1.447985	1.423955
C	1.059271	0.301958	-0.688828
H	0.963291	1.040670	-1.488368
H	1.068409	-0.674280	-1.175817
C	1.552232	-0.124354	2.182190
H	1.653963	0.909355	2.536615
H	1.695924	-0.764832	3.059509
C	2.435980	0.482500	-0.041371
H	2.601825	1.513826	0.265133
C	2.705525	-0.383105	1.193979
Cl	2.678787	-2.176695	0.733960
C	4.063988	-0.107728	1.834988
H	4.876022	-0.316375	1.136087
H	4.194883	-0.724368	2.728466
H	4.122836	0.947575	2.130421
Br	3.818604	0.247271	-1.460237

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56949361**

Number of imaginary frequencies = 0

1j_C002

B3LYP/6-31G* Geometry

C	-1.429982	-0.313358	-0.478027
C	-3.056595	1.393721	0.621525
C	-0.182542	0.383937	0.275585
C	-2.671829	-0.067986	0.414932
H	-3.701907	1.449310	1.512788
H	-2.496076	-0.507643	1.396649
C	-1.820706	2.225970	0.829455
H	-2.016917	3.262151	1.111059
C	-0.551012	1.845303	0.625694
O	-3.788744	1.876394	-0.510666
H	-3.943084	2.824065	-0.371196
Br	-4.290194	-1.075456	-0.190943
C	-1.236464	-1.841381	-0.638860
H	-1.968615	-2.223693	-1.353453
H	-1.393433	-2.390216	0.294617
H	-0.241954	-2.095419	-1.014783
C	-1.624248	0.285012	-1.889338
H	-2.592240	-0.034261	-2.284800
H	-0.847075	-0.073536	-2.571656
H	-1.617557	1.376528	-1.887131
C	0.520800	2.908973	0.762820
H	0.067268	3.872944	1.011741
H	1.078460	3.046042	-0.171652
H	1.253129	2.685977	1.546794
C	0.149929	-0.394594	1.593150
H	-0.588543	-0.150268	2.363670
H	0.065116	-1.465616	1.401165
C	1.054462	0.313374	-0.683171
H	0.959878	1.062831	-1.472935
H	1.061472	-0.655985	-1.183628
C	1.547499	-0.159527	2.180870
H	1.653126	0.866897	2.554950
H	1.689451	-0.816590	3.046143
C	2.431508	0.482111	-0.033322
H	2.599665	1.508090	0.289757
C	2.700384	-0.403589	1.188151
Cl	2.671875	-2.189233	0.699754
C	4.059352	-0.140130	1.833178
H	4.871023	-0.340482	1.131415
H	4.188804	-0.769957	2.717618
H	4.120579	0.910657	2.143962
Br	3.814313	0.268512	-1.455840

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56499789**

Number of imaginary frequencies = 0

1j_C003

B3LYP/6-31G* Geometry

C	1.574032	0.975136	-1.053902
C	3.419652	0.646233	0.699559
C	0.415742	1.052370	0.061671
C	2.801304	0.143051	-0.607233
H	3.970199	1.562424	0.439753
H	3.548046	0.136265	-1.402238
C	2.358769	1.005998	1.700428
H	2.743661	1.147971	2.709125
C	1.060739	1.244249	1.455122
O	4.424067	-0.196589	1.234382
H	4.023330	-1.078479	1.336617
Br	2.444771	-1.835812	-0.422787
C	2.149687	2.402797	-1.310442
H	3.077167	2.338690	-1.890796
H	2.364284	2.941339	-0.383312
H	1.449558	3.002857	-1.896750
C	1.091541	0.441099	-2.421101
H	1.860983	0.640582	-3.176447
H	0.171187	0.928851	-2.753571
H	0.923471	-0.637505	-2.409980
C	0.223374	1.730937	2.622435
H	0.823633	1.742839	3.536754
H	-0.652725	1.104632	2.819445
H	-0.142421	2.752595	2.462256
C	-0.518090	2.255465	-0.310486
H	-0.041396	3.198002	-0.021658
H	-0.619330	2.284933	-1.398263
C	-0.444721	-0.269447	0.053063
H	0.088987	-1.057307	0.582164
H	-0.563028	-0.611409	-0.975322
C	-1.947305	2.255306	0.254987
H	-1.951039	2.459627	1.331056
H	-2.510491	3.070341	-0.213593
C	-1.853957	-0.170576	0.638086
H	-1.837663	-0.026976	1.718919
C	-2.726375	0.944451	0.056558
Cl	-2.965639	0.681870	-1.762694
C	-4.117299	1.022499	0.681447
H	-4.677105	0.101797	0.508075
H	-4.675924	1.864349	0.262788
H	-4.024724	1.172309	1.764663
Br	-2.708996	-1.968051	0.480498

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56534936**

Number of imaginary frequencies = 0

1j_C004

B3LYP/6-31G* Geometry

C	-1.432088	-0.308004	-0.411720
C	-3.079908	1.437107	0.611694
C	-0.205634	0.390289	0.355964
C	-2.689772	-0.036658	0.442019
H	-3.744370	1.498244	1.490145
H	-2.574700	-0.481294	1.431121
C	-1.849013	2.253556	0.872847
H	-2.048420	3.285349	1.156007
C	-0.581996	1.838151	0.745493
O	-3.734106	2.018527	-0.509539
H	-4.512724	1.463213	-0.694894
Br	-4.325530	-1.007095	-0.230031
C	-1.234962	-1.833315	-0.548494
H	-2.022493	-2.249087	-1.181674
H	-1.293034	-2.350894	0.415110
H	-0.277143	-2.080065	-1.014910
C	-1.595209	0.280717	-1.832336
H	-2.531601	-0.081303	-2.266641
H	-0.781079	-0.046680	-2.485405
H	-1.634333	1.370930	-1.830749
C	0.520596	2.831295	1.058156
H	0.094124	3.814923	1.273419
H	1.227077	2.952643	0.229404
H	1.108111	2.537930	1.938905
C	0.198660	-0.349048	1.685920
H	0.571777	0.396128	2.398231
H	-0.686555	-0.777179	2.166933
C	1.043065	0.392677	-0.594335
H	1.027999	1.274024	-1.237896
H	1.020994	-0.473077	-1.260407
C	1.252710	-1.464919	1.545790
H	1.476872	-1.865303	2.541410
H	0.838828	-2.291195	0.970862
C	2.357140	0.334887	0.181543
H	2.385371	1.096773	0.958582
C	2.593009	-1.013946	0.882774
Cl	3.056956	-2.304766	-0.364947
C	3.740441	-0.935429	1.888290
H	4.658811	-0.588582	1.408754
H	3.921641	-1.913314	2.342151
H	3.475560	-0.229314	2.686533
Br	3.867863	0.888974	-0.983004

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56152036**

Number of imaginary frequencies = 0

1j_C005

B3LYP/6-31G* Geometry

C	1.577663	0.952641	-1.061939
C	3.419956	0.651784	0.674550
C	0.419531	1.041659	0.053871
C	2.802121	0.111224	-0.607564
H	3.939003	1.583578	0.383892
H	3.547292	0.108953	-1.404376
C	2.366651	1.004283	1.684781
H	2.742558	1.155108	2.697833
C	1.067605	1.238877	1.445021
O	4.393212	-0.261848	1.166679
H	4.812183	0.150724	1.938353
Br	2.439769	-1.846204	-0.409326
C	2.146799	2.378443	-1.338935
H	3.077450	2.307752	-1.913507
H	2.354872	2.935763	-0.421101
H	1.447754	2.966404	-1.938993
C	1.090955	0.403901	-2.421505
H	1.856667	0.599663	-3.181793
H	0.167630	0.885978	-2.754464
H	0.929831	-0.675216	-2.397430
C	0.233300	1.723900	2.614997
H	0.834618	1.736347	3.528893
H	-0.640524	1.095361	2.813254
H	-0.135053	2.744754	2.456037
C	-0.508759	2.247607	-0.322373
H	-0.025852	3.189981	-0.043117
H	-0.613840	2.268650	-1.409960
C	-0.449095	-0.274785	0.052483
H	0.082351	-1.065431	0.579488
H	-0.571219	-0.617213	-0.975123
C	-1.935843	2.260163	0.248181
H	-1.934927	2.469574	1.323343
H	-2.495128	3.076844	-0.222306
C	-1.856776	-0.165485	0.639995
H	-1.838362	-0.020254	1.720636
C	-2.724428	0.953614	0.058528
Cl	-2.974564	0.687178	-1.758634
C	-4.111923	1.043248	0.689516
H	-4.678214	0.125427	0.522091
H	-4.667083	1.887173	0.270355
H	-4.013378	1.196337	1.771795
Br	-2.725006	-1.957222	0.488237

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55988488**

Number of imaginary frequencies = 0

1j_C006

B3LYP/6-31G* Geometry

C	-1.438337	-0.297714	-0.417510
C	-3.086174	1.441735	0.593418
C	-0.210780	0.390799	0.354207
C	-2.709929	-0.027009	0.425935
H	-3.784414	1.512327	1.442717
H	-2.578384	-0.446574	1.423765
C	-1.851150	2.246313	0.891596
H	-2.038643	3.271157	1.216607
C	-0.582441	1.835406	0.758212
O	-3.741221	1.925987	-0.583408
H	-3.879357	2.878893	-0.464382
Br	-4.318271	-1.024488	-0.220616
C	-1.244518	-1.823544	-0.554600
H	-2.028271	-2.235110	-1.194201
H	-1.314025	-2.342910	0.407274
H	-0.282717	-2.070772	-1.012837
C	-1.588484	0.287983	-1.841008
H	-2.546834	-0.029326	-2.260611
H	-0.795093	-0.079130	-2.498960
H	-1.576210	1.379119	-1.847104
C	0.520542	2.822844	1.085787
H	0.096870	3.804447	1.316762
H	1.226859	2.954723	0.258341
H	1.108230	2.515138	1.961171
C	0.189155	-0.357810	1.680733
H	0.560774	0.380483	2.401052
H	-0.698909	-0.788665	2.153807
C	1.040245	0.398236	-0.592857
H	1.028594	1.283986	-1.230575
H	1.016692	-0.462337	-1.265378
C	1.241967	-1.474240	1.535369
H	1.463934	-1.880585	2.529077
H	0.826972	-2.296180	0.955283
C	2.352770	0.331752	0.184877
H	2.382537	1.087653	0.967677
C	2.584441	-1.022472	0.876867
Cl	3.047311	-2.304966	-0.379014
C	3.730684	-0.953879	1.884545
H	4.650860	-0.606559	1.408779
H	3.908352	-1.935360	2.332011
H	3.466727	-0.252589	2.687370
Br	3.867500	0.891468	-0.972829

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55722656**

Number of imaginary frequencies = 0

1k_C001

B3LYP/6-31G* Geometry

C	-1.278948	-0.328556	-0.436922
C	-3.229256	1.318265	-0.055410
C	-0.228401	0.713121	0.204717
C	-2.642318	-0.052898	0.243554
H	-3.559943	1.345822	-1.106783
H	-2.585253	-0.186231	1.323582
C	-2.172794	2.357784	0.157001
H	-2.557852	3.372212	0.240465
C	-0.853957	2.135436	0.226006
O	-4.323570	1.628599	0.797276
H	-5.002775	0.953017	0.625374
Br	-4.072350	-1.394457	-0.252191
C	-0.909132	-1.808014	-0.199463
H	-1.604375	-2.448158	-0.747617
H	-0.979925	-2.092134	0.854698
H	0.094595	-2.042318	-0.557487
C	-1.404895	-0.116292	-1.964658
H	-2.309372	-0.614312	-2.327644
H	-0.557268	-0.558183	-2.496710
H	-1.463413	0.941739	-2.237508
C	0.050489	3.342075	0.397128
H	-0.541781	4.219204	0.672336
H	0.588643	3.590836	-0.526076
H	0.807410	3.201335	1.178246
C	0.136830	0.383454	1.695544
H	0.436907	1.316755	2.183792
H	-0.758247	0.058955	2.236120
C	1.106471	0.785629	-0.617578
H	1.587050	1.742956	-0.413990
H	0.901139	0.790748	-1.689151
C	1.249782	-0.656649	1.935386
H	1.490171	-0.678362	3.004435
H	0.909729	-1.659968	1.675561
C	2.167365	-0.287408	-0.333364
H	1.872000	-1.273442	-0.681863
C	2.546371	-0.368488	1.152150
Cl	3.644427	-1.838666	1.392299
C	3.308027	0.842906	1.689513
H	3.548069	0.691996	2.745392
H	2.702386	1.751464	1.603488
H	4.234075	0.997041	1.132899
Br	3.738279	0.115753	-1.499252

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56668975**

Number of imaginary frequencies = 0

1k_C002

B3LYP/6-31G* Geometry

C	1.422382	0.323039	-0.661309
C	2.771990	-1.597607	0.386071
C	0.047748	-0.248980	-0.015753
C	2.553038	-0.096023	0.299971
H	3.248006	-1.943036	-0.546488
H	2.389050	0.303957	1.300194
C	1.449856	-2.286339	0.537740
H	1.530289	-3.331020	0.831830
C	0.239830	-1.751842	0.315488
O	3.588884	-1.954419	1.495230
H	4.447075	-1.519059	1.349111
Br	4.345530	0.714218	-0.173744
C	1.431597	1.863187	-0.802362
H	2.259912	2.161451	-1.449935
H	1.579481	2.373281	0.153875
H	0.509485	2.248776	-1.243115
C	1.658062	-0.284283	-2.065117
H	2.691266	-0.095205	-2.373573
H	1.006209	0.179189	-2.811263
H	1.483762	-1.363609	-2.088016
C	-0.953395	-2.665921	0.469873
H	-0.624843	-3.651722	0.812079
H	-1.493843	-2.802776	-0.471536
H	-1.688300	-2.291590	1.188658
C	-0.259432	0.502758	1.328372
H	0.285397	0.014699	2.142111
H	0.118935	1.524538	1.267035
C	-1.089690	0.009421	-1.077551
H	-1.161967	-0.837191	-1.763800
H	-0.773557	0.852275	-1.695690
C	-1.735724	0.600978	1.733555
H	-2.151592	-0.386368	1.969830
H	-1.815917	1.200176	2.647375
C	-2.523716	0.405355	-0.651700
H	-2.982557	0.972845	-1.459396
C	-2.643012	1.199117	0.660583
Cl	-2.006313	2.908787	0.216493
C	-4.068974	1.425548	1.159010
H	-4.058292	2.138644	1.987705
H	-4.498862	0.483199	1.507672
H	-4.708313	1.822620	0.365329
Br	-3.774042	-1.178748	-0.596640

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55993370**

Number of imaginary frequencies = 0

1k_C003

B3LYP/6-31G* Geometry

C	-1.290391	-0.327594	-0.445888
C	-3.244465	1.314997	-0.045405
C	-0.234916	0.712823	0.185858
C	-2.661742	-0.065820	0.238612
H	-3.645040	1.335388	-1.065455
H	-2.580096	-0.209683	1.317900
C	-2.173592	2.355547	0.107601
H	-2.553272	3.375812	0.148930
C	-0.853702	2.136402	0.184986
O	-4.371084	1.617442	0.771977
H	-4.052616	1.707129	1.685384
Br	-4.060563	-1.415387	-0.249645
C	-0.908706	-1.804777	-0.212491
H	-1.603633	-2.449206	-0.754698
H	-0.970475	-2.090558	0.841967
H	0.094787	-2.030032	-0.577112
C	-1.428295	-0.116460	-1.973083
H	-2.333044	-0.620101	-2.327046
H	-0.583161	-0.554845	-2.511990
H	-1.494365	0.940835	-2.247350
C	0.051957	3.345463	0.328720
H	-0.538191	4.229892	0.584898
H	0.588683	3.572611	-0.600643
H	0.810475	3.219778	1.111016
C	0.126460	0.402408	1.682062
H	0.425887	1.341853	2.159667
H	-0.769946	0.082661	2.223719
C	1.102819	0.770062	-0.634547
H	1.583387	1.731157	-0.449844
H	0.898677	0.753115	-1.706211
C	1.238030	-0.634855	1.939049
H	1.472805	-0.645599	3.009537
H	0.898883	-1.640477	1.686967
C	2.165911	-0.295543	-0.328851
H	1.875520	-1.287565	-0.663840
C	2.537967	-0.353722	1.159314
Cl	3.638934	-1.816247	1.427283
C	3.292858	0.867903	1.682954
H	3.527287	0.733873	2.742397
H	2.685446	1.773440	1.579131
H	4.221596	1.016201	1.129312
Br	3.741307	0.095672	-1.492344

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56415515**

Number of imaginary frequencies = 0

1k_C004

B3LYP/6-31G* Geometry

C	-1.278974	-0.328472	-0.437155
C	-3.229234	1.318297	-0.055372
C	-0.228387	0.712986	0.204907
C	-2.642347	-0.052891	0.243481
H	-3.559723	1.346016	-1.106810
H	-2.585105	-0.186299	1.323478
C	-2.172738	2.357723	0.157481
H	-2.557753	3.372145	0.241245
C	-0.853928	2.135277	0.226639
O	-4.323652	1.628523	0.797097
H	-5.002794	0.952834	0.625149
Br	-4.072411	-1.394361	-0.252254
C	-0.909246	-1.808010	-0.200135
H	-1.604205	-2.448016	-0.748820
H	-0.980437	-2.092521	0.853889
H	0.094637	-2.042130	-0.557840
C	-1.405024	-0.115670	-1.964744
H	-2.309603	-0.613446	-2.327813
H	-0.557521	-0.557450	-2.497073
H	-1.463473	0.942463	-2.237231
C	0.050541	3.341871	0.398184
H	-0.541655	4.218806	0.674169
H	0.588283	3.591129	-0.525142
H	0.807774	3.200721	1.178888
C	0.136824	0.382806	1.695614
H	0.436816	1.315963	2.184182
H	-0.758220	0.058031	2.236070
C	1.106488	0.785783	-0.617370
H	1.587034	1.743106	-0.413610
H	0.901153	0.791168	-1.688944
C	1.249884	-0.657294	1.935175
H	1.490231	-0.679271	3.004225
H	0.909843	-1.660561	1.675087
C	2.167468	-0.287273	-0.333472
H	1.872114	-1.273222	-0.682230
C	2.546393	-0.368814	1.152056
Cl	3.644500	-1.839164	1.391775
C	3.308091	0.842334	1.689936
H	3.547961	0.691058	2.745811
H	2.702553	1.750973	1.604081
H	4.234229	0.996576	1.133525
Br	3.738288	0.116293	-1.499248

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56669081**

Number of imaginary frequencies = 0

1k_C005

B3LYP/6-31G* Geometry

C	-1.29550	-0.51267	-0.46398
C	-3.18104	1.23944	-0.31302
C	-0.21666	0.67192	-0.30810
C	-2.54041	-0.00670	0.29597
H	-3.76572	0.93103	-1.19566
H	-2.31375	0.17917	1.34434
C	-2.14134	2.21643	-0.78258
H	-2.54990	3.16500	-1.12612
C	-0.82719	1.97359	-0.88664
O	-4.03863	1.89433	0.61502
H	-4.74623	1.25949	0.82362
Br	-4.01465	-1.37892	0.44529
C	-0.80969	-1.85290	0.12508
H	-1.59479	-2.60489	0.01116
H	-0.57377	-1.80013	1.19232
H	0.06988	-2.22242	-0.41053
C	-1.64124	-0.77361	-1.95023
H	-2.53414	-1.40414	-2.00949
H	-0.83361	-1.31046	-2.45659
H	-1.83563	0.14647	-2.50675
C	0.04356	3.01875	-1.55156
H	-0.53786	3.92494	-1.74483
H	0.42876	2.66745	-2.51795
H	0.91437	3.30822	-0.95261
C	0.11322	0.94934	1.20894
H	-0.64196	1.61590	1.63321
H	0.07143	0.02014	1.78722
C	1.12456	0.28257	-1.02214
H	1.58694	1.15711	-1.48531
H	0.94109	-0.41728	-1.83851
C	1.49538	1.57922	1.41236
H	1.56694	2.50684	0.83432
H	1.63413	1.86130	2.45959
C	2.14480	-0.34158	-0.06233
H	1.71211	-1.18949	0.45824
C	2.67232	0.66496	0.98069
Cl	3.21017	-0.32618	2.45859
C	3.87078	1.50545	0.54670
H	4.10293	2.24412	1.31955
H	3.63120	2.03974	-0.38090
H	4.75079	0.88688	0.36831
Br	3.59704	-1.19993	-1.12237

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56367623**

Number of imaginary frequencies = 0

1k_C006

B3LYP/6-31G* Geometry

C	1.431446	0.317229	-0.657762
C	2.780386	-1.602336	0.403669
C	0.053971	-0.251931	-0.018805
C	2.576198	-0.095312	0.300386
H	3.315781	-1.955214	-0.485283
H	2.400659	0.321798	1.293946
C	1.451696	-2.295125	0.503547
H	1.529644	-3.350784	0.760788
C	0.239211	-1.757199	0.296725
O	3.634936	-1.969427	1.484647
H	3.154011	-1.785606	2.308384
Br	4.340309	0.723542	-0.188593
C	1.435783	1.858110	-0.798916
H	2.264375	2.159399	-1.443574
H	1.581654	2.368472	0.157645
H	0.512884	2.241349	-1.240079
C	1.670398	-0.287488	-2.062200
H	2.700804	-0.085875	-2.371220
H	1.012097	0.168657	-2.807318
H	1.508857	-1.368863	-2.086393
C	-0.954225	-2.672705	0.437301
H	-0.626746	-3.665726	0.759336
H	-1.497721	-2.790238	-0.504788
H	-1.686912	-2.310053	1.164592
C	-0.253963	0.491577	1.329489
H	0.289293	-0.001435	2.141820
H	0.126851	1.512691	1.274656
C	-1.083587	0.015704	-1.078900
H	-1.158532	-0.826988	-1.769578
H	-0.763795	0.859769	-1.693068
C	-1.730176	0.588559	1.735330
H	-2.148282	-0.400364	1.961304
H	-1.810142	1.179466	2.654595
C	-2.516468	0.414193	-0.651303
H	-2.972894	0.988754	-1.455363
C	-2.634646	1.198893	0.666638
Cl	-1.992328	2.909108	0.238152
C	-4.060322	1.425134	1.166261
H	-4.048110	2.131476	2.000706
H	-4.493528	0.481276	1.506617
H	-4.697745	1.830811	0.375423
Br	-3.772784	-1.165999	-0.607340

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55771598**

Number of imaginary frequencies = 0

1k_C007

B3LYP/6-31G* Geometry

C	1.422389	0.323065	-0.661355
C	2.771896	-1.597472	0.386200
C	0.047746	-0.248870	-0.015742
C	2.553000	-0.095888	0.299962
H	3.247841	-1.943022	-0.546362
H	2.389131	0.304262	1.300145
C	1.449775	-2.286179	0.538046
H	1.530185	-3.330783	0.832388
C	0.239764	-1.751704	0.315580
O	3.588895	-1.954178	1.495317
H	4.447093	-1.518816	1.349171
Br	4.345607	0.714107	-0.173867
C	1.431773	1.863149	-0.802631
H	2.259858	2.161119	-1.450646
H	1.580174	2.373388	0.153442
H	0.509546	2.248831	-1.243094
C	1.658027	-0.284444	-2.065103
H	2.691267	-0.095612	-2.373587
H	1.006269	0.179083	-2.811302
H	1.483507	-1.363740	-2.087879
C	-0.953474	-2.665697	0.470233
H	-0.624999	-3.651354	0.812899
H	-1.493725	-2.802978	-0.471252
H	-1.688584	-2.291078	1.188655
C	-0.259478	0.502963	1.328353
H	0.285420	0.015078	2.142147
H	0.118719	1.524793	1.266923
C	-1.089646	0.009572	-1.077560
H	-1.161787	-0.836908	-1.763991
H	-0.773561	0.852571	-1.695527
C	-1.735771	0.600990	1.733492
H	-2.151492	-0.386453	1.969610
H	-1.816093	1.200025	2.647413
C	-2.523717	0.405330	-0.651745
H	-2.982649	0.972689	-1.459486
C	-2.643100	1.199125	0.660511
Cl	-2.006638	2.908798	0.216406
C	-4.069106	1.425324	1.158904
H	-4.058534	2.138280	1.987715
H	-4.498923	0.482873	1.507392
H	-4.708455	1.822463	0.365260
Br	-3.773863	-1.178862	-0.596543

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55993712**

Number of imaginary frequencies = 0

1k_C008

B3LYP/6-31G* Geometry

C	1.549761	0.632829	1.219427
C	2.263267	-1.531458	-0.147437
C	0.076442	0.053959	0.939176
C	2.594657	-0.085594	0.310278
H	1.897302	-1.493645	-1.183246
H	3.546625	-0.125252	0.838083
C	1.208106	-2.151439	0.716347
H	1.327340	-3.216364	0.901362
C	0.163135	-1.471970	1.208538
O	3.427365	-2.350582	-0.103764
H	4.022770	-2.023754	-0.798456
Br	3.127865	0.921207	-1.361181
C	1.986530	0.304047	2.676566
H	2.968783	0.748207	2.874099
H	2.058499	-0.769191	2.862354
H	1.287008	0.732733	3.401057
C	1.662683	2.169169	1.093118
H	2.713736	2.465257	1.168168
H	1.128641	2.666410	1.907510
H	1.290412	2.563652	0.146344
C	-0.832411	-2.204720	2.079912
H	-0.466855	-3.213722	2.294297
H	-1.803308	-2.309268	1.585219
H	-0.997746	-1.703364	3.040608
C	-0.953013	0.779651	1.852686
H	-0.829528	0.467542	2.893845
H	-0.742945	1.851270	1.829663
C	-0.307554	0.354326	-0.549066
H	0.259995	-0.271929	-1.237737
H	-0.029150	1.386496	-0.779755
C	-2.432750	0.608428	1.472160
H	-2.760560	-0.425507	1.619131
H	-3.049000	1.228551	2.132438
C	-1.782717	0.251339	-0.938300
H	-1.923623	0.621716	-1.953410
C	-2.755166	0.959122	0.019535
Cl	-2.410422	2.785860	-0.238833
C	-4.232716	0.774517	-0.317110
H	-4.844161	1.417208	0.322148
H	-4.523781	-0.266705	-0.156115
H	-4.432709	1.031452	-1.361585
Br	-2.321838	-1.680350	-1.132268

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56329332**

Number of imaginary frequencies = 0

1k_C009

B3LYP/6-31G* Geometry

C	-1.612642	-0.596151	1.190530
C	-2.554260	1.474958	-0.133257
C	-0.155249	0.024777	0.923427
C	-2.658433	-0.033886	0.190448
H	-2.478554	1.600602	-1.221995
H	-3.654561	-0.200592	0.596723
C	-1.393451	2.153000	0.541473
H	-1.498792	3.234773	0.632380
C	-0.304870	1.560318	1.048581
O	-3.796026	2.043118	0.317403
H	-3.808455	2.974544	0.045497
Br	-2.800726	-1.052754	-1.545425
C	-2.139376	-0.167427	2.592077
H	-3.086883	-0.678074	2.797019
H	-2.315866	0.906503	2.670087
H	-1.436736	-0.461442	3.378014
C	-1.651545	-2.142163	1.188419
H	-2.693545	-2.478756	1.197196
H	-1.174964	-2.546883	2.085764
H	-1.178731	-2.595487	0.316014
C	0.695493	2.414031	1.796404
H	0.888431	2.031941	2.805765
H	0.312991	3.434137	1.900556
H	1.652830	2.475286	1.272213
C	0.856564	-0.571823	1.945643
H	0.683340	-0.154961	2.942392
H	0.673635	-1.645231	2.029354
C	0.311235	-0.369140	-0.519935
H	-0.232731	0.207751	-1.268626
H	0.048275	-1.414762	-0.697857
C	2.347116	-0.401629	1.608233
H	2.650533	0.648515	1.669320
H	2.945991	-0.941681	2.349989
C	1.801998	-0.289101	-0.852564
H	1.986578	-0.762982	-1.815990
C	2.738776	-0.883165	0.211508
Cl	2.426037	-2.731685	0.116422
C	4.228247	-0.708419	-0.073414
H	4.815688	-1.273389	0.655558
H	4.497915	0.348697	-0.004522
H	4.482019	-1.064974	-1.076057
Br	2.343285	1.614614	-1.246651

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55924526**

Number of imaginary frequencies = 0

1k_C010

B3LYP/6-31G* Geometry

C	1.630501	0.906022	0.931254
C	2.919405	-1.292982	0.326385
C	0.229805	0.117105	0.845955
C	2.748651	0.222558	0.100036
H	3.238680	-1.755391	-0.610945
H	3.702048	0.699236	0.323383
C	1.682686	-1.953144	0.853990
H	1.825634	-3.007339	1.087638
C	0.509373	-1.375479	1.159277
O	4.016172	-1.540515	1.222502
H	3.686093	-1.418095	2.126661
Br	2.644756	0.547746	-1.892453
C	2.136060	0.892820	2.406578
H	3.173332	1.240174	2.460324
H	2.080874	-0.098669	2.864767
H	1.537602	1.572368	3.020217
C	1.559331	2.397096	0.527427
H	2.530641	2.864068	0.730086
H	0.810621	2.946066	1.103958
H	1.356269	2.545498	-0.533705
C	-0.509339	-2.230700	1.886521
H	-0.100754	-3.230532	2.060892
H	-1.435933	-2.348702	1.321191
H	-0.766138	-1.808148	2.865784
C	-0.753611	0.744844	1.885449
H	-0.498505	0.405988	2.894305
H	-0.614635	1.828128	1.887689
C	-0.374062	0.292370	-0.594552
H	0.128149	-0.371758	-1.297048
H	-0.149439	1.308131	-0.926972
C	-2.254222	0.494615	1.661572
H	-2.511616	-0.556216	1.828030
H	-2.823754	1.074065	2.396830
C	-1.885027	0.168444	-0.810761
H	-2.136487	0.566777	-1.792958
C	-2.757502	0.840376	0.261374
Cl	-2.494631	2.678414	-0.021777
C	-4.259082	0.617045	0.104290
H	-4.592161	0.874755	-0.905374
H	-4.804913	1.238238	0.819705
H	-4.499790	-0.433212	0.288397
Br	-2.433164	-1.758897	-1.041588

