Condensed 2- and 3-Dimensional Aromatic Systems: A Theoretical Study on the Relative Stabilities of Isomers of $CB_{19}H_{16}^{+}$, $B_{20}H_{15}Cl$ and $B_{20}H_{14}Cl_2$ and Comparison to $B_{12}H_{10}Cl_2^{2-}$, $C_6H_4Cl_2$, $C_{10}H_7Cl$ and $C_{10}H_6Cl_2$

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Total energies (a.u) and Cartesian coordinates of all structures at B3LYP/6-31G* level of theory.

$B_{20}H_{16}$

Total Energy = -506.908509

H	0.00000	2.50367	2.49562
H	-2.45863	-1.63951	1.23050
B	-0.88034	0.00000	2.65666
B	-1.55015	0.88116	1.25538
H	0.00000	-2.50367	2.49562
H	-2.45863	1.63951	1.23050
B	1.55015	-0.88116	1.25538
B	0.00000	1.19378	0.25736
B	0.00000	1.42344	2.00355
B	0.00000	-1.42344	2.00355
H	0.00000	1.47550	-3.68358
H	0.00000	-1.47550	-3.68358
B	-1.55015	-0.88116	1.25538
H	2.45863	1.63951	1.23050
B	0.88116	1.55015	-1.25538
B	0.00000	-1.19378	0.25736
B	1.55015	0.88116	1.25538
H	1.47550	0.00000	3.68358
H	2.45863	-1.63951	1.23050
H	-1.47550	0.00000	3.68358
B	0.88034	0.00000	2.65666
H	2.50367	0.00000	-2.49562
H	-1.63951	-2.45863	-1.23050
B	0.00000	-0.88034	-2.65666
B	0.88116	-1.55015	-1.25538
H	-2.50367	0.00000	-2.49562
H	1.63951	-2.45863	-1.23050
B	-0.88116	1.55015	-1.25538
B	1.19378	0.00000	-0.25736
B	1.42344	0.00000	-2.00355
B	-1.42344	0.00000	-2.00355
H	-1.63951	2.45863	-1.23050
B	0.00000	0.88034	-2.65666
B	-0.88116	-1.55015	-1.25538
H	1.63951	2.45863	-1.23050
B	-1.19378	0.00000	-0.25736

$1\text{-}CB_{19}H_{16}^{1+}$

Total Energy = -519.862607

B	1.21373	-0.88516	-1.52134
C	2.48167	0.00000	-0.80669
B	1.99076	-1.43440	0.01058
B	1.24032	-0.88630	1.54767
B	1.24032	0.88630	1.54767
B	2.63661	0.00000	0.87713
B	1.99076	1.43440	0.01058
B	0.24119	1.25286	0.00242
B	1.21373	0.88516	-1.52134
B	-0.26449	0.00000	-1.13161
B	-1.28842	-1.57223	-0.88259
B	-1.27980	-1.57183	0.88847
B	-0.25920	0.00000	1.14633
B	-1.27980	1.57183	0.88847
B	-2.67829	0.87685	0.00239
B	-2.00303	0.00000	1.42259
B	-2.67829	-0.87685	0.00239
B	-2.01099	0.00000	-1.41763
B	-1.28842	1.57223	-0.88259
B	0.24119	-1.25286	0.00242
H	2.60930	-2.43690	-0.07161
H	1.33005	1.58660	-2.46146
H	2.60930	2.43690	-0.07161
H	1.33005	-1.58660	-2.46146
H	-3.69831	-1.47831	0.00394
H	-3.69831	1.47831	0.00394
H	1.23821	-1.62908	2.46503
H	3.71889	0.00000	1.34781
H	1.23821	1.62908	2.46503
H	3.42549	0.00000	-1.34437
H	-2.46244	0.00000	2.51455

H	-1.23564	2.45359	-1.66837
H	-2.46729	0.00000	-2.51083
H	-1.24058	2.45767	1.66896
H	-1.23564	-2.45359	-1.66837
H	-1.24058	-2.45767	1.66896

2-$CB_{19}H_{16}^{1+}$
Total Energy = -519.853508

B	1.16633	-0.22897	0.00000
B	1.56550	1.27250	0.88945
B	1.56550	1.27250	-0.88945
B	-0.01050	0.27227	-1.18998
B	-0.89194	-1.24343	-1.55329
B	0.86577	-1.23606	-1.55654
C	1.28780	-1.88574	0.00000
H	2.26265	-2.36489	0.00000
B	-0.01050	0.27227	1.18998
B	-1.22371	-0.25650	0.00000
B	-1.43573	-2.00316	0.00000
B	-0.00401	-2.63532	0.87823
B	-0.00401	-2.63532	-0.87823
B	0.86577	-1.23606	1.55654
B	-0.89194	-1.24343	1.55329
B	-1.56863	1.27218	0.88370
B	-0.87866	2.66809	0.00000
B	-1.56863	1.27218	-0.88370
B	-0.00309	2.01003	-1.42454
B	0.87978	2.66714	0.00000
B	-0.00309	2.01003	1.42454
H	-1.63122	-1.24642	2.47317
H	-2.49156	-2.53713	0.00000
H	1.68897	-1.27817	2.39886
H	1.48311	3.68575	0.00000
H	-1.47438	3.69114	0.00000
H	1.68897	-1.27817	-2.39886
H	0.15580	-3.67134	-1.42179
H	-1.63122	-1.24642	-2.47317
H	0.15580	-3.67134	1.42179
H	-0.00542	2.48533	-2.51036
H	-2.46513	1.22689	1.65132
H	-0.00542	2.48533	2.51036
H	-2.46513	1.22689	-1.65132
H	2.46817	1.22613	1.64999
H	2.46817	1.22613	-1.64999

3-$CB_{19}H_{16}^{1+}$
Total Energy = -519.837004

B	0.24036	-1.24925	-0.16176
B	-0.25525	0.12845	-1.05803
B	-1.24523	1.69445	-0.65949
B	-1.98670	0.19423	-1.41583
B	-2.69254	-0.84989	-0.13042
B	-2.00921	-0.17833	1.39586
B	-0.25820	-0.14923	1.12860
B	-1.27010	1.44118	1.09886
B	-2.65729	0.89036	0.09655
C	1.21473	-0.56565	-1.48742
B	1.25006	1.11261	-1.36124
B	0.26428	1.26745	0.20563
B	2.02251	1.41796	0.21943
B	2.64966	-0.15065	0.87432
B	1.22450	-1.10438	1.39761
B	1.99417	-1.42850	-0.20224
B	2.64264	0.11613	-0.86585
B	-1.32300	-1.68576	0.66967
B	-1.30944	-1.44019	-1.07467
B	1.26619	0.64673	1.66255
H	2.47517	-2.47106	-0.48472
H	1.20551	1.85163	-2.27769
H	2.55280	2.46813	0.35947
H	1.21216	-1.09080	-2.43891
H	-3.72824	-1.41806	-0.21159
H	-3.66728	1.50656	0.15471
H	1.20874	-1.97770	2.19204
H	3.68534	-0.25389	1.43606
H	1.24652	1.23041	2.68869
H	3.59980	0.13485	-1.55671
H	-2.47017	-0.32316	2.47760
H	-1.19213	2.66178	-1.33439
H	-2.41646	0.35638	-2.50718
H	-1.24160	2.20573	1.99884
H	-1.21545	-2.18487	-1.99080
H	-1.28011	-2.66883	1.32137

4-$CB_{19}H_{16}^{1+}$
Total Energy = -519.809852

B	1.21241	-1.54275	0.89509
B	2.61790	-0.89323	-0.00000
B	1.98538	0.01059	1.42501
B	1.24988	1.56367	0.88199
B	1.24988	1.56367	-0.88199
B	2.65334	0.87128	0.00000
B	1.98538	0.01059	-1.42501
B	0.24912	0.02599	-1.19392
B	1.21241	-1.54275	-0.89510
C	-0.19149	-1.07989	-0.00000

B	-1.23713	-0.84846	1.59863
B	-1.25551	0.91187	1.54471
B	-0.29364	1.33053	0.00000
B	-1.25551	0.91187	-1.54471
B	-2.62628	-0.05523	-0.87762
B	-2.04415	1.40442	0.00000
B	-2.62628	-0.05523	0.87762
B	-1.86141	-1.44356	-0.00000
B	-1.23713	-0.84846	-1.59863
B	0.24912	0.02599	1.19392
H	2.46470	0.00530	2.50814
H	1.12299	-2.48051	-1.60252
H	2.46470	0.00530	-2.50814
H	1.12299	-2.48051	1.60251
H	-3.65312	-0.12768	1.46224
H	-3.65312	-0.12768	-1.46224
H	1.19754	2.44805	1.66452
H	3.67999	1.45964	0.00000
H	1.19754	2.44806	-1.66452
H	3.62772	-1.50969	-0.00000
H	-2.59871	2.45230	0.00000
H	-1.12276	-1.66930	-2.43677
H	-2.22897	-2.56761	-0.00000
H	-1.24433	1.64447	-2.47038
H	-1.12276	-1.66930	2.43677
H	-1.24433	1.64447	2.47038

