Supporting Material for

"Molecular electrostatic potentials of divalent carbon(0) compounds"

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Table S1 Geometries and SCF energies of investigated molecules

1

9			
E(SCF) =	-226.030912		
C	-0.000008	-1.286975	0.000059
N	-1.053597	-0.404208	0.000332
H	-2.020495	-0.728898	0.000923
N	1.053592	-0.404226	-0.000409
H	2.020505	-0.728881	-0.000483
C	-0.685606	0.941510	-0.000933
H	-1.400799	1.770304	-0.000040
C	0.685617	0.941500	0.000727
H	1.400805	1.770302	0.001016

2

9			
E(SCF) =	-724.115527		
C	0.000000	0.000000	0.713832
P	0.000000	1.466791	-0.073006
P	0.000000	-1.466791	-0.073006
H	0.000000	2.574721	0.834194
H	-1.088629	1.904551	-0.940296
H	1.088629	1.904551	-0.940296
H	0.000000	-2.574721	0.834194
H	-1.088629	-1.904551	-0.940296
H	1.088629	-1.904551	-0.940296

3

19			
E(SCF) =	-490.164355		
C	1.075562	2.471345	1.767275
C	0.755340	1.255548	2.308906
C	1.364631	2.728318	0.454093
N	0.928477	0.865988	3.647620
N	0.085791	0.130598	1.765074
N	1.971419	1.931142	-0.548710
N	1.219405	3.959143	-0.207680
C	0.336580	-0.364048	3.918150
C	-0.204363	-0.819647	2.747127
C	2.255198	2.675710	-1.696148
C	1.770680	3.937564	-1.485247
H	1.349468	1.503772	4.319837
H	0.359965	-0.825059	4.909639
H	-0.747974	-1.745074	2.534196
H	-0.333476	0.163528	0.838304
H	2.360393	1.016085	-0.331657
H	2.754665	2.248915	-2.571155
H	1.761155	4.808217	-2.147081
H	0.846512	4.768266	0.284407

4

5			
E(SCF) =	-264.559533		
C	-0.005334	0.000000	0.159729
C	0.006353	0.000000	1.449935
C	0.017187	0.000000	2.740152
O	0.027082	0.000000	3.916645
O	-0.015968	0.000000	-1.016716

5

39			
E(SCF) =	-652.084895		
C	-0.227019	0.045700	0.055863
C	-0.577232	0.089412	-1.237230
C	0.123738	0.005606	1.348915
N	0.225494	-0.421267	-2.300490
N	-1.798017	0.652423	-1.715725
N	1.040579	0.914652	1.956641
N	-0.375489	-0.950110	2.283228

C	-0.419342	-1.412218	-3.161172
H	0.100625	-1.465302	-4.140646
H	-1.472986	-1.125968	-3.329001
H	-0.406720	-2.436658	-2.708559
C	1.594718	-0.767889	-1.974068
H	2.147106	-0.989840	-2.910088
H	1.676095	-1.659911	-1.302130
H	2.092326	0.080060	-1.467817
C	-2.810511	0.951268	-0.722298
H	-2.999261	0.062989	-0.091160
H	-3.755477	1.222877	-1.235940
H	-2.527926	1.796281	-0.044104
C	0.529818	1.647965	3.114338
H	1.372252	2.019979	3.734416
H	-0.099203	0.978353	3.727756
H	-0.092803	2.529454	2.814681
C	1.818662	1.749656	1.062803
H	1.202923	2.515343	0.525810
H	2.320362	1.126685	0.299144
H	2.597186	2.281495	1.647234
C	0.636807	-1.735960	2.987711
H	1.497938	-1.090577	3.237040
H	1.012723	-2.591236	2.369995
H	0.214056	-2.152249	3.926069
C	-1.507988	-1.747909	1.856107
H	-1.895773	-2.322536	2.722108
H	-1.254599	-2.473921	1.042094
H	-2.316339	-1.092723	1.481620
C	-1.657343	1.709867	-2.716071
H	-0.837209	1.454762	-3.410877
H	-1.421669	2.701571	-2.251906
H	-2.599100	1.818401	-3.293852