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55745208**

Number of imaginary frequencies = 0

1k_C011

B3LYP/6-31G* Geometry

C	-1.31460	-0.53879	-0.44893
C	-3.16538	1.25869	-0.27685
C	-0.22467	0.63917	-0.35635
C	-2.55331	-0.00935	0.31246
H	-3.88033	0.97115	-1.06247
H	-2.31318	0.17436	1.35830
C	-2.13104	2.16408	-0.89465
H	-2.53333	3.08600	-1.31647
C	-0.82195	1.90553	-1.01398
O	-3.86569	1.90538	0.79285
H	-4.47477	2.55204	0.40514
Br	-4.02321	-1.36642	0.46809
C	-0.82186	-1.85346	0.19109
H	-1.60943	-2.60778	0.12299
H	-0.57169	-1.75179	1.25165
H	0.05142	-2.24639	-0.33837
C	-1.67975	-0.86200	-1.91794
H	-2.54969	-1.52563	-1.93568
H	-0.86267	-1.38453	-2.42460
H	-1.92040	0.03125	-2.49953
C	0.04551	2.88510	-1.77453
H	-0.53178	3.77728	-2.03504
H	0.41815	2.45287	-2.71247
H	0.92475	3.21560	-1.20922
C	0.09667	1.00103	1.14323
H	-0.66782	1.67987	1.52980
H	0.06384	0.10412	1.77094
C	1.11681	0.19826	-1.03977
H	1.58158	1.03441	-1.56675
H	0.93198	-0.56037	-1.80151
C	1.47212	1.65417	1.31129
H	1.53694	2.54730	0.67960
H	1.60745	1.99872	2.34009
C	2.13721	-0.35401	-0.03798
H	1.70799	-1.16819	0.53706
C	2.65683	0.72461	0.93560
Cl	3.20940	-0.16310	2.47267
C	3.84606	1.54664	0.44424
H	4.07498	2.33348	1.16905
H	3.59793	2.02084	-0.51342
H	4.73059	0.92564	0.30015
Br	3.59754	-1.27039	-1.03636

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56101940**

Number of imaginary frequencies = 0

1k_C012

B3LYP/6-31G* Geometry

C	-1.307398	-0.518148	-0.450031
C	-3.190689	1.244490	-0.305914
C	-0.223870	0.663287	-0.320248
C	-2.562241	-0.011866	0.307067
H	-3.837580	0.940437	-1.137028
H	-2.322673	0.170352	1.355086
C	-2.146569	2.189203	-0.838676
H	-2.556121	3.121618	-1.225422
C	-0.829575	1.950937	-0.929524
O	-4.081624	1.899451	0.595053
H	-3.540998	2.317639	1.284987
Br	-4.006998	-1.391999	0.456104
C	-0.813897	-1.848060	0.157051
H	-1.597805	-2.602825	0.060697
H	-0.572301	-1.777921	1.222256
H	0.064290	-2.222763	-0.377376
C	-1.658667	-0.805683	-1.930490
H	-2.543486	-1.448316	-1.972400
H	-0.847499	-1.339706	-2.434352
H	-1.869469	0.102211	-2.500899
C	0.039962	2.978454	-1.622608
H	-0.542337	3.878063	-1.842441
H	0.425785	2.599923	-2.578232
H	0.910674	3.284927	-1.031719
C	0.110942	0.970188	1.189690
H	-0.642911	1.643853	1.606175
H	0.071140	0.052631	1.786026
C	1.116948	0.256100	-1.026668
H	1.579815	1.118012	-1.512363
H	0.929785	-0.462988	-1.825082
C	1.492087	1.607011	1.377453
H	1.561693	2.521378	0.778189
H	1.632926	1.912381	2.417884
C	2.139909	-0.346118	-0.055924
H	1.709329	-1.183427	0.483259
C	2.668314	0.683555	0.964466
Cl	3.206831	-0.273935	2.463899
C	3.866145	1.515151	0.511774
H	4.745947	0.892921	0.345907
H	4.098870	2.269928	1.268753
H	3.625908	2.029441	-0.426911
Br	3.591155	-1.223072	-1.100567

SCF Energy (PCM/mPW1PW91/6-31+G) =** -6264.56165703

Number of imaginary frequencies = 0

1k_C013

B3LYP/6-31G* Geometry

C	-1.465474	-0.647838	-1.031507
C	-3.570220	-0.264789	0.472195
C	-0.561481	-1.014865	0.243924
C	-2.691781	0.238043	-0.671898
H	-4.117859	0.586686	0.896105
H	-3.311786	0.351192	-1.560943
C	-2.760644	-0.921183	1.544823
H	-3.305333	-1.130629	2.466641
C	-1.472277	-1.285366	1.470576
O	-4.527357	-1.169995	-0.113576
H	-4.846840	-1.754556	0.591951
Br	-2.248364	2.159489	-0.257607
C	-2.069002	-1.946398	-1.644221
H	-2.843604	-1.695368	-2.374854
H	-2.530868	-2.589479	-0.893725
H	-1.295377	-2.511985	-2.172447
C	-0.730048	0.066626	-2.189398
H	-1.440242	0.224425	-3.010200
H	0.090486	-0.529086	-2.592323
H	-0.354289	1.050867	-1.906464
C	-0.884139	-1.983211	2.685364
H	-1.539094	-1.851365	3.551178
H	0.103792	-1.600644	2.964341
H	-0.773396	-3.062427	2.522160
C	0.316567	-2.292378	0.017932
H	0.643911	-2.652573	0.995294
H	-0.278241	-3.106847	-0.402323
C	0.424447	0.130701	0.686188
H	0.711346	-0.042052	1.727406
H	-0.090319	1.090204	0.675963
C	1.587052	-2.105887	-0.827303
H	2.131659	-3.056173	-0.870344
H	1.348550	-1.844147	-1.860262
C	1.724047	0.268496	-0.125863
H	1.538244	0.651820	-1.124075
C	2.528092	-1.034136	-0.238432
Cl	3.880201	-0.780978	-1.478912
C	3.201549	-1.487848	1.056865
H	3.729865	-2.431348	0.894140
H	2.459327	-1.640516	1.847766
H	3.912776	-0.736835	1.403711
Br	2.787010	1.743300	0.702919

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55789874**

Number of imaginary frequencies = 0

1k_C014

B3LYP/6-31G* Geometry

C	1.468802	-0.531694	1.102930
C	3.489984	-0.434327	-0.542519
C	0.499686	-1.054897	-0.054753
C	2.697466	0.254410	0.572313
H	3.969039	0.334178	-1.162899
H	3.378235	0.443964	1.401323
C	2.631891	-1.305418	-1.407186
H	3.144043	-1.726998	-2.273880
C	1.343196	-1.622369	-1.215342
O	4.521475	-1.196188	0.116844
H	4.891825	-1.812190	-0.535514
Br	2.309952	2.136497	-0.033228
C	2.080079	-1.751802	1.858461
H	2.835675	-1.410661	2.573064
H	2.567338	-2.458852	1.185691
H	1.309916	-2.278066	2.428607
C	0.762290	0.335158	2.167567
H	1.487669	0.614445	2.940752
H	-0.041850	-0.211281	2.670358
H	0.360180	1.264542	1.758909
C	0.693693	-2.545396	-2.226799
H	1.418015	-2.841007	-2.991226
H	-0.148059	-2.071040	-2.746517
H	0.309825	-3.462519	-1.765080
C	-0.454626	-2.154468	0.533887
H	0.036406	-3.132533	0.520285
H	-0.651980	-1.936429	1.587935
C	-0.417618	0.070209	-0.671372
H	-0.644610	-0.172948	-1.715327
H	0.114805	1.018328	-0.697052
C	-1.813873	-2.257307	-0.169779
H	-1.679792	-2.473960	-1.233114
H	-2.385247	-3.093841	0.242929
C	-1.738465	0.240825	0.085278
H	-1.553735	0.407910	1.140235
C	-2.677616	-0.974532	-0.074024
Cl	-3.698811	-1.076562	1.480494
C	-3.656289	-0.912629	-1.244066
H	-4.199352	-1.859265	-1.323111
H	-3.103766	-0.749874	-2.177592
H	-4.371701	-0.098712	-1.125522
Br	-2.589566	1.961883	-0.455171

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55594840**

Number of imaginary frequencies = 0

1k_C015

B3LYP/6-31G* Geometry

C	-1.460087	-0.653729	-1.030392
C	-3.571914	-0.286484	0.472265
C	-0.557586	-1.012890	0.247950
C	-2.688638	0.226643	-0.672097
H	-4.118251	0.564821	0.898533
H	-3.295079	0.347718	-1.571092
C	-2.762786	-0.937577	1.543823
H	-3.322134	-1.174949	2.446466
C	-1.469790	-1.281696	1.473612
O	-4.519792	-1.258722	0.000821
H	-5.231123	-0.778171	-0.452993
Br	-2.255500	2.155732	-0.253418
C	-2.064808	-1.954459	-1.638188
H	-2.827738	-1.703455	-2.382275
H	-2.539585	-2.589046	-0.888521
H	-1.289757	-2.527345	-2.156020
C	-0.725528	0.059684	-2.189128
H	-1.434323	0.214291	-3.012048
H	0.097139	-0.534757	-2.589560
H	-0.352216	1.045295	-1.907402
C	-0.879082	-1.971328	2.692252
H	-1.536811	-1.838118	3.555507
H	0.106824	-1.583119	2.971453
H	-0.764799	-3.051017	2.535201
C	0.321311	-2.290763	0.027895
H	0.648736	-2.644921	1.007268
H	-0.273400	-3.108273	-0.386531
C	0.427761	0.135535	0.682762
H	0.713839	-0.032387	1.724902
H	-0.086307	1.095326	0.668473
C	1.591690	-2.108351	-0.818450
H	2.136849	-3.058523	-0.856597
H	1.353564	-1.852000	-1.852963
C	1.727833	0.269746	-0.129181
H	1.543186	0.648014	-1.129557
C	2.532168	-1.033278	-0.234744
Cl	3.884892	-0.785778	-1.476537
C	3.205337	-1.480144	1.063057
H	3.733366	-2.424688	0.905493
H	2.462764	-1.628223	1.854419
H	3.916686	-0.727487	1.406001
Br	2.790314	1.749513	0.692212

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55902661**

Number of imaginary frequencies = 0

1k_C016

B3LYP/6-31G* Geometry

C	1.463896	-0.537384	1.104339
C	3.490470	-0.452650	-0.542071
C	0.496255	-1.055948	-0.056290
C	2.693359	0.244813	0.574247
H	3.961138	0.316855	-1.167672
H	3.361467	0.443737	1.412966
C	2.633371	-1.322743	-1.402545
H	3.161925	-1.765875	-2.244197
C	1.341029	-1.624249	-1.215256
O	4.515362	-1.295208	0.010689
H	5.239071	-0.720200	0.308013
Br	2.313377	2.133811	-0.036123
C	2.077231	-1.759155	1.856400
H	2.819617	-1.416542	2.585041
H	2.577709	-2.457902	1.184500
H	1.305279	-2.295221	2.414665
C	0.757902	0.328420	2.169934
H	1.482309	0.605804	2.944969
H	-0.047531	-0.217709	2.670925
H	0.357148	1.258864	1.762174
C	0.689785	-2.543539	-2.229281
H	0.299201	-3.459046	-1.770034
H	1.416841	-2.842800	-2.989290
H	-0.146959	-2.064349	-2.753182
C	-0.459723	-2.155497	0.529932
H	0.030276	-3.133932	0.513042
H	-0.657671	-1.940398	1.584623
C	-0.419479	0.071854	-0.669620
H	-0.645888	-0.169660	-1.713988
H	0.113055	1.019880	-0.694062
C	-1.818588	-2.254693	-0.174910
H	-1.683259	-2.468003	-1.238697
H	-2.391240	-3.091973	0.234535
C	-1.740720	0.242468	0.086416
H	-1.557104	0.407031	1.141944
C	-2.681066	-0.971482	-0.076238
Cl	-3.702847	-1.075957	1.478299
C	-3.659585	-0.905642	-1.246125
H	-4.374086	-0.091176	-1.125778
H	-4.203662	-1.851494	-1.327462
H	-3.106617	-0.741486	-2.179111
Br	-2.589672	1.966220	-0.450280

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55703213**

Number of imaginary frequencies = 0

1k_C017

B3LYP/6-31G* Geometry

C	1.466183	-0.533297	1.101265
C	3.501931	-0.427364	-0.533912
C	0.503586	-1.047866	-0.065402
C	2.696079	0.258096	0.581457
H	3.993348	0.346166	-1.129823
H	3.370573	0.454537	1.414043
C	2.646964	-1.282685	-1.415020
H	3.173481	-1.705412	-2.269539
C	1.356141	-1.601496	-1.227961
O	4.593807	-1.183151	0.013731
H	4.248838	-2.049175	0.279733
Br	2.297085	2.142054	-0.022264
C	2.067106	-1.767142	1.846651
H	2.902696	-1.463229	2.485360
H	2.421931	-2.541215	1.159602
H	1.318561	-2.229551	2.495656
C	0.759120	0.319197	2.176715
H	1.479894	0.574338	2.962716
H	-0.058148	-0.225630	2.659394
H	0.375224	1.260943	1.779631
C	0.711592	-2.517942	-2.249041
H	1.440439	-2.807332	-3.011208
H	-0.126560	-2.038310	-2.769912
H	0.323366	-3.438516	-1.797709
C	-0.446760	-2.157694	0.511630
H	0.045810	-3.134917	0.485185
H	-0.644928	-1.953336	1.568413
C	-0.417206	0.077974	-0.673267
H	-0.643862	-0.160751	-1.718149
H	0.112356	1.027627	-0.694421
C	-1.805716	-2.255774	-0.192735
H	-1.670546	-2.455932	-1.259242
H	-2.373977	-3.100386	0.207626
C	-1.738260	0.241174	0.084999
H	-1.553446	0.406553	1.140199
C	-2.673481	-0.977755	-0.077161
Cl	-3.678890	-1.099882	1.486188
C	-3.663203	-0.910305	-1.237477
H	-4.201834	-1.859121	-1.320465
H	-3.120178	-0.735519	-2.174342
H	-4.381887	-0.101518	-1.104627
Br	-2.594940	1.960523	-0.450525

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55737798**

Number of imaginary frequencies = 0

1k_C018

B3LYP/6-31G* Geometry

C	-1.460107	-0.653643	-1.030312
C	-3.571916	-0.286569	0.472267
C	-0.557600	-1.012885	0.247965
C	-2.688605	0.226715	-0.672024
H	-4.117959	0.564808	0.898766
H	-3.295142	0.347923	-1.570927
C	-2.762872	-0.938023	1.543659
H	-3.322307	-1.175703	2.446161
C	-1.469788	-1.281933	1.473523
O	-4.519983	-1.258390	0.000554
H	-5.231474	-0.777642	-0.452782
Br	-2.255353	2.155827	-0.253303
C	-2.064900	-1.954300	-1.638218
H	-2.827593	-1.703273	-2.382547
H	-2.539962	-2.588833	-0.888664
H	-1.289861	-2.527407	-2.155850
C	-0.725568	0.059753	-2.189063
H	-1.434284	0.214114	-3.012089
H	0.097195	-0.534675	-2.589350
H	-0.352402	1.045452	-1.907435
C	-0.879017	-1.971370	2.692251
H	-0.764686	-3.051082	2.535373
H	-1.536657	-1.838024	3.555544
H	0.106857	-1.582967	2.971301
C	0.321282	-2.290788	0.027756
H	0.648687	-2.645087	1.007090
H	-0.273562	-3.108195	-0.386669
C	0.427826	0.135407	0.682905
H	0.714040	-0.032787	1.724982
H	-0.086293	1.095173	0.668955
C	1.591594	-2.108267	-0.818624
H	2.136710	-3.058463	-0.856879
H	1.353501	-1.851747	-1.853112
C	1.727753	0.269649	-0.129153
H	1.543100	0.647979	-1.129503
C	2.532138	-1.033274	-0.234810
Cl	3.884862	-0.785653	-1.476529
C	3.205236	-1.480276	1.062938
H	3.733720	-2.424512	0.905147
H	2.462613	-1.629048	1.854140
H	3.916226	-0.727406	1.406253
Br	2.790325	1.749415	0.692226

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55902974**

Number of imaginary frequencies = 0

1k_C019

B3LYP/6-31G* Geometry

C	1.516629	0.375965	-0.643450
C	2.923797	-1.493143	0.425241
C	0.172022	-0.196122	0.046508
C	2.683510	0.004106	0.298296
H	3.351383	-1.870146	-0.518003
H	2.549681	0.424530	1.294514
C	1.616647	-2.179163	0.686245
H	1.716915	-3.198119	1.054627
C	0.397501	-1.656959	0.493637
O	3.801134	-1.800934	1.501260
H	4.647165	-1.366582	1.294671
Br	4.446931	0.823990	-0.254006
C	1.472353	1.908845	-0.822488
H	2.358407	2.240936	-1.368535
H	1.466164	2.443002	0.132874
H	0.598877	2.229013	-1.398604
C	1.744938	-0.266962	-2.033445
H	2.768857	-0.065715	-2.363518
H	1.072989	0.155225	-2.785632
H	1.594600	-1.350078	-2.018296
C	-0.802868	-2.521404	0.801854
H	-0.479779	-3.504308	1.156493
H	-1.449685	-2.670623	-0.067085
H	-1.437393	-2.085085	1.582267
C	-0.205140	0.638166	1.321113
H	-0.549011	-0.039761	2.108058
H	0.685841	1.117840	1.735756
C	-0.977320	-0.076333	-1.020322
H	-1.012535	-0.975004	-1.638651
H	-0.691055	0.726353	-1.703510
C	-1.275103	1.716508	1.092921
H	-1.415575	2.299139	2.009668
H	-0.957030	2.421304	0.319766
C	-2.436607	0.305374	-0.629437
H	-2.816895	0.919953	-1.439614
C	-2.625705	1.099947	0.695508
Cl	-3.768515	2.525030	0.317761
C	-3.280188	0.356753	1.860720
H	-3.330895	1.018320	2.730107
H	-2.705992	-0.533158	2.132051
H	-4.288433	0.034048	1.600609
Br	-3.691723	-1.252063	-0.794550

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55444964**

Number of imaginary frequencies = 0

1k_C020

B3LYP/6-31G* Geometry

C	1.329475	-0.390291	0.553440
C	2.846274	1.602235	-0.034942
C	-0.001046	0.442432	0.164550
C	2.476099	0.158833	-0.323749
H	3.373034	1.651045	0.932316
H	2.255047	0.051275	-1.385172
C	1.596308	2.420175	0.053232
H	1.773167	3.493481	0.025981
C	0.344598	1.959174	0.193764
O	3.670981	2.157555	-1.052547
H	4.483787	1.622299	-1.062645
Br	4.189599	-0.905899	-0.162318
C	1.198873	-1.904502	0.300004
H	2.047889	-2.423824	0.751670
H	1.214008	-2.146881	-0.767294
H	0.288584	-2.319618	0.734235
C	1.670409	-0.188603	2.051509
H	2.690581	-0.537045	2.241219
H	1.005575	-0.774549	2.692677
H	1.600468	0.858243	2.359940
C	-0.750136	2.998519	0.307064
H	-0.306699	3.997658	0.342272
H	-1.363821	2.874982	1.204942
H	-1.441546	2.970028	-0.539943
C	-0.536264	0.139903	-1.275774
H	-1.161953	0.987535	-1.570990
H	0.291547	0.126966	-1.991664
C	-1.148033	0.074744	1.182648
H	-1.270290	0.854105	1.938059
H	-0.851812	-0.821048	1.735450
C	-1.372524	-1.142417	-1.488684
H	-1.809587	-1.079588	-2.492186
H	-0.736593	-2.026253	-1.497512
C	-2.538319	-0.297903	0.639199
H	-3.155369	-0.648753	1.464324
C	-2.532109	-1.359368	-0.480544
Cl	-2.252168	-2.971197	0.460519
C	-3.872610	-1.572427	-1.183000
H	-3.808479	-2.454349	-1.826521
H	-4.109068	-0.702700	-1.800767
H	-4.684540	-1.720159	-0.465482
Br	-3.608767	1.299442	0.037071

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55457809**

Number of imaginary frequencies = 0

1l_C001

B3LYP/6-31G* Geometry

C	-1.313417	-0.261700	-0.352736
C	-3.249101	1.286982	0.484711
C	-0.233403	0.651341	0.426345
C	-2.645147	-0.119149	0.425102
H	-3.978473	1.293243	1.311803
H	-2.523680	-0.489271	1.443656
C	-2.165225	2.276351	0.782867
H	-2.522895	3.274511	1.027898
C	-0.847463	2.045018	0.731431
O	-3.892186	1.714701	-0.709829
H	-4.583715	1.056082	-0.901932
Br	-4.101644	-1.340057	-0.257211
C	-0.940503	-1.760659	-0.385047
H	-1.658852	-2.297889	-1.008463
H	-0.969618	-2.223500	0.606223
H	0.047085	-1.929627	-0.817097
C	-1.484503	0.203488	-1.817519
H	-2.376318	-0.265558	-2.242170
H	-0.631016	-0.109551	-2.427335
H	-1.609654	1.284213	-1.905657
C	0.073780	3.208695	1.051502
H	-0.496342	4.027347	1.499206
H	0.561608	3.606673	0.153368
H	0.870774	2.942371	1.756439
C	0.199989	0.060983	1.815089
H	0.533184	0.893099	2.444548
H	-0.668758	-0.355676	2.335969
C	1.066264	0.880697	-0.424224
H	1.563192	1.780222	-0.061461
H	0.812350	1.091239	-1.463714
C	1.315820	-1.004158	1.809920
H	1.606649	-1.217765	2.844911
H	0.955195	-1.944259	1.391019
C	2.129433	-0.225808	-0.395353
H	1.811868	-1.129856	-0.907640
C	2.576445	-0.578013	1.029963
Cl	3.670560	-2.068183	0.947076
C	3.373007	0.514323	1.743263
H	4.273437	0.767589	1.180978
H	3.660453	0.172681	2.741241
H	2.772281	1.423566	1.853524
Br	3.648883	0.389236	-1.537899

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56285906**

Number of imaginary frequencies = 0

1l_C002

B3LYP/6-31G* Geometry

C	1.449065	0.273315	-0.573082
C	2.758537	-1.487049	0.832555
C	0.053604	-0.232579	0.085552
C	2.539890	-0.011806	0.479518
H	3.260736	-1.519213	1.814392
H	2.324831	0.543421	1.392771
C	1.432847	-2.181046	0.930895
H	1.499869	-3.205949	1.290482
C	0.237102	-1.692445	0.570254
O	3.532541	-2.219716	-0.111229
H	4.377192	-1.743733	-0.205847
Br	4.341080	0.752987	-0.020898
C	1.450108	1.789590	-0.883561
H	2.313522	2.027033	-1.509607
H	1.531935	2.408275	0.015182
H	0.554679	2.108520	-1.421754
C	1.736016	-0.480296	-1.893018
H	2.759274	-0.266743	-2.215054
H	1.064886	-0.142739	-2.688991
H	1.645045	-1.562110	-1.786479
C	-0.951033	-2.614533	0.713370
H	-0.631964	-3.570692	1.138552
H	-1.429246	-2.820872	-0.248642
H	-1.734969	-2.207194	1.358978
C	-0.302562	0.649099	1.335520
H	0.217617	0.252607	2.213118
H	0.067626	1.664953	1.185652
C	-1.048518	-0.086133	-1.032202
H	-1.089221	-0.991369	-1.641615
H	-0.714959	0.699980	-1.712012
C	-1.792287	0.766668	1.680233
H	-2.207082	-0.200906	1.989829
H	-1.910245	1.445036	2.532639
C	-2.499143	0.336233	-0.697251
H	-2.930596	0.818938	-1.572205
C	-2.665980	1.253527	0.525837
Cl	-2.020081	2.915027	-0.062692
C	-4.107344	1.519522	0.955993
H	-4.725213	1.825806	0.107101
H	-4.123693	2.315771	1.705140
H	-4.542718	0.616427	1.390994
Br	-3.747882	-1.241712	-0.532265

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55668059**

Number of imaginary frequencies = 0

1l_C003

B3LYP/6-31G* Geometry

C	-1.335228	-0.842216	-1.090093
C	-3.570692	-0.766822	0.191068
C	-0.482048	-1.038669	0.261144
C	-2.679912	-0.102928	-0.856917
H	-3.948419	-1.693055	-0.265389
H	-3.212107	-0.008751	-1.804080
C	-2.767357	-1.109381	1.410247
H	-3.365336	-1.286801	2.302675
C	-1.436272	-1.257386	1.467707
O	-4.751063	-0.043214	0.487990
H	-4.470045	0.842273	0.780720
Br	-2.478564	1.842954	-0.349136
C	-1.753422	-2.225979	-1.669032
H	-2.498276	-2.097849	-2.462853
H	-2.177122	-2.890415	-0.910639
H	-0.893677	-2.730698	-2.118988
C	-0.609749	-0.096645	-2.233509
H	-1.275757	-0.051344	-3.103796
H	0.297902	-0.609713	-2.556597
H	-0.362555	0.933487	-1.970344
C	-0.849357	-1.693297	2.801080
H	-0.615528	-2.765388	2.813723
H	-1.569888	-1.512397	3.603623
H	0.072330	-1.164589	3.066937
C	0.470050	-2.279766	0.200782
H	0.780171	-2.510264	1.222582
H	-0.065387	-3.168636	-0.141781
C	0.426714	0.196705	0.618057
H	0.676021	0.144557	1.680780
H	-0.132311	1.122686	0.493949
C	1.753195	-2.108586	-0.627819
H	2.345828	-3.028857	-0.572343
H	1.528566	-1.952238	-1.685919
C	1.754349	0.325277	-0.149958
H	1.598480	0.611898	-1.184712
C	2.622266	-0.940404	-0.116109
Cl	3.999770	-0.733266	-1.337516
C	3.273658	-1.239224	1.234236
H	3.942331	-0.428210	1.526372
H	3.845906	-2.169288	1.176498
H	2.514417	-1.348673	2.016091
Br	2.709984	1.918458	0.585765

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56480242**

Number of imaginary frequencies = 0

1l_C004

B3LYP/6-31G* Geometry

C	-1.320494	-0.255374	-0.358695
C	-3.254408	1.286930	0.467870
C	-0.239183	0.643796	0.432020
C	-2.667412	-0.116840	0.404677
H	-4.021146	1.292919	1.258525
H	-2.537183	-0.463168	1.430301
C	-2.167491	2.261949	0.817052
H	-2.514797	3.253224	1.112321
C	-0.848570	2.033124	0.762678
O	-3.871704	1.625354	-0.778392
H	-4.164186	2.548106	-0.713938
Br	-4.095699	-1.353488	-0.257872
C	-0.951498	-1.755211	-0.395064
H	-1.664209	-2.285924	-1.029487
H	-0.995463	-2.224558	0.592652
H	0.041515	-1.922560	-0.815511
C	-1.472708	0.213923	-1.824370
H	-2.382213	-0.219518	-2.248069
H	-0.627882	-0.127338	-2.431722
H	-1.558399	1.298667	-1.913731
C	0.073803	3.186876	1.113227
H	-0.493758	3.995315	1.582926
H	0.562613	3.606429	0.225391
H	0.870787	2.900809	1.809890
C	0.190848	0.031854	1.813189
H	0.520008	0.852282	2.459937
H	-0.679832	-0.396176	2.321384
C	1.061246	0.885684	-0.414067
H	1.558484	1.781014	-0.040986
H	0.807131	1.107091	-1.451242
C	1.308535	-1.031351	1.793983
H	1.597907	-1.259544	2.826293
H	0.949621	-1.965365	1.360698
C	2.124642	-0.220772	-0.398386
H	1.807478	-1.117599	-0.923485
C	2.569939	-0.591957	1.022526
Cl	3.667703	-2.078096	0.921074
C	3.362682	0.492124	1.752322
H	4.262206	0.757250	1.193975
H	3.651191	0.136481	2.745069
H	2.758307	1.397174	1.876279
Br	3.645839	0.410381	-1.530482

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55867049**

Number of imaginary frequencies = 0

1l_C005

B3LYP/6-31G* Geometry

C	-1.336558	-0.378605	-0.423553
C	-3.167122	1.360799	0.223403
C	-0.217863	0.725287	-0.075647
C	-2.531899	-0.020055	0.485556
H	-3.677608	1.667044	1.152262
H	-2.235433	-0.083323	1.531722
C	-2.112756	2.372944	-0.134300
H	-2.509322	3.371606	-0.306303
C	-0.814438	2.126117	-0.354000
O	-4.097793	1.390335	-0.853291
H	-4.761050	0.700926	-0.670275
Br	-4.014058	-1.386666	0.438043
C	-0.852341	-1.816028	-0.134895
H	-1.648611	-2.524093	-0.376699
H	-0.583569	-1.986144	0.912554
H	0.006423	-2.074110	-0.761820
C	-1.747831	-0.332225	-1.914198
H	-2.626582	-0.967163	-2.061366
H	-0.951792	-0.725608	-2.554206
H	-2.010110	0.671085	-2.250195
C	0.051208	3.260467	-0.861714
H	-0.509456	4.199413	-0.844956
H	0.366426	3.089254	-1.899246
H	0.964665	3.410834	-0.275103
C	0.188055	0.681628	1.447194
H	-0.537142	1.244434	2.040868
H	0.170127	-0.346784	1.822712
C	1.082480	0.464634	-0.914623
H	1.539225	1.405640	-1.228366
H	0.848682	-0.068698	-1.836571
C	1.583088	1.260727	1.707773
H	1.633009	2.287309	1.329135
H	1.774123	1.322820	2.782572
C	2.137676	-0.336051	-0.142018
H	1.718155	-1.264092	0.233368
C	2.730813	0.456367	1.041013
Cl	3.354579	-0.793849	2.266794
C	3.902819	1.374655	0.702822
H	4.767997	0.809147	0.355916
H	4.185241	1.954804	1.586376
H	3.608141	2.073620	-0.089653
Br	3.524086	-0.984739	-1.415722

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56077054**

Number of imaginary frequencies = 0

1l_C006

B3LYP/6-31G* Geometry

C	1.540106	1.395912	0.459114
C	3.148865	-0.481742	1.149755
C	0.234074	0.491832	0.743259
C	2.789353	0.560493	0.087045
H	3.629661	0.079931	1.964847
H	3.634531	1.225868	-0.093529
C	1.923036	-1.141101	1.713287
H	2.146695	-2.000233	2.343962
C	0.652526	-0.717205	1.618470
O	4.152633	-1.400360	0.756128
H	3.831840	-1.834220	-0.054376
Br	2.678684	-0.368581	-1.705851
C	1.945874	2.145973	1.766359
H	2.946742	2.579810	1.660216
H	1.947512	1.492391	2.642359
H	1.260302	2.974274	1.961828
C	1.341154	2.483353	-0.621767
H	2.161801	3.207722	-0.556340
H	0.405931	3.033625	-0.490425
H	1.360228	2.074407	-1.634191
C	-0.380932	-1.441876	2.456286
H	0.081523	-2.286911	2.974930
H	-1.209155	-1.829469	1.860131
H	-0.805578	-0.784000	3.225513
C	-0.804162	1.387212	1.501269
H	-0.536509	1.439458	2.561305
H	-0.732781	2.409362	1.122055
C	-0.387226	0.013424	-0.628522
H	0.106077	-0.899042	-0.959766
H	-0.146146	0.768290	-1.378548
C	-2.283146	0.985943	1.400128
H	-2.474275	0.036082	1.910717
H	-2.891682	1.743136	1.907269
C	-1.904339	-0.179601	-0.795202
H	-2.146316	-0.139540	-1.856195
C	-2.795501	0.806669	-0.026129
Cl	-2.577769	2.429150	-0.948985
C	-4.292345	0.512762	-0.081017
H	-4.630378	0.374058	-1.112074
H	-4.849042	1.344599	0.359158
H	-4.514103	-0.399040	0.479417
Br	-2.459824	-2.078148	-0.385822