1,1a-$B_{20}H_{14}Cl_2$

Total Energy = -1426.172561

B	0.84370	-1.29550	0.49441
B	2.52672	-1.12662	1.06323
B	2.21350	-1.68751	-0.58027
B	0.87450	-0.47932	-1.07107
B	-0.81762	0.00934	-1.30076
B	-0.45043	-1.64173	-0.80540
B	-0.79014	-1.76629	0.96676
B	-1.55723	-0.24789	1.54328
B	-1.87696	-0.81529	-0.10473
Cl	-3.52355	-1.33213	-0.60605
B	1.29527	0.27956	1.15402
B	0.34271	0.94299	-0.17376
B	-1.39989	0.91178	0.17045
B	-0.27691	0.99152	1.59697
B	0.08872	-0.65382	2.08430
B	1.87469	1.78156	0.19501
B	3.20570	1.07634	-0.76352
B	1.56269	1.22047	-1.44856
B	2.51278	-0.29528	-1.69201
B	3.57572	-0.57274	-0.27156
B	3.01418	0.60864	0.95941
H	-1.04876	-2.84842	1.37716
H	-0.26601	1.99668	2.21921
Cl	-2.48722	2.31454	-0.10618
H	0.42649	-1.07369	3.13770
H	4.68791	-0.97979	-0.34518
H	4.06834	1.78299	-1.16897
H	-0.44649	-2.63675	-1.44438
H	-1.13637	0.43678	-2.35539
H	-2.45504	-0.21086	2.31575
H	2.79509	-0.56633	-2.81225
H	1.79081	2.86892	0.65372
H	3.67724	1.02341	1.85196
H	1.21126	1.82523	-2.40274
H	2.82579	-1.73888	2.03083
H	2.24436	-2.78156	-1.03034

1,1b- $B_{20}H_{14}Cl_2$

Total Energy = -1426.175381

B	0.00028	-0.65686	1.19438
B	0.88221	-2.17048	1.55137
B	-0.88241	-2.17045	1.55147
B	-1.19243	-1.17324	0.00000
B	-1.55070	0.33267	-0.88288
B	-1.55070	0.33267	0.88288
B	-0.00005	1.08532	1.42853
B	0.89138	1.73951	0.00000
B	-0.89163	1.73916	0.00000
Cl	-1.80227	3.28755	0.00000
B	1.19287	-1.17313	0.00000
B	0.00028	-0.65686	-1.19438
B	-0.00005	1.08532	-1.42853
B	1.55085	0.33325	-0.88292
B	1.55085	0.33325	0.88292
B	0.88221	-2.17048	-1.55137
B	0.00002	-3.57061	-0.88069
B	-0.88241	-2.17045	-1.55147
B	-1.42291	-2.91823	0.00000
B	0.00002	-3.57061	0.88069
B	1.42299	-2.91834	0.00000
H	-0.00013	1.59643	2.49776
H	2.45919	0.32649	-1.64002
H	-0.00013	1.59643	-2.49776
H	2.45919	0.32649	1.64002
H	-0.00004	-4.59699	1.47616
H	-0.00004	-4.59699	-1.47616
H	-2.45895	0.32645	1.64009
H	-2.45895	0.32645	-1.64009
Cl	1.80208	3.28773	0.00000
H	-2.50365	-3.40829	0.00000
H	1.64130	-2.14367	-2.45870

H	2.50358	-3.40872	0.00000
H	-1.64136	-2.14358	-2.45889
H	1.64130	-2.14367	2.45870
H	-1.64136	-2.14358	2.45889

1,3a-$B_{20}H_{14}Cl_2$

Energy = -1426.173232

B	0.65004	-1.03109	-0.92312
B	2.40841	-1.36180	-0.93393
B	1.77034	-0.02305	-1.88699
B	0.57843	0.70661	-0.63814
B	-1.06250	0.93103	0.06967
B	-0.85539	-0.04521	-1.39131
B	-0.93601	-1.78677	-0.90237
B	-1.35799	-1.90833	0.84249
B	-2.01746	-0.58608	-0.11887
Cl	-3.78376	-0.46634	-0.43070
B	1.44793	-1.10826	0.65270
B	0.41768	0.27501	1.06524
B	-1.22440	-0.22857	1.46293
B	0.08572	-1.42841	1.76398
B	0.26506	-2.39237	0.30212
B	2.11060	0.32334	1.65038
B	3.15198	1.12615	0.44187
B	1.47522	1.66561	0.70065
B	2.11682	1.49834	-0.97870
B	3.32131	0.16860	-1.02485
B	3.14899	-0.66535	0.55600
H	-1.29557	-2.54557	-1.73966
H	0.35636	-1.69360	2.88486
H	-1.80656	0.19143	2.40631
H	0.69122	-3.48614	0.15518
H	4.33072	0.20861	-1.64750
H	4.04522	1.81553	0.80918
H	-1.10511	0.23316	-2.51286
Cl	-1.77037	2.56055	0.18461
H	-2.10801	-2.71298	1.28413
H	2.18404	2.49333	-1.62159
H	2.27189	0.23232	2.81910
H	3.99472	-1.31566	1.07612
H	1.08580	2.72578	1.04932
H	2.74138	-2.44377	-1.27847
H	1.56021	0.04883	-3.04921

1,3b- $B_{20}H_{14}Cl_2$

Energy = -1426.173775

B	0.32454	-0.82430	1.14611
B	1.99732	-0.51953	1.69540
B	1.61024	-2.04631	0.90231
B	0.55875	-1.41046	-0.50799
B	-0.99490	-1.01380	-1.28719
B	-0.97469	-1.83697	0.27737
B	-1.37393	-0.60882	1.54239
B	-1.83760	0.93391	0.75438
B	-2.21896	-0.58912	-0.04828
Cl	-3.92826	-1.10067	-0.29933
B	1.07559	0.66094	0.56822
B	0.30765	0.28275	-0.97269
B	-1.40043	0.71680	-0.97919
B	-0.34898	1.68851	0.13941
B	-0.31084	0.84757	1.68428
B	1.97495	0.90885	-1.05830
B	3.14998	-0.42822	-1.00795
B	1.58539	-0.61830	-1.84966
B	2.21122	-1.94271	-0.79558
B	3.16417	-1.23893	0.55398
B	2.83221	0.52370	0.48195
H	-1.85542	-1.01681	2.54626
Cl	-0.13723	3.43716	-0.14435
H	-1.90178	1.31563	-1.87069
H	-0.09014	1.27721	2.76404
H	4.17011	-1.71170	0.96959
H	4.14669	-0.34888	-1.64692
H	-1.15663	-2.97568	0.53876
H	-1.19503	-1.44996	-2.36797
H	-2.72225	1.62773	1.12790
H	2.45376	-2.97339	-1.33170
H	2.10451	1.99027	-1.51818
H	3.54838	1.36512	0.91438
H	1.38604	-0.85136	-2.99245
H	2.14387	-0.27923	2.84475
H	1.42275	-3.11693	1.36993

1,1′a- $B_{20}H_{14}Cl_2$

Energy = -1426.175025

B	0.43565	1.12683	-0.76898
B	-1.12271	2.00030	-0.74116
B	-0.84918	0.75478	-1.95553
B	-0.06920	-0.56366	-0.87949
B	1.31927	-1.44185	-0.18516
B	1.59332	-0.19191	-1.40542
B	2.17317	1.28813	-0.54417
B	2.44971	0.90483	1.19119
B	2.72908	-0.34478	-0.02670
Cl	4.38079	-1.00022	-0.32706
B	-0.43541	1.12618	0.76798
B	0.06907	-0.56396	0.88107
B	1.73372	-0.72743	1.42403
B	0.84949	0.75578	1.95523

B	1.12266	2.00084	0.74037
B	-1.59385	-0.19155	1.40550
B	-2.72926	-0.34480	0.02670
B	-1.31957	-1.44204	0.18618
B	-1.73341	-0.72824	-1.42326
B	-2.44971	0.90391	-1.19153
B	-2.17304	1.28803	0.54366
H	2.83024	2.04257	-1.18097
H	0.57030	0.85859	3.10038
H	2.05836	-1.49182	2.27050
H	1.07834	3.17923	0.83746
H	-3.37284	1.30907	-1.81550
Cl	-4.38083	-0.99973	0.32689
H	1.84118	-0.30168	-2.55652
H	1.33467	-2.61941	-0.29266
H	3.37304	1.31027	1.81460
H	-2.05729	-1.49337	-2.26938
H	-1.84158	-0.30000	2.55679
H	-2.82961	2.04296	1.18042
H	-1.33453	-2.61959	0.29405
H	-1.07876	3.17873	-0.83808
H	-0.56981	0.85650	-3.10074