(H+)-1

10

E(SCF) = -226.449739

C	0.069789	-1.203752	0.000217
N	-1.031637	-0.432938	0.000538
H	-1.992320	-0.794635	0.000468
N	1.127712	-0.373739	0.000158
H	2.106338	-0.683581	-0.000274
C	-0.676422	0.905813	0.000383
H	-1.416436	1.712344	0.000339
C	0.700083	0.943239	0.000096
H	1.394205	1.789640	-0.000216
H	0.099828	-2.299065	-0.000480

(H+)-2

10

E(SCF) = -724.536965

C	-0.000030	0.035627	1.195657
P	-1.535122	-0.010082	1.969227
P	1.535225	-0.010317	1.968895
H	-0.000234	-0.101785	0.101760
H	-2.514362	0.696544	1.216438
H	-1.503577	0.604179	3.253053
H	-2.195172	-1.256909	2.242243
H	1.502877	0.601096	3.254030
H	2.196248	-1.257211	2.239085
H	2.514136	0.698857	1.217993

(H+)-3

20

-490.644721

C	1.017311	2.552947	1.806545
C	0.700363	1.295610	2.356555
C	1.344224	2.798719	0.458731
N	0.637227	0.985155	3.691867
N	0.368291	0.123598	1.709037
N	1.693906	1.900085	-0.527754
N	1.401018	4.026022	-0.152817
C	0.249507	-0.340907	3.877731

C	0.071592	-0.881912	2.636992
C	1.994823	2.571993	-1.718604
C	1.801950	3.902686	-1.482205
H	0.884221	1.638243	4.436620
H	0.145440	-0.784648	4.871666
H	-0.228688	-1.887868	2.331488
H	0.091657	0.091409	0.726288
H	1.976892	0.939030	-0.328665
H	2.308220	2.044208	-2.623396
H	1.903819	4.767372	-2.143709
H	1.142232	4.899739	0.307436
H	1.009170	3.414637	2.486098

(H+)-4

6

E(SCF) = -264.846645

H	-1.695664	0.103693	1.348650
C	0.102691	0.039195	0.193924
C	-0.584189	0.068327	1.379336
C	0.036769	0.055822	2.600855
O	0.512053	0.046889	3.641205
O	0.634200	0.016074	-0.818629

(H+)-5

40

E(SCF) = -652.555884

C	0.068097	0.027856	-0.019596
C	-0.418217	0.054987	-1.355760
C	0.180363	1.093497	0.915537
N	0.028625	-0.883992	-2.252287
N	-1.354729	0.954784	-1.805874
N	0.358046	2.407490	0.553421
N	0.152302	0.813431	2.259345
C	-0.856572	-1.508463	-3.239636
H	-0.560428	-1.269325	-4.282494
H	-1.900035	-1.188483	-3.077576
H	-0.815235	-2.611174	-3.117240
C	1.318692	-1.548560	-2.079596
H	1.759766	-1.749863	-3.076876
H	1.220764	-2.521613	-1.548907
H	2.011103	-0.901443	-1.512302
C	-2.355414	1.546780	-0.924679
H	-2.416800	0.975180	0.017967
H	-3.347746	1.514397	-1.420929
H	-2.129358	2.609178	-0.688938
C	-0.152630	3.521403	1.355408
H	0.657227	4.085330	1.865490
H	-0.863474	3.150396	2.114171
H	-0.688635	4.233202	0.693485
C	1.023220	2.792810	-0.686484
H	0.304931	3.166001	-1.448103
H	1.574775	1.932555	-1.104731
H	1.747910	3.607174	-0.477337
C	1.016084	1.503268	3.221883
H	1.720897	2.170583	2.697030
H	1.610998	0.749915	3.779736
H	0.436014	2.095229	3.960493
C	-0.497300	-0.390732	2.773022
H	-0.944879	-0.167734	3.762755
H	0.221326	-1.229661	2.906457
H	-1.300822	-0.715413	2.088213
C	-1.387967	1.430637	-3.190594
H	-0.454497	1.154318	-3.711160
H	-1.475867	2.537142	-3.195036
H	-2.251624	1.025259	-3.759658
H	0.404768	-0.953986	0.340658