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55841394**

Number of imaginary frequencies = 0

1l_C007

B3LYP/6-31G* Geometry

C	-1.322859	-0.252447	-0.366459
C	-3.261060	1.271696	0.516139
C	-0.238749	0.647394	0.414317
C	-2.661175	-0.136736	0.415652
H	-3.988590	1.261226	1.335341
H	-2.514618	-0.511366	1.429524
C	-2.171386	2.258478	0.816487
H	-2.528676	3.252153	1.082734
C	-0.851073	2.039802	0.729941
O	-4.031025	1.699158	-0.605463
H	-3.418151	1.891937	-1.331229
Br	-4.086637	-1.361254	-0.267373
C	-0.940401	-1.747133	-0.438290
H	-1.656681	-2.274104	-1.072021
H	-0.968417	-2.232417	0.541904
H	0.049353	-1.896799	-0.872904
C	-1.502053	0.240327	-1.823964
H	-2.446532	-0.140413	-2.224111
H	-0.702302	-0.135767	-2.469436
H	-1.496921	1.332930	-1.907241
C	0.070265	3.207074	1.034149
H	-0.496597	4.026612	1.484459
H	0.551279	3.602168	0.130805
H	0.873951	2.943980	1.732738
C	0.188684	0.051098	1.802603
H	0.521256	0.880317	2.436257
H	-0.683447	-0.364778	2.317545
C	1.063320	0.871504	-0.435443
H	1.556458	1.777220	-0.083191
H	0.814060	1.067835	-1.479438
C	1.301897	-1.016048	1.797541
H	1.583069	-1.239470	2.833065
H	0.943612	-1.951711	1.366402
C	2.133019	-0.229562	-0.395367
H	1.826009	-1.135131	-0.911250
C	2.569030	-0.582698	1.032689
Cl	3.669910	-2.067210	0.955525
C	3.353862	0.511489	1.755888
H	4.260795	0.766553	1.204925
H	3.629578	0.170652	2.757433
H	2.750026	1.419583	1.858430
Br	3.658446	0.396473	-1.523948

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56043422**

Number of imaginary frequencies = 0

1l_C008

B3LYP/6-31G* Geometry

C	1.357778	-0.667601	1.224644
C	3.516091	-0.862484	-0.154406
C	0.432203	-1.082079	-0.014162
C	2.693392	-0.000509	0.806245
H	3.941455	-1.672398	0.455628
H	3.276167	0.233179	1.697778
C	2.642527	-1.472352	-1.212543
H	3.195325	-1.873139	-2.060668
C	1.310662	-1.626140	-1.163978
O	4.660746	-0.217987	-0.682851
H	4.349957	0.595415	-1.119020
Br	2.505517	1.843726	0.005147
C	1.804360	-1.947290	1.998636
H	2.599691	-1.701707	2.711561
H	2.172337	-2.731887	1.332181
H	0.975477	-2.360498	2.578048
C	0.658348	0.247628	2.251592
H	1.344241	0.446134	3.083766
H	-0.230100	-0.226682	2.680386
H	0.375307	1.215163	1.830546
C	0.652766	-2.365745	-2.312817
H	0.182441	-3.300167	-1.983221
H	1.398356	-2.626214	-3.069291
H	-0.123933	-1.774610	-2.812315
C	-0.600818	-2.169644	0.458898
H	-0.151235	-3.166776	0.410626
H	-0.849827	-2.003466	1.511998
C	-0.409898	0.119783	-0.596147
H	-0.587289	-0.040065	-1.664612
H	0.154222	1.046181	-0.531152
C	-1.920689	-2.171697	-0.322189
H	-1.733837	-2.323385	-1.388605
H	-2.544905	-3.009655	0.001683
C	-1.764470	0.297897	0.096558
H	-1.635966	0.396002	1.168413
C	-2.740205	-0.864122	-0.187953
Cl	-3.845925	-1.020794	1.302863
C	-3.651868	-0.690019	-1.400205
H	-4.344033	0.141377	-1.265447
H	-4.222329	-1.608358	-1.568720
H	-3.044532	-0.489354	-2.291301
Br	-2.513611	2.083661	-0.383066

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56191906**

Number of imaginary frequencies = 0

1l_C009

B3LYP/6-31G* Geometry

C	1.456680	0.266327	-0.570909
C	2.767277	-1.493210	0.820282
C	0.060035	-0.230834	0.086638
C	2.563641	-0.023389	0.472449
H	3.303929	-1.541570	1.781541
H	2.332024	0.510121	1.394482
C	1.432724	-2.171557	0.950163
H	1.479933	-3.185939	1.350455
C	0.236263	-1.686955	0.583151
O	3.564075	-2.135349	-0.182299
H	3.503848	-3.091166	-0.026647
Br	4.337162	0.766970	-0.014615
C	1.461210	1.784041	-0.875933
H	2.312961	2.018095	-1.518169
H	1.569132	2.398233	0.023040
H	0.555394	2.110399	-1.392238
C	1.731481	-0.479915	-1.897837
H	2.766279	-0.302710	-2.202372
H	1.080375	-0.110338	-2.696585
H	1.599082	-1.559234	-1.806402
C	-0.954289	-2.603114	0.738950
H	-0.640946	-3.554934	1.178774
H	-1.431964	-2.820057	-0.221049
H	-1.738049	-2.183641	1.376401
C	-0.296102	0.657343	1.332274
H	0.226343	0.268502	2.211906
H	0.074281	1.671547	1.173391
C	-1.042302	-0.086839	-1.030937
H	-1.082949	-0.992204	-1.640313
H	-0.707232	0.698361	-1.710980
C	-1.785362	0.777190	1.678465
H	-2.200446	-0.187693	1.996036
H	-1.901746	1.461445	2.526403
C	-2.492882	0.336479	-0.697953
H	-2.924142	0.816564	-1.574405
C	-2.661421	1.257010	0.522726
Cl	-2.021213	2.917809	-0.071357
C	-4.103291	1.519812	0.953436
H	-4.722871	1.821843	0.104261
H	-4.121232	2.318247	1.700211
H	-4.535693	0.616796	1.391620
Br	-3.742598	-1.242255	-0.532176

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55222128**

Number of imaginary frequencies = 0

1l_C010

B3LYP/6-31G* Geometry

C	1.452180	0.272993	-0.566954
C	2.766231	-1.481635	0.851294
C	0.057752	-0.230369	0.086055
C	2.560719	-0.006470	0.478252
H	3.276324	-1.510510	1.820965
H	2.330364	0.546894	1.389423
C	1.435638	-2.171687	0.948367
H	1.499592	-3.194257	1.317452
C	0.239809	-1.690804	0.570484
O	3.641361	-2.218421	-0.001345
H	3.187380	-2.352908	-0.847313
Br	4.332181	0.765657	-0.034937
C	1.453352	1.787599	-0.886302
H	2.311770	2.021694	-1.519782
H	1.548580	2.407016	0.010075
H	0.551933	2.106528	-1.414696
C	1.731531	-0.479903	-1.891635
H	2.781201	-0.348212	-2.172332
H	1.124709	-0.080171	-2.709798
H	1.513894	-1.550793	-1.821600
C	-0.945569	-2.618601	0.697539
H	-0.627643	-3.574572	1.124140
H	-1.415703	-2.823856	-0.268973
H	-1.736781	-2.214989	1.336394
C	-0.296777	0.650690	1.336241
H	0.227170	0.256414	2.212341
H	0.070859	1.667083	1.183843
C	-1.044875	-0.081863	-1.031491
H	-1.087984	-0.985912	-1.642828
H	-0.711416	0.705452	-1.710005
C	-1.786066	0.763622	1.683363
H	-2.198235	-0.205732	1.991184
H	-1.904237	1.439365	2.537750
C	-2.495759	0.339369	-0.695029
H	-2.927362	0.825400	-1.568038
C	-2.662393	1.252211	0.531544
Cl	-2.020333	2.915960	-0.053474
C	-4.103677	1.513734	0.964654
H	-4.723485	1.821955	0.117886
H	-4.120295	2.307243	1.716650
H	-4.536645	0.608298	1.397247
Br	-3.743374	-1.240191	-0.537019

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55428764**

Number of imaginary frequencies = 0

1l_C011

B3LYP/6-31G* Geometry

C	-1.344530	-0.370012	-0.426099
C	-3.181351	1.350048	0.218221
C	-0.224272	0.723240	-0.061813
C	-2.557836	-0.026442	0.475604
H	-3.739588	1.639672	1.122738
H	-2.252473	-0.068602	1.520212
C	-2.115706	2.372640	-0.085861
H	-2.490845	3.390105	-0.209151
C	-0.816312	2.131067	-0.310839
O	-4.094473	1.273107	-0.882855
H	-4.433466	2.168690	-1.038825
Br	-4.004055	-1.405930	0.437065
C	-0.865402	-1.811584	-0.149184
H	-1.656596	-2.514702	-0.418020
H	-0.620812	-1.998788	0.901285
H	0.007079	-2.058601	-0.761481
C	-1.739669	-0.311105	-1.921012
H	-2.651118	-0.896520	-2.070717
H	-0.958849	-0.747344	-2.552320
H	-1.945120	0.703267	-2.264811
C	0.053915	3.277066	-0.782825
H	-0.501492	4.218654	-0.739020
H	0.370713	3.134848	-1.824310
H	0.966952	3.405184	-0.190944
C	0.183521	0.653649	1.459866
H	-0.541635	1.204354	2.064764
H	0.164100	-0.381699	1.814750
C	1.075474	0.477028	-0.906714
H	1.531928	1.422136	-1.208942
H	0.839549	-0.044079	-1.835081
C	1.578822	1.226482	1.733400
H	1.629089	2.262632	1.381912
H	1.769880	1.261169	2.809452
C	2.133217	-0.333689	-0.148008
H	1.715460	-1.268074	0.213360
C	2.727616	0.440130	1.046284
Cl	3.364598	-0.828270	2.245964
C	3.893248	1.370520	0.718894
H	4.758832	0.815885	0.355765
H	4.178507	1.934884	1.611723
H	3.590472	2.083255	-0.058190
Br	3.518987	-0.959351	-1.434270

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55620953**

Number of imaginary frequencies = 0

1l_C012

B3LYP/6-31G* Geometry

C	-1.340228	-0.827581	-1.090555
C	-3.563323	-0.760564	0.177622
C	-0.486208	-1.031260	0.259866
C	-2.681093	-0.073268	-0.850725
H	-3.902289	-1.701098	-0.292934
H	-3.213440	0.012580	-1.798889
C	-2.770043	-1.090177	1.406600
H	-3.359084	-1.261020	2.308442
C	-1.440775	-1.246431	1.466547
O	-4.706993	0.043498	0.439542
H	-5.266547	-0.443494	1.064663
Br	-2.466449	1.852166	-0.343527
C	-1.752322	-2.208175	-1.679320
H	-2.498957	-2.075526	-2.470801
H	-2.172400	-2.882752	-0.927598
H	-0.891639	-2.706524	-2.135100
C	-0.611651	-0.077201	-2.228853
H	-1.276323	-0.028962	-3.100090
H	0.296357	-0.589656	-2.552132
H	-0.368440	0.952088	-1.960605
C	-0.856858	-1.681385	2.801297
H	-1.576691	-1.497198	3.603976
H	0.065415	-1.153958	3.066446
H	-0.624658	-2.753866	2.815457
C	0.459425	-2.277065	0.198342
H	0.769887	-2.510440	1.219584
H	-0.079989	-3.163124	-0.145474
C	0.427867	0.199784	0.619455
H	0.677259	0.146209	1.682091
H	-0.129118	1.126882	0.493908
C	1.742308	-2.110400	-0.631574
H	2.330516	-3.033752	-0.579387
H	1.516235	-1.949972	-1.688718
C	1.755994	0.322528	-0.148592
H	1.600755	0.613063	-1.182303
C	2.617415	-0.947722	-0.118218
Cl	3.995811	-0.746176	-1.340255
C	3.268475	-1.252983	1.230888
H	3.942277	-0.446495	1.523716
H	3.834836	-2.186543	1.171027
H	2.509176	-1.358737	2.013209
Br	2.721596	1.907855	0.591037

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55945497**

Number of imaginary frequencies = 0

1l_C013

B3LYP/6-31G* Geometry

C	1.364879	-0.653097	1.223799
C	3.510579	-0.848767	-0.145755
C	0.436804	-1.078615	-0.009735
C	2.694126	0.029766	0.792823
H	3.912541	-1.662375	0.484864
H	3.278143	0.256321	1.685644
C	2.645027	-1.462469	-1.207709
H	3.187933	-1.868393	-2.062279
C	1.315246	-1.626785	-1.157070
O	4.608032	-0.109539	-0.667764
H	5.146021	-0.722992	-1.192557
Br	2.487414	1.855970	0.000402
C	1.810798	-1.926116	2.007517
H	2.610731	-1.674752	2.713341
H	2.173143	-2.720088	1.348714
H	0.984692	-2.332060	2.596300
C	0.662799	0.265818	2.245606
H	1.348525	0.468780	3.076934
H	-0.224723	-0.208662	2.676382
H	0.381455	1.231229	1.819748
C	0.660255	-2.375698	-2.301187
H	0.192906	-3.309416	-1.965509
H	1.405260	-2.638365	-3.057796
H	-0.118313	-1.789542	-2.803157
C	-0.591770	-2.166685	0.471152
H	-0.139357	-3.163026	0.430236
H	-0.840114	-1.993501	1.523183
C	-0.409170	0.116832	-0.599653
H	-0.587105	-0.049770	-1.667079
H	0.154632	1.043922	-0.539365
C	-1.912561	-2.178796	-0.308443
H	-1.726680	-2.337708	-1.374044
H	-2.533973	-3.016216	0.022237
C	-1.763338	0.294116	0.093677
H	-1.633415	0.399106	1.164704
C	-2.735559	-0.872532	-0.183112
Cl	-3.841826	-1.023659	1.308657
C	-3.647674	-0.709105	-1.396458
H	-4.341767	0.121528	-1.267231
H	-4.215700	-1.630037	-1.559129
H	-3.040618	-0.512406	-2.288657
Br	-2.520845	2.073736	-0.395352

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55659758**

Number of imaginary frequencies = 0

1l_C014

B3LYP/6-31G* Geometry

C	1.546196	0.331305	-0.560633
C	2.920113	-1.358540	0.874365
C	0.180542	-0.166373	0.148114
C	2.676261	0.099475	0.466823
H	3.477137	-1.340909	1.826237
H	2.492723	0.685179	1.367674
C	1.603279	-2.040845	1.093062
H	1.682049	-3.029809	1.540162
C	0.395106	-1.565610	0.761458
O	3.643343	-2.134183	-0.074117
H	4.485456	-1.669488	-0.228395
Br	4.452847	0.852139	-0.123956
C	1.492572	1.833624	-0.918040
H	2.398971	2.114115	-1.459516
H	1.434021	2.477378	-0.034562
H	0.644986	2.069455	-1.568565
C	1.825255	-0.460731	-1.860371
H	2.835647	-0.231384	-2.210582
H	1.131401	-0.172577	-2.655488
H	1.767151	-1.539832	-1.711345
C	-0.811069	-2.420390	1.073177
H	-0.500568	-3.355260	1.548457
H	-1.389526	-2.671578	0.180236
H	-1.508446	-1.921490	1.756334
C	-0.246392	0.800000	1.310251
H	-0.613464	0.207233	2.154169
H	0.623683	1.334475	1.701628
C	-0.933998	-0.175295	-0.960507
H	-0.943195	-1.135631	-1.478548
H	-0.627619	0.548479	-1.718161
C	-1.317466	1.835240	0.932560
H	-1.494154	2.509963	1.777125
H	-0.979706	2.458478	0.099635
C	-2.407448	0.234992	-0.664556
H	-2.759456	0.758001	-1.548543
C	-2.649053	1.163532	0.559789
Cl	-3.791369	2.525941	-0.002715
C	-3.333632	0.539887	1.776937
H	-4.330132	0.178861	1.522619
H	-3.417335	1.288887	2.569565
H	-2.759494	-0.308907	2.157341
Br	-3.652424	-1.338505	-0.708700

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55105401**

Number of imaginary frequencies = 0

1l_C015

B3LYP/6-31G* Geometry

C	1.355693	-0.324374	0.472005
C	2.820044	1.614996	-0.471638
C	0.003014	0.460913	0.055842
C	2.452288	0.129502	-0.516303
H	3.304073	1.864497	-1.431100
H	2.167324	-0.131902	-1.535286
C	1.570773	2.427454	-0.322474
H	1.734854	3.500174	-0.402428
C	0.337415	1.975183	-0.052877
O	3.682754	1.989200	0.596851
H	4.474540	1.426619	0.522965
Br	4.173140	-0.910970	-0.327323
C	1.217943	-1.857484	0.375261
H	2.083732	-2.330724	0.845034
H	1.190486	-2.208610	-0.661233
H	0.326919	-2.225131	0.885344
C	1.756252	0.020557	1.926975
H	2.764240	-0.357874	2.119605
H	1.084711	-0.461899	2.644072
H	1.766639	1.094448	2.116844
C	-0.751401	3.019992	0.069300
H	-0.310586	4.019509	0.016340
H	-1.304060	2.950894	1.011311
H	-1.496612	2.940400	-0.727606
C	-0.585722	0.040269	-1.333556
H	-1.238987	0.854359	-1.662526
H	0.209250	-0.015646	-2.083906
C	-1.104375	0.171787	1.140145
H	-1.204424	1.007626	1.835404
H	-0.781634	-0.674635	1.752889
C	-1.407967	-1.265336	-1.409806
H	-1.873268	-1.298652	-2.402021
H	-0.759420	-2.138301	-1.355972
C	-2.509740	-0.249753	0.677418
H	-3.095343	-0.534618	1.549529
C	-2.535411	-1.399657	-0.351912
Cl	-2.222480	-2.930065	0.704679
C	-3.896570	-1.668723	-0.994042
H	-4.686275	-1.755447	-0.242620
H	-3.850101	-2.601515	-1.563121
H	-4.154048	-0.854056	-1.675407
Br	-3.612148	1.289714	-0.012576

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55081144**

Number of imaginary frequencies = 0

1m_C001

B3LYP/6-31G* Geometry

C	1.482903	0.689219	0.538605
C	2.457443	-1.652430	-0.082146
C	-0.002205	0.038807	0.604446
C	2.272472	-0.177370	-0.464906
H	2.655194	-2.213353	-1.011242
H	1.802368	-0.122836	-1.446325
C	1.215213	-2.174259	0.579792
H	1.282128	-3.225216	0.853706
C	0.142795	-1.464380	0.957245
O	3.511245	-1.895430	0.845129
H	4.318331	-1.514074	0.455406
Br	4.100687	0.570192	-0.885986
C	2.140325	0.682561	1.936636
H	3.197947	0.944645	1.838981
H	2.087721	-0.293405	2.420996
H	1.671784	1.429567	2.585306
C	1.480479	2.153175	0.032284
H	2.452377	2.606879	0.241136
H	0.720634	2.763197	0.526291
H	1.325161	2.234033	-1.048333
C	-0.896301	-2.179259	1.797891
H	-1.026672	-1.697310	2.774308
H	-0.578046	-3.208737	1.985811
H	-1.872727	-2.219589	1.310646
C	-0.825783	0.801454	1.687238
H	-0.527639	0.461241	2.683271
H	-0.571644	1.862181	1.646107
C	-0.685510	0.226087	-0.801164
H	-0.325053	-0.532172	-1.500347
H	-0.376009	1.195354	-1.200033
C	-2.356777	0.707008	1.578687
H	-2.708851	-0.304382	1.805375
H	-2.808279	1.368399	2.326487
C	-2.214271	0.261864	-0.904714
H	-2.500053	0.655813	-1.879365
C	-2.923069	1.058094	0.203401
Cl	-2.489111	2.845577	-0.175837
C	-4.447591	0.993745	0.161295
H	-4.869677	1.696949	0.884319
H	-4.784593	-0.016112	0.409358
H	-4.825376	1.248286	-0.833387
Br	-2.973682	-1.602095	-1.015381

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56334019**

Number of imaginary frequencies = 0

1m_C002

B3LYP/6-31G* Geometry

C	-1.355130	0.161943	0.748433
C	-3.016100	0.810932	-1.156580
C	-0.190142	1.009414	0.033201
C	-2.315482	-0.302421	-0.368903
H	-3.366425	0.368737	-2.104307
H	-1.788262	-0.948026	-1.071889
C	-2.035139	1.904109	-1.459818
H	-2.409206	2.661135	-2.146474
C	-0.809725	2.040707	-0.935794
O	-4.116414	1.417605	-0.489298
H	-4.733309	0.698467	-0.262845
Br	-3.756088	-1.549792	0.294225
C	-2.099010	1.033887	1.787153
H	-2.981407	0.495730	2.145063
H	-2.440218	1.981603	1.367959
H	-1.461628	1.235011	2.653144
C	-0.806594	-1.082638	1.480061
H	-1.618798	-1.575836	2.018919
H	-0.045203	-0.816688	2.219069
H	-0.383642	-1.823663	0.793184
C	0.009087	3.237636	-1.374409
H	-0.572975	3.862695	-2.057269
H	0.925545	2.946926	-1.903742
H	0.311443	3.867064	-0.529790
C	0.680776	1.710382	1.131710
H	0.220685	2.658183	1.427367
H	0.695472	1.094633	2.036022
C	0.771319	0.105415	-0.830301
H	1.145050	0.677302	-1.686503
H	0.228240	-0.739101	-1.258874
C	2.137009	1.958709	0.716849
H	2.174901	2.582274	-0.180270
H	2.657728	2.517804	1.499605
C	1.970962	-0.434448	-0.043275
H	1.636578	-0.982249	0.829615
C	2.947883	0.674546	0.406217
Cl	3.736268	0.085279	1.985836
C	4.083269	0.995168	-0.563417
H	4.652087	1.854088	-0.194947
H	3.667488	1.249650	-1.546097
H	4.756976	0.147111	-0.686745
Br	2.850538	-1.871450	-1.112276

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56321003**

Number of imaginary frequencies = 0

1m_C003

B3LYP/6-31G* Geometry

C	-1.367526	0.096090	0.759800
C	-3.056018	0.827225	-1.100374
C	-0.228001	1.042040	0.116052
C	-2.308586	-0.310613	-0.401207
H	-3.411586	0.437649	-2.068719
H	-1.752326	-0.874787	-1.150380
C	-2.105860	1.957831	-1.348510
H	-2.492314	2.734677	-2.005410
C	-0.887091	2.098637	-0.811964
O	-4.159527	1.355462	-0.374184
H	-4.758238	0.607035	-0.199702
Br	-3.704808	-1.665264	0.142216
C	-2.149859	0.846307	1.862149
H	-3.053320	0.282871	2.111092
H	-2.462061	1.844660	1.550443
H	-1.552661	0.926259	2.776258
C	-0.809358	-1.201364	1.387120
H	-1.619023	-1.736252	1.888770
H	-0.044937	-0.998713	2.137421
H	-0.396598	-1.886242	0.639216
C	-0.104492	3.344083	-1.188572
H	-0.581745	3.846906	-2.034137
H	0.930505	3.127391	-1.480036
H	-0.060358	4.066371	-0.364350
C	0.610476	1.793713	1.202194
H	1.062283	2.668746	0.732210
H	-0.044097	2.193946	1.980436
C	0.780830	0.257976	-0.803658
H	1.218842	0.964672	-1.514769
H	0.250245	-0.473543	-1.418961
C	1.760681	1.016190	1.867213
H	2.310993	1.696490	2.527197
H	1.391534	0.208926	2.502538
C	1.945213	-0.468372	-0.107565
H	1.607907	-1.341349	0.442520
C	2.752647	0.429060	0.840684
Cl	3.925901	-0.640280	1.792132
C	3.595036	1.500983	0.150130
H	4.134959	2.090171	0.896293
H	2.960163	2.180088	-0.428694
H	4.314584	1.045252	-0.531990
Br	3.076654	-1.276132	-1.542244

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56365564**

Number of imaginary frequencies = 0

1m_C004

B3LYP/6-31G* Geometry

C	1.489919	0.676518	0.541327
C	2.471699	-1.651804	-0.084556
C	0.004807	0.031760	0.604656
C	2.296237	-0.183835	-0.463623
H	2.710437	-2.213680	-1.001672
H	1.806112	-0.145951	-1.435903
C	1.212840	-2.181919	0.545620
H	1.247972	-3.247040	0.782032
C	0.143179	-1.475526	0.939921
O	3.559541	-1.790602	0.838346
H	3.547528	-2.705999	1.159914
Br	4.091438	0.586313	-0.899948
C	2.140577	0.674179	1.942680
H	3.205053	0.904407	1.845540
H	2.060574	-0.293022	2.441593
H	1.686077	1.440366	2.579255
C	1.485639	2.141354	0.036407
H	2.451657	2.600143	0.258494
H	0.713566	2.745128	0.519394
H	1.347933	2.221459	-1.046574
C	-0.898637	-2.198397	1.769464
H	-1.024078	-1.730426	2.753335
H	-0.588801	-3.233762	1.940614
H	-1.875895	-2.223690	1.283314
C	-0.817392	0.784972	1.695284
H	-0.519139	0.435307	2.688153
H	-0.559661	1.845084	1.664093
C	-0.681069	0.231448	-0.798067
H	-0.322221	-0.520018	-1.505238
H	-0.369161	1.203571	-1.187683
C	-2.348964	0.696203	1.587675
H	-2.705017	-0.315460	1.807001
H	-2.797575	1.353238	2.341062
C	-2.209604	0.272380	-0.900048
H	-2.495195	0.675982	-1.870775
C	-2.916330	1.059733	0.215978
Cl	-2.481209	2.849234	-0.148354
C	-4.441071	0.997262	0.175540
H	-4.861210	1.694647	0.905321
H	-4.779028	-0.014312	0.415259
H	-4.820118	1.260997	-0.816254
Br	-2.975627	-1.589030	-1.030183

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55886529**

Number of imaginary frequencies = 0

1m_C005

B3LYP/6-31G* Geometry

C	1.164017	-0.190581	-1.089919
C	3.264966	-1.472929	-0.326316
C	0.419692	-0.420520	0.317915
C	2.710845	-0.200897	-0.964925
H	3.142577	-2.270716	-1.073101
H	3.156732	-0.043002	-1.947469
C	2.477995	-1.823243	0.901129
H	2.984080	-2.516684	1.570865
C	1.236419	-1.410592	1.193904
O	4.662972	-1.445988	-0.102566
H	4.841204	-0.670274	0.458639
Br	3.473390	1.379351	0.041732
C	0.787861	1.105798	-1.843265
H	1.325703	1.125718	-2.798898
H	1.074641	2.005692	-1.296638
H	-0.276904	1.159880	-2.078819
C	0.851249	-1.364451	-2.066164
H	1.522281	-1.327686	-2.931951
H	-0.168438	-1.284728	-2.453872
H	0.957824	-2.346236	-1.596694
C	0.603004	-1.974257	2.456188
H	1.375086	-2.399073	3.103750
H	-0.108068	-2.779287	2.231674
H	0.060111	-1.226565	3.044362
C	0.212291	0.890188	1.156507
H	0.049540	0.595981	2.197952
H	1.130915	1.477073	1.162137
C	-1.004958	-1.057070	0.142074
H	-1.327272	-1.445933	1.109430
H	-0.971230	-1.922611	-0.520092
C	-0.958123	1.804766	0.740934
H	-1.064632	2.600591	1.487238
H	-0.749283	2.302181	-0.205930
C	-2.110134	-0.109943	-0.336508
H	-1.933460	0.260796	-1.343708
C	-2.313202	1.075911	0.618296
Cl	-3.488143	2.266683	-0.175857
C	-2.909520	0.711004	1.977843
H	-3.048480	1.616393	2.574500
H	-2.239429	0.041495	2.527706
H	-3.872599	0.211220	1.860242
Br	-3.772266	-1.193895	-0.571371

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56342693**

Number of imaginary frequencies = 0

1m_C006

B3LYP/6-31G* Geometry

C	-1.363166	0.163483	0.749559
C	-3.027315	0.810530	-1.142945
C	-0.197168	1.010085	0.038044
C	-2.337730	-0.303266	-0.362407
H	-3.414961	0.372899	-2.076415
H	-1.797261	-0.920757	-1.080281
C	-2.033170	1.890800	-1.467939
H	-2.384645	2.635857	-2.183684
C	-0.811820	2.038990	-0.935647
O	-4.124036	1.341713	-0.391452
H	-4.498388	2.072987	-0.907470
Br	-3.735723	-1.576856	0.288806
C	-2.099560	1.031067	1.797174
H	-3.000992	0.508751	2.128605
H	-2.412675	1.995022	1.392652
H	-1.468396	1.202008	2.674440
C	-0.811605	-1.083711	1.474624
H	-1.620970	-1.576520	2.016955
H	-0.043577	-0.819793	2.207649
H	-0.396546	-1.824680	0.782821
C	0.007093	3.234771	-1.376008
H	-0.569722	3.855981	-2.067265
H	0.928073	2.942721	-1.896125
H	0.302269	3.868684	-0.532101
C	0.674157	1.710779	1.136208
H	0.214039	2.658155	1.433777
H	0.687823	1.093870	2.039543
C	0.764084	0.106875	-0.827389
H	1.136932	0.677484	-1.684968
H	0.219312	-0.737671	-1.253542
C	2.130770	1.960047	0.723291
H	2.170329	2.587733	-0.170970
H	2.651187	2.515449	1.508900
C	1.965261	-0.432231	-0.042485
H	1.632368	-0.982741	0.829257
C	2.941790	0.676853	0.407547
Cl	3.734994	0.085066	1.983499
C	4.074602	1.001334	-0.563939
H	4.643258	1.859991	-0.194584
H	3.656303	1.257742	-1.545089
H	4.748939	0.154358	-0.691080
Br	2.845933	-1.865310	-1.116378

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55892973**

Number of imaginary frequencies = 0

1m_C007

B3LYP/6-31G* Geometry

C	-1.372691	0.090260	0.754065
C	-3.081123	0.838370	-1.069222
C	-0.236416	1.039720	0.112554
C	-2.338067	-0.307691	-0.397597
H	-3.494599	0.457976	-2.016181
H	-1.776367	-0.831147	-1.171750
C	-2.112859	1.950263	-1.353259
H	-2.477891	2.717469	-2.037701
C	-0.891602	2.093346	-0.820829
O	-4.157842	1.290130	-0.241197
H	-4.576825	2.037571	-0.695996
Br	-3.684423	-1.693876	0.128117
C	-2.137504	0.823381	1.879538
H	-3.052916	0.272634	2.110694
H	-2.431225	1.836051	1.596545
H	-1.535292	0.868658	2.793122
C	-0.806404	-1.215853	1.356536
H	-1.608102	-1.752716	1.867533
H	-0.025147	-1.023595	2.092285
H	-0.413303	-1.895072	0.592957
C	-0.102888	3.330166	-1.212347
H	-0.057002	4.062296	-0.396792
H	-0.574552	3.825117	-2.066042
H	0.931749	3.105251	-1.497508
C	0.598873	1.796467	1.197779
H	1.050339	2.672108	0.728036
H	-0.058485	2.195338	1.974403
C	0.774574	0.255622	-0.805578
H	1.211352	0.958464	-1.521197
H	0.243963	-0.480769	-1.415129
C	1.748559	1.021853	1.866575
H	2.296446	1.703772	2.526964
H	1.378079	0.215327	2.502038
C	1.940705	-0.465126	-0.106464
H	1.604980	-1.338896	0.442875
C	2.743744	0.435255	0.842805
Cl	3.917556	-0.630019	1.798043
C	3.585594	1.508137	0.153036
H	4.122309	2.099586	0.899746
H	2.950710	2.184966	-0.428502
H	4.307789	1.052873	-0.526589
Br	3.077946	-1.269524	-1.538875