1,1′b- $B_{20}H_{14}Cl_2$

Energy = -1426.173094

B	0.77643	-0.82234	0.00000
B	0.05766	-1.58617	1.55450
B	-1.53069	-0.83151	1.55012
B	-1.34015	-2.47446	0.88192
B	-1.34015	-2.47446	-0.88192
B	-2.34057	-1.27751	0.00000
B	-1.37950	0.20670	0.00000
B	-1.04690	1.71413	-0.88500
B	0.67893	1.72413	-1.42597
B	1.75638	1.92914	0.00000
B	0.67893	1.72413	1.42597
B	0.16399	2.69717	0.00000
Cl	-0.00232	4.49248	0.00000
B	1.75709	0.38148	0.88031
B	-0.07905	0.15207	1.19481
B	-1.04690	1.71413	0.88500
B	1.75709	0.38148	-0.88031
B	-0.07905	0.15207	-1.19481
B	0.05766	-1.58617	-1.55450
B	0.22770	-2.51392	0.00000
Cl	1.36081	-3.91357	0.00000
B	-1.53069	-0.83151	-1.55012
H	-2.20506	-0.48365	2.45803
H	-3.52701	-1.25412	0.00000
H	0.75649	-1.90416	2.45360
H	2.72225	2.61599	0.00000
H	0.75649	-1.90416	-2.45360
H	-1.77660	-3.40508	-1.47357
H	-2.20506	-0.48365	-2.45803
H	-1.77660	-3.40508	1.47357
H	0.89014	2.17985	-2.50014
H	-1.86933	2.09712	1.64350
H	0.89014	2.17985	2.50014
H	-1.86933	2.09712	-1.64350
H	2.56411	-0.03218	1.63992
H	2.56411	-0.03218	-1.63992

1,3′a-$B_{20}H_{14}Cl_2$

Energy = -1426.173948

B	-0.18496	-1.43498	-0.63927
B	1.31952	-2.37281	-0.47756
B	1.14415	-1.24727	-1.82351
B	0.41212	0.21311	-0.91266
B	-0.94507	1.21704	-0.35303
B	-1.25631	-0.14232	-1.44003
B	-1.93097	-1.48739	-0.43923
B	-2.21831	-0.90526	1.23905
B	-2.40835	0.21775	-0.11159
Cl	-4.01790	0.91834	-0.52045
B	0.65919	-1.30537	0.90872
B	0.24671	0.40515	0.83188
B	-1.42070	0.70588	1.31447
B	-0.62759	-0.75543	2.02044
B	-0.94012	-2.10585	0.93674
B	1.87966	0.00016	1.44265
B	3.04974	-0.06652	0.08085
B	1.73291	1.13953	0.10411
B	2.10171	0.22383	-1.41914
B	2.72247	-1.40756	-1.00469
B	2.38742	-1.59016	0.74914
H	-2.61472	-2.27313	-1.00642
H	-0.37508	-0.75304	3.17639
H	-1.72326	1.57121	2.06649
H	-0.95390	-3.26772	1.15983
H	3.61939	-1.93867	-1.57153
H	4.15955	0.31481	0.25018
H	-1.47700	-0.14369	-2.60178
H	-0.89263	2.37440	-0.58547
H	-3.17314	-1.19677	1.87841
H	2.47909	0.88430	-2.32914
H	2.09799	0.21479	2.58526
H	2.97609	-2.31468	1.48167

Cl	1.96914	2.90676	0.15964
H	1.20779	-3.55031	-0.44833
H	0.88267	-1.45585	-2.95845

1,3′b-$B_{20}H_{14}Cl_2$

Energy = -1426.173907

B	0.30812	1.26845	0.79916
B	-1.29916	1.72684	1.43321
B	-0.67483	2.50887	-0.01918
B	-0.02153	1.00729	-0.91892
B	1.27279	-0.11550	-1.40995
B	1.67489	1.32607	-0.46962
B	1.94578	0.80428	1.23900
B	1.90119	-0.99177	1.33048
B	2.52319	-0.21645	-0.12972
Cl	4.25243	-0.38499	-0.60881
B	-0.85245	-0.05021	1.04961
B	-0.24045	-0.68319	-0.47701
B	1.29422	-1.52483	-0.27808
B	0.20336	-1.48185	1.16030
B	0.60141	-0.04427	2.09503
B	-2.03198	-0.80063	-0.25035
B	-2.81657	0.68206	-0.85822
B	-1.37967	-0.01282	-1.68645
B	-1.51921	1.77300	-1.43595
B	-2.40894	2.10368	0.08839
B	-2.51825	0.51097	0.90551
H	2.65040	1.49647	1.89549
H	-0.31048	-2.49115	1.49939
H	1.51016	-2.58582	-0.76140
H	0.43612	0.18158	3.24464
H	-3.20514	2.97402	0.21662
H	-3.88264	0.58182	-1.36736
H	2.15335	2.34783	-0.82395
H	1.41055	-0.32414	-2.56573
H	2.64147	-1.63454	1.99701
H	-1.58406	2.43375	-2.41937
Cl	-2.80919	-2.40384	-0.15839
H	-3.34945	0.20995	1.69632
H	-1.30023	-0.42273	-2.79322
H	-1.33896	2.12068	2.54831
H	-0.17584	3.57224	-0.16058

2,2a- $B_{20}H_{14}Cl_2$

Energy = -1426.171791

B	-0.35867	1.19290	0.00000
B	0.64468	0.87577	1.55227
B	0.64624	-0.87590	1.55215
B	2.05259	0.00117	0.88362
B	2.05259	0.00117	-0.88362
B	1.41243	-1.42776	0.00000
Cl	2.18132	-3.05590	0.00000
B	-1.86444	1.55219	0.88209
B	-2.61049	-0.00058	1.42435
B	-3.26423	0.87921	0.00000
B	-2.61049	-0.00058	-1.42435
B	-1.86342	-1.55272	-0.88240
B	-3.26376	-0.88100	0.00000
B	-1.86342	-1.55272	0.88240
B	-0.35833	-1.19454	0.00000
B	-0.86360	-0.00011	1.19436
B	-1.86444	1.55219	-0.88209
B	-0.86360	-0.00011	-1.19436
B	0.64468	0.87577	-1.55227
B	1.40971	1.42901	0.00000
Cl	2.17959	3.05649	0.00000
B	0.64624	-0.87590	-1.55215
H	0.63362	-1.64091	2.45343
H	0.63300	1.64269	2.45200
H	-4.29221	1.47184	0.00000
H	-4.29120	-1.47453	0.00000
H	0.63300	1.64269	-2.45200
H	3.08094	0.00234	-1.47298
H	0.63362	-1.64091	-2.45343
H	3.08094	0.00234	1.47298
H	-3.10326	-0.00092	-2.50385
H	-1.83530	-2.45902	1.64259
H	-3.10326	-0.00091	2.50385
H	-1.83531	-2.45902	-1.64259
H	-1.83579	2.45843	1.64231
H	-1.83579	2.45843	-1.64230

2,3a- $B_{20}H_{14}Cl_2$

Energy = -1426.171172

B	-0.07951	0.08575	-0.75025
B	-0.40642	-1.73860	-1.04407
B	0.45923	-2.42124	0.32311
B	-1.30108	-2.17315	0.44235
B	-1.70741	-0.76359	1.41267
B	-0.25628	-1.72410	1.82638
B	1.09543	-0.84580	1.10911
B	2.34015	0.39772	1.40071
B	2.08113	1.77062	0.25654
B	2.52237	1.25330	-1.40704
B	2.73091	-0.52683	-1.29829
B	3.38559	0.57163	-0.03497
B	2.73972	-1.02395	0.43650
B	1.21148	-1.12035	-0.63547
B	1.21649	0.17659	-1.98139

B	0.81855	1.60066	-1.02212
B	0.66241	0.80810	0.67150
B	-1.13754	0.77017	0.68868
Cl	-2.05343	2.29549	0.67951
B	-1.67592	-0.62191	-0.38457
Cl	-3.13081	-0.35172	-1.40500
B	-0.24223	0.07024	2.03016
H	1.06030	-3.43646	0.41119
H	-0.13607	-2.36222	2.81963
H	-0.57104	-2.15984	-2.13635
H	3.09426	1.94226	-2.18565
H	4.54124	0.79795	0.11208
H	-2.70704	-0.74305	2.04913
H	-0.06160	0.51600	3.11081
H	-2.03394	-3.10543	0.42726
H	2.25208	2.86066	0.69294
H	3.33298	-2.00211	0.73952
H	3.39277	-1.18033	-2.03547
H	2.59202	0.64726	2.52982
H	0.91760	-0.09455	-3.09361
H	0.17306	2.54945	-1.30575