(H+)2-1

11

E(SCF) = -226.537096

C	-0.000456	-1.181503	-0.000002

N	-1.120188	-0.259988	-0.000114
H	-2.113827	-0.579534	-0.000169
N	1.120035	-0.260798	0.000009
H	2.113409	-0.581088	0.000093
C	-0.737258	0.990296	0.000022
H	-1.424112	1.858701	0.000058
C	0.738004	0.989737	-0.000026
H	1.425436	1.857688	0.000054
H	-0.001507	-1.850210	0.903309
H	-0.000071	-1.851239	-0.902571

(H+)2-2

11

E(SCF) = -724.733361

C	-0.132712	0.000030	1.100518
P	-0.867661	-1.624784	1.610958
P	-0.867795	1.624760	1.610960
H	-0.093268	0.000046	-0.014495
H	0.925984	0.000046	1.452658
H	-0.048156	-2.641321	1.042669
H	-2.196165	-1.773144	1.122329
H	-0.875057	-1.772578	3.026475
H	-0.048136	2.641353	1.042995
H	-0.875547	1.772461	3.026487
H	-2.196168	1.773131	1.121987

(H+)2-3

21

E(SCF) = -490.893399

C	0.843258	2.662179	1.879247
C	0.540162	1.262103	2.352212
C	1.325574	2.820654	0.458769
N	0.999991	0.693411	3.491479
N	-0.312195	0.360412	1.808266
N	2.396046	2.237182	-0.132158
N	0.819565	3.677158	-0.459483
C	0.442793	-0.559685	3.673249
C	-0.391769	-0.773793	2.598576
C	2.567135	2.721128	-1.418154
C	1.563452	3.641454	-1.625298
H	1.648523	1.140818	4.151900
H	0.677892	-1.191920	4.537277
H	-1.025011	-1.630612	2.341000
H	-0.850637	0.500449	0.945258
H	3.017328	1.551415	0.312950
H	3.375592	2.380546	-2.075333
H	1.326768	4.262086	-2.497281
H	0.013543	4.296327	-0.304892
H	1.596471	3.102013	2.568610
H	-0.064411	3.291523	2.005789

(H+)2-4

7

E(SCF) = -264.882049

C	0.148378	0.037282	0.147582
C	-0.668015	0.070851	1.377038
C	0.079993	0.054697	2.649587
O	0.576804	0.045000	3.657090
O	0.699795	0.014153	-0.830879
H	-1.316922	1.002927	1.352721
H	-1.375534	-0.817770	1.363891

(H+)2-5

41

E(SCF) = -652.807050

C	0.153519	-0.098415	0.023426
C	-0.419297	0.021003	-1.386961
C	0.239748	1.112443	0.949493
N	0.142099	-0.724325	-2.359935
N	-1.510161	0.778586	-1.619912
N	0.614005	2.315446	0.469016
N	0.022564	0.915741	2.265344

C	-0.631514	-1.270107	-3.497009
H	-0.400604	-0.751632	-4.448173
H	-1.713015	-1.224416	-3.290758
H	-0.347813	-2.335167	-3.607426
C	1.531175	-1.225044	-2.319539
H	1.923770	-1.235508	-3.354212
H	1.572558	-2.260864	-1.924101
H	2.193612	-0.570446	-1.726426
C	-2.472509	1.145415	-0.570273
H	-2.286553	0.594001	0.365331
H	-3.492990	0.879392	-0.913106
H	-2.450859	2.236681	-0.376565
C	0.268345	3.594647	1.120239
H	1.135203	4.052055	1.636550
H	-0.561883	3.457021	1.832449
H	-0.061258	4.294691	0.327266
C	1.382336	2.480501	-0.773939
H	0.776151	2.989742	-1.549912
H	1.750520	1.515598	-1.157969
H	2.269024	3.112433	-0.563946
C	0.708942	1.699871	3.315727
H	1.579462	2.231881	2.899222
H	1.076295	0.982229	4.075345
H	0.027638	2.414383	3.817915
C	-0.776136	-0.199419	2.813193
H	-1.297408	0.162852	3.719787
H	-0.127972	-1.051322	3.105082
H	-1.552000	-0.543394	2.106893
C	-1.839622	1.345058	-2.942931
H	-0.955830	1.334754	-3.601890
H	-2.149886	2.397278	-2.787754
H	-2.679542	0.812967	-3.431452
H	-0.415544	-0.898462	0.538650
H	1.172862	-0.529527	-0.043682