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55958942**

Number of imaginary frequencies = 0

1m_C008

B3LYP/6-31G* Geometry

C	-1.42910	0.21968	1.28309
C	-3.03825	-1.58141	0.43652
C	-0.24167	-0.22943	0.28027
C	-2.84264	-0.09573	0.73969
H	-3.14318	-2.08234	1.40919
H	-3.59515	0.25481	1.44726
C	-1.83901	-2.13401	-0.27672
H	-2.02669	-3.08889	-0.76486
C	-0.60678	-1.60284	-0.33902
O	-4.25730	-1.88608	-0.21871
H	-4.27633	-1.35281	-1.03344
Br	-3.35734	0.96213	-0.90065
C	-1.38692	1.71111	1.68083
H	-2.06972	1.87654	2.52290
H	-1.71130	2.36593	0.86963
H	-0.39060	2.02993	1.99717
C	-1.34926	-0.60047	2.61198
H	-2.28669	-0.50457	3.17136
H	-0.55886	-0.22069	3.26381
H	-1.16261	-1.66331	2.43771
C	0.42464	-2.37501	-1.13036
H	-0.02010	-3.29117	-1.52991
H	1.29084	-2.65648	-0.52825
H	0.80894	-1.80223	-1.98171
C	-0.05114	0.80278	-0.89140
H	-0.73539	0.55019	-1.70308
H	-0.34732	1.79462	-0.54912
C	1.06917	-0.27485	1.16806
H	1.16929	-1.25229	1.64591
H	0.92125	0.43769	1.98258
C	1.36228	0.94509	-1.47627
H	1.67808	0.03306	-1.99695
H	1.35213	1.74486	-2.22526
C	2.45730	0.13542	0.62792
H	3.07292	0.45382	1.46756
C	2.45483	1.22873	-0.45148
Cl	2.01914	2.79559	0.48899
C	3.80946	1.51729	-1.09439
H	3.73598	2.41270	-1.71748
H	4.11487	0.67494	-1.72017
H	4.58143	1.68147	-0.33699
Br	3.54516	-1.44299	-0.00516

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55416994**

Number of imaginary frequencies = 0

1m_C009

B3LYP/6-31G* Geometry

C	1.127053	-0.499007	-1.049916
C	3.210793	-1.552532	0.014132
C	0.401032	-0.314644	0.381074
C	2.667933	-0.475935	-0.922641
H	3.063528	-2.516522	-0.492060
H	3.129578	-0.551687	-1.908071
C	2.451330	-1.520516	1.308815
H	2.982511	-1.964407	2.148787
C	1.244271	-0.969978	1.504919
O	4.613419	-1.488896	0.205063
H	4.808755	-0.592382	0.532347
Br	3.377792	1.304631	-0.286147
C	0.741526	0.545753	-2.125036
H	1.154359	0.227087	-3.089678
H	1.151024	1.535260	-1.914434
H	-0.337969	0.642694	-2.255797
C	0.805735	-1.892361	-1.671406
H	1.489408	-2.099367	-2.502638
H	-0.207148	-1.909382	-2.084659
H	0.892848	-2.711301	-0.952045
C	0.721136	-0.936990	2.929513
H	1.438512	-1.415495	3.601937
H	-0.236824	-1.452927	3.060658
H	0.582656	0.091411	3.284850
C	0.162887	1.203479	0.741687
H	0.981557	1.570468	1.365349
H	0.186632	1.814725	-0.161049
C	-1.011141	-1.012491	0.393032
H	-1.305654	-1.226476	1.422457
H	-0.976852	-1.980268	-0.102309
C	-1.174219	1.473521	1.440912
H	-1.241861	0.904180	2.374794
H	-1.241380	2.529818	1.719112
C	-2.120401	-0.162542	-0.230825
H	-1.877460	0.116932	-1.249363
C	-2.423775	1.110458	0.606070
Cl	-2.731445	2.495436	-0.600742
C	-3.649643	1.039928	1.514242
H	-3.708498	1.947930	2.121635
H	-3.565165	0.175733	2.183516
H	-4.569926	0.934781	0.939072
Br	1.127053	-0.499007	-1.049916

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55845564**

Number of imaginary frequencies = 0

1m_C010

B3LYP/6-31G* Geometry

C	1.169353	-0.183227	-1.085528
C	3.255541	-1.460832	-0.332241
C	0.422133	-0.415140	0.321039
C	2.720444	-0.180599	-0.951044
H	3.091634	-2.251468	-1.086462
H	3.161289	-0.032484	-1.937632
C	2.484840	-1.805538	0.906708
H	2.987372	-2.491006	1.590003
C	1.241345	-1.400907	1.199207
O	4.655975	-1.338489	-0.113790
H	4.974310	-2.195778	0.209865
Br	3.462720	1.391169	0.046434
C	0.792427	1.114737	-1.835749
H	1.330240	1.135513	-2.791463
H	1.082451	2.012346	-1.287952
H	-0.272449	1.168358	-2.071248
C	0.851235	-1.351418	-2.065569
H	1.525729	-1.314913	-2.928730
H	-0.166764	-1.264702	-2.456790
H	0.949055	-2.336981	-1.601572
C	0.612289	-1.961767	2.464636
H	1.385897	-2.381922	3.113741
H	-0.097885	-2.768808	2.244290
H	0.069125	-1.212755	3.050392
C	0.210309	0.895182	1.159410
H	0.048144	0.602368	2.201379
H	1.127710	1.483889	1.161770
C	-0.999755	-1.057278	0.144544
H	-1.322777	-1.446423	1.111715
H	-0.962916	-1.922818	-0.517508
C	-0.963081	1.804941	0.741838
H	-1.073333	2.600582	1.487813
H	-0.754174	2.302751	-0.204708
C	-2.106776	-0.113669	-0.336430
H	-1.928802	0.257177	-1.343326
C	-2.315587	1.071618	0.617511
Cl	-3.494422	2.257560	-0.179001
C	-2.912998	0.705079	1.976120
H	-3.056529	1.610283	2.571935
H	-2.240884	0.038837	2.527474
H	-3.873847	0.201248	1.857171
Br	-3.765450	-1.203483	-0.574821

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55869850**

Number of imaginary frequencies = 0

1m_C011

B3LYP/6-31G* Geometry

C	-1.435949	0.254598	1.271461
C	-3.021212	-1.567091	0.486749
C	-0.253638	-0.188912	0.257549
C	-2.853905	-0.075974	0.737260
H	-3.059549	-2.041724	1.482770
H	-3.598610	0.271543	1.454868
C	-1.846231	-2.100589	-0.279586
H	-2.031180	-3.042167	-0.797995
C	-0.631210	-1.542108	-0.394241
O	-4.263432	-1.808863	-0.165839
H	-4.354740	-2.769690	-0.263397
Br	-3.373184	0.947008	-0.900023
C	-1.399920	1.751387	1.647382
H	-2.067613	1.923310	2.500328
H	-1.747147	2.388292	0.831734
H	-0.399437	2.081277	1.940627
C	-1.332991	-0.541518	2.613631
H	-2.273637	-0.459314	3.169642
H	-0.554497	-0.131464	3.261499
H	-1.119130	-1.602780	2.460756
C	0.346667	-2.233860	-1.318958
H	-0.020371	-3.230775	-1.581579
H	1.343431	-2.342776	-0.891244
H	0.459964	-1.678988	-2.259301
C	-0.037224	0.860111	-0.891454
H	-0.738284	0.651660	-1.701352
H	-0.292153	1.855233	-0.527108
C	1.053958	-0.268001	1.150408
H	1.130471	-1.249671	1.623572
H	0.912835	0.445330	1.965198
C	1.378604	0.953765	-1.481270
H	1.661958	0.031465	-2.002489
H	1.393716	1.753300	-2.230456
C	2.455023	0.117241	0.627129
H	3.062763	0.435795	1.472105
C	2.484879	1.201873	-0.461667
Cl	2.105350	2.786522	0.474629
C	3.845222	1.439669	-1.112174
H	3.799436	2.331975	-1.742336
H	4.117037	0.581746	-1.732507
H	4.626614	1.582217	-0.360153
Br	3.531818	-1.491217	0.044923

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56334019**

Number of imaginary frequencies = 0

1n_C001

B3LYP/6-31G* Geometry

C	1.480490	0.451870	-0.849249
C	2.825451	0.631953	1.339504
C	0.140217	0.938072	-0.089614
C	2.342584	-0.264835	0.209825
H	3.616547	1.295669	0.952206
H	1.819140	-1.123118	0.630124
C	1.695300	1.484940	1.832884
H	1.908967	2.002094	2.766564
C	0.527100	1.690145	1.207866
O	3.330530	-0.117948	2.437171
H	4.081199	-0.631702	2.090813
Br	3.992403	-1.137353	-0.567089
C	2.237698	1.668287	-1.433125
H	3.243947	1.359530	-1.733616
H	2.331161	2.488967	-0.715827
H	1.731528	2.052770	-2.323213
C	1.192699	-0.528746	-2.010639
H	2.082926	-0.617788	-2.638529
H	0.370734	-0.189982	-2.646856
H	0.952832	-1.536852	-1.660272
C	-0.425234	2.691652	1.830470
H	0.009056	3.104989	2.745191
H	-1.392984	2.255023	2.101658
H	-0.631003	3.533105	1.157926
C	-0.671446	1.847498	-1.067483
H	-0.224037	2.846668	-1.097218
H	-0.574481	1.444892	-2.077860
C	-0.720799	-0.324130	0.284137
H	-0.291433	-0.819375	1.158329
H	-0.694704	-1.040349	-0.538133
C	-2.177698	2.003102	-0.794598
H	-2.358671	2.641199	0.076668
H	-2.640782	2.512553	-1.647055
C	-2.195602	-0.052505	0.575238
H	-2.326826	0.527933	1.489807
C	-2.939757	0.690211	-0.540974
Cl	-2.899237	-0.310094	-2.100580
C	-4.408849	0.956395	-0.220375
H	-4.957126	0.022144	-0.087480
H	-4.874744	1.532493	-1.024740
H	-4.482167	1.536104	0.708536
Br	-3.062952	-1.785082	1.049440

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57154775**

Number of imaginary frequencies = 0

1n_C002

B3LYP/6-31G* Geometry

C	1.499323	0.532715	-0.799916
C	2.800353	0.458274	1.430358
C	0.146751	0.943658	-0.019381
C	2.356873	-0.301903	0.183786
H	3.651007	1.100251	1.173635
H	1.816514	-1.203907	0.477271
C	1.681069	1.313493	1.954523
H	1.896339	1.767761	2.921089
C	0.518933	1.582720	1.340318
O	3.315637	-0.400899	2.444363
H	2.574295	-0.930431	2.781469
Br	3.998618	-1.067132	-0.673713
C	2.266230	1.800808	-1.243127
H	3.271890	1.520691	-1.571111
H	2.360250	2.536237	-0.438711
H	1.766868	2.284868	-2.087557
C	1.224719	-0.319633	-2.061978
H	2.127769	-0.361203	-2.675150
H	0.423388	0.096353	-2.677566
H	0.962107	-1.354221	-1.822062
C	-0.422810	2.549801	2.030162
H	0.013043	2.890722	2.973643
H	-1.398969	2.110353	2.265519
H	-0.612780	3.440119	1.418765
C	-0.664808	1.931044	-0.918944
H	-0.217526	2.929249	-0.866487
H	-0.568589	1.613581	-1.959130
C	-0.712101	-0.347602	0.234694
H	-0.281477	-0.923205	1.057632
H	-0.687234	-0.984655	-0.650566
C	-2.171026	2.062688	-0.634329
H	-2.352767	2.625927	0.286806
H	-2.634534	2.640392	-1.441775
C	-2.184955	-0.101540	0.556147
H	-2.310035	0.401915	1.516113
C	-2.932990	0.732539	-0.490849
Cl	-2.896981	-0.132386	-2.128478
C	-4.400649	0.971059	-0.143021
H	-4.947561	0.028605	-0.081339
H	-4.871081	1.607929	-0.897349
H	-4.469407	1.476412	0.828761
Br	-3.050544	-1.867289	0.890474

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56928023**

Number of imaginary frequencies = 0

1n_C003

B3LYP/6-31G* Geometry

C	1.480410	0.450955	-0.849447
C	2.825653	0.633266	1.338856
C	0.140247	0.937910	-0.090269
C	2.342599	-0.264639	0.210146
H	3.616727	1.296586	0.950855
H	1.819313	-1.122536	0.631427
C	1.695540	1.486633	1.831652
H	1.909296	2.004561	2.764880
C	0.527204	1.691068	1.206628
O	3.330811	-0.115641	2.437237
H	4.081534	-0.629586	2.091267
Br	3.992283	-1.137929	-0.566248
C	2.237561	1.666868	-1.434607
H	3.243672	1.357799	-1.735230
H	2.331420	2.488234	-0.718143
H	1.731106	2.050631	-2.324853
C	1.192774	-0.530639	-2.010040
H	2.083214	-0.620508	-2.637513
H	0.371172	-0.192125	-2.646820
H	0.952489	-1.538396	-1.658934
C	-0.425203	2.692950	1.828462
H	0.009168	3.107227	2.742728
H	-1.392787	2.256296	2.100248
H	-0.631290	3.533711	1.155203
C	-0.671313	1.846800	-1.068749
H	-0.223884	2.845955	-1.098925
H	-0.574295	1.443773	-2.078940
C	-0.720861	-0.323896	0.284754
H	-0.291590	-0.818032	1.159631
H	-0.694648	-1.041241	-0.536531
C	-2.177588	2.002548	-0.796067
H	-2.358620	2.641264	0.074725
H	-2.640651	2.511383	-1.648905
C	-2.195751	-0.052035	0.575313
H	-2.327119	0.529117	1.489423
C	-2.939668	0.689895	-0.541507
Cl	-2.898976	-0.311724	-2.100414
C	-4.408803	0.956337	-0.221380
H	-4.957089	0.022221	-0.087559
H	-4.874634	1.531579	-1.026394
H	-4.482205	1.537036	0.706916
Br	-3.063169	-1.784203	1.050766

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.57154775**

Number of imaginary frequencies = 0

1n_C004

B3LYP/6-31G* Geometry

C	-1.42360	0.38518	-1.07404
C	-3.28042	1.31602	0.50996
C	-0.37172	0.36611	0.13783
C	-2.89104	0.30457	-0.58549
H	-4.05406	0.86479	1.14485
H	-3.54997	0.44492	-1.44301
C	-2.12174	1.72993	1.35948
H	-2.38760	2.44430	2.13620
C	-0.83819	1.37007	1.21603
O	-3.80135	2.52077	-0.07617
H	-4.70831	2.33549	-0.36890
Br	-3.48466	-1.52635	0.03295
C	-1.19110	-0.72310	-2.12590
H	-1.86410	-0.55313	-2.97480
H	-1.40406	-1.72265	-1.74515
H	-0.17020	-0.71315	-2.51651
C	-1.32887	1.74192	-1.83760
H	-2.13799	1.81618	-2.57155
H	-0.38716	1.80288	-2.39020
H	-1.40821	2.60592	-1.17610
C	0.15992	2.00751	2.16304
H	-0.35406	2.68116	2.85464
H	0.90620	2.60504	1.62516
H	0.70581	1.27674	2.77013
C	-0.25905	-1.06637	0.76353
H	-1.12739	-1.25579	1.39664
H	-0.29736	-1.80520	-0.03866
C	1.02754	0.77320	-0.44913
H	1.06665	1.85208	-0.61856
H	1.15176	0.30506	-1.42711
C	1.01097	-1.35868	1.57200
H	1.03593	-0.77423	2.50067
H	1.00474	-2.41193	1.87466
C	2.26012	0.38905	0.37497
H	2.34469	0.99153	1.27796
C	2.32541	-1.07278	0.82293
Cl	2.40759	-2.18762	-0.65377
C	3.54483	-1.38699	1.68630
H	4.47133	-1.20047	1.14016
H	3.52375	-2.43232	2.00665
H	3.53528	-0.75095	2.58073
Br	3.88031	0.95387	-0.64775

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56268033**

Number of imaginary frequencies = 0

1n_C005

B3LYP/6-31G* Geometry

C	-1.428027	0.383152	-1.072330
C	-3.286198	1.310653	0.502849
C	-0.374922	0.362338	0.138863
C	-2.897957	0.303960	-0.586538
H	-4.076658	0.873015	1.126346
H	-3.561734	0.456595	-1.436741
C	-2.128619	1.713681	1.364870
H	-2.389959	2.401350	2.171501
C	-0.842185	1.361934	1.221223
O	-3.831656	2.449323	-0.193808
H	-3.867139	3.188500	0.434261
Br	-3.487373	-1.520078	0.034201
C	-1.197555	-0.726251	-2.123578
H	-1.866245	-0.551062	-2.974628
H	-1.419058	-1.724488	-1.744314
H	-0.174907	-0.722654	-2.509820
C	-1.325173	1.737822	-1.837778
H	-2.141925	1.823177	-2.561063
H	-0.387579	1.788527	-2.398479
H	-1.388316	2.601878	-1.174715
C	0.154090	1.992759	2.174160
H	-0.359282	2.660979	2.871953
H	0.900979	2.593713	1.640949
H	0.699575	1.257287	2.775445
C	-0.260281	-1.071307	0.762385
H	-1.128486	-1.263626	1.394735
H	-0.299554	-1.806708	-0.042808
C	1.024260	0.772097	-0.446198
H	1.062951	1.851306	-0.613898
H	1.148131	0.306216	-1.425244
C	1.010840	-1.366786	1.567986
H	1.037188	-0.787379	2.499857
H	1.005094	-2.421480	1.865499
C	2.257397	0.386474	0.376619
H	2.341715	0.985298	1.282099
C	2.324515	-1.077107	0.818814
Cl	2.406595	-2.185731	-0.661726
C	3.544827	-1.393282	1.680292
H	4.470829	-1.204304	1.134149
H	3.524746	-2.439750	1.996956
H	3.535613	-0.760484	2.577046
Br	3.876661	0.957680	-0.643890

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56155160**

Number of imaginary frequencies = 0

1n_C006

B3LYP/6-31G* Geometry

C	-1.426404	0.382519	-1.074015
C	-3.291289	1.324558	0.493056
C	-0.379555	0.351908	0.142204
C	-2.898850	0.309510	-0.595072
H	-4.103653	0.898942	1.087775
H	-3.562019	0.453854	-1.447335
C	-2.141528	1.698366	1.376568
H	-2.409480	2.388373	2.175606
C	-0.854931	1.339692	1.233672
O	-3.875202	2.499197	-0.092530
H	-3.150212	3.075778	-0.379250
Br	-3.486959	-1.515768	0.033550
C	-1.197565	-0.719468	-2.133203
H	-1.844854	-0.521670	-2.996063
H	-1.451231	-1.714522	-1.766253
H	-0.166870	-0.736990	-2.497247
C	-1.303240	1.741068	-1.832898
H	-2.160821	1.889840	-2.497122
H	-0.406367	1.750319	-2.458415
H	-1.237690	2.599170	-1.157347
C	0.138292	1.954025	2.201085
H	-0.377574	2.615328	2.903238
H	0.893607	2.557645	1.682607
H	0.674607	1.207434	2.796976
C	-0.262000	-1.089091	0.748015
H	-1.129197	-1.290308	1.378609
H	-0.300447	-1.814668	-0.066247
C	1.020204	0.771790	-0.435399
H	1.057957	1.853006	-0.591315
H	1.147810	0.316151	-1.418942
C	1.010035	-1.392212	1.549578
H	1.034286	-0.825927	2.489379
H	1.006131	-2.450940	1.832235
C	2.253210	0.380344	0.384713
H	2.332721	0.966659	1.298722
C	2.323830	-1.089138	0.806114
Cl	2.410546	-2.176153	-0.690225
C	3.543982	-1.414204	1.664451
H	4.470122	-1.214695	1.122302
H	3.526526	-2.465199	1.965802
H	3.531720	-0.794570	2.570259
Br	3.871020	0.971769	-0.625753

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56318040**

Number of imaginary frequencies = 0

1o_C001

B3LYP/6-31G* Geometry

C	-1.365152	0.211813	0.884448
C	-2.978432	1.021492	-0.959707
C	-0.132074	0.998174	0.203339
C	-2.338811	-0.166853	-0.258132
H	-3.696720	1.500862	-0.274157
H	-1.858208	-0.800768	-1.002952
C	-1.906846	2.002116	-1.324485
H	-2.208359	2.733089	-2.072257
C	-0.672521	2.046155	-0.806846
O	-3.644769	0.639680	-2.155914
H	-4.341512	0.013823	-1.891430
Br	-3.864963	-1.349168	0.350852
C	-2.091940	1.111875	1.911711
H	-3.070116	0.680401	2.146016
H	-2.244930	2.129350	1.539813
H	-1.531213	1.173732	2.849123
C	-0.944105	-1.082371	1.613216
H	-1.805998	-1.504086	2.135938
H	-0.173496	-0.892681	2.362286
H	-0.587624	-1.852428	0.921669
C	0.253680	3.149428	-1.285981
H	-0.139589	3.597741	-2.202833
H	1.268035	2.792783	-1.496140
H	0.348221	3.954331	-0.546034
C	0.759113	1.741917	1.253533
H	1.288411	2.541764	0.735113
H	0.134724	2.238370	2.000658
C	0.795640	0.050670	-0.647859
H	1.298587	0.649736	-1.410839
H	0.192698	-0.677145	-1.196708
C	1.845823	0.925912	1.968040
H	2.457947	1.604874	2.572387
H	1.419290	0.196814	2.666652
C	1.886061	-0.708453	0.113829
H	1.464616	-1.486544	0.748024
C	2.778000	0.148498	1.017788
Cl	3.718104	1.379784	-0.000984
C	3.811001	-0.667751	1.791424
H	3.298295	-1.414149	2.411406
H	4.396978	-0.017621	2.446935
H	4.486264	-1.189560	1.110923
Br	-1.365152	0.211813	0.884448

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56931482**

Number of imaginary frequencies = 0

1o_C002

B3LYP/6-31G* Geometry

C	-1.417935	0.138513	0.920305
C	-2.938273	1.152091	-0.895619
C	-0.151288	0.946228	0.346120
C	-2.359321	-0.114117	-0.278787
H	-3.681654	1.579609	-0.202856
H	-1.870389	-0.695922	-1.059890
C	-1.838365	2.147267	-1.112377
H	-2.103511	2.963704	-1.781169
C	-0.622629	2.110458	-0.550818
O	-3.551660	0.898437	-2.152787
H	-4.276270	0.271804	-1.981154
Br	-3.936196	-1.293281	0.179942
C	-2.150246	0.968954	2.000996
H	-3.118314	0.508870	2.222642
H	-2.325572	2.000839	1.683228
H	-1.578379	0.996984	2.932767
C	-1.015046	-1.213826	1.546369
H	-1.900204	-1.705670	1.956667
H	-0.309125	-1.084033	2.372916
H	-0.574496	-1.901758	0.817543
C	0.344433	3.231045	-0.869413
H	1.283905	2.863690	-1.299205
H	0.604994	3.815183	0.022006
H	-0.100546	3.920991	-1.592046
C	0.702308	1.462684	1.555468
H	0.280172	2.399432	1.934045
H	0.613771	0.749898	2.381067
C	0.762452	0.023756	-0.547197
H	1.173963	0.595817	-1.383807
H	0.175700	-0.778846	-0.996632
C	2.204070	1.690524	1.286210
H	2.341486	2.542492	0.623433
H	2.684179	1.962496	2.233398
C	1.928369	-0.577135	0.233425
H	1.573120	-1.080609	1.131998
C	2.964578	0.462461	0.688184
Cl	3.935732	1.061200	-0.775234
C	3.970578	-0.128805	1.674296
H	3.442170	-0.447841	2.582463
H	4.716768	0.618953	1.955966
H	4.477810	-0.995784	1.245128
Br	2.726886	-2.081827	-0.790805

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56534231**

Number of imaginary frequencies = 0

1o_C003

B3LYP/6-31G* Geometry

C	-1.377137	0.218450	0.884018
C	-2.976065	1.003490	-0.987841
C	-0.138564	0.999607	0.211331
C	-2.353388	-0.182155	-0.257806
H	-3.747612	1.455311	-0.353770
H	-1.849405	-0.826691	-0.980762
C	-1.910313	2.011579	-1.306515
H	-2.217966	2.764935	-2.030926
C	-0.673385	2.054071	-0.792359
O	-3.681387	0.615870	-2.163304
H	-3.024079	0.302855	-2.806696
Br	-3.854013	-1.357390	0.364473
C	-2.116046	1.126138	1.896160
H	-3.092669	0.690045	2.127639
H	-2.273160	2.138523	1.512090
H	-1.563276	1.202189	2.837235
C	-0.954393	-1.064767	1.631353
H	-1.817765	-1.486188	2.150465
H	-0.189594	-0.861345	2.382809
H	-0.588575	-1.841014	0.951389
C	0.249342	3.165255	-1.259051
H	-0.144289	3.623289	-2.171041
H	1.265125	2.813422	-1.470994
H	0.340356	3.961897	-0.510074
C	0.753939	1.737600	1.266044
H	1.281578	2.542531	0.754005
H	0.128877	2.226445	2.017578
C	0.788848	0.053634	-0.642077
H	1.292970	0.653677	-1.403852
H	0.185506	-0.674492	-1.190406
C	1.844213	0.920348	1.974207
H	2.457770	1.598927	2.577506
H	1.421454	0.189320	2.672713
C	1.878456	-0.708946	0.116893
H	1.455265	-1.486210	0.750951
C	2.773694	0.145481	1.019576
Cl	3.710629	1.378742	-0.000655
C	3.809147	-0.672387	1.788055
H	3.298285	-1.420506	2.407400
H	4.396513	-0.023694	2.443702
H	4.482862	-1.192138	1.104478
Br	2.919217	-1.772925	-1.213210

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56683223**

Number of imaginary frequencies = 0

1o_C004

B3LYP/6-31G* Geometry

C	-1.365212	0.212236	0.884556
C	-2.978478	1.021358	-0.959689
C	-0.132089	0.998362	0.203235
C	-2.338740	-0.166768	-0.257991
H	-3.696620	1.500912	-0.274157
H	-1.858032	-0.800599	-1.002806
C	-1.906922	2.001892	-1.324837
H	-2.208414	2.732739	-2.072734
C	-0.672593	2.046163	-0.807151
O	-3.645179	0.639248	-2.155692
H	-4.341456	0.012957	-1.890979
Br	-3.864787	-1.349368	0.350984
C	-2.091989	1.112835	1.911365
H	-3.069852	0.681110	2.146504
H	-2.245632	2.129929	1.538673
H	-1.530857	1.175762	2.848473
C	-0.944255	-1.081665	1.613851
H	-1.806216	-1.503262	2.136558
H	-0.173845	-0.891547	2.362998
H	-0.587563	-1.851945	0.922669
C	0.253468	3.149415	-1.286547
H	0.347935	3.954446	-0.546725
H	-0.139885	3.597533	-2.203448
H	1.267871	2.792873	-1.496700
C	0.759189	1.742244	1.253298
H	1.288399	2.542075	0.734775
H	0.134785	2.238733	2.000399
C	0.795514	0.050665	-0.647802
H	1.298403	0.649600	-1.410911
H	0.192502	-0.677224	-1.196483
C	1.846030	0.926405	1.967824
H	2.458185	1.605554	2.571931
H	1.419677	0.197435	2.666649
C	1.885997	-0.708351	0.113929
H	1.464596	-1.486299	0.748339
C	2.778151	0.148630	1.017700
Cl	3.718750	1.379288	-0.001230
C	3.810852	-0.667712	1.791645
H	3.297901	-1.413767	2.411843
H	4.396959	-0.017540	2.446985
H	4.486000	-1.189911	1.111321
Br	2.932052	-1.772224	-1.211757

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56931238**

Number of imaginary frequencies = 0

1o_C005

B3LYP/6-31G* Geometry

C	-1.431191	0.140817	0.919209
C	-2.930116	1.138481	-0.930411
C	-0.157303	0.942238	0.355478
C	-2.375740	-0.128100	-0.281785
H	-3.727982	1.546705	-0.299589
H	-1.867460	-0.727998	-1.039366
C	-1.835608	2.154509	-1.094953
H	-2.104527	2.991228	-1.738571
C	-0.618589	2.113646	-0.534229
O	-3.576284	0.877996	-2.173041
H	-2.890555	0.610271	-2.807093
Br	-3.935276	-1.294326	0.190145
C	-2.172502	0.976946	1.988935
H	-3.135396	0.508234	2.213682
H	-2.359146	2.002827	1.658135
H	-1.602594	1.022975	2.921255
C	-1.030601	-1.207076	1.557569
H	-1.918115	-1.697976	1.962314
H	-0.330087	-1.071510	2.387777
H	-0.584183	-1.898828	0.835602
C	0.347845	3.239264	-0.834635
H	0.603816	3.811227	0.065686
H	-0.094563	3.938822	-1.549738
H	1.289915	2.877654	-1.263808
C	0.694403	1.451557	1.569410
H	0.272988	2.387297	1.951166
H	0.600097	0.735454	2.391036
C	0.755670	0.019206	-0.538158
H	1.167357	0.590072	-1.375811
H	0.168557	-0.785570	-0.983612
C	2.198372	1.677541	1.309507
H	2.343208	2.540296	0.662345
H	2.674595	1.931614	2.263598
C	1.923001	-0.582290	0.239529
H	1.568781	-1.089207	1.136708
C	2.958445	0.457371	0.694711
Cl	3.914061	1.070927	-0.774356
C	3.976496	-0.136519	1.666522
H	3.457332	-0.468782	2.575213
H	4.718988	0.614153	1.950174
H	4.487075	-0.995004	1.224669
Br	2.721494	-2.081367	-0.793390