2,3b- $B_{20}H_{14}Cl_2$

Energy = -1426.171932

B	0.30140	-0.99744	-0.42888
B	1.03016	0.55989	-1.15726
B	0.27707	1.77568	-0.13376
Cl	-0.13964	3.45089	-0.58359
B	-0.89976	-1.20758	-1.73296
B	-2.27133	-0.06958	-1.44603
B	-2.43601	-1.81501	-1.05883
B	-2.22298	-1.91702	0.72183
B	-2.25692	-0.25676	1.43040
B	-3.22286	-0.62735	-0.02720
B	-2.29172	0.88521	0.08673
B	-0.76876	0.61542	0.96596
B	0.70780	1.37739	1.58147
B	1.93308	0.07015	1.60957
B	1.91876	1.20795	0.26870
B	1.98434	-0.55272	-0.07810
Cl	3.40105	-1.38511	-0.81315
B	-0.86836	-2.34847	-0.38884
B	-0.66829	-1.15513	1.04144
B	1.07192	-1.44533	1.21874
B	0.29646	-0.24755	2.24239
B	-0.70487	0.39953	-0.78126
H	0.67168	2.28837	2.34020
H	1.35146	0.61871	-2.29321
H	-3.08898	-2.57830	-1.69052
H	-4.40715	-0.58523	0.03471
H	1.41724	-2.55258	1.44681
H	2.86448	0.04073	2.34305
H	-0.04400	-0.32636	3.37282
H	2.83217	1.94300	0.09578
H	-2.64490	-2.79047	1.40573
H	-2.68203	2.00052	0.04483
H	-2.73292	0.45636	-2.40418
H	-2.62811	-0.12565	2.54643
H	-0.47948	-1.32233	-2.83286
H	-0.41904	-3.44165	-0.33563

2,2′a- $B_{20}H_{14}Cl_2$

Energy = -1426.171099

B	-0.58985	-0.37159	0.65349
B	-1.86653	0.95174	1.01544
B	-1.33628	2.19279	-0.11180
B	-2.66635	1.09739	-0.57783
B	-2.13343	-0.14911	-1.70435
B	-1.38198	1.47764	-1.76951
B	0.13321	1.31811	-0.87235
B	1.86654	0.95295	-1.01449
B	2.25404	-0.53895	-0.04872
Cl	3.44813	-1.68653	-0.75613
B	0.39817	-0.00272	2.09458
B	1.38174	1.47520	1.77110
B	2.13316	-0.15140	1.70415
B	2.66640	1.09669	0.57912
B	1.33601	2.19230	0.11436
B	-0.13330	1.31671	0.87369
B	0.92525	-1.24813	0.97046
B	0.58946	-0.37129	-0.65479
B	-0.92548	-1.24672	-0.97201
B	-2.25390	-0.53915	0.04836
Cl	-3.44771	-1.68782	0.75470
B	-0.39846	0.00003	-2.09508
H	-1.35939	3.37132	-0.00716
H	-1.49935	2.24166	-2.66994
H	-2.35865	1.04048	2.08693
H	2.88661	-0.57697	2.51508
H	3.77740	1.50784	0.63570
H	-0.87117	-2.42514	-1.04869
H	-2.88671	-0.57342	-2.51612
H	0.12850	-0.10750	-3.14884
H	-3.77727	1.50889	-0.63403
H	1.35992	3.37101	0.01172
H	1.49993	2.23799	2.67246
H	2.35880	1.04338	-2.08578
H	-0.12843	-0.11128	3.14841
H	0.87055	-2.42663	1.04552

2,3′a- $B_{20}H_{14}Cl_2$

Energy = -1426.171642

B	-0.26336	0.36569	-0.35996
B	-1.22931	-0.77506	-1.49869
B	-0.70932	-2.33056	-0.87036
B	-2.25874	-1.63989	-0.32148
B	-2.13790	-0.95336	1.29680
B	-1.15882	-2.39451	0.87648
B	0.44413	-1.75774	0.48955
B	2.04514	-1.34115	1.15489
B	2.33650	0.42582	0.95924
B	2.60884	0.80150	-0.77877
B	2.13722	-0.69188	-1.64775
B	3.11820	-0.75370	-0.14472
B	1.91889	-2.03582	-0.46150
B	0.49231	-1.02799	-1.12330
B	0.99997	0.71208	-1.57651
B	1.14519	1.43075	0.02800
Cl	0.87675	3.13529	0.47434
B	0.65328	-0.09464	1.06929
B	-1.01781	0.43342	1.35598
B	-2.01491	0.13250	-0.13391
Cl	-3.24296	1.37409	-0.57164
B	-0.49669	-1.12644	1.97616
H	-0.52063	-3.34920	-1.44208
H	-1.30405	-3.47560	1.34427
H	-1.50543	-0.44325	-2.59937
H	3.40880	1.58225	-1.17406
H	4.27267	-1.02622	-0.11475
H	-1.16752	1.46924	1.90417
H	-3.07904	-0.96881	2.01828
H	-0.18671	-1.43518	3.07551
H	-3.28060	-2.11914	-0.68600
H	2.88175	0.98181	1.85382
H	2.10968	-3.14190	-0.83590
H	2.53062	-0.99221	-2.72626
H	2.34639	-1.84997	2.18002
H	0.65552	1.21374	-2.59079

2,3′b- $B_{20}H_{14}Cl_2$

Energy = -1426.171892

B	0.88136	0.79337	-0.25748
B	1.70646	0.45705	1.39420
B	0.57629	-0.70951	2.06289
B	2.05427	-1.29102	1.25325
B	1.72425	-1.90051	-0.36740
B	0.49169	-2.10318	0.92008
B	-0.66313	-0.78706	0.65731
B	-2.21061	-0.31963	-0.14484
Cl	-3.40084	-1.57687	-0.57672
B	0.16438	2.33448	0.26462
B	-1.28626	2.00243	1.28775
B	-1.47261	2.52117	-0.42045
B	-1.83403	1.01277	-1.32049
B	-2.61076	1.37164	0.26078
B	-1.83576	0.28822	1.46716
B	-0.04435	0.75455	1.24577
B	-0.17846	1.72260	-1.35420
B	-0.49677	-0.07897	-0.94774
B	1.12480	-0.61708	-1.46031
B	2.33907	-0.22165	-0.16736
Cl	3.96301	0.33957	-0.70909
B	-0.00150	-1.78454	-0.78522
H	0.24269	-0.87768	3.18560
H	0.16026	-3.14491	1.38149
H	2.35672	1.28937	1.92561
H	-1.85026	3.59658	-0.75012
H	-3.75356	1.66020	0.38969
H	1.43997	-0.41123	-2.58109
H	2.37957	-2.78279	-0.81322
H	-0.68085	-2.58272	-1.33206
H	2.93384	-1.76131	1.89502
H	-2.41646	0.96013	-2.35234
H	-2.25899	-0.06024	2.51554
H	-1.44550	2.70316	2.23198
H	0.91471	3.17784	0.61823
H	0.27921	2.04215	-2.39729

3,3a- $B_{20}H_{14}Cl_2$

Energy = -1426.172334

B	0.45077	0.46745	1.19484
B	1.62304	1.06049	0.00000
B	2.18495	0.18233	-1.54892
B	3.10625	0.11543	0.00000
B	2.68949	-1.39419	0.87918
B	1.27469	-2.06927	0.00000
B	0.07689	-0.77033	0.00000
B	1.05697	-1.17094	-1.55045
B	2.68949	-1.39419	-0.87917
B	0.68921	2.29481	0.88155
B	0.68921	2.29481	-0.88155
B	0.45077	0.46745	-1.19484
B	-0.88209	1.59930	-1.41886
B	-1.95266	1.36622	0.00000
B	-1.34334	-0.07421	0.88438
B	-0.88209	1.59930	1.41886
B	-0.80844	2.69419	0.00000
B	1.05697	-1.17094	1.55045
B	2.18495	0.18233	1.54892
B	-1.34334	-0.07421	-0.88438

H	-1.27128	1.90627	2.49635
H	1.28956	2.97201	-1.64361
H	-1.27128	1.90627	-2.49635
H	1.28956	2.97201	1.64361
H	3.47712	-2.05273	1.47434
H	3.47712	-2.05274	-1.47434
Cl	-2.33093	-1.10510	1.94947
H	-3.12037	1.56748	0.00000
Cl	-2.33093	-1.10510	-1.94947
H	-1.20988	3.81065	0.00000
H	0.96386	-3.21412	0.00000
H	2.64660	0.78258	-2.45806
H	4.17610	0.62972	0.00000
H	0.54976	-1.73283	-2.45861
H	2.64660	0.78258	2.45806
H	0.54976	-1.73283	2.45861