BH3-1

13

E(SCF) =	-252.704911		
C	1.162688	0.811839	5.326949
N	1.306774	0.006638	4.235704
N	0.948399	-0.072785	6.342561
B	1.274493	2.393071	5.405575
H	0.931213	2.871330	4.317872
H	2.473210	2.646226	5.615917
H	0.589948	2.794280	6.354241
C	0.969900	-1.392467	5.907560
C	1.199850	-1.341495	4.555594
H	1.473841	0.398923	3.307730
H	1.285487	-2.140198	3.813825
H	0.815790	-2.244319	6.575454
H	0.794828	0.248432	7.299728

BH3-2

13

E(SCF) =	-750.760546		
C	0.099857	-0.449569	-0.057058
P	1.410142	-0.032175	0.928679
P	-0.099607	0.057016	-1.659020
B	-1.330599	-0.166840	0.787808
H	-1.056393	0.477215	1.822703
H	-1.867168	-1.247394	1.057017
H	-2.072469	0.547582	0.080520
H	2.735772	-0.206582	0.399864
H	1.441004	-0.837817	2.104575
H	1.525635	1.278667	1.532094
H	1.007044	-0.106300	-2.562293
H	-0.526924	1.400443	-1.988168
H	-1.132944	-0.684699	-2.303201

BH3-3

23

E(SCF)	-516.8480481		

C	1.05301711	2.53311605	1.77335458
C	0.76469029	1.26214072	2.27929843
C	1.3211941	2.72513683	0.41596943
N	0.67414197	0.99422248	3.62606471
N	0.48989751	0.03974708	1.65556709
N	1.49814201	1.82645908	-0.64281226
N	1.51281379	3.9682553	-0.14624145
C	0.32863344	-0.328151	3.85071698
C	0.18392709	-0.92720312	2.62836741
C	1.88592631	2.52909193	-1.79628904
C	1.877585	3.86037272	-1.47938685
H	0.89065449	1.76637871	4.27491017
H	0.22448971	-0.74524534	4.85625541
H	-0.08100833	-1.95524762	2.36677211
H	0.12215582	0.0071494	0.70318964
H	1.76675804	0.85631503	-0.46634014
H	2.0883448	2.02520568	-2.74549378
H	2.0702745	4.73502762	-2.10705576
H	1.54267453	4.77275466	0.49896243
B	1.05542972	3.80972219	2.80228994
H	1.76386039	4.73742166	2.34625024
H	-0.09954472	4.22764283	2.98755148
H	1.5498173	3.46926865	3.90571565

BH3-4

9

E(SCF) =	-291.149278		
C	0.287417	-0.000037	0.258991
C	-0.220312	0.000005	1.490460
C	0.383005	0.000050	2.677207
O	0.792863	0.000101	3.765721
O	0.643565	-0.000072	-0.848872
B	-2.031839	-0.000006	1.455617
H	-2.260424	0.000098	0.246705
H	-2.313349	-1.051029	2.015697
H	-2.313372	1.050890	2.015919