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56332234**

Number of imaginary frequencies = 0

1o_C006

B3LYP/6-31G* Geometry

C	-1.417957	0.138406	0.920164
C	-2.938463	1.152278	-0.895305
C	-0.151254	0.946157	0.346014
C	-2.359412	-0.114024	-0.278902
H	-3.681501	1.579752	-0.202162
H	-1.870521	-0.695588	-1.060185
C	-1.838434	2.147299	-1.112308
H	-2.103584	2.963788	-1.781033
C	-0.622613	2.110371	-0.550946
O	-3.552429	0.899043	-2.152297
H	-4.276552	0.271817	-1.980607
Br	-3.936202	-1.293434	0.179903
C	-2.150245	0.968721	2.000932
H	-3.118354	0.508651	2.222471
H	-2.325484	2.000692	1.683383
H	-1.578383	0.996507	2.932713
C	-1.015160	-1.214019	1.546071
H	-1.900331	-1.705840	1.956378
H	-0.309211	-1.084315	2.372606
H	-0.574693	-1.901922	0.817171
C	0.344445	3.230987	-0.869438
H	-0.100407	3.920868	-1.592209
H	1.284052	2.863675	-1.298976
H	0.604750	3.815209	0.022007
C	0.702220	1.462749	1.555369
H	0.280097	2.399590	1.933735
H	0.613505	0.750099	2.381066
C	0.762529	0.023711	-0.547196
H	1.174070	0.595724	-1.383825
H	0.175856	-0.778953	-0.996616
C	2.204079	1.690477	1.286317
H	2.341674	2.542505	0.623653
H	2.684038	1.962326	2.233616
C	1.928467	-0.577164	0.233431
H	1.573214	-1.080709	1.131966
C	2.964603	0.462451	0.688331
Cl	3.935872	1.061253	-0.775080
C	3.970589	-0.128820	1.674442
H	3.442107	-0.448190	2.582449
H	4.716546	0.619053	1.956409
H	4.478086	-0.995566	1.245125
Br	2.727068	-2.081718	-0.790939

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56533994**

Number of imaginary frequencies = 0

1o_C007

B3LYP/6-31G* Geometry

C	-1.571561	-0.872967	0.528113
C	-2.568011	1.505175	0.360598
C	-0.084754	-0.233479	0.643210
C	-2.394757	0.140747	-0.293668
H	-3.340621	1.419428	1.143226
H	-1.972088	0.272197	-1.288492
C	-1.301759	1.943070	1.033474
H	-1.351118	2.949272	1.445250
C	-0.216574	1.187695	1.257118
O	-2.961996	2.494061	-0.583679
H	-3.831719	2.216407	-0.920608
Br	-4.256838	-0.509963	-0.743038
C	-2.181341	-1.077292	1.933753
H	-3.248616	-1.302097	1.839894
H	-2.071179	-0.194693	2.568791
H	-1.709542	-1.923144	2.443308
C	-1.607377	-2.243671	-0.187955
H	-2.604716	-2.677916	-0.082661
H	-0.899712	-2.955474	0.245946
H	-1.413207	-2.175372	-1.262760
C	0.852168	1.752446	2.170961
H	0.551300	2.743087	2.523970
H	1.817748	1.857870	1.672946
H	0.999814	1.123913	3.057922
C	0.787584	-1.162970	1.545224
H	0.562757	-0.967601	2.598050
H	0.496841	-2.202998	1.378851
C	0.531511	-0.146655	-0.806327
H	0.166053	0.751678	-1.308187
H	0.161638	-0.995917	-1.388221
C	2.315430	-1.071358	1.351224
H	2.702161	-0.110095	1.695247
H	2.796719	-1.843999	1.960773
C	2.060450	-0.187808	-0.990212
H	2.283708	-0.380960	-2.039995
C	2.724648	-1.261961	-0.111467
Cl	4.562337	-1.139061	-0.214930
C	2.385529	-2.659143	-0.656945
H	1.307544	-2.842000	-0.656440
H	2.861863	-3.424473	-0.037571
H	2.752473	-2.772187	-1.681138
Br	2.849153	1.629267	-0.749747

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56134413**

Number of imaginary frequencies = 0

1o_C008

B3LYP/6-31G* Geometry

C	-1.585392	-0.874923	0.511827
C	-2.539640	1.529677	0.329649
C	-0.091115	-0.258159	0.635717
C	-2.410458	0.147045	-0.310937
H	-3.365842	1.504226	1.050052
H	-1.990447	0.248300	-1.312047
C	-1.288992	1.916122	1.065446
H	-1.339255	2.905683	1.517895
C	-0.208008	1.150097	1.278695
O	-2.936197	2.525585	-0.612170
H	-2.155624	2.742728	-1.147766
Br	-4.266166	-0.495584	-0.726121
C	-2.200371	-1.083998	1.914782
H	-3.266544	-1.309095	1.814166
H	-2.095364	-0.203970	2.554295
H	-1.729813	-1.931230	2.423478
C	-1.631619	-2.242638	-0.210883
H	-2.637627	-2.659208	-0.124584
H	-0.942637	-2.967935	0.230670
H	-1.419884	-2.173318	-1.282584
C	0.851558	1.682524	2.221786
H	0.548349	2.661245	2.604890
H	1.822336	1.802304	1.737111
H	0.988846	1.024135	3.088185
C	0.777828	-1.211020	1.516351
H	0.547089	-1.046408	2.573034
H	0.489137	-2.245744	1.318111
C	0.524762	-0.159248	-0.811510
H	0.153102	0.736566	-1.313411
H	0.162393	-1.009759	-1.396268
C	2.306817	-1.112376	1.332823
H	2.691279	-0.159865	1.702475
H	2.786093	-1.899111	1.925704
C	2.053197	-0.183607	-0.992758
H	2.282309	-0.354759	-2.045124
C	2.724143	-1.267963	-0.131873
Cl	4.559983	-1.124041	-0.227535
C	2.398502	-2.657127	-0.706044
H	1.322599	-2.852720	-0.702466
H	2.887204	-3.429254	-0.105129
H	2.761050	-2.744575	-1.734295
Br	2.819990	1.638994	-0.715861

SCF Energy (PCM/mPW1PW91/6-31+G) = --6264.55998262**

Number of imaginary frequencies = 0

1o_C009

B3LYP/6-31G* Geometry

C	1.633357	0.938449	0.440107
C	2.193857	-1.599285	-0.021351
C	0.110298	0.405401	0.578922
C	2.379001	-0.119258	-0.417113
H	3.145100	-1.991075	0.359774
H	2.079866	-0.025402	-1.458942
C	1.146526	-1.807112	1.036347
H	1.218022	-2.746043	1.585593
C	0.189485	-0.927549	1.362325
O	1.870276	-2.282813	-1.251034
H	1.508492	-3.151795	-1.014427
Br	4.349000	0.266227	-0.553445
C	2.273674	1.118673	1.835288
H	3.310737	1.445696	1.725384
H	2.274648	0.196709	2.420619
H	1.741423	1.886400	2.405866
C	1.744579	2.301652	-0.282741
H	2.799699	2.519751	-0.469194
H	1.348037	3.120030	0.324690
H	1.240627	2.320030	-1.254690
C	-0.714742	-1.236597	2.533747
H	-0.392113	-2.162502	3.019532
H	-1.753804	-1.373200	2.222394
H	-0.691132	-0.443802	3.290809
C	-0.750383	1.483787	1.301008
H	-0.510209	1.508357	2.368062
H	-0.472145	2.468097	0.917192
C	-0.478786	0.154849	-0.857114
H	-0.059337	-0.759266	-1.282298
H	-0.165722	0.974125	-1.513610
C	-2.280656	1.344845	1.155951
H	-2.651205	0.461805	1.679831
H	-2.762221	2.212926	1.619613
C	-2.005767	0.080665	-1.001969
H	-2.268434	0.056379	-2.060155
C	-2.713879	1.257689	-0.310515
Cl	-4.544594	1.027771	-0.359957
C	-2.453438	2.556207	-1.092571
H	-1.389161	2.806545	-1.118367
H	-2.986257	3.385287	-0.618751
H	-2.810637	2.465509	-2.122486
Br	-2.666062	-1.697618	-0.374008

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55746117**

Number of imaginary frequencies = 0

1o_C010

B3LYP/6-31G* Geometry

C	1.292496	-0.437879	-0.969415
C	3.355680	-1.269860	0.416384
C	0.388259	-0.354690	0.351747
C	2.814330	-0.328925	-0.668999
H	4.260839	-0.824706	0.838041
H	3.368702	-0.513929	-1.588348
C	2.353303	-1.521124	1.496410
H	2.741464	-2.076019	2.349359
C	1.053455	-1.186435	1.480661
O	3.812399	-2.502952	-0.164423
H	3.054573	-3.106105	-0.204485
Br	3.458201	1.535206	-0.224137
C	0.973636	0.601730	-2.066520
H	1.627676	0.419640	-2.928051
H	1.158800	1.624885	-1.738653
H	-0.053842	0.520750	-2.428260
C	1.115177	-1.835058	-1.640892
H	1.921619	-2.027140	-2.355406
H	0.174703	-1.879242	-2.198474
H	1.102430	-2.652490	-0.913994
C	0.210941	-1.610059	2.670915
H	0.855152	-1.915593	3.500112
H	-0.435436	-2.463177	2.428568
H	-0.445051	-0.812121	3.034747
C	0.207319	1.089623	0.938092
H	-0.074259	0.986821	1.990325
H	1.164272	1.610559	0.931870
C	-1.054196	-0.937950	0.123131
H	-1.493427	-1.166704	1.093875
H	-1.019070	-1.883793	-0.418633
C	-0.856162	1.980183	0.277294
H	-0.959976	2.901573	0.861105
H	-0.547524	2.286759	-0.727444
C	-2.054023	-0.010692	-0.568190
H	-1.780277	0.202850	-1.601146
C	-2.249391	1.339065	0.133404
Cl	-2.937052	1.071530	1.835613
C	-3.219679	2.265871	-0.595159
H	-2.854308	2.450750	-1.613375
H	-3.291485	3.225417	-0.075616
H	-4.214427	1.820928	-0.660549
Br	-3.767267	-1.010209	-0.796971

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56534231**

Number of imaginary frequencies = 0

1o_C011

B3LYP/6-31G* Geometry

C	1.281871	-0.442314	-0.959233
C	3.335892	-1.290739	0.425787
C	0.387022	-0.322203	0.367076
C	2.805061	-0.352722	-0.667560
H	4.252972	-0.855243	0.843158
H	3.342703	-0.544170	-1.597310
C	2.342766	-1.491768	1.521249
H	2.729161	-2.037917	2.379440
C	1.056853	-1.115916	1.517893
O	3.641539	-2.587288	-0.115700
H	4.488633	-2.516648	-0.585075
Br	3.485547	1.504084	-0.236538
C	0.975162	0.592361	-2.064728
H	1.627214	0.396163	-2.924763
H	1.168096	1.617568	-1.747299
H	-0.052459	0.517447	-2.427370
C	1.089119	-1.843991	-1.613044
H	1.836853	-2.001188	-2.397281
H	0.107065	-1.911562	-2.091299
H	1.193869	-2.660711	-0.897074
C	0.227724	-1.474189	2.739299
H	0.882170	-1.743906	3.572878
H	-0.424253	-2.335371	2.546323
H	-0.419588	-0.656886	3.074270
C	0.196710	1.142349	0.897902
H	-0.078860	1.078027	1.954601
H	1.149082	1.671725	0.867485
C	-1.051967	-0.924887	0.171816
H	-1.487163	-1.105578	1.154471
H	-1.008255	-1.897165	-0.319392
C	-0.878022	1.998798	0.209341
H	-0.994045	2.936395	0.764519
H	-0.573057	2.279138	-0.803975
C	-2.054971	-0.036861	-0.562801
H	-1.775872	0.135706	-1.602190
C	-2.264367	1.338639	0.083315
Cl	-2.958956	1.133741	1.792006
C	-3.238699	2.227869	-0.685606
H	-2.871318	2.372838	-1.709556
H	-3.318740	3.207568	-0.206374
H	-4.230041	1.773504	-0.735465
Br	-3.760837	-1.056129	-0.761618

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56041187**

Number of imaginary frequencies = 0

1o_C012

B3LYP/6-31G* Geometry

C	1.391696	-0.246090	1.128939
C	3.167751	1.215150	-0.185371
C	0.352592	0.619946	0.285967
C	2.817859	-0.128366	0.517281
H	3.174729	1.039154	-1.271070
H	3.550380	-0.281065	1.308628
C	2.172104	2.299409	0.109565
H	2.581962	3.306792	0.110645
C	0.865027	2.079805	0.306575
O	4.456347	1.673097	0.215146
H	5.105306	1.062760	-0.171629
Br	3.330252	-1.607279	-0.762172
C	0.956550	-1.717246	1.294376
H	1.732816	-2.280109	1.822910
H	0.791072	-2.229009	0.344242
H	0.042049	-1.784156	1.892612
C	1.542220	0.325481	2.569787
H	2.178692	-0.340418	3.163056
H	0.575505	0.386487	3.079190
H	1.992526	1.319872	2.579345
C	-0.055750	3.247682	0.569611
H	0.492648	4.189534	0.473273
H	-0.478838	3.214400	1.582312
H	-0.905774	3.283325	-0.122928
C	0.300569	0.139772	-1.207781
H	1.168262	0.514395	-1.754267
H	0.366878	-0.950832	-1.267129
C	-1.094018	0.487873	0.883576
H	-1.607510	1.450427	0.892735
H	-1.062798	0.156381	1.922112
C	-0.965083	0.623316	-1.931624
H	-1.010671	1.713508	-1.880195
H	-0.909561	0.366341	-2.995305
C	-1.963559	-0.479749	0.083876
H	-1.473339	-1.448189	-0.017549
C	-2.274314	0.019329	-1.340498
Cl	-3.536263	1.373988	-1.284290
C	-2.846899	-1.094833	-2.214360
H	-2.090217	-1.880250	-2.342047
H	-3.112834	-0.711186	-3.202842
H	-3.732528	-1.538053	-1.752596
Br	-3.590353	-0.954194	1.119279

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55746357**

Number of imaginary frequencies = 0

1o_C013

B3LYP/6-31G* Geometry

C	1.427735	-0.096979	1.127680
C	3.373788	1.155841	-0.086692
C	0.408223	0.571230	0.099868
C	2.867045	-0.153055	0.555910
H	3.934604	0.910121	-0.998294
H	3.558026	-0.401563	1.359622
C	2.285589	2.143372	-0.407653
H	2.652041	3.117876	-0.735685
C	0.963608	1.960248	-0.285900
O	4.284403	1.716766	0.879788
H	4.561142	2.587596	0.552005
Br	3.221153	-1.682376	-0.707851
C	0.980544	-1.495787	1.600591
H	1.735066	-1.914409	2.276076
H	0.860577	-2.209395	0.783201
H	0.041996	-1.439616	2.161880
C	1.570520	0.775234	2.412725
H	2.243128	0.277085	3.118926
H	0.609157	0.898715	2.919403
H	1.982806	1.763428	2.207150
C	0.041500	3.132123	-0.544708
H	0.598668	3.963752	-0.986746
H	-0.405072	3.499494	0.388934
H	-0.792494	2.893443	-1.212858
C	0.280366	-0.264657	-1.227176
H	1.148583	-0.081762	-1.862076
H	0.302414	-1.334467	-1.004158
C	-1.026564	0.663709	0.740244
H	-1.497475	1.624034	0.524894
H	-0.977178	0.593366	1.826427
C	-0.989505	0.051773	-2.031830
H	-0.994334	1.106019	-2.312126
H	-0.973649	-0.513736	-2.970395
C	-1.963113	-0.427545	0.226295
H	-1.517585	-1.413395	0.362340
C	-2.305216	-0.292251	-1.269061
Cl	-3.490358	1.109627	-1.529014
C	-2.976183	-1.552654	-1.811284
H	-2.273228	-2.393435	-1.744011
H	-3.252735	-1.420228	-2.860582
H	-3.870458	-1.800428	-1.234545
Br	-3.570957	-0.544307	1.387893

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55301610**

Number of imaginary frequencies = 0

1o_C014

B3LYP/6-31G* Geometry

C	1.424499	-0.032866	1.130822
C	3.399832	1.172275	-0.092532
C	0.416001	0.535820	0.031945
C	2.878299	-0.110192	0.597586
H	4.066588	0.881271	-0.908492
H	3.552976	-0.334560	1.422180
C	2.308180	2.069672	-0.599296
H	2.676136	3.003956	-1.021454
C	0.983807	1.872519	-0.499557
O	4.253231	1.904681	0.801484
H	3.682988	2.430203	1.384547
Br	3.254405	-1.688997	-0.602406
C	1.001230	-1.399711	1.708841
H	1.718275	-1.707929	2.478887
H	0.983249	-2.193844	0.960278
H	0.019500	-1.340262	2.190259
C	1.499158	0.940215	2.350042
H	2.342489	0.674777	2.996393
H	0.598461	0.869145	2.965931
H	1.609078	1.985806	2.050981
C	0.060343	2.992472	-0.933568
H	0.622872	3.758467	-1.475348
H	-0.403691	3.482119	-0.066759
H	-0.761876	2.660737	-1.574845
C	0.273013	-0.436572	-1.196844
H	1.139551	-0.333654	-1.851168
H	0.287399	-1.474648	-0.854458
C	-1.016297	0.715590	0.660197
H	-1.474430	1.653290	0.342662
H	-0.965370	0.762788	1.747391
C	-0.997866	-0.209739	-2.031257
H	-0.988942	0.795154	-2.454785
H	-0.990124	-0.897291	-2.884728
C	-1.970996	-0.410579	0.268290
H	-1.539027	-1.383698	0.504617
C	-2.319194	-0.428326	-1.230890
Cl	-3.463666	0.974105	-1.632628
C	-3.033239	-1.717255	-1.632413
H	-2.358149	-2.568503	-1.473774
H	-3.307915	-1.690472	-2.690245
H	-3.933534	-1.870853	-1.032720
Br	-3.573281	-0.376122	1.442385

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55386673**

Number of imaginary frequencies = 0

1p_C001

B3LYP/6-31G* Geometry

C	1.475436	0.794893	0.561979
C	2.521815	-1.554775	0.344938
C	-0.000200	0.131079	0.669692
C	2.313871	-0.184844	-0.283595
H	3.277766	-1.462475	1.142962
H	1.887110	-0.308136	-1.278052
C	1.254179	-2.041680	0.979741
H	1.312823	-3.064893	1.346164
C	0.150783	-1.315787	1.212461
O	2.959805	-2.513998	-0.610630
H	3.818937	-2.195375	-0.938746
Br	4.157247	0.518973	-0.730267
C	2.086829	0.974912	1.970386
H	3.153609	1.202778	1.878080
H	1.978704	0.080891	2.590386
H	1.615363	1.811552	2.494759
C	1.478916	2.180342	-0.128071
H	2.436220	2.673944	0.058485
H	0.689727	2.835595	0.248358
H	1.371698	2.114474	-1.214929
C	-0.930122	-1.948822	2.065341
H	-1.119840	-1.368740	2.977004
H	-0.618389	-2.949577	2.378259
H	-1.877052	-2.050960	1.531002
C	-0.863774	1.011533	1.625178
H	-0.603115	0.789615	2.664712
H	-0.607761	2.061489	1.471007
C	-0.639142	0.122376	-0.769595
H	-0.263441	-0.729991	-1.340075
H	-0.304155	1.022645	-1.290929
C	-2.388983	0.898451	1.472351
H	-2.747676	-0.082786	1.799398
H	-2.868235	1.638562	2.122871
C	-2.164108	0.157646	-0.931408
H	-2.408392	0.435377	-1.955956
C	-2.904068	1.086205	0.045838
Cl	-2.440966	2.812801	-0.528811
C	-4.426914	1.025915	-0.040292
H	-4.865109	1.819087	0.571467
H	-4.782185	0.058665	0.324280
H	-4.768610	1.152235	-1.071799
Br	-2.948022	-1.696524	-0.852692

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56585401**

Number of imaginary frequencies = 0

1p_C002

B3LYP/6-31G* Geometry

C	-1.323726	0.211607	0.870709
C	-3.068284	1.006205	-0.848402
C	-0.167947	1.049592	0.132823
C	-2.354761	-0.178022	-0.212682
H	-3.772557	1.434538	-0.116346
H	-1.902754	-0.782883	-0.998707
C	-2.061233	2.050259	-1.225760
H	-2.442249	2.808410	-1.907326
C	-0.798390	2.123080	-0.783916
O	-3.774259	0.634905	-2.025339
H	-4.436849	-0.022230	-1.748985
Br	-3.803594	-1.411539	0.467066
C	-2.001055	1.075435	1.961617
H	-2.914220	0.579596	2.304989
H	-2.267197	2.072006	1.597668
H	-1.346545	1.197602	2.829020
C	-0.790434	-1.070867	1.543564
H	-1.595951	-1.550772	2.104361
H	0.011939	-0.853297	2.254389
H	-0.426557	-1.804692	0.816796
C	0.047326	3.286079	-1.260754
H	-0.539126	3.932977	-1.919080
H	0.927178	2.958844	-1.828812
H	0.411287	3.904262	-0.431620
C	0.765800	1.700093	1.212087
H	0.345869	2.654470	1.545333
H	0.799793	1.064073	2.101963
C	0.729348	0.138280	-0.789104
H	1.084576	0.715711	-1.649230
H	0.141776	-0.679380	-1.210688
C	2.210851	1.919471	0.742956
H	2.228273	2.569156	-0.135927
H	2.779605	2.440099	1.518734
C	1.942005	-0.449534	-0.059396
H	1.626578	-0.995392	0.821721
C	2.970452	0.622866	0.360182
Cl	3.827507	-0.022676	1.880508
C	4.058047	0.935759	-0.665055
H	4.700964	0.073736	-0.844044
H	4.669780	1.771753	-0.312891
H	3.594683	1.221846	-1.617318
Br	2.732170	-1.900633	-1.176013

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56679309**

Number of imaginary frequencies = 0

1p_C003

B3LYP/6-31G* Geometry

C	1.489195	0.796400	0.553224
C	2.495910	-1.577302	0.307205
C	0.005660	0.154206	0.666408
C	2.330328	-0.185725	-0.299938
H	3.307063	-1.545437	1.044233
H	1.902779	-0.273182	-1.299655
C	1.240908	-2.019581	1.003156
H	1.300688	-3.030141	1.405553
C	0.141555	-1.284486	1.231476
O	2.940079	-2.538922	-0.648727
H	2.186283	-2.739407	-1.227506
Br	4.165400	0.513632	-0.712172
C	2.105646	0.971565	1.960072
H	3.171877	1.198229	1.863073
H	2.000215	0.076094	2.578431
H	1.636857	1.807171	2.488768
C	1.503081	2.183530	-0.134940
H	2.469777	2.662112	0.037931
H	0.728986	2.850055	0.253020
H	1.380857	2.120998	-1.220571
C	-0.928317	-1.891524	2.116757
H	-0.613707	-2.883882	2.452856
H	-1.883843	-2.005938	1.600312
H	-1.102354	-1.285824	3.014467
C	-0.856221	1.053464	1.605657
H	-0.591178	0.856000	2.648911
H	-0.603389	2.100015	1.426586
C	-0.631827	0.140588	-0.771762
H	-0.246438	-0.704135	-1.347244
H	-0.307269	1.046763	-1.289490
C	-2.381939	0.932462	1.460961
H	-2.736764	-0.042288	1.810204
H	-2.861236	1.684492	2.097549
C	-2.156121	0.154889	-0.932468
H	-2.406737	0.414260	-1.960303
C	-2.904213	1.089300	0.033240
Cl	-2.463592	2.810458	-0.571912
C	-4.426319	1.007107	-0.046313
H	-4.873083	1.802841	0.555809
H	-4.767005	0.040536	0.333956
H	-4.773574	1.114078	-1.078124
Br	-2.911752	-1.710180	-0.824767

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56420330**

Number of imaginary frequencies = 0

1p_C004

B3LYP/6-31G* Geometry

C	1.535995	0.847859	0.553167
C	2.146886	-1.628768	-0.108272
C	0.019960	0.284481	0.651749
C	2.286039	-0.121360	-0.397329
H	3.102840	-2.010696	0.272742
H	1.961835	0.043632	-1.422503
C	1.084225	-1.947905	0.906760
H	1.161326	-2.934759	1.364368
C	0.114532	-1.114164	1.306721
O	1.878929	-2.235615	-1.389037
H	1.628251	-3.159271	-1.227999
Br	4.244786	0.314985	-0.546811
C	2.186518	0.905364	1.953941
H	3.221564	1.245738	1.864946
H	2.195072	-0.065526	2.453803
H	1.657282	1.617080	2.595506
C	1.622728	2.272048	-0.043118
H	2.673535	2.520935	-0.214608
H	1.217364	3.023876	0.638967
H	1.106981	2.373223	-1.002446
C	-0.797303	-1.547178	2.432164
H	-0.817992	-0.815913	3.248645
H	-0.451270	-2.497255	2.850724
H	-1.824874	-1.695221	2.088625
C	-0.847135	1.287440	1.465347
H	-0.581962	1.246469	2.526201
H	-0.609430	2.299425	1.132482
C	-0.576416	0.161114	-0.795222
H	-0.142945	-0.697924	-1.311637
H	-0.296304	1.052969	-1.364219
C	-2.371444	1.126483	1.339350
H	-2.713481	0.198141	1.808236
H	-2.863510	1.945470	1.875684
C	-2.097168	0.080488	-0.940565
H	-2.371371	0.173145	-1.991039
C	-2.887112	1.096792	-0.099697
Cl	-2.503144	2.751001	-0.899664
C	-4.404716	0.951350	-0.178163
H	-4.886284	1.786862	0.337234
H	-4.713852	0.015855	0.295245
H	-4.745627	0.941263	-1.217667
Br	-2.744177	-1.783954	-0.523924

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56167755**

Number of imaginary frequencies = 0

1p_C005

B3LYP/6-31G* Geometry

C	-1.334976	0.080965	0.881781
C	-3.124056	1.040292	-0.713044
C	-0.206287	1.056100	0.263156
C	-2.359386	-0.189080	-0.248773
H	-3.815201	1.357290	0.085227
H	-1.888879	-0.659315	-1.112238
C	-2.145261	2.138038	-0.991458
H	-2.544695	2.945968	-1.601426
C	-0.881292	2.192987	-0.552941
O	-3.852956	0.798741	-1.908907
H	-4.482619	0.085129	-1.705294
Br	-3.758868	-1.562040	0.249786
C	-2.042629	0.753564	2.081206
H	-1.417464	0.716368	2.978458
H	-2.968507	0.215575	2.307321
H	-2.293251	1.800750	1.886235
C	-0.786121	-1.279820	1.364330
H	-1.584630	-1.837303	1.859360
H	0.022760	-1.166638	2.086855
H	-0.434259	-1.903878	0.536742
C	-0.069868	3.422429	-0.921995
H	0.043827	4.111593	-0.075967
H	-0.569281	3.973906	-1.723439
H	0.939751	3.179903	-1.274055
C	0.690535	1.714750	1.363925
H	1.143974	2.610183	0.934482
H	0.076109	2.075723	2.192925
C	0.743441	0.315808	-0.750112
H	1.162959	1.055666	-1.437409
H	0.168177	-0.366769	-1.381528
C	1.844515	0.868629	1.927477
H	2.434730	1.485903	2.614467
H	1.478626	0.024769	2.515867
C	1.922899	-0.473680	-0.152698
H	1.591174	-1.377516	0.348201
C	2.783591	0.340076	0.823322
Cl	3.970965	-0.814190	1.649987
C	3.620499	1.442979	0.175980
H	4.190066	1.978535	0.940380
H	2.979490	2.163751	-0.342722
H	4.313792	1.021436	-0.553762
Br	2.982781	-1.197501	-1.682876

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56708918**

Number of imaginary frequencies = 0

1p_C006

B3LYP/6-31G* Geometry

C	-1.334142	0.210457	0.867463
C	-3.070755	0.990647	-0.872998
C	-0.174742	1.049203	0.139044
C	-2.371279	-0.194260	-0.213580
H	-3.826936	1.390179	-0.187638
H	-1.898669	-0.809088	-0.982618
C	-2.067950	2.059880	-1.203584
H	-2.455892	2.839152	-1.858632
C	-0.801674	2.130229	-0.768252
O	-3.818645	0.615915	-2.026150
H	-3.184480	0.336524	-2.707030
Br	-3.793691	-1.421263	0.481975
C	-2.020012	1.073290	1.953729
H	-2.925223	0.566526	2.301301
H	-2.300998	2.063454	1.583285
H	-1.365858	1.210998	2.819099
C	-0.796434	-1.067637	1.546247
H	-1.601211	-1.549590	2.105050
H	0.004730	-0.844969	2.256940
H	-0.429140	-1.802432	0.821846
C	0.040022	3.301962	-1.230092
H	-0.548859	3.957859	-1.877429
H	0.920208	2.984683	-1.803477
H	0.404355	3.908100	-0.392523
C	0.757874	1.694204	1.222864
H	0.338039	2.647220	1.559878
H	0.788249	1.054236	2.109679
C	0.724553	0.143607	-0.786745
H	1.081719	0.725482	-1.643505
H	0.138099	-0.673706	-1.211150
C	2.204225	1.914430	0.758540
H	2.225256	2.568615	-0.117109
H	2.771563	2.430449	1.538435
C	1.936543	-0.449411	-0.060291
H	1.619088	-1.004159	0.814471
C	2.964056	0.619367	0.371280
Cl	3.812968	-0.037144	1.890880
C	4.057339	0.938176	-0.646227
H	4.667772	1.771154	-0.284822
H	3.599485	1.231313	-1.599029
H	4.700597	0.076919	-0.827612
Br	2.728579	-1.889012	-1.191048

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56452212**

Number of imaginary frequencies = 0

1p_C007

B3LYP/6-31G* Geometry

C	-1.323750	0.211546	0.870624
C	-3.068392	1.006231	-0.848308
C	-0.167957	1.049472	0.132657
C	-2.354834	-0.178028	-0.212749
H	-3.772573	1.434556	-0.116198
H	-1.902917	-0.782759	-0.998912
C	-2.061328	2.050173	-1.225864
H	-2.442252	2.808373	-1.907426
C	-0.798419	2.122909	-0.784151
O	-3.774597	0.634929	-2.025165
H	-4.437069	-0.022245	-1.748616
Br	-3.803612	-1.411562	0.467097
C	-2.000935	1.075453	1.961543
H	-2.914164	0.579721	2.304927
H	-2.266937	2.072098	1.597690
H	-1.346404	1.197468	2.828957
C	-0.790433	-1.070862	1.543529
H	-1.595941	-1.550793	2.104325
H	0.011877	-0.853163	2.254392
H	-0.426472	-1.804706	0.816830
C	0.047259	3.286005	-1.260778
H	-0.539094	3.932847	-1.919247
H	0.927279	2.958887	-1.828630
H	0.410963	3.904230	-0.431549
C	0.765698	1.700086	1.211933
H	0.345723	2.654473	1.545107
H	0.799712	1.064149	2.101873
C	0.729318	0.138044	-0.789085
H	1.084443	0.715261	-1.649401
H	0.141818	-0.679803	-1.210408
C	2.210780	1.919500	0.742853
H	2.228171	2.569077	-0.136116
H	2.779454	2.440208	1.518624
C	1.942103	-0.449581	-0.059386
H	1.626747	-0.995428	0.821759
C	2.970452	0.622910	0.360187
Cl	3.827353	-0.022555	1.880733
C	4.058205	0.935747	-0.664854
H	4.669759	1.771875	-0.312705
H	3.594969	1.221656	-1.617235
H	4.701246	0.073767	-0.843621
Br	2.732378	-1.900535	-1.176082