3, 3a- $B_{20}H_{14}Cl_2$

Energy = -1426.172914

B	-0.20540	-0.74682	0.00000
B	0.66617	0.20879	1.20894
B	2.11481	1.35257	0.88124
B	2.32134	-0.35479	1.42599
B	2.64692	-1.39728	0.00000
B	2.32134	-0.35479	-1.42599
B	0.66617	0.20879	-1.20894
B	2.11481	1.35257	-0.88124
B	3.22116	0.26584	0.00000
B	-1.07878	-0.10780	1.57320
B	-0.46398	1.54413	1.55221
B	0.56413	1.49000	0.00000
B	-0.99538	2.30169	0.00000
B	-2.08863	1.18603	-0.87574
B	-1.07878	-0.10780	-1.57320
B	-1.93516	-0.37561	0.00000
B	-2.08863	1.18603	0.87574
B	1.10954	-1.57501	-0.88074
B	1.10954	-1.57501	0.88074
B	-0.46398	1.54413	-1.55221
H	-2.75924	-1.22781	0.00000
H	-0.19395	2.26029	2.45401
H	-1.09706	3.48380	0.00000
Cl	-1.51927	-1.08297	3.00041
H	3.42252	-2.29537	0.00000
H	4.38574	0.49373	0.00000
Cl	-1.51927	-1.08297	-3.00041
H	-3.05630	1.52323	-1.47214
H	-0.19395	2.26029	-2.45401
H	-3.05630	1.52323	1.47214
H	2.79185	-0.51538	-2.50361
H	2.38210	2.22667	1.63273
H	2.79185	-0.51538	2.50361
H	2.38210	2.22667	-1.63273
H	0.78488	-2.42572	1.63498
H	0.78488	-2.42572	-1.63498

3,3b- $B_{20}H_{14}Cl_2$

Energy = -1426.172308

B	-0.00036	1.19361	0.04318
B	1.19631	-0.00180	0.55577
B	0.87240	-1.55147	1.55844
B	1.42521	-0.00443	2.30331
B	0.00407	0.87996	2.95497
B	-1.42521	0.00443	2.30331
B	-1.19631	0.00180	0.55577
B	-0.88975	-1.54729	1.55515
B	-0.00407	-0.87996	2.95497
B	1.54771	0.89313	-0.95410
B	1.57395	-0.86925	-0.97840
B	0.00036	-1.19361	0.04318
B	0.00407	-1.42003	-1.70499
B	-0.87649	-0.00832	-2.36516
B	-1.57395	0.86925	-0.97840
B	-0.00407	1.42003	-1.70499
B	0.87649	0.00832	-2.36516
B	-0.87240	1.55147	1.55844
B	0.88975	1.54729	1.55515
B	-1.54771	-0.89313	-0.95410
H	-0.01779	2.49821	-2.19874
Cl	3.00701	-1.93014	-1.06736
H	0.01779	-2.49821	-2.19874
H	2.45407	1.65297	-0.93560
H	0.00355	1.47584	3.98113
H	-0.00355	-1.47584	3.98113
Cl	-3.00701	1.93014	-1.06736
H	-1.47419	-0.01001	-3.38898
H	-2.45407	-1.65297	-0.93560
H	1.47419	0.01001	-3.38898
H	-2.50489	0.00946	2.79564
H	1.62804	-2.45989	1.52330
H	2.50489	-0.00946	2.79564
H	-1.64839	-2.45487	1.52756
H	1.64839	2.45487	1.52756
H	-1.62804	2.45989	1.52330

3,3′a- $B_{20}H_{14}Cl_2$

Energy = -1426.170076

B	0.10495	-0.12377	0.86949
B	-1.59320	0.38390	0.80188
B	-2.46930	1.15614	-0.66395

B	-1.77824	2.12670	0.68996
B	-0.16417	2.73418	0.22235
B	0.25030	1.83834	-1.28412
B	0.10495	0.12377	-0.86949
B	-1.21258	0.98146	-1.88890
B	-1.38663	2.52670	-1.01612
B	-1.21260	-0.98143	1.88890
B	-2.46932	-1.15608	0.66396
B	-1.59321	-0.38387	-0.80188
B	-1.77829	-2.12665	-0.68995
B	-0.16423	-2.73418	-0.22235
B	0.97059	-1.36645	-0.31613
B	0.25026	-1.83834	1.28412
B	-1.38669	-2.52667	1.01612
B	0.97062	1.36643	0.31613
B	-0.30244	1.49978	1.52516
B	-0.30248	-1.49977	-1.52516
H	1.02095	-2.22762	2.09721
H	-3.64671	-1.10255	0.76731
H	-2.54722	-2.72284	-1.36956
H	-1.31631	-0.78285	3.05074
H	0.25156	3.81228	0.48779
H	-1.81000	3.47579	-1.58895
Cl	2.71482	-1.56886	-0.60524
H	0.25147	-3.81229	-0.48779
H	-0.20033	-1.66081	-2.69251
H	-1.81008	-3.47575	1.58895
H	1.02100	2.22759	-2.09721
H	-3.64668	1.10264	-0.76731
H	-2.54715	2.72290	1.36956
H	-1.31629	0.78289	-3.05074
H	-0.20028	1.66081	2.69251
Cl	2.71487	1.56879	0.60524

3,3′b- $B_{20}H_{14}Cl_2$

Energy = -1426.172680

B	-0.90049	0.81125	0.79226
B	0.36496	1.71323	-0.06634
B	2.02228	1.07491	-0.64507
B	1.80049	1.94892	0.92105
B	1.63571	0.76045	2.25551
B	1.43963	-0.82493	1.43747
B	0.05087	-0.61905	0.36303
B	1.83239	-0.64709	-0.32530
B	2.65737	0.37524	0.88154
B	-1.31944	2.25169	-0.33085
B	-0.29734	1.86226	-1.71236
B	0.48040	0.27784	-1.08888
B	-0.78962	0.23014	-2.30784
B	-2.25635	-0.30646	-1.42944
B	-1.74691	-0.78915	0.21296
B	-2.43630	0.86320	-0.07637
B	-2.02027	1.40560	-1.73564
B	0.01380	0.04139	2.11635
B	0.23175	1.76013	1.79276
B	-0.70659	-1.16306	-1.15950
H	-3.45956	1.09348	0.47772
H	0.28192	2.57690	-2.45628
H	-0.56361	-0.01288	-3.44689
H	-1.61711	3.30617	0.11605
H	2.12008	0.89485	3.33033
H	3.82836	0.24820	1.01787
Cl	-2.61884	-1.94830	1.25236
H	-3.15935	-0.88972	-1.92962
H	-0.36810	-2.21596	-1.57631
H	-2.77047	1.98523	-2.44926
H	1.71059	-1.87508	1.91713
H	2.62237	1.61043	-1.51239
H	2.33793	3.00319	1.01043
Cl	2.59502	-1.99656	-1.20985
H	-0.21418	2.70336	2.35040
H	-0.62566	-0.49822	2.95156

3,3b- $B_{20}H_{14}Cl_2$

Energy = -1426.172680

B	-0.05087	-0.61905	0.36303
B	0.90049	0.81125	0.79226
B	1.31944	2.25169	-0.33085
B	2.43630	0.86320	-0.07637
B	2.25635	-0.30646	-1.42944
B	0.78962	0.23014	-2.30784
B	-0.48040	0.27784	-1.08888
B	0.29734	1.86226	-1.71236
B	2.02027	1.40560	-1.73564
B	-0.01380	0.04139	2.11635
B	-0.23175	1.76013	1.79276
B	-0.36496	1.71323	-0.06634
B	-1.80049	1.94892	0.92105
B	-2.65737	0.37524	0.88154
B	-1.83239	-0.64709	-0.32530
B	-1.43963	-0.82493	1.43747
B	-1.63571	0.76045	2.25551
B	0.70659	-1.16306	-1.15950
B	1.74691	-0.78915	0.21296
B	-2.02228	1.07491	-0.64507
H	-1.71059	-1.87508	1.91713
H	0.21418	2.70336	2.35040
H	-2.33793	3.00319	1.01043
H	0.62566	-0.49822	2.95156
H	3.15935	-0.88972	-1.92962

H	2.77047	1.98523	-2.44926
Cl	-2.59502	-1.99656	-1.20985
H	-3.82836	0.24820	1.01787
H	-2.62237	1.61043	-1.51239
H	-2.12008	0.89485	3.33033
H	0.56361	-0.01288	-3.44689
H	1.61711	3.30617	0.11605
H	3.45956	1.09348	0.47772
H	-0.28192	2.57690	-2.45628
Cl	2.61884	-1.94830	1.25236
H	0.36810	-2.21596	-1.57631

3,3′d-$B_{20}H_{14}Cl_2$

Energy = -1426.172876

B	0.30678	-0.83612	1.02105
B	-0.30678	0.83612	1.02105
B	-0.01070	2.15443	-0.32880
B	1.00046	2.01209	1.17010
B	2.49541	1.09443	0.79618
B	2.20893	0.39235	-0.83198
B	0.70939	-0.51984	-0.66913
B	0.72327	1.12508	-1.55533
B	1.76688	2.08638	-0.45510
B	-1.28032	-0.38757	1.89489
B	-2.02957	0.61599	0.65442
B	-0.70939	0.51984	-0.66913
B	-2.20893	-0.39235	-0.83198
B	-1.76688	-2.08638	-0.45510
B	0.01070	-2.15443	-0.32880
B	-1.00046	-2.01209	1.17010
B	-2.49541	-1.09443	0.79618
B	2.02957	-0.61599	0.65442
B	1.28032	0.38757	1.89489
B	-0.72327	-1.12508	-1.55533
H	-0.93286	-2.92938	1.91916
H	-2.71118	1.57628	0.75808
H	-3.06134	-0.07679	-1.59448
H	-1.32486	-0.29266	3.07342
H	3.56873	1.37368	1.21805
H	2.33529	3.03747	-0.87737
Cl	1.00046	-3.61383	-0.60265
H	-2.33529	-3.03747	-0.87737
H	-0.64197	-1.19599	-2.73328
H	-3.56873	-1.37368	1.21805
H	3.06134	0.07679	-1.59448
Cl	-1.00046	3.61383	-0.60265
H	0.93286	2.92938	1.91916
H	0.64197	1.19599	-2.73328
H	1.32486	0.29266	3.07342
H	2.71118	-1.57628	0.75808