BH3-5

43

E(SCF) =	-678.724100		
C	0.093867	-0.332439	0.014769
C	-0.341552	0.026557	-1.294335
C	0.196234	0.696489	0.984230
N	0.182844	-0.539194	-2.438301
N	-1.395919	0.905520	-1.520328
N	0.556393	2.014867	0.667434
N	0.054162	0.471497	2.339590
C	-0.661718	-1.016175	-3.527141
H	-0.425056	-0.524325	-4.497362
H	-1.725595	-0.843023	-3.288956
H	-0.515168	-2.111465	-3.654229
C	1.563258	-0.993966	-2.503964
H	2.030992	-0.618164	-3.442115
H	1.629617	-2.101369	-2.477147
H	2.122294	-0.615723	-1.630749
C	-2.468308	1.088398	-0.555722
H	-2.429207	0.281834	0.197006
H	-3.452313	1.050474	-1.075290
H	-2.404889	2.068400	-0.031460
C	-0.016194	3.159878	1.357589
H	0.742116	3.738756	1.935122
H	-0.803846	2.825690	2.056332
H	-0.477375	3.863014	0.626425
C	1.441562	2.349260	-0.431337
H	0.904859	2.780913	-1.307829
H	1.979434	1.444897	-0.765212
H	2.189378	3.105445	-0.098645
C	0.920682	1.097728	3.327480
H	1.729303	1.657520	2.824944
H	1.384887	0.310742	3.961278
H	0.373783	1.794445	4.003930
C	-0.881903	-0.513111	2.863530

H	-1.721800	-0.008919	3.396758
H	-0.370326	-1.189438	3.578721
H	-1.261799	-1.147019	2.040706
C	-1.477698	1.759434	-2.697139
H	-0.533756	1.704259	-3.268344
H	-1.640298	2.816422	-2.388874
H	-2.317069	1.480512	-3.374823
B	0.313255	-1.929932	0.383978
H	1.045913	-2.043961	1.380475
H	-0.806690	-2.440065	0.625293
H	0.787286	-2.559975	-0.571898

(BH3)2-2

17

E(SCF) =	-777.399488		
C	-0.091552	0.000474	0.982621
P	-0.770183	-1.525635	1.516479
P	-0.778439	1.512337	1.545591
B	-0.431418	0.041754	-0.680661
H	-0.426411	1.239640	-1.020496
H	-1.575129	-0.418962	-0.869298
H	0.440447	-0.599860	-1.263643
B	1.458674	-0.027896	1.675449
H	1.805333	-1.222254	1.736383
H	1.388993	0.424093	2.836045
H	2.209800	0.627531	0.955838
H	-0.153156	-2.541177	0.747227
H	-2.170868	-1.754951	1.319615
H	-0.555775	-1.914703	2.875456
H	0.094286	2.543182	1.121768
H	-0.894016	1.724990	2.957867
H	-2.062716	1.891337	1.044431

(BH3)2-3

27

E(SCF)	-543.4643208		
C	1.26424202	2.48521783	1.90253124
C	0.61249058	1.22633429	2.28240977
C	1.52830816	2.61212078	0.45768538
N	1.00599885	0.46178911	3.32588592
N	-0.53312201	0.64636515	1.8189207
N	2.66661633	2.25581051	-0.18678372
N	0.76322736	3.24197785	-0.46519136
C	0.10641509	-0.56550658	3.55956286
C	-0.87333373	-0.45123466	2.60302424
C	2.6282445	2.66705082	-1.50727798
C	1.41395964	3.29446053	-1.68654228
H	1.84797088	0.79586552	3.83917201
H	0.2338892	-1.29194684	4.36636478
H	-1.76584761	-1.05454402	2.41633246
H	-1.1365949	1.12828418	1.14907222
H	3.4348962	1.8819375	0.40268199
H	3.45259837	2.49794277	-2.20565657
H	0.98168419	3.77287617	-2.5695889
H	-0.11869842	3.66854225	-0.119357
B	0.03995512	3.6322868	2.27015186
H	0.49878662	4.76502167	2.10508923
H	-0.9118719	3.41831049	1.4447287
H	-0.4024397	3.44652038	3.40488813
B	2.76528529	2.56868633	2.66756394
H	2.65395837	2.31164334	3.88527231
H	3.51725435	1.67791239	2.16661505
H	3.27183238	3.67902167	2.51723109