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56679337**

Number of imaginary frequencies = 0

1p_C008

B3LYP/6-31G* Geometry

C	-1.348152	0.092348	0.888095
C	-3.119939	1.019609	-0.749756
C	-0.212694	1.058747	0.273121
C	-2.369782	-0.208106	-0.246086
H	-3.869040	1.316794	-0.007055
H	-1.869315	-0.695438	-1.085616
C	-2.146856	2.138496	-0.980497
H	-2.552344	2.961614	-1.567752
C	-0.882968	2.198757	-0.539275
O	-3.884758	0.758853	-1.922526
H	-3.260746	0.564038	-2.641273
Br	-3.743926	-1.574134	0.266533
C	-2.073385	0.780585	2.068126
H	-2.996096	0.237010	2.292976
H	-2.331362	1.822061	1.852735
H	-1.458418	0.764437	2.973043
C	-0.797395	-1.256286	1.401622
H	-1.598821	-1.809812	1.894940
H	0.002481	-1.124235	2.130858
H	-0.432180	-1.893364	0.589680
C	-0.077314	3.436239	-0.892497
H	0.031162	4.115063	-0.037689
H	-0.577620	3.995960	-1.687770
H	0.934524	3.202100	-1.244338
C	0.688110	1.712452	1.375004
H	1.139059	2.611514	0.950738
H	0.075040	2.065960	2.208148
C	0.734968	0.318552	-0.742350
H	1.155100	1.058855	-1.429341
H	0.158388	-0.364075	-1.372689
C	1.846861	0.866883	1.930917
H	2.440052	1.485346	2.614284
H	1.486382	0.022387	2.521184
C	1.913995	-0.473882	-0.149058
H	1.580988	-1.376104	0.354137
C	2.780546	0.339260	0.821866
Cl	3.972437	-0.815124	1.640504
C	3.613688	1.442627	0.170360
H	4.189628	1.975533	0.931769
H	2.969711	2.165858	-0.341311
H	4.301114	1.022174	-0.565604
Br	2.964807	-1.201154	-1.684247

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56464698**

Number of imaginary frequencies = 0

1p_C009

B3LYP/6-31G* Geometry

C	-1.334947	0.081313	0.881721
C	-3.123762	1.039717	-0.714080
C	-0.206287	1.056223	0.262900
C	-2.359282	-0.189378	-0.248840
H	-3.815387	1.356909	0.083780
H	-1.888733	-0.660392	-1.111842
C	-2.145029	2.137574	-0.992367
H	-2.544539	2.945343	-1.602504
C	-0.881203	2.192883	-0.553536
O	-3.852075	0.797442	-1.910120
H	-4.481829	0.083843	-1.706389
Br	-3.758976	-1.561618	0.250610
C	-2.043008	0.754181	2.080711
H	-2.969133	0.216393	2.306305
H	-2.293236	1.801421	1.885556
H	-1.418378	0.716818	2.978327
C	-0.786116	-1.279238	1.364934
H	-1.584615	-1.836423	1.860318
H	0.022877	-1.165835	2.087310
H	-0.434370	-1.903735	0.537630
C	-0.069899	3.422473	-0.922359
H	-0.569325	3.973920	-1.723809
H	0.939775	3.180040	-1.274329
H	0.043671	4.111592	-0.076279
C	0.690579	1.715047	1.363559
H	1.143988	2.610432	0.933976
H	0.076215	2.076055	2.192568
C	0.743535	0.315723	-0.750201
H	1.163155	1.055512	-1.437511
H	0.168291	-0.366856	-1.381623
C	1.844572	0.868994	1.927253
H	2.434827	1.486452	2.614053
H	1.478781	0.025235	2.515853
C	1.922856	-0.473715	-0.152568
H	1.590973	-1.377338	0.348595
C	2.783621	0.340310	0.823184
Cl	3.971311	-0.813510	1.650076
C	3.620122	1.443432	0.175681
H	4.189785	1.979026	0.939977
H	2.978745	2.164116	-0.342707
H	4.313267	1.022108	-0.554317
Br	2.982548	-1.198317	-1.682587

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.56708913**

Number of imaginary frequencies = 0

1p_C010

B3LYP/6-31G* Geometry

C	1.274870	-0.279486	-0.985813
C	3.449308	-1.233712	0.122388
C	0.449109	-0.465315	0.376990
C	2.805679	-0.146713	-0.749313
H	4.358727	-0.823778	0.569470
H	3.311866	-0.138497	-1.713937
C	2.524418	-1.717377	1.192116
H	2.984463	-2.394987	1.909821
C	1.215101	-1.445188	1.307120
O	3.922848	-2.323165	-0.685563
H	3.181108	-2.931662	-0.824547
Br	3.390685	1.639500	-0.008712
C	0.851380	0.909018	-1.876832
H	1.447908	0.888512	-2.797316
H	1.034245	1.873410	-1.402900
H	-0.196329	0.852755	-2.177974
C	1.110611	-1.553335	-1.872611
H	1.878154	-1.582866	-2.652245
H	0.140667	-1.547733	-2.378914
H	1.172828	-2.480955	-1.295655
C	0.470006	-2.111499	2.450644
H	1.178927	-2.550474	3.158032
H	-0.183360	-2.920385	2.100565
H	-0.161797	-1.413983	3.012537
C	0.236182	0.847535	1.209730
H	0.010996	0.552285	2.240539
H	1.168938	1.408877	1.262700
C	-0.980283	-1.068680	0.130229
H	-1.348268	-1.477890	1.071672
H	-0.941174	-1.915772	-0.555503
C	-0.885541	1.790896	0.733723
H	-0.991135	2.607840	1.456762
H	-0.628175	2.256592	-0.218359
C	-2.060144	-0.096155	-0.361763
H	-1.869398	0.268199	-1.367542
C	-2.255614	1.097437	0.584459
Cl	-3.382092	2.312777	-0.240938
C	-2.892138	0.753369	1.931107
H	-3.004801	1.661427	2.529360
H	-2.262565	0.053236	2.490764
H	-3.872625	0.294858	1.792253
Br	-3.738516	-1.152520	-0.613637

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55883905**

Number of imaginary frequencies = 0

1p_C011

B3LYP/6-31G* Geometry

C	1.260893	-0.264284	-0.981230
C	3.424408	-1.269313	0.096162
C	0.448094	-0.432590	0.392408
C	2.794871	-0.163013	-0.760931
H	4.355717	-0.885283	0.532131
H	3.280909	-0.143367	-1.737423
C	2.513165	-1.709596	1.192532
H	2.971291	-2.388850	1.908537
C	1.219405	-1.392748	1.336080
O	3.724877	-2.428534	-0.698549
H	4.533565	-2.238331	-1.201219
Br	3.429768	1.601391	-0.002397
C	0.853665	0.940421	-1.858385
H	1.444841	0.918651	-2.782324
H	1.052393	1.898351	-1.377179
H	-0.195877	0.902797	-2.156100
C	1.069677	-1.529364	-1.872030
H	1.773624	-1.510795	-2.710281
H	0.063702	-1.543335	-2.302468
H	1.239221	-2.459435	-1.327296
C	0.490375	-2.008637	2.518356
H	1.210013	-2.423868	3.229192
H	-0.169932	-2.828339	2.209335
H	-0.129673	-1.288786	3.064788
C	0.225864	0.898239	1.193782
H	0.010710	0.627035	2.233110
H	1.152496	1.471729	1.227458
C	-0.976475	-1.055890	0.170778
H	-1.339754	-1.429277	1.128831
H	-0.928010	-1.929298	-0.479880
C	-0.909700	1.818812	0.703276
H	-1.027467	2.644397	1.414640
H	-0.657950	2.274737	-0.254677
C	-2.060111	-0.107448	-0.355416
H	-1.863736	0.232622	-1.368811
C	-2.271487	1.106709	0.561368
Cl	-3.405563	2.292636	-0.297862
C	-2.912411	0.788009	1.912199
H	-3.046381	1.709988	2.484205
H	-2.273993	0.115630	2.495335
H	-3.883010	0.307398	1.778760
Br	-3.729726	-1.181298	-0.593326

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55844531**

Number of imaginary frequencies = 0

1p_C012

B3LYP/6-31G* Geometry

C	-1.51140	-0.03416	1.16101
C	-3.06364	-1.56367	-0.26687
C	-0.26252	-0.30465	0.18061
C	-2.87985	-0.22272	0.45964
H	-3.78712	-1.42319	-1.07442
H	-3.67736	-0.11712	1.19448
C	-1.77537	-2.09126	-0.81451
H	-1.88804	-2.99651	-1.40954
C	-0.53709	-1.60980	-0.60769
O	-3.69101	-2.52946	0.59335
H	-2.99240	-2.95667	1.11228
Br	-3.36667	1.24121	-0.84092
C	-1.50610	1.35449	1.83902
H	-2.29844	1.37905	2.59692
H	-1.70908	2.16565	1.13893
H	-0.56316	1.57047	2.34784
C	-1.49913	-1.08329	2.31922
H	-2.46962	-1.11069	2.82471
H	-0.75349	-0.81866	3.07393
H	-1.26522	-2.09275	1.96920
C	0.60289	-2.37494	-1.23877
H	0.21408	-3.21852	-1.81690
H	1.29800	-2.76993	-0.49306
H	1.20261	-1.75857	-1.91536
C	-0.08533	0.86324	-0.85381
H	-0.74922	0.69207	-1.70274
H	-0.41752	1.79659	-0.39923
C	1.01383	-0.40226	1.11042
H	1.14297	-1.42400	1.47525
H	0.80381	0.19819	1.99773
C	1.33422	1.10752	-1.38041
H	1.69379	0.26304	-1.98156
H	1.31789	1.97850	-2.04507
C	2.39929	0.12601	0.66987
H	2.96878	0.38385	1.56100
C	2.38165	1.32435	-0.29269
Cl	1.84793	2.76472	0.78760
C	3.74112	1.73422	-0.85523
H	3.64774	2.69203	-1.37416
H	4.09709	0.98234	-1.56427
H	4.48542	1.83843	-0.06052
Br	3.58656	-1.32569	-0.07823

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55053192**

Number of imaginary frequencies = 0

1p_C013

B3LYP/6-31G* Geometry

C	-1.505960	-0.052173	1.162636
C	-3.045770	-1.563603	-0.298911
C	-0.253167	-0.318855	0.186246
C	-2.868198	-0.231080	0.449202
H	-3.725384	-1.402388	-1.145879
H	-3.662454	-0.130178	1.189904
C	-1.751404	-2.112545	-0.803654
H	-1.862910	-3.031117	-1.376273
C	-0.517271	-1.630071	-0.591994
O	-3.613052	-2.562154	0.566982
H	-4.561407	-2.371321	0.650166
Br	-3.367292	1.255824	-0.825762
C	-1.498328	1.333045	1.847822
H	-2.321791	1.372309	2.571049
H	-1.647588	2.156342	1.148274
H	-0.574918	1.520872	2.401495
C	-1.519217	-1.112063	2.308704
H	-2.446440	-1.029365	2.884839
H	-0.694275	-0.936714	3.004792
H	-1.456918	-2.135432	1.937249
C	0.628349	-2.405952	-1.198815
H	0.243555	-3.253191	-1.774162
H	1.307332	-2.798997	-0.437250
H	1.243794	-1.800108	-1.870780
C	-0.085827	0.842968	-0.856648
H	-0.748490	0.659047	-1.704200
H	-0.423737	1.778487	-0.411268
C	1.023385	-0.403478	1.115611
H	1.158646	-1.423406	1.482730
H	0.810229	0.197186	2.001876
C	1.331463	1.092453	-1.386261
H	1.696269	0.244751	-1.979772
H	1.309967	1.957689	-2.058337
C	2.404069	0.133916	0.670989
H	2.972397	0.402193	1.559783
C	2.376415	1.325563	-0.299510
Cl	1.828910	2.768620	0.771430
C	3.732198	1.744805	-0.863985
H	3.629866	2.698206	-1.389365
H	4.095803	0.991467	-1.567550
H	4.474925	1.861431	-0.069513
Br	3.604208	-1.311671	-0.069854

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.54990660**

Number of imaginary frequencies = 0

1p_C014

B3LYP/6-31G* Geometry

C	-1.511384	-0.033743	1.161020
C	-3.063890	-1.563579	-0.266297
C	-0.262609	-0.304558	0.180624
C	-2.879923	-0.222451	0.459772
H	-3.787707	-1.423394	-1.073572
H	-3.677406	-0.116390	1.194592
C	-1.775773	-2.091186	-0.814231
H	-1.888459	-2.996389	-1.409315
C	-0.537463	-1.609686	-0.607586
O	-3.690853	-2.529214	0.594458
H	-2.991973	-2.956366	1.113085
Br	-3.366434	1.241024	-0.841396
C	-1.505941	1.355108	1.838614
H	-2.297954	1.379828	2.596850
H	-1.709251	2.166068	1.138380
H	-0.562788	1.571264	2.346974
C	-1.499071	-1.082483	2.319611
H	-2.469738	-1.110162	2.824744
H	-0.753842	-0.817323	3.074543
H	-1.264563	-2.091946	1.969991
C	0.602438	-2.374742	-1.238911
H	0.213678	-3.218294	-1.817084
H	1.297678	-2.769707	-0.493312
H	1.201969	-1.758203	-1.915521
C	-0.085107	0.863214	-0.853921
H	-0.748793	0.691984	-1.703016
H	-0.417379	1.796614	-0.399510
C	1.013737	-0.402317	1.110469
H	1.142730	-1.424069	1.475339
H	0.803743	0.198231	1.997720
C	1.334542	1.107463	-1.380295
H	1.694159	0.263018	-1.981434
H	1.318219	1.978474	-2.044926
C	2.399285	0.125753	0.669953
H	2.968836	0.383374	1.561130
C	2.381836	1.324250	-0.292452
Cl	1.848214	2.764587	0.787772
C	3.741458	1.733881	-0.854860
H	3.648286	2.691633	-1.373911
H	4.097501	0.981875	-1.563728
H	4.485598	1.838121	-0.059993
Br	3.586201	-1.325940	-0.078458

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55053288**

Number of imaginary frequencies = 0

1p_C015

B3LYP/6-31G* Geometry

C	1.335466	0.382834	1.101070
C	3.211959	0.871849	-0.704944
C	0.369363	0.807307	-0.093244
C	2.765348	0.085774	0.559662
H	3.167583	0.185744	-1.563278
H	3.486539	0.301336	1.346706
C	2.323468	2.046434	-0.993917
H	2.819986	2.894271	-1.460226
C	1.004695	2.053998	-0.756484
O	4.547718	1.344557	-0.560972
H	5.124675	0.563198	-0.573591
Br	3.165038	-1.860465	0.198983
C	0.783040	-0.789744	1.939189
H	1.515841	-1.084782	2.697113
H	0.566071	-1.680984	1.347156
H	-0.127271	-0.488561	2.467936
C	1.536929	1.564590	2.095155
H	2.123766	1.221564	2.954416
H	0.581006	1.929096	2.484171
H	2.062165	2.408132	1.642910
C	0.193323	3.277060	-1.113054
H	0.827111	4.020113	-1.606289
H	-0.245361	3.753080	-0.226386
H	-0.638201	3.050583	-1.793212
C	0.262828	-0.327751	-1.173256
H	1.137537	-0.312269	-1.826157
H	0.257862	-1.316755	-0.704915
C	-1.080827	1.093268	0.435644
H	-1.522230	1.951262	-0.075542
H	-1.068892	1.358967	1.493539
C	-0.996408	-0.173295	-2.031715
H	-1.023759	0.837017	-2.459546
H	-0.977078	-0.865303	-2.877913
C	-2.022484	-0.100781	0.248941
H	-1.607795	-0.992559	0.708935
C	-2.312951	-0.386749	-1.238565
Cl	-2.784139	-2.179577	-1.361218
C	-3.452218	0.418727	-1.858482
H	-3.513606	0.206358	-2.929953
H	-3.260207	1.491260	-1.730477
H	-4.409615	0.184014	-1.392362
Br	-3.675229	0.195906	1.321287

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55843754**

Number of imaginary frequencies = 0

1p_C016

B3LYP/6-31G* Geometry

C	1.366189	-0.516649	-1.004009
C	3.454467	-0.850721	0.529312
C	0.437084	-0.651508	0.287659
C	2.803515	-0.071998	-0.632129
H	4.018131	-0.148024	1.157084
H	3.447029	-0.196709	-1.501416
C	2.475802	-1.616913	1.375540
H	2.942961	-2.266815	2.117721
C	1.139540	-1.612798	1.273758
O	4.382404	-1.757083	-0.099817
H	4.771455	-2.309967	0.596845
Br	3.019422	1.900356	-0.295360
C	0.782372	0.418295	-2.083232
H	1.495788	0.512865	-2.909738
H	0.583985	1.429051	-1.721483
H	-0.140508	0.004410	-2.502698
C	1.567571	-1.901079	-1.693070
H	2.187648	-1.775619	-2.586884
H	0.614459	-2.323643	-2.023632
H	2.064656	-2.626413	-1.048427
C	0.350386	-2.557539	2.154707
H	1.012292	-3.043745	2.877580
H	-0.127871	-3.350936	1.565552
H	-0.446285	-2.061753	2.720727
C	0.239771	0.724014	1.029095
H	1.108058	0.934997	1.655145
H	0.187144	1.543532	0.308312
C	-0.992779	-1.165446	-0.115791
H	-1.385115	-1.860529	0.629722
H	-0.960623	-1.728287	-1.048542
C	-1.029190	0.760025	1.886535
H	-1.025775	-0.068853	2.603068
H	-1.056939	1.676506	2.482347
C	-2.006003	-0.026413	-0.279166
H	-1.637543	0.717261	-0.979098
C	-2.338572	0.663308	1.059669
Cl	-2.901453	2.386874	0.650862
C	-3.449394	0.015626	1.882766
H	-3.540551	0.527126	2.845598
H	-3.204278	-1.036683	2.072904
H	-4.408095	0.055948	1.364884
Br	-3.620539	-0.722788	-1.218114

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55383500**

Number of imaginary frequencies = 0

1p_C017

B3LYP/6-31G* Geometry

C	1.357583	-0.541696	-0.983573
C	3.485423	-0.884870	0.499733
C	0.446305	-0.590045	0.327931
C	2.812026	-0.113162	-0.657720
H	4.152150	-0.201693	1.032226
H	3.432036	-0.244801	-1.543202
C	2.507099	-1.509763	1.450819
H	2.980291	-2.104878	2.230665
C	1.167133	-1.471070	1.377704
O	4.370070	-1.891317	-0.017961
H	3.828414	-2.656231	-0.268711
Br	3.053022	1.863006	-0.341909
C	0.794000	0.351066	-2.108897
H	1.483723	0.336745	-2.961136
H	0.678760	1.395457	-1.813735
H	-0.167393	-0.026029	-2.471743
C	1.490469	-1.968967	-1.603906
H	2.284262	-1.981998	-2.358398
H	0.569686	-2.263631	-2.115267
H	1.710197	-2.736994	-0.857544
C	0.381744	-2.304465	2.369940
H	1.051239	-2.721558	3.127838
H	-0.120293	-3.148749	1.879241
H	-0.396344	-1.739036	2.893907
C	0.231927	0.833831	0.968038
H	1.094909	1.097062	1.580851
H	0.178013	1.597089	0.187833
C	-0.979524	-1.154586	-0.020514
H	-1.359054	-1.783249	0.787521
H	-0.944575	-1.800344	-0.897671
C	-1.041973	0.928267	1.814508
H	-1.031522	0.165401	2.600244
H	-1.079612	1.892763	2.328237
C	-2.009011	-0.048123	-0.277652
H	-1.652685	0.641733	-1.036369
C	-2.350086	0.745993	0.999373
Cl	-2.937569	2.421028	0.449485
C	-3.451136	0.153625	1.875952
H	-3.547952	0.742203	2.793030
H	-3.190975	-0.875597	2.152710
H	-4.411150	0.137461	1.359095
Br	-3.613476	-0.843128	-1.152879

SCF Energy (PCM/mPW1PW91/6-31+G) = -6264.55471525**

Number of imaginary frequencies = 0

2a_C001

B3LYP/6-31G* Geometry

C	-0.397120	1.367775	-1.155147
C	1.533622	0.136570	-0.065899
C	-0.755700	-0.166344	0.904960
C	0.598822	-0.888361	0.615255
C	-1.335038	0.560353	-0.287482
C	0.969746	0.705188	-1.363931
H	-1.450784	-0.926774	1.258921
H	1.665390	1.426779	-1.798131
H	-0.864434	1.556355	-2.122382
H	1.773386	0.937779	0.634446
H	0.846031	-0.101181	-2.095902
Cl	-0.155447	3.069290	-0.465765
Br	3.320722	-0.654588	-0.481153
C	0.267515	-2.084459	-0.309845
H	-0.344239	-1.805102	-1.172741
H	-0.285003	-2.846830	0.249396
H	1.194483	-2.534213	-0.676636
C	1.215904	-1.435241	1.914239
H	2.064671	-2.081994	1.678374
H	0.477370	-2.024872	2.469102
H	1.567898	-0.633061	2.567451
Cl	-0.646113	0.999769	2.338655
C	-2.632970	0.490048	-0.632322
H	-2.953644	1.009370	-1.534183
C	-3.725755	-0.214304	0.098106
H	-3.448108	-0.554182	1.094260
H	-4.610923	0.419653	0.176783
Cl	-4.274412	-1.701914	-0.825598

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95069880**

Number of imaginary frequencies = 0

2a_C002

B3LYP/6-31G* Geometry

C	-0.434366	1.486628	-0.751790
C	1.615371	0.230366	0.058852
C	-0.633308	-0.807080	0.436641
C	0.863263	-1.119343	0.112664
C	-1.247408	0.244922	-0.459805
C	1.055649	1.199882	-0.977590
H	-1.179239	-1.745814	0.353341
H	1.617116	2.136752	-0.964219
H	-0.844310	1.993541	-1.626077
H	1.621064	0.687347	1.049082
H	1.169625	0.772167	-1.980528
Cl	-0.621036	2.745605	0.590158

Br	3.557032	-0.022216	-0.339283
C	0.878268	-1.849048	-1.251611
H	0.322613	-1.315377	-2.028509
H	0.433007	-2.844773	-1.149164
H	1.910037	-1.971089	-1.592700
C	1.467980	-2.058769	1.170858
H	2.454388	-2.399406	0.846056
H	0.828532	-2.937791	1.310952
H	1.578212	-1.564097	2.138765
Cl	-0.888706	-0.334565	2.204704
C	-2.444329	0.108451	-1.057433
H	-2.787223	0.914548	-1.704627
C	-3.407882	-1.026729	-0.939764
H	-3.600248	-1.488160	-1.911795
H	-3.103865	-1.796299	-0.232288
Cl	-5.031155	-0.418078	-0.364245

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94945428**

Number of imaginary frequencies = 0

2b_C001

B3LYP/6-31G* Geometry

C	0.924839	-0.077654	1.164690
C	-1.474658	-0.036955	0.304365
C	0.309005	0.925934	-1.146588
C	-1.028339	0.125001	-1.166146
C	1.359693	0.370796	-0.210249
C	-0.451068	-0.760204	1.173665
H	0.706788	0.951386	-2.162683
H	-0.810886	-0.837077	2.202116
H	1.652390	-0.768740	1.587369
H	-1.718238	0.939882	0.723928
H	-0.317265	-1.784062	0.805917
Cl	0.935304	1.332209	2.362805
Br	-3.198304	-1.036913	0.450187
C	-0.721489	-1.234656	-1.838325
H	0.148682	-1.740492	-1.409673
H	-0.524065	-1.087269	-2.905533
H	-1.586462	-1.896659	-1.739277
C	-2.095870	0.851241	-2.002931
H	-2.961448	0.200061	-2.148648
H	-1.693823	1.115743	-2.987512
H	-2.436007	1.769755	-1.518809
Cl	0.041319	2.718320	-0.757786
C	2.626498	0.262778	-0.648065
H	2.844731	0.555181	-1.673896
C	3.809167	-0.201946	0.132276
H	3.627050	-0.292708	1.201694
H	4.662215	0.460999	-0.023896
Cl	4.364572	-1.852884	-0.445242

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95085642**

Number of imaginary frequencies = 0

2b_C002

B3LYP/6-31G* Geometry

C	0.782156	-1.214873	-0.070197
C	-1.575087	-0.272813	0.157219
C	0.330737	1.333479	0.070309
C	-1.153891	1.121579	-0.358320
C	1.259033	0.198763	-0.309833
C	-0.709819	-1.408460	-0.379858
H	0.686578	2.259311	-0.385187
H	-1.043724	-2.365533	0.027178
H	1.351498	-1.920299	-0.672944
H	-1.581605	-0.274540	1.247779
H	-0.821880	-1.468627	-1.468833
Cl	1.138703	-1.759565	1.658816
Br	-3.471184	-0.692561	-0.312108
C	-1.189279	1.210409	-1.902494
H	-0.442836	0.573370	-2.386131
H	-1.000051	2.241028	-2.221631
H	-2.177994	0.916798	-2.266207
C	-2.057795	2.229574	0.210831
H	-3.052864	2.167486	-0.237391
H	-1.638992	3.216681	-0.015750
H	-2.165678	2.149889	1.295110
Cl	0.488186	1.672232	1.882824
C	2.434159	0.496783	-0.891417
H	2.675020	1.546481	-1.052690
C	3.499405	-0.447868	-1.343163
H	3.700682	-0.340349	-2.412144
H	3.290660	-1.493033	-1.120751
Cl	5.078694	-0.056696	-0.512527

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94950874**

Number of imaginary frequencies = 0

2c_C001

B3LYP/6-31G* Geometry

C	-0.14450	1.44752	-0.99747
C	1.35710	-0.67043	-1.08666
C	-0.62880	-0.57200	0.56608
C	0.28320	-1.47452	-0.31392
C	-1.11877	0.67143	-0.14138
C	0.80188	0.55748	-1.81168

H	-1.48009	-1.18588	0.85761
H	1.61687	1.15619	-2.22451
H	-0.70520	2.07864	-1.68818
H	1.81705	-1.33381	-1.82030
H	0.21648	0.18997	-2.66642
Cl	0.78595	2.68038	0.01162
Br	2.93879	-0.15586	0.02438
C	-0.65952	-2.11398	-1.37665
H	-1.24496	-1.37852	-1.93503
H	-1.36785	-2.78984	-0.88618
H	-0.07756	-2.70580	-2.09166
C	0.89945	-2.62596	0.49722
H	1.42113	-3.31569	-0.17650
H	0.11469	-3.18919	1.01456
H	1.61431	-2.26697	1.23715
Cl	0.10838	-0.11211	2.19403
C	-2.39559	1.08958	-0.08224
H	-2.67796	1.96477	-0.66549
C	-3.50004	0.49668	0.72513
H	-3.16516	-0.20024	1.49142
H	-4.09983	1.27687	1.19664
Cl	-4.67115	-0.43182	-0.34490

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94416274**

Number of imaginary frequencies = 0

2c_C002

B3LYP/6-31G* Geometry

C	-0.246847	-1.173855	1.240947
C	1.748660	0.468389	0.955037
C	-0.491792	0.937617	-0.248575
C	0.789392	1.546384	0.392417
C	-1.139921	-0.134843	0.598944
C	1.052690	-0.592745	1.811367
H	-1.186002	1.764203	-0.393873
H	1.748637	-1.398764	2.054304
H	-0.792923	-1.655736	2.052891
H	2.504910	0.968600	1.561530
H	0.782977	-0.113804	2.763787
Cl	0.084316	-2.575161	0.090813
Br	2.884243	-0.414315	-0.435049
C	0.293484	2.389824	1.604219
H	-0.324782	1.817840	2.301659
H	-0.304659	3.235755	1.247850
H	1.145907	2.799391	2.157154
C	1.505395	2.508792	-0.568895
H	2.324877	3.015521	-0.046032
H	0.809221	3.275207	-0.928157
H	1.921310	1.987451	-1.430473
Cl	-0.247955	0.315658	-1.964396
C	-2.458024	-0.176744	0.862507
H	-2.826058	-0.976078	1.504241
C	-3.526957	0.739719	0.364193
H	-4.044969	1.234233	1.190105
H	-3.176304	1.492321	-0.339997
Cl	-4.817956	-0.212282	-0.511195

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94269525**

Number of imaginary frequencies = 0

2c_C003

B3LYP/6-31G* Geometry

C	-0.282005	1.572540	-1.088772
C	1.714349	0.198808	-0.405018
C	-0.360783	-0.865610	-1.167627
C	0.871682	-1.098709	-0.219765
C	-1.168232	0.367185	-0.785843
C	0.968250	1.517963	-0.191495
H	0.035190	-0.699481	-2.175595
H	0.659384	1.621698	0.852695
H	0.017121	1.554119	-2.142139
H	2.159977	0.184727	-1.403376
H	1.632040	2.354521	-0.425066
Cl	-1.077590	3.193945	-0.888822
Br	3.318552	0.217592	0.783570
C	1.700767	-2.300987	-0.707027
H	1.944146	-2.213018	-1.773297
H	1.159566	-3.238079	-0.560142
H	2.639355	-2.351682	-0.148869
C	0.423671	-1.319222	1.233513
H	1.296550	-1.452128	1.877475
H	-0.191362	-2.221683	1.301412
H	-0.163104	-0.482564	1.622784
Cl	-1.345894	-2.388357	-1.402615
C	-2.368410	0.494654	-0.205964
H	-2.720201	1.510610	-0.050952
C	-3.333259	-0.537156	0.288966
H	-4.258223	-0.527365	-0.293234
H	-2.942245	-1.546455	0.329948
Cl	-3.836145	-0.116513	2.000708

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94182893**

Number of imaginary frequencies = 0

2c_C004

B3LYP/6-31G* Geometry

C	-0.371751	1.086850	-1.463470

C	1.283480	-0.522633	-0.381434
C	-0.717543	0.053710	0.910031
C	0.845508	-0.059141	1.029816
C	-1.268347	0.412152	-0.458205
C	1.077877	0.537925	-1.465733
H	-1.125916	-0.920021	1.183640
H	1.791706	1.350766	-1.324424
H	-0.812409	0.982472	-2.454139
H	0.764959	-1.449113	-0.641168
H	1.293282	0.096087	-2.443112
Cl	-0.381442	2.924169	-1.214414
Br	3.202635	-1.067641	-0.440241
C	1.150398	-1.135237	2.089556
H	0.781662	-2.121071	1.780276
H	0.670723	-0.870788	3.037764
H	2.226460	-1.218773	2.259524
C	1.547522	1.253040	1.429685
H	2.626365	1.135157	1.287597
H	1.363512	1.474295	2.483287
H	1.210198	2.113270	0.848175
Cl	-1.422088	1.163619	2.208496
C	-2.509708	0.065563	-0.842817
H	-2.823273	0.304566	-1.857703
C	-3.549977	-0.608610	-0.013812
H	-3.269337	-0.743563	1.028564
H	-4.495805	-0.064345	-0.055535
Cl	-3.915241	-2.276212	-0.683846