1,12- $B_{12}H_{10}Cl_2^{2-}$

Energy =-1225.004785

B	-0.004914	0.895916	-1.446405
B	-0.004914	-0.895916	-1.446405
B	1.422066	0.000000	-0.879085
Cl	3.033427	0.000000	-1.875235
B	0.891314	1.449270	0.002886
B	0.004914	0.895916	1.446405
B	-1.422066	0.000000	0.879085
Cl	-3.033427	0.000000	1.875235
B	-0.891314	1.449270	-0.002886
B	-1.444590	0.000000	-0.899048
B	-0.891314	-1.449270	-0.002886
B	0.004914	-0.895916	1.446405
B	1.444590	0.000000	0.899048
B	0.891314	-1.449270	0.002886
H	0.010334	1.523394	-2.470673
H	0.010334	-1.523394	-2.470673
H	-0.010334	1.523394	2.470673
H	-0.010334	-1.523394	2.470673
H	2.474638	0.000000	1.517261
H	-2.474638	0.000000	-1.517261
H	-1.534001	2.464096	0.006546
H	1.534001	2.464096	-0.006546
H	1.534001	-2.464096	-0.006546
H	-1.534001	-2.464096	0.006546

1,2-$B_{12}H_{10}Cl_2^{2-}$

Energy =-1225.002674

B	-0.943644	-1.446248	0.895875
B	-0.943651	-1.446261	-0.895854
B	-2.383337	-0.892314	0.000001
B	-1.832379	0.000013	1.444278
B	-0.943636	1.446259	0.895853
B	0.487431	0.891271	0.000000
B	0.487434	-0.891274	0.000000
B	-0.046466	-0.000014	-1.451665
B	-0.943644	1.446246	-0.895875
B	-2.383338	0.892313	0.000000
B	-1.832372	-0.000001	-1.444283
B	-0.046471	0.000001	1.451671
H	-0.924128	-2.469584	1.525088
H	0.606607	-0.000009	2.457362
H	-2.459169	0.000008	-2.472310
H	-0.924139	2.469583	-1.525088
H	-3.405279	1.528866	0.000009
H	0.606630	-0.000027	-2.457344
H	-2.459193	0.000027	2.472295
Cl	2.083313	-1.889564	-0.000001

H -3.405270 -1.528879 -0.000005
H -0.924158 -2.469614 -1.525041
Cl 2.083309 1.889567 0.000000
H -0.924108 2.469611 1.525041

1,2-$C_6H_4Cl_2$
Energy =-1151.435730
C 1.131613 -1.438586 0.000000
C -0.053361 -0.699149 0.000000
C 0.000000 0.701124 0.000000
C 1.237863 1.348264 0.000000
C 2.416946 0.605995 0.000000
C 2.363826 -0.788295 0.000000
Cl -1.578353 -1.554643 0.000000
Cl -1.455180 1.670324 0.000000
H 1.263142 2.432782 0.000000
H 3.373256 1.120386 0.000000
H 3.278168 -1.374047 0.000000
H 1.074184 -2.521807 0.000000

12- C10H6Cl2
Energy =-1305.078092
C 2.026139 -2.973120 0.000000
C 2.770028 -1.770246 0.000000
C 2.133946 -0.548807 0.000000
C 0.715439 -0.467654 0.000000
C -0.040059 -1.687614 0.000000
C 0.651305 -2.927855 0.000000
C -1.457740 -1.630220 0.000000
C -2.115811 -0.426575 0.000000
C -1.382382 0.784474 0.000000
C 0.000000 0.770672 0.000000
H -2.023186 -2.558149 0.000000
H -3.199087 -0.378186 0.000000
Cl -2.291565 2.277937 0.000000
Cl 0.893738 2.275901 0.000000
H 0.067650 -3.845101 0.000000
H 3.855736 -1.809634 0.000000
H 2.542598 -3.928776 0.000000
H 2.714148 0.366267 0.000000

13- $C_6H_4Cl_2$
Energy =-1151.439542
C 1.214262 -1.393191 0.000000
C 1.196103 0.001022 0.000000
C 0.000000 0.717758 0.000000
C -1.196104 0.001028 0.000000
C -1.214262 -1.393184 0.000000
C 0.000000 -2.080080 0.000000
Cl 2.714059 0.885179 0.000000
H 0.000002 1.800944 0.000000
Cl -2.714059 0.885193 0.000000
H -2.158776 -1.925553 0.000000
H -0.000002 -3.166274 0.000000
H 2.158776 -1.925563 0.000000

13-C10H6Cl2
Energy =-1305.082114
C -0.015262 2.401512 0.000000
C 0.000000 0.982172 0.000000
C -1.250006 0.275068 0.000000
C -2.458819 1.022502 0.000000
C -2.440056 2.397840 0.000000
C -1.206796 3.091514 0.000000
C -1.267653 -1.144368 0.000000
C -0.084130 -1.839769 0.000000
C 1.164886 -1.178546 0.000000
C 1.189822 0.196430 0.000000
Cl 2.762213 0.986687 0.000000
H -3.402232 0.482641 0.000000
H -3.372505 2.955283 0.000000
H -1.200677 4.177758 0.000000
H 0.926927 2.937714 0.000000
H -2.216756 -1.670213 0.000000
H 2.085009 -1.749880 0.000000
Cl -0.092312 -3.596065 0.000000

1,4- $C_6H_4Cl_2$
Energy =-1151.439679
C 0.000000 1.213776 0.697216
C 0.000000 0.000000 1.383710
C 0.000000 -1.213776 0.697216
C 0.000000 -1.213776 -0.697216
C 0.000000 0.000000 -1.383710
C 0.000000 1.213776 -0.697216
Cl 0.000000 0.000000 3.139496
H 0.000000 -2.150112 1.244490
H 0.000000 -2.150112 -1.244490
Cl 0.000000 0.000000 -3.139496
H 0.000000 2.150112 -1.244490
H 0.000000 2.150112 1.244490

14- C10H6Cl2
Energy =-1305.080966
C 0.726510 2.056434 0.000000
C 0.000000 0.836292 0.000000
C 0.732322 -0.403992 0.000000
C 2.151727 -0.356582 0.000000
C 2.820869 0.845494 0.000000
C 2.102293 2.062315 0.000000
C -0.007846 -1.622754 0.000000

C -1.382005 -1.635948 0.000000
C -2.099710 -0.420774 0.000000
C -1.424358 0.775826 0.000000
Cl -2.368791 2.262031 0.000000
H 2.704270 -1.289039 0.000000
H 3.907081 0.859058 0.000000
H 2.638539 3.007003 0.000000
H 0.175946 2.990031 0.000000
Cl 0.836859 -3.166241 0.000000
H -3.183899 -0.434688 0.000000
H -1.917913 -2.578676 0.000000

15- C10H6Cl2
Energy =-1305.081196
C 1.233106 1.422998 0.000000
C 0.000000 0.720426 0.000000
C 0.000123 -0.720467 0.000000
C 1.270170 -1.370465 0.000000
C 2.453263 -0.670286 0.000000
C 2.427441 0.741690 0.000000
C -1.232908 -1.423003 0.000000
C -2.427278 -0.741700 0.000000
C -2.453114 0.670248 0.000000
C -1.270094 1.370528 0.000000
Cl -1.349862 3.131109 0.000000
Cl 1.349584 -3.131058 0.000000
H 3.397254 -1.204276 0.000000
H 3.366230 1.287703 0.000000
H 1.221213 2.506258 0.000000
H -1.221046 -2.506291 0.000000
H -3.397294 1.203922 0.000000
H -3.365886 -1.288005 0.000000

16- C10H6Cl2
Energy =-1305.083038
C -1.383461 0.313676 0.000000
C 0.000000 0.633943 0.000000
C 0.954993 -0.438785 0.000000
C 0.487635 -1.780084 0.000000
C -0.861132 -2.039461 0.000000
C -1.812191 -0.993273 0.000000
C 2.344774 -0.146489 0.000000
C 2.785107 1.155905 0.000000
C 1.861496 2.226721 0.000000
C 0.511005 1.964054 0.000000
Cl -0.604285 3.328124 0.000000
H 1.205315 -2.594238 0.000000
Cl -1.434906 -3.700383 0.000000
H -2.870494 -1.230609 0.000000
H -2.111607 1.116757 0.000000
H 3.053454 -0.970177 0.000000
H 2.211610 3.253206 0.000000
H 3.848620 1.376208 0.000000