(BH3)2-4

13

E(SCF) =	-317.729243		
C	1.211688	0.000177	-0.481750
C	0.000206	0.001902	0.111533
C	-1.210672	-0.004489	-0.482960
O	-2.299077	-0.029817	-0.870840
O	2.300530	0.021363	-0.868640

B	-0.011834	1.616184	1.140392
B	0.009905	-1.605986	1.154371
H	0.704809	1.264189	2.060780
H	0.399962	2.448967	0.346944
H	-1.207483	1.682356	1.402627
H	1.205225	-1.670504	1.418175
H	-0.707878	-1.245696	2.070566
H	-0.401671	-2.444188	0.366557

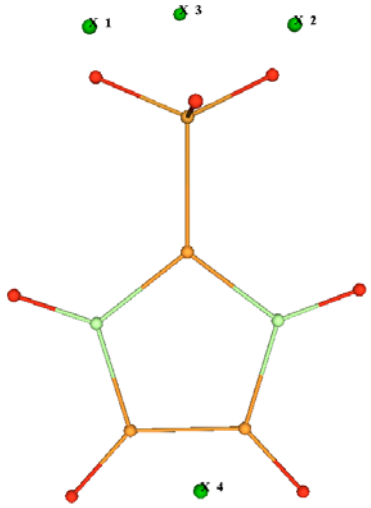
(BH3)2-5

47

E(SCF) = -705.316749

C	-0.159263	-0.368310	0.067795
C	-0.497662	0.067935	-1.292222
C	-0.003961	0.716115	1.044581
N	-0.067454	-0.541649	-2.438347
N	-1.402295	1.092109	-1.506787
N	0.636492	1.893834	0.704141
N	-0.351805	0.635165	2.364678
C	-1.020780	-0.898163	-3.490637
H	-0.778614	-0.419044	-4.464368
H	-2.048135	-0.631073	-3.191461
H	-0.989625	-2.000034	-3.627381
C	1.214983	-1.226463	-2.572641
H	1.672982	-0.933452	-3.542695
H	1.075526	-2.327646	-2.561548
H	1.885336	-0.967889	-1.736427
C	-2.374698	1.528880	-0.512639
H	-2.524403	0.723628	0.228239
H	-3.348404	1.709742	-1.015426
H	-2.067551	2.474444	-0.014301
C	0.387458	3.148097	1.407399
H	1.242599	3.465942	2.044385
H	-0.510825	3.058188	2.043137
H	0.211725	3.951792	0.660309
C	1.541287	2.019398	-0.431679
H	1.059426	2.526815	-1.295937
H	1.908091	1.017625	-0.717108
H	2.420395	2.626352	-0.127460
C	0.595819	1.034867	3.406545
H	1.553397	1.351607	2.960373
H	0.802685	0.149646	4.044862
H	0.198699	1.846654	4.054300
C	-1.455977	-0.172125	2.874916
H	-2.021944	0.431280	3.618015
H	-1.075616	-1.087990	3.373514
H	-2.118372	-0.491925	2.053610
C	-1.400355	1.891200	-2.727861
H	-0.470601	1.716910	-3.297419
H	-1.450165	2.967284	-2.454976
H	-2.268014	1.674571	-3.389954
B	1.303703	-1.262352	0.502125
H	2.309869	-0.604069	0.164224
H	1.287624	-1.391272	1.728503
H	1.281200	-2.359055	-0.046027
B	-1.358620	-1.663046	0.185557
H	-1.122601	-2.338812	1.181348
H	-2.504275	-1.167814	0.232025
H	-1.244904	-2.344061	-0.836342

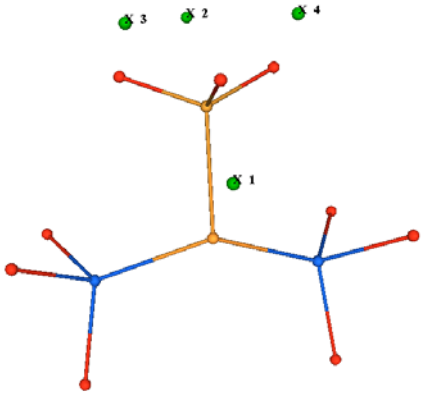
Figure S1. MESP isosurfaces of **1-BH_3 - 5-BH_3** at the MP2/6-311G(2d,2p)//BP86/SVP level of theory.