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94082416**

Number of imaginary frequencies = 0

2c_C005

B3LYP/6-31G* Geometry

C	-0.247585	1.612001	-0.779098
C	1.779566	0.152391	-0.460376
C	-0.445482	-0.821339	-0.824313
C	0.927920	-1.104057	-0.113406
C	-1.120434	0.446655	-0.318137
C	1.143391	1.503644	-0.127702
H	-0.229457	-0.670661	-1.887799
H	1.039678	1.624731	0.954512
H	-0.148604	1.582986	-1.869440
H	2.035601	0.117069	-1.522771
H	1.788020	2.309387	-0.488528
Cl	-0.919402	3.267865	-0.446920
Br	3.571438	0.100175	0.419397
C	1.600245	-2.345329	-0.728260
H	1.639480	-2.276716	-1.822530
H	1.057481	-3.256163	-0.467171
H	2.625050	-2.433324	-0.357573
C	0.742515	-1.298858	1.399865
H	1.706959	-1.495690	1.874465
H	0.087137	-2.154839	1.588069
H	0.300596	-0.421458	1.880695
Cl	-1.511175	-2.302964	-0.866989
C	-2.195927	0.633167	0.459520
H	-2.466092	1.666490	0.657934
C	-3.098753	-0.344612	1.137223
H	-2.808882	-1.383855	1.036117
H	-3.189625	-0.089061	2.195629
Cl	-4.801799	-0.213547	0.471414

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95069880**

Number of imaginary frequencies = 0

2d_C001

B3LYP/6-31G* Geometry

C	-0.016877	1.561504	0.079447
C	1.437364	-0.105142	-1.143099
C	-0.418496	-0.900155	0.470015
C	0.495243	-1.264302	-0.737722
C	-1.035988	0.479490	0.380776
C	0.748626	1.259627	-1.214551
H	-1.195726	-1.660662	0.517861
H	1.491045	2.039858	-1.396086
H	0.695912	1.615180	0.906971
H	1.896910	-0.342078	-2.103496
H	0.048211	1.268416	-2.057994
Cl	-0.719949	3.236346	-0.030998
Br	3.043461	0.083614	0.048198
C	-0.469028	-1.497905	-1.938329
H	-1.138673	-0.654588	-2.124634
H	-1.094236	-2.376336	-1.747744
H	0.106118	-1.691145	-2.850468
C	1.260731	-2.576374	-0.500662
H	1.790763	-2.867005	-1.414977
H	0.563100	-3.381968	-0.246206
H	1.992065	-2.484586	0.302492
Cl	0.408236	-1.059551	2.119636
C	-2.348354	0.703662	0.547085
H	-2.717011	1.716945	0.421760
C	-3.384287	-0.306848	0.910758
H	-2.984452	-1.220702	1.347514
H	-4.115511	0.119059	1.599126
Cl	-4.363183	-0.831396	-0.557070

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94905315**

Number of imaginary frequencies = 0

2d_C002

B3LYP/6-31G* Geometry

C	0.266436	1.825250	-0.517055
C	-1.651753	0.251277	0.011618
C	0.498720	0.022709	1.187614
C	-0.709780	-0.820223	0.638484
C	1.204869	0.812465	0.102016
C	-1.008753	1.152257	-1.039310
H	0.096683	0.749887	1.898161
H	-0.725394	0.558728	-1.916516
H	0.760802	2.361600	-1.326644
H	-2.079889	0.860374	0.809637
H	-1.723782	1.907675	-1.375142
Cl	-0.173480	3.163735	0.689870
Br	-3.265914	-0.578519	-0.823702
C	-1.446014	-1.505775	1.804755
H	-1.706973	-0.783924	2.588381
H	-0.828609	-2.286180	2.254512
H	-2.371146	-1.962036	1.442884
C	-0.239062	-1.870051	-0.380759
H	-1.098335	-2.411401	-0.784519
H	0.424654	-2.591351	0.105156
H	0.307329	-1.425985	-1.218457
Cl	1.602749	-0.980492	2.245251
C	2.435790	0.723679	-0.428745
H	2.681932	1.462723	-1.190200
C	3.561368	-0.230004	-0.176606
H	4.413063	0.276509	0.285068
H	3.293881	-1.099565	0.411239
Cl	4.182016	-0.861973	-1.780183

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94565429**

Number of imaginary frequencies = 0

2d_C003

B3LYP/6-31G* Geometry

C	0.130702	1.367775	-1.155147
C	-1.787441	0.136570	-0.065899
C	0.350111	-0.166344	0.904960
C	-0.902244	-0.888361	0.615255
C	1.070040	0.560353	-0.287482
C	-1.001033	0.705188	-1.363931
H	1.015345	-0.926774	1.258921
H	-1.675511	1.426779	-1.798131
H	-0.302065	1.556355	-2.122382
H	-2.513816	0.937779	0.634446
H	-0.572059	-0.101181	-2.095902
Cl	0.944841	3.069290	-0.465765
Br	-2.978492	-0.654588	-0.481153
C	-0.348366	-2.084459	-0.309845
H	0.316527	-1.805102	-1.172741
H	0.214190	-2.846830	0.249396
H	-1.173543	-2.534213	-0.676636
C	-1.706730	-1.435241	1.914239
H	-2.505813	-2.081994	1.678374
H	-1.057796	-2.024872	2.469102
H	-2.161926	-0.633061	2.567451
Cl	-0.000045	0.999769	2.338655
C	2.383352	0.490048	-0.632322
H	2.802489	1.009370	-1.534183
C	3.378219	-0.214304	0.098106
H	3.909694	-0.554182	1.094260
H	2.963428	0.419653	0.176783
Cl	4.678053	-1.701914	-0.825598

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94815150**

Number of imaginary frequencies = 0

2d_C004

B3LYP/6-31G* Geometry

C	0.288661	1.785963	-0.259913
C	-1.720998	0.301008	0.155272
C	0.537569	-0.456405	0.799361
C	-0.848809	-0.984414	0.273568
C	1.170165	0.560381	-0.132326
C	-1.129328	1.412558	-0.705957
H	0.355343	0.056329	1.747657
H	-1.067545	1.082458	-1.749793
H	0.723493	2.497559	-0.961390
H	-1.933684	0.680656	1.156150
H	-1.777559	2.292285	-0.681678
Cl	0.217926	2.730634	1.333013
Br	-3.543538	-0.100646	-0.559451
C	-1.485254	-1.919918	1.318506
H	-1.515363	-1.447515	2.307980
H	-0.924372	-2.852702	1.405988
H	-2.511223	-2.158033	1.026056
C	-0.688907	-1.719298	-1.067600
H	-1.665218	-2.036275	-1.442888
H	-0.066123	-2.608773	-0.934552
H	-0.218840	-1.092345	-1.831862
Cl	1.629129	-1.830533	1.304466
C	2.276261	0.535653	-0.896469
H	2.486735	1.446850	-1.455865

C	3.286936	-0.533802	-1.153988
H	3.103911	-1.465337	-0.632053
H	3.366699	-0.721253	-2.227795
Cl	4.949992	0.038625	-0.645002

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94549286**

Number of imaginary frequencies = 0

2e_C001

B3LYP/6-31G* Geometry

C	-0.417544	1.670760	0.537106
C	1.588043	0.178243	0.242987
C	-0.612094	-0.811598	0.900346
C	0.714388	-1.090946	0.126529
C	-1.319092	0.451555	0.467118
C	0.898504	1.458358	-0.232853
H	-1.253198	-1.683244	0.784379
H	1.556139	2.315707	-0.068767
H	-0.192239	1.869716	1.588748
H	1.927390	0.288260	1.274229
H	0.690318	1.406611	-1.305207
Cl	-1.195317	3.208675	-0.049495
Br	3.300922	-0.006076	-0.767875
C	0.316862	-1.396246	-1.336770
H	-0.292942	-0.609549	-1.788256
H	-0.258946	-2.326487	-1.384905
H	1.219303	-1.520271	-1.941395
C	1.434822	-2.320087	0.707564
H	2.296448	-2.576175	0.085568
H	0.760020	-3.183387	0.730815
H	1.789924	-2.140260	1.725580
Cl	-0.346893	-0.722070	2.741177
C	-2.599151	0.482824	0.067059
H	-3.004170	1.429830	-0.276368
C	-3.561739	-0.656908	0.041436
H	-3.245027	-1.527755	0.613309
H	-4.542674	-0.340498	0.399963
Cl	-3.848414	-1.250463	-1.673164

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95231952**

Number of imaginary frequencies = 0

2e_C002

B3LYP/6-31G* Geometry

C	-0.424208	1.447535	0.630667
C	1.666939	0.069777	0.345960
C	-0.573644	-1.030947	0.238401
C	0.891382	-1.102932	-0.296413
C	-1.235435	0.311740	0.030353
C	1.029608	1.442519	0.122332
H	-1.142175	-1.832044	-0.230283
H	1.601809	2.206427	0.654867
H	-0.428575	1.335245	1.718448
H	1.789809	-0.123585	1.412575
H	1.046143	1.704818	-0.939416
Cl	-1.131034	3.100979	0.350456
Br	3.552919	0.156846	-0.306868
C	0.808595	-0.976834	-1.835452
H	0.274672	-0.079793	-2.160429
H	0.290780	-1.846097	-2.256144
H	1.816929	-0.944874	-2.256539
C	1.536045	-2.455582	0.051826
H	2.517231	-2.534337	-0.423353
H	0.912021	-3.281353	-0.308621
H	1.667543	-2.577049	1.129954
Cl	-0.675930	-1.448910	2.046379
C	-2.399324	0.480494	-0.614696
H	-2.787225	1.490290	-0.710321
C	-3.259831	-0.570031	-1.234418
H	-3.482457	-0.329407	-2.276481
H	-2.852780	-1.578671	-1.185324
Cl	-4.888132	-0.639929	-0.400360

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95169674**

Number of imaginary frequencies = 0

2e_C003

B3LYP/6-31G* Geometry

C	-0.005538	1.726364	-0.391773
C	-1.437910	-0.308797	-1.155994
C	0.220503	-0.508696	0.698987
C	-0.421673	-1.284984	-0.495906
C	0.956276	0.730944	0.226184
C	-0.876734	1.079126	-1.479540
H	-0.594968	-0.181004	1.349175
H	-0.220376	0.965993	-2.354258
H	0.551854	2.549209	-0.838830
H	-1.821947	-0.766209	-2.069083
H	-1.682819	1.755052	-1.775082
Cl	-1.012097	2.563543	0.910371
Br	-3.108754	-0.104642	-0.061098
C	-1.124841	-2.574741	-0.032135
H	-1.775941	-2.401683	0.827119
H	-0.387960	-3.334525	0.238144
H	-1.741425	-2.972560	-0.846317
C	0.637364	-1.672906	-1.553569
H	0.164305	-2.213683	-2.380777

H	1.380193	-2.339076	-1.103568
H	1.173666	-0.813944	-1.964349
Cl	1.185008	-1.611523	1.791335
C	2.260668	1.052130	0.191243
H	2.497605	2.040047	-0.202119
C	3.486141	0.289339	0.580496
H	4.037400	0.804956	1.370787
H	3.308787	-0.739200	0.868971
Cl	4.636058	0.232828	-0.849315

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94208026**

Number of imaginary frequencies = 0

2f_C001

B3LYP/6-31G* Geometry

C	0.824359	-0.946357	-0.564330
C	-1.310688	0.410626	-1.192191
C	0.092057	1.108832	0.852566
C	-0.850113	1.580620	-0.288647
C	1.179106	0.155152	0.406058
C	-0.170294	-0.501805	-1.645416
H	0.560572	1.996544	1.281312
H	-0.567731	-1.376797	-2.164612
H	1.723050	-1.290598	-1.073581
H	-1.796168	0.829999	-2.074622
H	0.418637	0.060217	-2.384434
Cl	0.252583	-2.460189	0.321307
Br	-2.791813	-0.686799	-0.414928
C	0.008037	2.531284	-1.175510
H	0.943256	2.078110	-1.515847
H	0.266917	3.432428	-0.609017
H	-0.561817	2.847236	-2.056194
C	-2.035604	2.401765	0.243720
H	-2.602371	2.822064	-0.595287
H	-1.674252	3.234617	0.857502
H	-2.714014	1.797245	0.845197
Cl	-0.795282	0.386152	2.301025
C	2.434052	0.348485	0.848537
H	2.629793	1.204064	1.492872
C	3.619308	-0.511789	0.566112
H	3.365536	-1.503822	0.196202
H	4.246749	-0.616148	1.452495
Cl	4.703522	0.254149	-0.706739

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94413393**

Number of imaginary frequencies = 0

2f_C002

B3LYP/6-31G* Geometry

C	0.676081	-0.767913	-1.035379
C	-1.714635	0.273907	-1.046266
C	0.108143	1.256390	0.489358
C	-1.180697	1.540444	-0.331540
C	1.144671	0.432401	-0.246619
C	-0.636215	-0.515002	-1.791280
H	0.549540	2.219807	0.751022
H	-1.042609	-1.461946	-2.153651
H	1.426722	-1.043533	-1.774163
H	-2.479738	0.581200	-1.760794
H	-0.366526	0.070921	-2.681962
Cl	0.580774	-2.271299	0.024295
Br	-2.756937	-0.952478	0.141229
C	-0.763210	2.548207	-1.442326
H	0.079242	2.199766	-2.046437
H	-0.470981	3.500999	-0.987727
H	-1.606908	2.746967	-2.112177
C	-2.265256	2.224168	0.516827
H	-3.106882	2.518842	-0.120902
H	-1.864399	3.129441	0.986591
H	-2.643976	1.566972	1.298926
Cl	-0.217636	0.504513	2.141658
C	2.427132	0.834635	-0.210677
H	2.667863	1.734498	0.353383
C	3.610898	0.177565	-0.843214
H	4.086026	0.830287	-1.580427
H	3.390578	-0.784447	-1.303092
Cl	4.897648	-0.145089	0.412582

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94272419**

Number of imaginary frequencies = 0

2f_C003

B3LYP/6-31G* Geometry

C	0.615842	-1.037331	-1.278447
C	-1.640003	-0.327227	-0.452200
C	0.110035	1.328690	-0.966137
C	-1.138431	1.086380	-0.038430
C	1.200858	0.268914	-0.769570
C	-0.591330	-1.440901	-0.413435
H	-0.235287	1.288550	-2.005085
H	-0.258946	-1.630663	0.611020
H	0.277383	-0.877579	-2.307758
H	-2.072246	-0.267420	-1.454913
H	-1.027850	-2.366400	-0.797619
Cl	1.731253	-2.469272	-1.444072
Br	-3.192885	-0.923094	0.651815
C	-2.237317	2.117613	-0.354511

H	-2.462578	2.144478	-1.428212
H	-1.932839	3.120575	-0.048060
H	-3.156447	1.856437	0.176786
C	-0.752410	1.162242	1.447914
H	-1.629758	0.968968	2.070120
H	-0.374871	2.160616	1.686040
H	0.023166	0.440127	1.716973
Cl	0.725801	3.039304	-0.812393
C	2.366014	0.553331	-0.172400
H	2.511202	1.590442	0.115452
C	3.527032	-0.312938	0.194901
H	4.456762	0.097764	-0.205394
H	3.434632	-1.354608	-0.084919
Cl	3.745118	-0.290952	2.018579

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94111977**

Number of imaginary frequencies = 0

2f_C004

B3LYP/6-31G* Geometry

C	0.615826	-1.037337	-1.278435
C	-1.640035	-0.327205	-0.452221
C	0.110038	1.328678	-0.966122
C	-1.138461	1.086370	-0.038420
C	1.200830	0.268899	-0.769516
C	-0.591390	-1.440898	-0.413472
H	-0.235288	1.288503	-2.005071
H	-0.259036	-1.630708	0.610983
H	0.277404	-0.877562	-2.307756
H	-2.072330	-0.267385	-1.454911
H	-1.027908	-2.366379	-0.797704
Cl	1.731216	-2.469276	-1.444012
Br	-3.192917	-0.923070	0.651834
C	-2.237337	2.117617	-0.354506
H	-2.462496	2.144572	-1.428224
H	-1.932914	3.120558	-0.047932
H	-3.156509	1.856375	0.176689
C	-0.752446	1.162192	1.447922
H	-1.629798	0.968929	2.070126
H	-0.374875	2.160545	1.686083
H	0.023104	0.440041	1.716969
Cl	0.725800	3.039271	-0.812401
C	2.366007	0.553305	-0.172370
H	2.511226	1.590423	0.115445
C	3.527065	-0.312953	0.194838
H	4.456763	0.097735	-0.205544
H	3.434637	-1.354631	-0.084946
Cl	3.745309	-0.290910	2.018495

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94112031**

Number of imaginary frequencies = 0

2g_C001

B3LYP/6-31G* Geometry

C	-0.861734	-1.091660	0.874181
C	1.486487	-0.319217	0.316817
C	-0.303012	1.349764	0.613378
C	1.003384	1.061756	-0.212361
C	-1.361823	0.269961	0.465399
C	0.464832	-1.444609	0.194419
H	-0.026755	1.405859	1.670745
H	0.247807	-1.641169	-0.861953
H	-1.590437	-1.869929	0.658917
H	1.807427	-0.217240	1.355252
H	0.865855	-2.368315	0.619253
Cl	-0.666419	-1.168291	2.719364
Br	3.154170	-0.927509	-0.600828
C	2.067396	2.126475	0.111526
H	2.240940	2.197737	1.192525
H	1.757966	3.110312	-0.248017
H	3.015408	1.864645	-0.365404
C	0.711801	1.042446	-1.722800
H	1.611158	0.753894	-2.272997
H	0.405515	2.036879	-2.058233
H	-0.088788	0.343983	-1.985284
Cl	-0.953117	3.019322	0.260081
C	-2.599905	0.470875	-0.010939
H	-2.865020	1.464084	-0.358537
C	-3.681717	-0.553232	-0.120532
H	-4.662577	-0.099239	0.024013
H	-3.576285	-1.386597	0.573119
Cl	-3.738841	-1.298526	-1.801148

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95162914**

Number of imaginary frequencies = 0

2g_C002

B3LYP/6-31G* Geometry

C	-0.712572	-1.368162	0.070576
C	1.625646	-0.409589	0.230322
C	-0.321774	1.042192	0.665586
C	1.131299	1.056318	0.064124
C	-1.245659	0.039597	-0.010346
C	0.736338	-1.464708	-0.418774
H	-0.246147	0.768759	1.722191
H	0.727617	-1.327119	-1.506541
H	-1.330559	-2.068773	-0.486391

H	1.751254	-0.630600	1.291587
H	1.130851	-2.464659	-0.221688
Cl	-0.824650	-1.989384	1.814538
Br	3.472443	-0.660061	-0.492580
C	2.031168	1.986610	0.898325
H	2.002653	1.716075	1.961064
H	1.712129	3.026858	0.804922
H	3.066975	1.908456	0.558087
C	1.120659	1.507290	-1.406205
H	2.126364	1.431387	-1.827438
H	0.792373	2.547636	-1.477392
H	0.446204	0.904160	-2.022199
Cl	-1.027546	2.724843	0.716734
C	-2.385427	0.364764	-0.639182
H	-2.674667	1.410790	-0.665141
C	-3.342746	-0.552424	-1.325870
H	-3.056498	-1.602920	-1.314628
H	-3.508915	-0.242115	-2.360223
Cl	-4.988789	-0.469996	-0.530521

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.95095901**

Number of imaginary frequencies = 0

2g_C003

B3LYP/6-31G* Geometry

C	-0.420891	1.151922	0.174059
C	1.390009	0.011484	-1.176192
C	0.065197	-1.248846	0.645918
C	0.950133	-1.369587	-0.631344
C	-1.021564	-0.188868	0.542047
C	0.274186	1.061540	-1.192907
H	-0.396175	-2.221299	0.819752
H	0.691454	2.035060	-1.458392
H	0.328188	1.405583	0.928276
H	1.797340	-0.115263	-2.179951
H	-0.464987	0.798077	-1.958932
Cl	-1.530826	2.597102	0.170598
Br	2.953185	0.805047	-0.195181
C	0.037142	-2.006673	-1.720540
H	-0.884214	-1.445114	-1.893489
H	-0.245375	-3.021828	-1.421403
H	0.579920	-2.081469	-2.668981
C	2.139387	-2.320278	-0.418010
H	2.672069	-2.468638	-1.364380
H	1.784393	-3.298381	-0.074640
H	2.847494	-1.932571	0.314118
Cl	1.028108	-0.972110	2.201423
C	-2.286733	-0.598184	0.735816
H	-2.412325	-1.651027	0.986421
C	-3.590774	0.125465	0.657523
H	-3.514120	1.178949	0.419280
H	-4.163149	-0.007735	1.578414
Cl	-4.626608	-0.628454	-0.659844

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94297146**

Number of imaginary frequencies = 0

2g_C004

B3LYP/6-31G* Geometry

C	-0.420674	1.152011	0.174119
C	1.389165	0.010706	-1.176487
C	0.065240	-1.248511	0.647308
C	0.949568	-1.370079	-0.630547
C	-1.021499	-0.188505	0.542896
C	0.273455	1.060891	-1.193305
H	-0.396278	-2.220829	0.821565
H	0.690758	2.034191	-1.459508
H	0.329156	1.405445	0.927670
H	1.796094	-0.116693	-2.180318
H	-0.466170	0.797077	-1.958751
Cl	-1.529928	2.597657	0.171481
Br	2.952767	0.804929	-0.196532
C	0.036191	-2.007946	-1.718857
H	-0.885160	-1.446496	-1.892069
H	-0.246353	-3.022831	-1.418809
H	0.578749	-2.083641	-2.667352
C	2.138984	-2.320472	-0.416908
H	2.671463	-2.469304	-1.363316
H	1.784160	-3.298417	-0.072912
H	2.847163	-1.932169	0.314811
Cl	1.028829	-0.971286	2.201846
C	-2.286757	-0.597614	0.736560
H	-2.412412	-1.650239	0.988036
C	-3.590686	0.126065	0.656891
H	-3.513835	1.179279	0.417685
H	-4.163769	-0.006530	1.577410
Cl	-4.625861	-0.628762	-0.660711

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94296976**

Number of imaginary frequencies = 0

2h_C001

B3LYP/6-31G* Geometry

C	0.670671	-1.285068	0.091235
C	-1.364330	-0.079446	1.173024
C	-0.083305	1.006104	-0.675767
C	-0.848147	1.290621	0.654475

C	1.082065	0.052518	-0.478468
C	-0.287872	-1.158935	1.283707
H	-0.789999	0.550313	-1.375507
H	0.342060	-0.899649	2.146214
H	1.542585	-1.843664	0.424657
H	-1.833485	0.066551	2.147234
H	-0.740165	-2.128410	1.505726
Cl	-0.018968	-2.348552	-1.255423
Br	-2.895144	-0.773854	0.074021
C	-2.019187	2.268311	0.442994
H	-2.658149	1.967557	-0.390132
H	-1.646011	3.276320	0.248485
H	-2.639842	2.303556	1.346048
C	0.091666	1.889046	1.727753
H	-0.455599	2.043880	2.664348
H	0.460189	2.862604	1.391537
H	0.963412	1.263404	1.936313
Cl	0.412197	2.556994	-1.501786
C	2.364243	0.348438	-0.740765
H	2.606291	1.347002	-1.089257
C	3.523316	-0.583391	-0.600982
H	4.316214	-0.329644	-1.304760
H	3.262846	-1.633448	-0.729105
Cl	4.302358	-0.458481	1.064516

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94806661**

Number of imaginary frequencies = 0

2h_C002

B3LYP/6-31G* Geometry

C	0.597086	-0.920827	1.011797
C	-1.699032	-0.162491	0.288414
C	0.216321	1.435945	0.259355
C	-1.135235	1.081476	-0.434354
C	1.201575	0.285107	0.323316
C	-0.730143	-1.345393	0.353587
H	0.663621	2.282487	-0.262646
H	-1.176602	-2.155392	0.936116
H	0.411039	-0.654967	2.055905
H	-2.020334	0.120191	1.291917
H	-0.533570	-1.735807	-0.649007
Cl	1.675761	-2.387699	1.122484
Br	-3.392010	-0.806678	-0.552790
C	-0.812539	0.799862	-1.920365
H	-0.056593	0.021582	-2.052190
H	-0.439960	1.710186	-2.402641
H	-1.721298	0.485363	-2.440275
C	-2.118887	2.262559	-0.362367
H	-3.012579	2.040672	-0.951572
H	-1.656781	3.169835	-0.767967
H	-2.429555	2.471581	0.664466
Cl	-0.042434	2.090195	1.984553
C	2.415755	0.478253	-0.214397
H	2.606196	1.465472	-0.628886
C	3.591911	-0.459648	-0.329621
H	3.348452	-1.386060	-0.846864
H	4.020633	-0.709611	0.641837
Cl	4.928838	0.319805	-1.288961

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94571486**

Number of imaginary frequencies = 0

2h_C003

B3LYP/6-31G* Geometry

C	0.695512	-0.459657	1.311068
C	-1.608073	-0.145704	0.325027
C	0.155797	1.582946	-0.018265
C	-1.112557	0.937625	-0.657306
C	1.239850	0.585664	0.357058
C	-0.540879	-1.168008	0.720888
H	0.555016	2.319963	-0.715431
H	-0.948847	-1.853145	1.468188
H	0.406242	0.056057	2.230453
H	-2.019356	0.335015	1.213919
H	-0.240184	-1.768155	-0.142632
Cl	1.848354	-1.745935	1.895699
Br	-3.177347	-1.147590	-0.397364
C	-0.673722	0.341828	-2.015536
H	0.153770	-0.366454	-1.926321
H	-0.352848	1.142574	-2.690825
H	-1.518416	-0.175744	-2.477518
C	-2.198745	1.996388	-0.915360
H	-3.033226	1.548243	-1.461094
H	-1.796435	2.818219	-1.518499
H	-2.586025	2.418045	0.015645
Cl	-0.263277	2.603966	1.480679
C	2.449599	0.776214	-0.196433
H	2.542403	1.647676	-0.843618
C	3.726280	0.005850	-0.102471
H	3.675469	-0.889231	0.504582
H	4.535739	0.648983	0.251637
Cl	4.240539	-0.530694	-1.779483

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94611341**

Number of imaginary frequencies = 0

2h_C004

B3LYP/6-31G* Geometry

C	0.548019	-1.178127	0.724555
C	-1.770578	-0.033460	1.014674
C	-0.024491	0.977509	-0.459487
C	-1.178030	1.319856	0.534596
C	1.066113	0.135338	0.185923
C	-0.734878	-1.021606	1.554134
H	-0.457165	0.408379	-1.287436
H	-0.414479	-0.646998	2.536902
H	1.294093	-1.661804	1.351234
H	-2.518779	0.162589	1.784353
H	-1.193751	-1.998310	1.725489
Cl	0.337360	-2.379333	-0.662508
Br	-2.865747	-0.925587	-0.410841
C	-2.266002	2.186063	-0.127458
H	-2.589369	1.773487	-1.085414
H	-1.898276	3.201204	-0.293188
H	-3.143497	2.243239	0.527045
C	-0.648690	2.080906	1.772614
H	-1.468943	2.289689	2.468445
H	-0.223488	3.038900	1.459351
H	0.130751	1.537206	2.313210
Cl	0.626939	2.483581	-1.258035
C	2.348385	0.516929	0.290852
H	2.630242	1.483645	-0.114456
C	3.479781	-0.244014	0.899757
H	3.215325	-1.231884	1.273438
H	3.951945	0.326497	1.703447
Cl	4.804451	-0.514051	-0.333807

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94701361**

Number of imaginary frequencies = 0

2h_C005

B3LYP/6-31G* Geometry

C	0.666797	-0.942936	0.788653
C	-1.688540	-0.130821	0.346330
C	0.247307	1.405167	0.038985
C	-1.188915	1.078915	-0.472728
C	1.213531	0.231495	-0.001150
C	-0.748037	-1.336112	0.315859
H	0.644452	2.231137	-0.551678
H	-1.134687	-2.120429	0.971545
H	0.622959	-0.640651	1.838326
H	-1.870427	0.182731	1.375274
H	-0.692319	-1.755326	-0.692855
Cl	1.670787	-2.465477	0.826006
Br	-3.490951	-0.745064	-0.254879
C	-1.062408	0.755260	-1.979410
H	-0.349782	-0.047947	-2.183683
H	-0.728985	1.643601	-2.527160
H	-2.036993	0.456351	-2.373912
C	-2.123693	2.289829	-0.308821
H	-3.089662	2.080034	-0.775873
H	-1.693162	3.174391	-0.791817
H	-2.297798	2.530054	0.743043
Cl	0.226802	2.093371	1.767151
C	2.345872	0.409923	-0.702774
H	2.468886	1.390032	-1.162159
C	3.501935	-0.493844	-0.990086
H	3.591798	-0.674762	-2.064470
H	3.482070	-1.438948	-0.461846
Cl	5.060285	0.340678	-0.512634

SCF Energy (PCM/mPW1PW91/6-31+G) = -4341.94596549**

Number of imaginary frequencies = 0

3a_C001

B3LYP/6-31G* Geometry

C	-2.2781	-0.2065	0.1678
C	-2.7301	0.9247	1.1404
H	-2.9350	0.4372	2.1051
C	-1.6241	1.9679	1.3070
H	-2.0276	2.9628	1.4995
C	-0.3177	1.8309	0.6346
C	-0.1041	0.5187	-0.2000
C	-0.1031	-0.6991	0.7780
H	0.1808	-0.3742	1.7795
O	-1.4809	-1.1365	0.8551
Br	-3.9429	-1.2038	-0.3652
C	-1.4289	0.2695	-1.0438
O	-3.8414	1.6694	0.6813
H	-4.5434	1.0307	0.4647
O	-0.4607	1.6408	2.0654
C	1.2256	0.5321	-0.9897
H	1.4291	1.5143	-1.4172
H	1.1946	-0.1668	-1.8287
C	2.3646	0.1292	-0.0428
H	2.3061	0.7093	0.8768
C	2.3100	-1.3816	0.3093
C	0.8242	-1.8329	0.3540
H	0.5591	-2.2005	-0.6408
H	0.7201	-2.6750	1.0432
C	3.0994	-2.2986	-0.6232
H	2.7756	-2.1426	-1.6593

H	2.9149	-3.3431	-0.3558
H	4.1696	-2.0994	-0.5653
Cl	3.0346	-1.5713	2.0045
Br	4.1118	0.7014	-0.7992
C	0.4459	3.0878	0.2685
H	0.1427	3.9009	0.9338
H	0.2411	3.3943	-0.7632
H	1.5283	2.9563	0.3735
C	-1.3079	-0.8523	-2.0976
H	-0.5261	-0.6227	-2.8274
H	-2.2488	-0.9311	-2.6478
H	-1.1129	-1.8321	-1.6599
C	-1.9791	1.5055	-1.7775
H	-1.3150	1.7668	-2.6101
H	-2.1061	2.3837	-1.1460
H	-2.9612	1.2685	-2.1988

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74961064**

Number of imaginary frequencies = 0

H	-3.827249	0.032497	-2.82678
H	-4.771434	0.041043	-1.322431
Cl	-2.78841	2.181277	-1.29869
Br	-3.016206	-1.766556	0.927987
C	0.272117	2.980688	1.95892
H	1.016186	3.759441	2.148504
H	0.141936	2.400802	2.878878
H	-0.673265	3.483802	1.729309
C	0.440785	-1.830422	0.781611
H	-0.39751	-1.93173	1.471334
H	1.208201	-2.548735	1.081596
H	0.106904	-2.117237	-0.216153
C	1.692654	-0.271405	2.220665
H	0.950887	-0.476157	3.00232
H	2.141344	0.701765	2.414481
H	2.486961	-1.017702	2.319543