17- C10H6Cl2
Energy =-1225.004914
B -0.892427 0.585865 1.448880
B -1.443952 1.481383 -0.000002
B -0.000009 2.028717 0.893149
B 0.892434 0.585878 1.448876
B 1.424320 -0.296484 0.000001
B 0.000010 -0.865183 -0.898341
B -1.424321 -0.296485 0.000000
B -0.892434 0.585846 -1.448874
B 0.892427 0.585861 -1.448880
B 1.443953 1.481386 -0.000002
B -0.000001 2.028701 -0.893174
B 0.000001 -0.865168 0.898367
H -1.533014 0.572940 2.465061
H -0.000004 -1.890418 1.519856
H 0.000004 3.051182 -1.528813
H 1.533014 0.572955 -2.465061
H 2.474795 2.098215 0.000008
H -1.533037 0.572914 -2.465044
H 1.533039 0.572979 2.465046
Cl -3.033638 -1.294451 -0.000001
H -0.000028 3.051216 1.528759
H -2.474788 2.098224 0.000003
H 0.000028 -1.890450 -1.519802
Cl 3.033637 -1.294452 0.000000

17- C10H6Cl2
Energy =-1305.082842
C 0.590858 -0.869035 0.000000
C 0.000000 0.421729 0.000000
C -1.431476 0.536717 0.000000
C -2.208238 -0.652896 0.000000
C -1.620564 -1.895184 0.000000
C -0.209507 -1.986544 0.000000
C -2.037283 1.819840 0.000000
C -1.266385 2.958591 0.000000
C 0.144636 2.867082 0.000000
C 0.752724 1.632866 0.000000
Cl 2.512732 1.567882 0.000000
H -3.291812 -0.567128 0.000000
H -2.218251 -2.800052 0.000000
Cl 0.525780 -3.582869 0.000000
H 1.668975 -0.968607 0.000000
H -3.122009 1.886234 0.000000
H 0.752014 3.765753 0.000000
H -1.732213 3.939602 0.000000

18- C10H6Cl2
Energy =-1305.067567

C	-1.296005	-0.387901	0.000000
C	0.000000	0.231111	0.000000
C	0.001049	1.681581	0.000000
C	-1.217530	2.409426	0.000000
C	-2.426886	1.764286	0.000000
C	-2.458046	0.357017	0.000000
C	1.220647	2.407615	0.000000
C	2.429255	1.760935	0.000000
C	2.458416	0.353603	0.000000
C	1.295050	-0.388968	0.000000
Cl	1.552797	-2.131347	0.000000
H	-1.165967	3.494666	0.000000
H	-3.358911	2.321471	0.000000
H	-3.408716	-0.164403	0.000000
Cl	-1.555312	-2.128917	0.000000
H	1.170419	3.492928	0.000000
H	3.408251	-0.169308	0.000000
H	3.361987	2.316895	0.000000

1-$B_{12}H_{11}Cl^{2-}$
Energy =-765.348680

B	0.100799	0.689236	1.359471
B	0.100443	-1.079967	1.075031
B	-1.415408	-0.241324	1.500588
B	-1.415873	1.352426	0.693288
B	-1.415304	1.077060	-1.071933
B	0.100416	0.242309	-1.504793
B	1.016054	0.000191	0.000052
B	0.100933	-1.356271	-0.695435
B	-1.415702	-0.686964	-1.355609
B	-2.352915	-0.000250	-0.000035
B	-1.415501	-1.502687	0.234156
B	0.100528	1.506847	-0.234824
H	0.656202	1.170412	2.311834
H	0.655816	2.561179	-0.398826
H	-1.952753	-2.569100	0.400032
H	-1.953464	-1.173455	-2.318763
H	-3.558485	0.000295	-0.000424
H	0.656835	-2.305789	-1.181759
H	-1.954058	2.312727	1.185048
Cl	2.917774	-0.000245	0.000028
H	-1.952688	-0.412645	2.566235
H	0.654599	-1.836715	1.828271
H	0.655512	0.411810	-2.558462
H	-1.952021	1.842417	-1.833454

1- B20H15Cl
Energy =-966.541565

B	0.300105	0.156282	1.195635
B	1.081059	1.196512	0.000000
B	1.979226	0.657218	-1.550890
B	2.831932	1.007350	0.000000
B	3.132212	-0.528310	0.879361
B	2.164708	-1.757473	0.000000
B	0.521487	-1.125235	0.000000
B	1.564973	-1.056386	-1.552705
B	3.132212	-0.528310	-0.879361
B	-0.306131	1.897986	0.879794
B	-0.306131	1.897985	-0.879794
B	0.300105	0.156282	-1.195635
B	-1.395514	0.566587	-1.426633
B	-2.238823	-0.138921	0.000000
B	-1.025690	-1.118574	0.883601
B	-1.395514	0.566587	1.426633
B	-1.819434	1.576420	0.000000
B	1.564973	-1.056386	1.552705
B	1.979226	0.657218	1.550890
B	-1.025690	-1.118574	-0.883601
H	-1.886556	0.677202	2.500509
H	-0.073914	2.775162	-1.639377
H	-1.886556	0.677202	-2.500509
H	-0.073914	2.775162	1.639377
H	4.130637	-0.769551	1.473814
H	4.130637	-0.769551	-1.473814
H	-1.229903	-2.005626	1.638877
Cl	-3.960460	-0.677565	0.000000
H	-1.229903	-2.005626	-1.638877
H	-2.692793	2.378287	0.000000
H	2.391048	-2.922524	0.000000
H	2.132465	1.400398	-2.459159
H	3.562383	1.942899	0.000000
H	1.362634	-1.788265	-2.460333
H	2.132465	1.400398	2.459159
H	1.362634	-1.788265	2.460333

1-C_6H_5Cl
Energy =-691.844974

C	0.000000	1.216130	-0.178540
C	0.000000	0.000000	0.503640
C	0.000000	-1.216130	-0.178540
C	0.000000	-1.207470	-1.574390
C	0.000000	0.000000	-2.274940
C	0.000000	1.207470	-1.574390
Cl	0.000000	0.000000	2.264660
H	0.000000	-2.149370	0.374650
H	0.000000	-2.151590	-2.112240
H	0.000000	0.000000	-3.361080
H	0.000000	2.151590	-2.112240
H	0.000000	2.149370	0.374650

1- C10H7Cl
Energy =-845.487506
C -0.257957 -2.536896 0.000000
C 1.023952 -1.939490 0.000000
C 1.139503 -0.568714 0.000000
C 0.000000 0.288240 0.000000
C -1.292770 -0.339171 0.000000
C -1.389437 -1.755918 0.000000
C -2.451423 0.483677 0.000000
C -2.349059 1.855316 0.000000
C -1.074188 2.469668 0.000000
C 0.071877 1.706691 0.000000
H -3.426795 0.003154 0.000000
H -3.244776 2.470238 0.000000
H -0.999620 3.553607 0.000000
H 1.045442 2.183843 0.000000
H -2.375977 -2.212146 0.000000
H 1.916423 -2.555897 0.000000
H -0.335578 -3.620333 0.000000
Cl 2.758700 0.129242 0.000000

23- C10H6Cl2
Energy =-1305.079165
C -2.511025 -1.409647 0.000000
C -1.274426 -0.710222 0.000000
C -0.053913 -1.457391 0.000000
C -0.114194 -2.876828 0.000000
C -1.327991 -3.525767 0.000000
C -2.536692 -2.785811 0.000000
C 1.178379 -0.755998 0.000000
C 1.214300 0.619800 0.000000
C 0.000000 1.362652 0.000000
C -1.209500 0.706295 0.000000
Cl 0.019820 3.111596 0.000000
H 0.814575 -3.441753 0.000000
H -1.363776 -4.611551 0.000000
H -3.487356 -3.311589 0.000000
H -3.436631 -0.839529 0.000000
H 2.110338 -1.312383 0.000000
Cl 2.762626 1.431352 0.000000
H -2.128364 1.284188 0.000000

26- C10H6Cl2
Energy =-1305.084309
C -1.246135 -1.398943 0.000000
C -0.000059 -0.716211 0.000000
C 0.000000 0.715988 0.000000
C -1.237397 1.411788 0.000000
C -2.417369 0.706719 0.000000
C -2.435625 -0.708501 0.000000
C 1.246034 1.399028 0.000000
C 2.435514 0.708559 0.000000
C 2.417285 -0.706584 0.000000
C 1.237491 -1.411827 0.000000
Cl 3.951040 -1.566079 0.000000
H -1.244489 2.497082 0.000000
Cl -3.950913 1.566065 0.000000
H -3.385908 -1.231213 0.000000
H -1.251685 -2.485819 0.000000
H 1.251179 2.485871 0.000000
H 3.385777 1.231355 0.000000
H 1.244532 -2.497131 0.000000