MESP at Minima

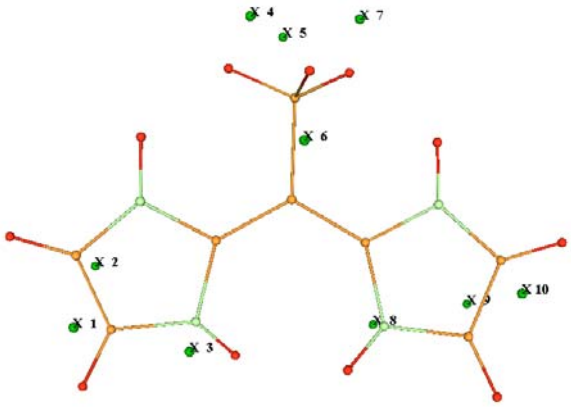
-0.08005
-0.08006
-0.08003
0.00446

1-BH_3



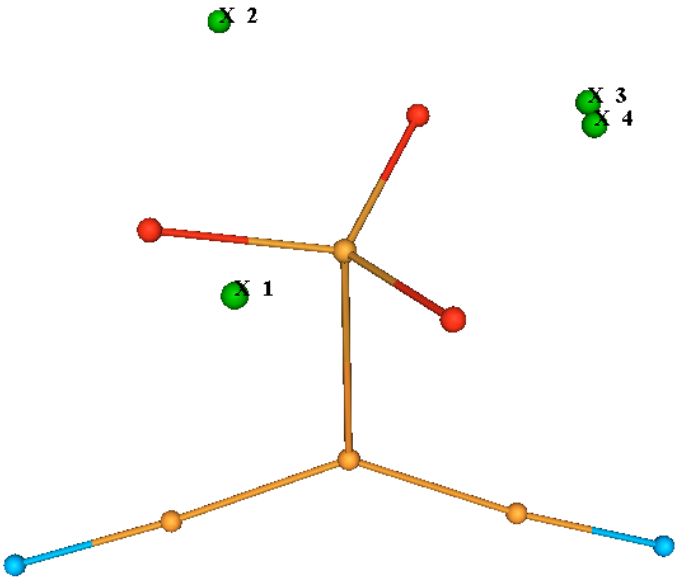
MESP at Minima
-0.07225
-0.07855
-0.08292
-0.08295

2-BH_3



MESP at Minima
-0.011431
-0.013452
-0.007137
-0.093446
-0.092635
-0.081314
-0.093010
-0.003960
-0.009548
-0.012117