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74482357**

Number of imaginary frequencies = 0

3a_C002

B3LYP/6-31G* Geometry

C	1.969065	-0.160547	-0.374869
C	2.906615	1.068811	-0.250693
H	3.202947	1.340157	-1.274812
C	2.153453	2.226052	0.397035
H	2.818062	2.883044	0.96033
C	0.737401	2.114034	0.802764
C	-0.00421	0.749707	0.48017
C	-0.106574	0.625922	-1.06869
H	-0.113248	1.620925	-1.508291
O	1.135449	0.003796	-1.487949
Br	3.164271	-1.73325	-0.801147
C	1.030157	-0.409748	0.837895
O	4.029498	0.863387	0.584038
H	4.474861	0.058823	0.264149
O	1.138696	2.89869	-0.346209
C	-1.389212	0.703706	1.201236
H	-1.670594	1.729902	1.440411
H	-1.300964	0.193064	2.164496
C	-2.636722	0.157162	0.470022
H	-3.522339	0.635272	0.885026
C	-2.631499	0.326193	-1.057446
C	-1.298234	-0.145537	-1.634962
H	-1.22572	-1.215083	-1.415143
H	-1.300059	-0.037745	-2.72451
C	-3.831334	-0.281184	-1.779592
H	-3.781154	-1.372256	-1.73737

3b_C001

B3LYP/6-31G* Geometry

C	-2.32248	-0.09307	0.03605
C	-2.77898	1.08677	0.93267
H	-3.59162	1.60931	0.42076
C	-1.65174	2.09975	1.13859
H	-2.00008	3.11703	1.32766
C	-0.31348	1.89901	0.54293
C	-0.10870	0.56976	-0.26841
C	-0.16635	-0.62801	0.73016
H	0.11867	-0.29527	1.72863
O	-1.56153	-1.01348	0.79833
Br	-3.97242	-1.05417	-0.52607
C	-1.41101	0.33212	-1.14750
O	-3.30814	0.63143	2.15411
H	-2.67213	-0.02368	2.49248
O	-0.54360	1.71977	1.96110
C	1.24419	0.53663	-1.01815
H	1.49069	1.50905	-1.44561
H	1.21627	-0.16643	-1.85364
C	2.34383	0.10491	-0.03803
H	2.28190	0.69535	0.87467
C	2.22956	-1.39968	0.32635
C	0.72848	-1.80081	0.34275
H	0.47381	-2.17514	-0.65188
H	0.58064	-2.62801	1.04187
C	3.00829	-2.35202	-0.57929
H	2.71162	-2.19729	-1.62373

H	2.78416	-3.38695	-0.30530
H	4.08307	-2.18693	-0.50032
Cl	2.90963	-1.59532	2.03943
Br	4.12742	0.61113	-0.75429
C	0.52458	3.11947	0.21688
H	0.23508	3.94146	0.87727
H	0.37606	3.44266	-0.81975
H	1.59465	2.93629	0.36176
C	-1.91596	1.56633	-1.91901
H	-1.26597	1.76124	-2.77948
H	-1.96438	2.48112	-1.32573
H	-2.92089	1.36360	-2.30530
C	-1.29000	-0.80827	-2.18110
H	-0.47111	-0.62049	-2.88189
H	-2.21152	-0.86150	-2.76564
H	-1.15271	-1.78803	-1.72231

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75147490**

Number of imaginary frequencies = 0

H	-3.631973	0.285137	-2.954396
H	-4.660460	0.212738	-1.508200
Cl	-2.646834	2.304010	-1.227394
Br	-3.084439	-1.775017	0.710653
C	0.223708	2.833520	2.219772
H	0.963464	3.589587	2.497531
H	0.015663	2.216614	3.100722
H	-0.693986	3.364083	1.944344
C	1.594993	-0.504488	2.348443
H	0.833114	-0.790924	3.082654
H	2.008519	0.457479	2.656330
H	2.397291	-1.248290	2.405315
C	0.366797	-1.918958	0.754378
H	-0.510627	-2.036474	1.390543
H	1.097805	-2.676949	1.046624
H	0.082900	-2.134468	-0.276016

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74677840**

Number of imaginary frequencies = 0

3b_C002

B3LYP/6-31G* Geometry

C	2.010725	-0.225859	-0.199170
C	2.966212	0.950317	0.105954
H	3.732987	0.604270	0.804079
C	2.209851	2.090086	0.782089
H	2.834070	2.720653	1.418606
C	0.759332	2.008768	1.063593
C	0.007302	0.688551	0.606871
C	-0.009633	0.681821	-0.949955
H	0.015277	1.707312	-1.311142
O	1.246290	0.073676	-1.349650
Br	3.166428	-1.782271	-0.671539
C	0.988898	-0.522832	0.931532
O	3.644428	1.384362	-1.048291
H	2.959150	1.482172	-1.733362
O	1.274268	2.831337	-0.007788
C	-1.418510	0.626916	1.243033
H	-1.693419	1.640143	1.537759
H	-1.397485	0.048896	2.171439
C	-2.633162	0.163178	0.405416
H	-3.530152	0.636978	0.800314
C	-2.535186	0.433617	-1.104194
C	-1.178299	-0.025536	-1.635835
H	-1.135961	-1.108770	-1.487599
H	-1.114498	0.156495	-2.713624
C	-3.701578	-0.098154	-1.933055
H	-3.673725	-1.190455	-1.962595

3c_C001

B3LYP/6-31G* Geometry

C	-2.249825	-0.178188	0.038380
C	-3.026017	1.159254	0.076057
H	-3.746312	1.171829	-0.745923
C	-2.069729	2.333743	-0.122297
H	-2.542360	3.226882	-0.536095
C	-0.617613	2.133243	-0.324677
C	-0.089425	0.643905	-0.306216
C	-0.211421	0.120957	1.155092
H	-0.111710	0.959270	1.842114
O	-1.578260	-0.358736	1.269210
Br	-3.612397	-1.629682	-0.096256
C	-1.164576	-0.237101	-1.071109
O	-3.772938	1.292929	1.260914
H	-3.152796	1.094660	1.985262
O	-1.144481	2.615793	0.932555
C	1.361556	0.566149	-0.853254
H	1.894222	1.480172	-0.588634
H	1.352812	0.523751	-1.947542
C	2.216842	-0.592227	-0.330188
H	1.906136	-1.550112	-0.747069
C	2.212418	-0.757278	1.194873
C	0.749453	-0.983661	1.610718
H	0.439645	-1.953218	1.210036
H	0.693589	-1.067337	2.701008
C	3.106330	-1.892838	1.687130
H	2.791116	-2.835524	1.222392

H	3.022424	-1.997027	2.772215
H	4.150219	-1.710589	1.426292
Cl	2.812887	0.800701	1.997034
Br	4.050215	-0.368350	-1.075065
C	0.153079	3.195252	-1.084699
H	-0.433793	4.117443	-1.118518
H	0.367965	2.884291	-2.112660
H	1.103061	3.427895	-0.592925
C	-0.714246	-1.683884	-1.359773
H	0.176196	-1.685715	-1.996465
H	-1.504551	-2.207452	-1.903080
H	-0.516048	-2.267424	-0.460455
C	-1.628514	0.330937	-2.427489
H	-0.837991	0.203280	-3.175718
H	-1.898054	1.387927	-2.409328
H	-2.500887	-0.233255	-2.774967

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75626575**

Number of imaginary frequencies = 0

H	-2.176294	-3.735378	0.539771
H	-3.205216	-2.822907	1.657250
Cl	-3.727415	-1.959350	-1.018790
Br	-3.144015	1.178431	-0.332052
C	-0.492657	3.007494	1.267158
H	-0.170411	4.007510	0.963393
H	-0.238200	2.874551	2.325098
H	-1.578162	2.955103	1.154271
C	1.336023	-1.583891	1.705755
H	0.678521	-1.667221	2.576757
H	2.336503	-1.878096	2.030697
H	1.024851	-2.309129	0.954326
C	2.064228	0.695959	2.284165
H	1.540944	0.551232	3.236361
H	2.101024	1.768340	2.086616
H	3.092919	0.343700	2.418788

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74423243**

Number of imaginary frequencies = 0

3c_C002

B3LYP/6-31G* Geometry

C	2.101472	-0.064767	-0.198695
C	2.551064	1.358104	-0.601244
H	3.448481	1.617267	-0.032997
C	1.470356	2.375200	-0.247748
H	1.851979	3.383196	-0.072685
C	0.196141	1.977288	0.392726
C	-0.015775	0.435687	0.668108
C	-0.172761	-0.283744	-0.705691
H	-0.612227	0.413447	-1.414916
O	1.181467	-0.547824	-1.155701
Br	3.721532	-1.227117	-0.318872
C	1.381775	-0.134335	1.178995
O	2.909813	1.423683	-1.960169
H	2.170588	1.016548	-2.446271
O	0.253126	2.351952	-1.000445
C	-1.234114	0.144177	1.585723
H	-1.480980	1.006822	2.205099
H	-0.989399	-0.658346	2.287080
C	-2.505664	-0.300280	0.845792
H	-3.329127	-0.422617	1.549641
C	-2.281635	-1.621495	0.080314
C	-0.972163	-1.600639	-0.757113
H	-0.336088	-2.426051	-0.432083
H	-1.203071	-1.797697	-1.805934
C	-2.275767	-2.790982	1.081413
H	-1.432058	-2.712461	1.774107

3d_C001

B3LYP/6-31G* Geometry

C	-2.329314	-0.08429	0.066428
C	-2.84865	1.276906	0.596551
H	-3.642245	1.62319	-0.071099
C	-1.747064	2.339048	0.577453
H	-2.118039	3.360806	0.476554
C	-0.379326	2.024283	0.113599
C	-0.114074	0.534233	-0.311027
C	-0.199156	-0.358142	0.967855
H	0.028208	0.240914	1.850642
O	-1.590125	-0.745476	1.080514
Br	-3.931717	-1.209652	-0.285628
C	-1.369097	0.037899	-1.147722
O	-3.430863	1.146215	1.871096
H	-2.806703	0.612674	2.394354
O	-0.675683	2.217628	1.519428
C	1.274822	0.349397	-0.968402
H	1.526458	1.187224	-1.618665
H	1.308884	-0.549018	-1.58841
C	2.311086	0.205145	0.148274
H	2.141362	0.968101	0.91204
C	2.221024	-1.166575	0.86304
C	0.719639	-1.582444	0.946638
H	0.477207	-2.221949	0.100416
H	0.555751	-2.17492	1.852737
C	2.899781	-1.12179	2.230701
H	3.933137	-0.776955	2.138494

H	2.894645	-2.110151	2.697094
H	2.357817	-0.427773	2.88631
Cl	3.0715	-2.468931	-0.133194
Br	4.1293	0.657018	-0.488524
C	0.457989	3.138428	-0.483076
H	0.128238	4.096481	-0.071796
H	0.353037	3.177629	-1.573131
H	1.522857	3.023397	-0.253477
C	-1.1801	-1.330359	-1.837064
H	-0.326958	-1.313126	-2.521277
H	-2.069158	-1.558898	-2.429717
H	-1.054072	-2.151302	-1.130734
C	-1.854409	1.011107	-2.238937
H	-1.161596	0.994695	-3.087749
H	-1.952931	2.047318	-1.910387
H	-2.83234	0.681647	-2.606751

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75000255**

Number of imaginary frequencies = 0

H	-2.404195	2.322014	-2.420433
H	-1.692410	2.720284	-0.850319
Cl	-3.939098	-0.044816	-1.854763
Br	-3.072088	-1.392713	1.007469
C	0.554729	3.115536	1.921957
H	1.353006	3.845598	2.082543
H	0.364208	2.600938	2.869786
H	-0.345522	3.678220	1.651204
C	0.348071	-1.755791	0.988454
H	-0.493884	-1.755407	1.681019
H	1.056965	-2.519461	1.317736
H	-0.011507	-2.057365	0.004627
C	1.724368	-0.240161	2.356826
H	0.978022	-0.368975	3.149227
H	2.223035	0.716688	2.521291
H	2.470458	-1.032457	2.481009

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74212982**

Number of imaginary frequencies = 0

3d_C002

B3LYP/6-31G* Geometry

C	2.034897	-0.288163	-0.221578
C	3.058478	0.866220	-0.114770
H	3.848374	0.566146	0.579149
C	2.401889	2.118012	0.460019
H	3.092433	2.776759	0.990337
C	0.970124	2.149384	0.826804
C	0.125496	0.835515	0.551559
C	0.038015	0.645449	-0.994664
H	0.127249	1.616680	-1.478802
O	1.227187	-0.095568	-1.366808
Br	3.091612	-1.946581	-0.543994
C	1.052957	-0.388325	0.978162
O	3.686298	1.120913	-1.348250
H	2.971227	1.132320	-2.009396
O	1.460199	2.828536	-0.353519
C	-1.273750	0.937397	1.246121
H	-1.467299	1.990847	1.456267
H	-1.246777	0.452102	2.225786
C	-2.556948	0.468213	0.508126
H	-3.403493	1.031823	0.899909
C	-2.464419	0.668443	-1.015599
C	-1.215059	-0.042313	-1.544723
H	-1.262952	-1.095755	-1.263961
H	-1.188021	0.007636	-2.637591
C	-2.502631	2.172495	-1.341589
H	-3.454377	2.605990	-1.022060

3e_C001

B3LYP/6-31G* Geometry

C	-2.218987	-0.208897	0.205082
C	-2.993016	1.092534	0.543180
H	-3.362328	0.974428	1.572561
C	-2.044480	2.286655	0.467737
H	-2.563424	3.208446	0.200515
C	-0.616405	2.133945	0.119351
C	-0.085964	0.664667	-0.119604
C	-0.135964	-0.088464	1.243012
H	-0.021116	0.631007	2.051791
O	-1.489801	-0.606172	1.333475
Br	-3.615574	-1.636464	-0.101940
C	-1.201392	-0.087405	-0.963076
O	-4.038696	1.402116	-0.356222
H	-4.609567	0.615134	-0.406400
O	-1.041107	2.433889	1.470648
C	1.336029	0.689765	-0.741712
H	1.875179	1.559259	-0.364073
H	1.273052	0.815776	-1.827555
C	2.222363	-0.524301	-0.446098
H	1.895476	-1.409937	-0.991209
C	2.295191	-0.923200	1.032965
C	0.856516	-1.233833	1.476064
H	0.537123	-2.134867	0.943622
H	0.854299	-1.486959	2.541356
C	3.219514	-2.108508	1.301059
H	2.892014	-2.970837	0.706812

H	3.183552	-2.383657	2.358710
H	4.249636	-1.872213	1.029374
Cl	2.922437	0.499750	2.038634
Br	4.016367	-0.166254	-1.234121
C	0.082900	3.302304	-0.548536
H	-0.516323	4.207709	-0.417384
H	0.220682	3.134326	-1.621796
H	1.064673	3.489675	-0.102041
C	-0.767326	-1.471925	-1.487046
H	0.097182	-1.371300	-2.150634
H	-1.577457	-1.907636	-2.076961
H	-0.532797	-2.185180	-0.696180
C	-1.712496	0.687008	-2.192803
H	-0.925825	0.722811	-2.956053
H	-2.038095	1.704665	-1.984125
H	-2.567196	0.158017	-2.625637

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75368963**

Number of imaginary frequencies = 0

H	3.183622	-2.382597	2.359597
H	4.249576	-1.871975	1.029841
Cl	2.922727	0.500705	2.038300
Br	4.016175	-0.166813	-1.234328
C	0.082113	3.302390	-0.549686
H	-0.516779	4.207892	-0.417699
H	0.218416	3.134310	-1.623126
H	1.064483	3.489652	-0.104545
C	-0.767070	-1.472250	-1.486429
H	0.097164	-1.371743	-2.150406
H	-1.577280	-1.908507	-2.075860
H	-0.532063	-2.185047	-0.695299
C	-1.712704	0.686311	-2.192736
H	-0.926077	0.722309	-2.956040
H	-2.038666	1.703894	-1.984193
H	-2.567254	0.156988	-2.625499

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75368600**

Number of imaginary frequencies = 0

3e_C002

B3LYP/6-31G* Geometry

C	-2.218869	-0.208917	0.205203
C	-2.993126	1.092447	0.542992
H	-3.362697	0.974370	1.572270
C	-2.044866	2.286767	0.467217
H	-2.563995	3.208291	0.199541
C	-0.616690	2.134153	0.118900
C	-0.085930	0.664962	-0.119610
C	-0.135892	-0.087795	1.243285
H	-0.021435	0.632015	2.051828
O	-1.489735	-0.605760	1.333728
Br	-3.615096	-1.636963	-0.101716
C	-1.201372	-0.087667	-0.962916
O	-4.038821	1.401932	-0.356463
H	-4.609451	0.614713	-0.406631
O	-1.041514	2.434606	1.470057
C	1.336076	0.689766	-0.741699
H	1.875296	1.559242	-0.364171
H	1.273155	0.815620	-1.827571
C	2.222242	-0.524320	-0.445799
H	1.895064	-1.410086	-0.990581
C	2.295300	-0.922546	1.033360
C	0.856667	-1.232918	1.476905
H	0.537020	-2.134248	0.945169
H	0.854734	-1.485280	2.542383
C	3.219442	-2.107947	1.301812
H	2.891644	-2.970491	0.708052

3e_C003

B3LYP/6-31G* Geometry

C	2.041982	-0.141484	-0.335558
C	2.492260	1.236623	-0.885131
H	2.571976	1.123620	-1.976356
C	1.442962	2.290903	-0.545682
H	1.882721	3.283435	-0.435337
C	0.206420	1.963729	0.195910
C	-0.023746	0.446050	0.572654
C	-0.238966	-0.358172	-0.745131
H	-0.674180	0.302870	-1.490836
O	1.095071	-0.690677	-1.208293
Br	3.665653	-1.343308	-0.436650
C	1.382848	-0.112661	1.074325
O	3.691969	1.727133	-0.319510
H	4.363422	1.031624	-0.434772
O	0.186002	2.265244	-1.218212
C	-1.213292	0.236604	1.546933
H	-1.412473	1.135753	2.130384
H	-0.964322	-0.537475	2.278198
C	-2.522117	-0.206377	0.874288
H	-3.326076	-0.261250	1.608543
C	-2.362645	-1.576746	0.181511
C	-1.074557	-1.651205	-0.685702
H	-0.452910	-2.468812	-0.315860
H	-1.336337	-1.915587	-1.712212
C	-2.369731	-2.685227	1.249762
H	-1.507986	-2.593059	1.918560

H	-2.312384	-3.662739	0.763550
H	-3.285799	-2.652747	1.846605
Cl	-3.846426	-1.927664	-0.861343
Br	-3.148559	1.223830	-0.367209
C	-0.402109	3.057743	1.051907
H	-0.061535	4.030059	0.684695
H	-0.099531	2.966642	2.101261
H	-1.493278	3.038970	0.993171
C	1.330876	-1.530483	1.682012
H	0.705366	-1.552800	2.579741
H	2.337082	-1.824690	1.989615
H	0.977775	-2.289882	0.984529
C	2.098331	0.772590	2.111591
H	1.550447	0.737993	3.061097
H	2.209639	1.813680	1.813895
H	3.103912	0.381496	2.295441

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74237063**

Number of imaginary frequencies = 0

H	3.055559	-2.220647	2.543242
H	2.474973	-0.569125	2.842609
Cl	3.161826	-2.414737	-0.306306
Br	4.116302	0.754552	-0.518951
C	0.386299	3.132737	-0.258409
H	0.046563	4.059290	0.212650
H	0.223511	3.217084	-1.338399
H	1.464789	3.044524	-0.087070
C	-1.205839	-1.254726	-1.819233
H	-0.395097	-1.164857	-2.547825
H	-2.120384	-1.471030	-2.377099
H	-1.013048	-2.116309	-1.179136
C	-1.920373	1.102686	-2.031933
H	-1.213610	1.203753	-2.864084
H	-2.096730	2.088692	-1.604162
H	-2.872685	0.758150	-2.447341

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74810020**

Number of imaginary frequencies = 0

3f_C001

B3LYP/6-31G* Geometry

C	-2.288826	-0.170083	0.216349
C	-2.801436	1.129084	0.907559
H	-3.045538	0.850460	1.943641
C	-1.717721	2.209547	0.899832
H	-2.142768	3.213355	0.862828
C	-0.380631	1.963758	0.326672
C	-0.110957	0.510160	-0.205699
C	-0.137021	-0.472685	1.009003
H	0.087954	0.070990	1.927604
O	-1.510312	-0.913651	1.120865
Br	-3.911222	-1.297100	-0.160050
C	-1.391473	0.059635	-1.031139
O	-3.899111	1.735580	0.254462
H	-4.579101	1.048200	0.140263
O	-0.587183	2.074262	1.760362
C	1.254821	0.393907	-0.923739
H	1.463269	1.271662	-1.535440
H	1.284928	-0.468764	-1.593010
C	2.332577	0.215982	0.147715
H	2.167842	0.929804	0.958547
C	2.302627	-1.196115	0.784720
C	0.817715	-1.662266	0.883482
H	0.568704	-2.254944	0.005151
H	0.698762	-2.316268	1.753612
C	3.018256	-1.207847	2.134136
H	4.037995	-0.826476	2.034242

3f_C002

B3LYP/6-31G* Geometry

C	1.988512	-0.255293	-0.393065
C	2.990911	0.927728	-0.480188
H	3.242241	1.044797	-1.544788
C	2.339829	2.201735	0.049881
H	3.071009	2.875148	0.498816
C	0.946308	2.228103	0.534327
C	0.112703	0.886174	0.404975
C	-0.056119	0.570871	-1.115343
H	0.009148	1.499362	-1.680465
O	1.112727	-0.199906	-1.485650
Br	3.077727	-1.933179	-0.642616
C	1.090725	-0.282094	0.875129
O	4.147238	0.771439	0.318996
H	4.529635	-0.096128	0.096944
O	1.326694	2.855427	-0.716642
C	-1.246332	1.021899	1.169499
H	-1.443833	2.086275	1.311972
H	-1.156354	0.611096	2.178870
C	-2.560359	0.485127	0.541350
H	-3.394222	1.061178	0.942279
C	-2.556217	0.581550	-0.994898
C	-1.333054	-0.157835	-1.544679
H	-1.355476	-1.190312	-1.191114
H	-1.367975	-0.182594	-2.638159
C	-2.622472	2.059487	-1.419403
H	-3.555815	2.513036	-1.074244

H	-2.587874	2.135906	-2.509767
H	-1.786804	2.638386	-1.014407
Cl	-4.071159	-0.193326	-1.697577
Br	-3.010144	-1.345858	1.192494
C	0.602606	3.241762	1.610977
H	1.403875	3.982776	1.680346
H	0.487185	2.769246	2.591949
H	-0.320392	3.785393	1.380918
C	0.409878	-1.654007	1.024382
H	-0.387538	-1.612260	1.766815
H	1.147566	-2.385013	1.365411
H	-0.007896	-2.027139	0.089073
C	1.825435	-0.013824	2.200978
H	1.108226	-0.048762	3.029979
H	2.360604	0.933965	2.243617
H	2.561604	-0.805470	2.371892

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74048021**

Number of imaginary frequencies = 0

H	2.134871	1.104498	2.120536
H	3.780084	0.496983	1.854855
Cl	3.297120	-2.277885	1.093858
Br	4.051073	0.357505	-0.990800
C	-0.089267	3.479389	-0.135572
H	-0.736563	4.334199	0.079184
H	0.127579	3.471405	-1.208985
H	0.852676	3.640622	0.398969
C	-0.642653	-1.172287	-1.748690
H	0.252409	-0.945982	-2.336492
H	-1.395901	-1.561021	-2.438191
H	-0.417493	-1.975035	-1.047282
C	-1.682078	1.004758	-2.220629
H	-0.886945	1.142432	-2.962210
H	-2.019335	1.994774	-1.910117
H	-2.517411	0.508976	-2.726977

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75406435**

Number of imaginary frequencies = 0

3g_C001

B3LYP/6-31G* Geometry

C	-2.261834	-0.214697	-0.005284
C	-3.114444	1.008390	0.405647
H	-3.841015	1.211455	-0.385474
C	-2.234008	2.247737	0.553353
H	-2.763918	3.189871	0.399705
C	-0.776209	2.201877	0.308707
C	-0.157605	0.799944	-0.077857
C	-0.240866	-0.120904	1.175326
H	-0.198004	0.494285	2.074024
O	-1.572373	-0.696638	1.132945
Br	-3.534632	-1.644102	-0.559444
C	-1.180053	0.105924	-1.073119
O	-3.857488	0.754206	1.573018
H	-3.225731	0.371618	2.207937
O	-1.312482	2.288925	1.649631
C	1.295310	0.966971	-0.600366
H	1.762431	1.813752	-0.094175
H	1.288029	1.228301	-1.663791
C	2.239618	-0.231688	-0.408343
H	2.015865	-1.047766	-1.091546
C	2.229081	-0.773925	1.028499
C	0.791496	-1.250946	1.304880
H	0.552416	-2.070173	0.626179
H	0.735410	-1.660696	2.318747
C	2.753990	0.200756	2.082356
H	2.729934	-0.267293	3.069882

3g_C002

B3LYP/6-31G* Geometry

C	-2.058871	-0.013511	-0.177901
C	-2.526527	-1.479870	-0.323111
H	-3.386960	-1.641385	0.331676
C	-1.421846	-2.435027	0.118649
H	-1.787636	-3.403172	0.467135
C	-0.114719	-1.947962	0.613918
C	0.105562	-0.383310	0.636376
C	0.182134	0.110841	-0.839330
H	0.586153	-0.691116	-1.453066
O	-1.194772	0.301470	-1.252118
Br	-3.684543	1.124344	-0.394112
C	-1.261684	0.270657	1.126475
O	-2.965633	-1.757881	-1.631314
H	-2.261560	-1.428706	-2.218170
O	-0.251800	-2.531843	-0.700763
C	1.370310	0.038483	1.430234
H	1.655010	-0.718820	2.160654
H	1.168422	0.946644	2.003840
C	2.591035	0.371002	0.568249
H	3.451077	0.605144	1.193645
C	2.347690	1.516053	-0.432229
C	0.970506	1.400475	-1.139932
H	0.359815	2.269972	-0.905944
H	1.133273	1.433775	-2.222653
C	3.491912	1.752582	-1.416042
H	3.310974	2.673776	-1.976549

H	3.551127	0.918820	-2.120652
H	4.451247	1.841093	-0.898048
Cl	2.329578	3.043019	0.667500
Br	3.204627	-1.269000	-0.420802
C	0.631986	-2.836548	1.590460
H	0.299250	-3.870108	1.459084
H	0.439877	-2.546733	2.630068
H	1.709253	-2.805403	1.408828
C	-1.184390	1.784993	1.413191
H	-0.466385	2.002500	2.208480
H	-2.161885	2.134554	1.753604
H	-0.921790	2.381020	0.540411
C	-1.876456	-0.370474	2.385986
H	-1.301678	-0.075766	3.271341
H	-1.917556	-1.460724	2.364582
H	-2.898005	0.002015	2.519832

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74854482**

Number of imaginary frequencies = 0

H	2.219271	1.005903	2.148122
H	3.866177	0.455943	1.782905
Cl	3.415273	-2.288339	0.898504
Br	4.014397	0.466668	-1.077559
C	-0.158216	3.447536	0.103161
H	-0.812698	4.273132	0.396285
H	-0.019263	3.487674	-0.982075
H	0.814235	3.616576	0.577291
C	-0.693147	-1.110882	-1.706339
H	0.163421	-0.836332	-2.330032
H	-1.475051	-1.479857	-2.374700
H	-0.412010	-1.941555	-1.059284
C	-1.766177	1.084156	-2.008999
H	-0.974116	1.323467	-2.728711
H	-2.170031	2.015257	-1.615693
H	-2.573015	0.592066	-2.560776

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.75184030**

Number of imaginary frequencies = 0

3h_C001

B3LYP/6-31G* Geometry

C	-2.229661	-0.278719	0.167845
C	-3.081820	0.886777	0.736531
H	-3.445001	0.552330	1.719501
C	-2.209844	2.129688	0.899490
H	-2.786301	3.050765	0.802117
C	-0.776526	2.134173	0.542852
C	-0.154171	0.767908	0.047973
C	-0.165420	-0.228940	1.245377
H	-0.109882	0.331792	2.178351
O	-1.481510	-0.837758	1.213488
Br	-3.532622	-1.700407	-0.423345
C	-1.215331	0.121886	-0.940212
O	-4.142110	1.300250	-0.101720
H	-4.657899	0.503399	-0.318599
O	-1.215557	2.155308	1.923825
C	1.268615	0.991954	-0.531575
H	1.742063	1.822292	-0.004397
H	1.206557	1.306823	-1.578552
C	2.243934	-0.193597	-0.446647
H	2.004859	-0.977099	-1.162283
C	2.310875	-0.810552	0.958244
C	0.898309	-1.337065	1.270806
H	0.648044	-2.125375	0.559701
H	0.896213	-1.800635	2.262799
C	2.858268	0.122221	2.038164
H	2.887948	-0.395589	3.000344

3h_C002

B3LYP/6-31G* Geometry

C	2.005185	-0.044994	-0.337223
C	2.477832	1.396599	-0.658746
H	2.617959	1.440392	-1.748951
C	1.406033	2.394447	-0.230879
H	1.832381	3.360641	0.043370
C	0.133382	1.967389	0.387803
C	-0.107545	0.412424	0.534690
C	-0.249532	-0.195252	-0.892947
H	-0.648600	0.567184	-1.558400
O	1.107422	-0.458963	-1.330401
Br	3.637325	-1.223437	-0.526236
C	1.271865	-0.218153	1.023456
O	3.641788	1.797783	0.036513
H	4.318524	1.118253	-0.131685
O	0.187730	2.466741	-0.969147
C	-1.342135	0.069988	1.408474
H	-1.574520	0.876150	2.104676
H	-1.132880	-0.807413	2.025805
C	-2.606933	-0.282091	0.622376
H	-3.446779	-0.445936	1.295625
C	-2.436794	-1.500504	-0.304407
C	-1.081805	-1.481488	-1.062298
H	-0.486133	-2.345054	-0.773682
H	-1.279610	-1.599829	-2.133128
C	-3.622285	-1.764847	-1.230102
H	-3.491741	-2.728440	-1.730066

H	-3.679691	-0.980047	-1.988953
H	-4.564988	-1.783648	-0.675609
Cl	-2.426415	-2.950200	0.896807
Br	-3.211370	1.304866	-0.454274
C	-0.528580	2.930374	1.354499
H	-0.179254	3.945299	1.144145
H	-0.278897	2.694163	2.395075
H	-1.615473	2.918758	1.239705
C	1.188895	-1.708294	1.417006
H	0.514539	-1.857016	2.264577
H	2.178796	-2.050526	1.728416
H	0.867762	-2.358044	0.603977
C	1.925360	0.506147	2.215035
H	1.333551	0.323830	3.120085
H	2.036183	1.581348	2.084147
H	2.926292	0.098340	2.386878

SCF Energy (PCM/mPW1PW91/6-31+G) = -6413.74423243**

Number of imaginary frequencies = 0