27- C10H6Cl2
Energy =-1305.084314
C -1.239011 0.905054 0.000000
C 0.000000 0.210127 0.000000
C -0.000350 -1.222162 0.000000
C -1.244809 -1.905574 0.000000
C -2.436097 -1.217938 0.000000
C -2.417333 0.197288 0.000000
C 1.243605 -1.906512 0.000000
C 2.435285 -1.219531 0.000000
C 2.417379 0.195635 0.000000
C 1.239633 0.904224 0.000000
Cl 3.952085 1.053130 0.000000
H -1.248161 -2.992619 0.000000
H -3.386095 -1.740956 0.000000
Cl -3.951358 1.055522 0.000000
H -1.248333 1.990187 0.000000
H 1.245932 -2.993528 0.000000
H 3.384962 -1.743176 0.000000
H 1.249519 1.989357 0.000000

2-B20H15Cl
Energy =-966.539695
B 0.272491 -0.775885 0.000000
B -0.701158 0.080749 -1.194329
B -2.269216 1.048915 -0.882216
B -2.276282 -0.673703 -1.422822
B -2.487174 -1.748125 0.000000
B -2.276282 -0.673703 1.422822
B -0.701158 0.080749 1.194329
B -2.269216 1.048915 0.882216
B -3.243545 -0.160032 0.000000
B 1.036978 -0.059227 -1.554182
B 0.284616 1.529359 -1.549229
B -0.755228 1.380640 0.000000
B 0.730290 2.338963 0.000000
B 1.927528 1.337905 0.881269
B 1.036978 -0.059227 1.554182

B 1.965102 -0.229231 0.000000
B 1.927528 1.337905 -0.881269
B -0.933281 -1.752907 0.881679
B -0.933281 -1.752907 -0.881679
B 0.284616 1.529359 1.549229
Cl 3.365793 -1.363100 0.000000
H -0.060443 2.204270 -2.458067
H 0.709469 3.525697 0.000000
H 1.355378 -0.758664 -2.452879
H -3.159124 -2.726247 0.000000
H -4.426709 -0.066683 0.000000
H 1.355378 -0.758664 2.452879
H 2.859354 1.772057 1.473043
H -0.060443 2.204270 2.458067
H 2.859354 1.772057 -1.473043
H -2.721673 -0.886206 2.502273
H -2.637501 1.877222 -1.643143
H -2.721673 -0.886206 -2.502273
H -2.637501 1.877222 1.643142
H -0.516938 -2.559998 -1.640195
H -0.516938 -2.559998 1.640195

2-C10H7Cl
Energy =-845.488839
C -0.085654 -1.958034 0.000000
C 1.147535 -1.263539 0.000000
C 1.202769 0.109533 0.000000
C 0.000000 0.865482 0.000000
C -1.258077 0.179248 0.000000
C -1.259714 -1.241391 0.000000
C -2.456580 0.941056 0.000000
C -2.416859 2.317191 0.000000
C -1.173064 2.995366 0.000000
C 0.007038 2.286636 0.000000
H -3.409397 0.417021 0.000000
H -3.340554 2.889202 0.000000
H -1.154178 4.081771 0.000000
H 0.962250 2.805974 0.000000
H -2.211896 -1.766306 0.000000
Cl 2.637594 -2.199755 0.000000
H -0.089614 -3.042602 0.000000
H 2.159928 0.621491 0.000000

3-B20H15Cl
Energy =-966.540571
B -0.507186 0.951789 1.002207
B -0.043591 -0.707628 0.638659
B -0.585632 -1.729874 -0.836499
B -1.407431 -1.819035 0.767869
B -2.863868 -0.769919 0.747131
B -2.717735 0.195062 -0.761378
B -1.147458 0.982686 -0.648055
B -1.390493 -0.478977 -1.781359
B -2.354290 -1.562183 -0.737694
B 1.123552 0.264410 1.583596
B 1.676435 -0.535223 0.111803
B 0.186803 -0.132210 -1.008933
B 1.718732 0.723221 -1.195144
B 1.442282 2.343622 -0.479160
B -0.298312 2.446370 -0.099057
B 0.883875 2.012975 1.194226
B 2.254740 1.114159 0.474573
B -2.288216 0.917143 0.835518
B -1.479887 -0.328734 1.782788
B 0.223229 1.648713 -1.581989
H 0.981170 2.768684 2.104107
Cl 2.718279 -1.979885 -0.007386
H 2.456802 0.496676 -2.095826
H 1.302986 -0.043542 2.711726
H -3.899353 -1.058926 1.249955
H -3.043552 -2.389306 -1.237003
H -0.957793 3.416874 0.053580
H 2.030192 3.321977 -0.803693
H 0.012051 1.933423 -2.711031
H 3.388204 1.250793 0.795203
H -3.628247 0.691691 -1.338713
H 0.050228 -2.660746 -1.193390
H -1.327605 -2.851181 1.347969
H -1.453492 -0.340967 -2.955014
H -1.375066 -0.438974 2.956337
H -2.875030 1.879722 1.195840

$B_{12}H_{12}^{2-}$
Energy =-305.690537
B 0.000000 0.893587 -1.445401
B 0.000000 -0.893587 -1.445401
B 0.000000 0.893587 1.445401
B 0.000000 -0.893587 1.445401
B -1.445401 0.000000 0.893587
B 1.445401 0.000000 0.893587
B -1.445401 0.000000 -0.893587
B 1.445401 0.000000 -0.893587
B -0.893587 1.445401 0.000000
B 0.893587 1.445401 0.000000
B 0.893587 -1.445401 0.000000
B -0.893587 -1.445401 0.000000
H 0.000000 1.528636 -2.472515
H 0.000000 -1.528636 -2.472515
H 0.000000 1.528636 2.472515
H 0.000000 -1.528636 2.472515

H -2.472515 0.000000 1.528636
H 2.472515 0.000000 1.528636
H -2.472515 0.000000 -1.528636
H 2.472515 0.000000 -1.528636
H -1.528636 2.472515 0.000000
H 1.528636 2.472515 0.000000
H 1.528636 -2.472515 0.000000
H -1.528636 -2.472515 0.000000

B20H16
Energy =-506.908509
H 0.000000 2.503671 2.495619
H -2.458630 -1.639507 1.230503
B -0.880343 0.000000 2.656663
B -1.550149 0.881155 1.255379
H 0.000000 -2.503671 2.495619
H -2.458630 1.639507 1.230503
B 1.550149 -0.881155 1.255379
B 0.000000 1.193782 0.257358
B 0.000000 1.423440 2.003546
B 0.000000 -1.423440 2.003546
H 0.000000 1.475501 -3.683578
H 0.000000 -1.475501 -3.683578
B -1.550149 -0.881155 1.255379
H 2.458630 1.639507 1.230503
B 0.881155 1.550149 -1.255379
B 0.000000 -1.193782 0.257358
B 1.550149 0.881155 1.255379
H 1.475501 0.000000 3.683578
H 2.458630 -1.639507 1.230503
H -1.475501 0.000000 3.683578
B 0.880343 0.000000 2.656663
H 2.503671 0.000000 -2.495619
H -1.639507 -2.458630 -1.230503
B 0.000000 -0.880343 -2.656663
B 0.881155 -1.550149 -1.255379
H -2.503671 0.000000 -2.495619
H 1.639507 -2.458630 -1.230503
B -0.881155 1.550149 -1.255379
B 1.193782 0.000000 -0.257358
B 1.423440 0.000000 -2.003546
B -1.423440 0.000000 -2.003546
H -1.639507 2.458630 -1.230503
B 0.000000 0.880343 -2.656663
B -0.881155 -1.550149 -1.255379
H 1.639507 2.458630 -1.230503
B -1.193782 0.000000 -0.257358

C6H6
Energy =-232.248661
C 0.000000 1.396616 0.000000
C 1.209505 0.698308 0.000000
C 1.209505 -0.698308 0.000000
C 0.000000 -1.396616 0.000000
C -1.209505 -0.698308 0.000000
C -1.209505 0.698308 0.000000
H 0.000000 2.483600 0.000000
H 2.150860 1.241800 0.000000
H 2.150860 -1.241800 0.000000
H 0.000000 -2.483600 0.000000
H -2.150860 -1.241800 0.000000
H -2.150860 1.241800 0.000000

C10H8
Energy =-385.892728
C 0.000000 1.245025 1.402523
C 0.000000 2.434289 0.708223
C 0.000000 2.434289 -0.708223
C 0.000000 1.245025 -1.402523
C 0.000000 0.000000 -0.717303
C 0.000000 0.000000 0.717303
C 0.000000 -1.245025 -1.402523
C 0.000000 -2.434289 -0.708223
C 0.000000 -1.245025 1.402523
C 0.000000 -2.434289 0.708223
H 0.000000 1.243057 2.490098
H 0.000000 3.378795 1.245647
H 0.000000 3.378795 -1.245647
H 0.000000 1.243057 -2.490098
H 0.000000 -1.243057 2.490098
H 0.000000 -3.378795 -1.245647
H 0.000000 -3.378795 1.245647
H 0.000000 -1.243057 -2.490098