3-BH_3

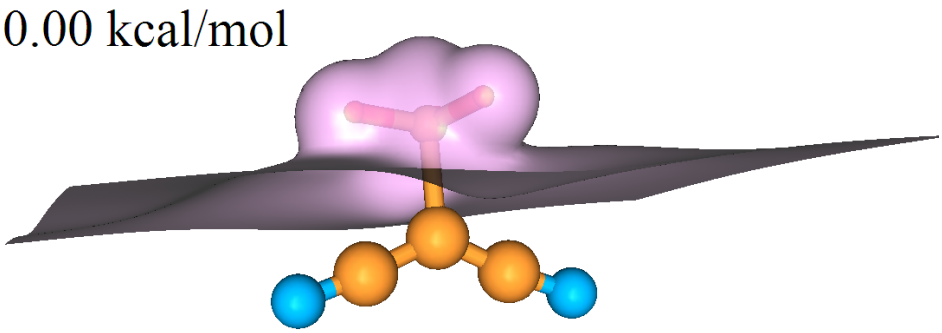


MESP at Minima

-0.04568
-0.04568
-0.04455
-0.04455

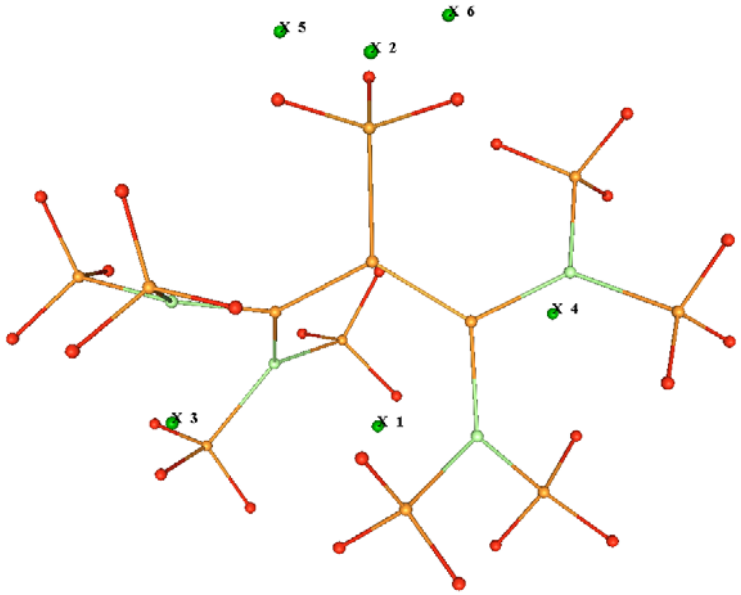
4-BH_3

MESP topography, a (3,+3) minima at central carbon atom is absent.



4-BH_3

MESP isosurface of 0.00 kcal/mol suggesting no negative valued MESP region near central carbon atom

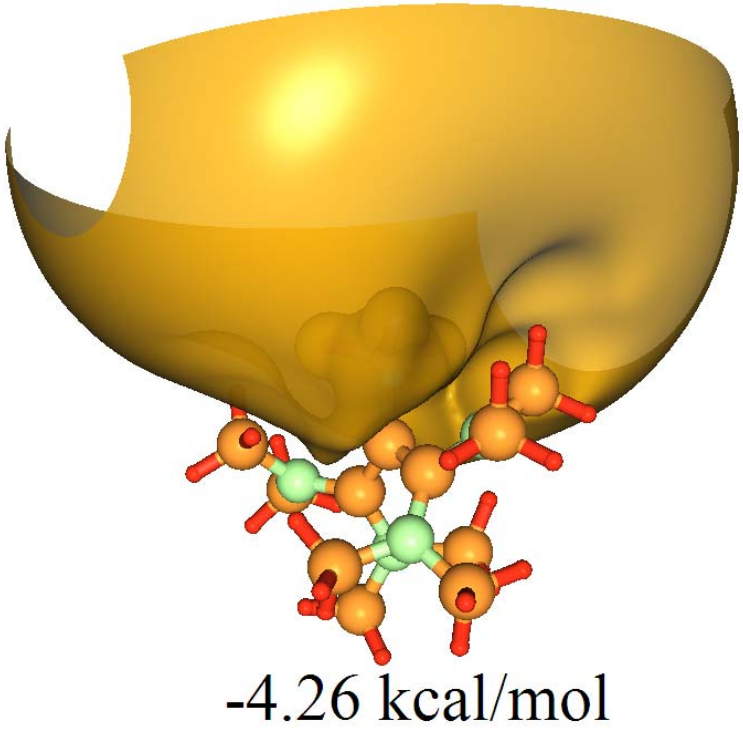


MESP at Minima

-0.00589
-0.10760
-0.00001
0.00044
-0.10692
-0.10360

5

MESP topography, non (3,+3) minima at central carbon atom



5

MESP isosurface of -4.26 kcal/mol suggesting that though a (3,+3) minima not seen near central carbon atom, the smaller negative valued MESP region at central carbon would be responsible for smaller binding energy of second BH3 adduct.