

Supporting Information for:

A Theoretical Study of the Aromaticity in Neutral and Anionic Borole Compounds

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A) List of Cartesian coordinates of the optimized geometries calculated at PBE0/6-31+G(d,p) level.

Borole 1

C	0.002835700	-1.257110927	0.388581962
C	0.002026070	-0.762294813	-0.878357138
C	-0.002835700	1.257110927	0.388581962
C	-0.002026070	0.762294813	-0.878357138
B	0.000000000	0.000000000	1.354130036
C	0.000000000	0.000000000	2.901835157
C	0.651245221	1.014573405	3.633461212
C	-0.651245221	-1.014573405	3.633461212
C	0.670712827	1.004423796	5.024423317
C	-0.670712827	-1.004423796	5.024423317
C	0.000000000	0.000000000	5.722150389
H	1.194998605	1.787144380	5.565832382
H	-1.194998605	-1.787144380	5.565832382
C	0.002719161	-1.551043330	-2.124934231
C	-0.933201189	-1.305506833	-3.140707312
C	0.941396504	-2.576509896	-2.312488248
C	-0.941181960	-2.075772140	-4.300075397
H	-1.664034738	-0.511636828	-3.016817303
C	0.944457467	-3.332779497	-3.479866335
H	1.671894846	-2.774412778	-1.533569188
C	0.000000000	-3.088475888	-4.476351413
H	-1.680416293	-1.877743351	-5.071235458
H	1.683759793	-4.118249131	-3.609846343
H	-0.000851073	-3.682713818	-5.385848457

C	-0.002719161	1.551043330	-2.124934231
C	-0.941396504	2.576509896	-2.312488248
C	0.933201189	1.305506833	-3.140707312
C	-0.944457467	3.332779497	-3.479866335
H	-1.671894846	2.774412778	-1.533569188
C	0.941181960	2.075772140	-4.300075397
H	1.664034738	0.511636828	-3.016817303
C	0.000000000	3.088475888	-4.476351413
H	-1.683759793	4.118249131	-3.609846343
H	1.680416293	1.877743351	-5.071235458
H	0.000851073	3.682713818	-5.385848457
C	0.038388490	2.682824272	0.759200989
C	1.007420960	3.552901686	0.234725949
C	-0.888517965	3.203260137	1.676242058
C	1.041397018	4.893729771	0.605520979
H	1.739893027	3.166849298	-0.468672105
C	-0.861785402	4.547333292	2.039037090
H	-1.639175165	2.543442864	2.103090090
C	0.104160152	5.399174146	1.506051045
H	1.803538280	5.546891858	0.188919945
H	-1.595669265	4.928450636	2.744167139
H	0.129839413	6.446623359	1.793275068
C	-0.038388490	-2.682824272	0.759200989
C	0.888517965	-3.203260137	1.676242058
C	-1.007420960	-3.552901686	0.234725949
C	0.861785402	-4.547333292	2.039037090
H	1.639175165	-2.543442864	2.103090090
C	-1.041397018	-4.893729771	0.605520979

H	-1.739893027	-3.166849298	-0.468672105
C	-0.104160152	-5.399174146	1.506051045
H	1.595669265	-4.928450636	2.744167139
H	-1.803538280	-5.546891858	0.188919945
H	-0.129839413	-6.446623359	1.793275068
H	1.156115936	1.816184791	3.102087168
H	0.000000000	0.000000000	6.809096439
H	-1.156115936	-1.816184791	3.102087168

Borole [1]⁻

C	0.049422865	-1.230913119	0.384071037
C	0.027761036	-0.734353752	-0.919848063
C	-0.049422865	1.230913119	0.384071037
C	-0.027761036	0.734353752	-0.919848063
B	0.000000000	0.000000000	1.335838108
C	0.000000000	0.000000000	2.907906227
C	0.747530234	0.935697594	3.652185281
C	-0.747530234	-0.935697594	3.652185281
C	0.756369743	0.935413711	5.045437390
C	-0.756369743	-0.935413711	5.045437390
C	0.000000000	0.000000000	5.752864471
H	1.351107185	1.672178982	5.582038435
H	-1.351107185	-1.672178982	5.582038435
C	0.045931377	-1.546254408	-2.149431158
C	-0.878414500	-1.334709611	-3.188414239
C	0.988499540	-2.575911597	-2.322522168
C	-0.863688424	-2.115478632	-4.340865321
H	-1.619031240	-0.547424074	-3.080335231

C	1.005619154	-3.356004176	-3.474431251
H	1.712762310	-2.756053132	-1.533257106
C	0.079070855	-3.132138556	-4.493840330
H	-1.593942205	-1.927275352	-5.124798383
H	1.748056676	-4.144380808	-3.576959258
H	0.092032502	-3.741330909	-5.394364401
C	-0.045931377	1.546254408	-2.149431158
C	-0.988499540	2.575911597	-2.322522168
C	0.878414500	1.334709611	-3.188414239
C	-1.005619154	3.356004176	-3.474431251
H	-1.712762310	2.756053132	-1.533257106
C	0.863688424	2.115478632	-4.340865321
H	1.619031240	0.547424074	-3.080335231
C	-0.079070855	3.132138556	-4.493840330
H	-1.748056676	4.144380808	-3.576959258
H	1.593942205	1.927275352	-5.124798383
H	-0.092032502	3.741330909	-5.394364401
C	-0.031280037	2.651013041	0.753977052
C	0.840485996	3.583940043	0.157006006
C	-0.878414500	3.134264367	1.770967130
C	0.854487111	4.920558317	0.544313031
H	1.519348396	3.241870465	-0.619147055
C	-0.865552916	4.470421787	2.160430160
H	-1.553290322	2.434899429	2.256734170
C	0.000000000	5.377999859	1.548758110
H	1.542569689	5.610399690	0.059773992
H	-1.536562992	4.804726159	2.949068216
H	0.012129189	6.422179656	1.851942129

C	0.031280037	-2.651013041	0.753977052
C	0.878414500	-3.134264367	1.770967130
C	-0.840485996	-3.583940043	0.157006006
C	0.865552916	-4.470421787	2.160430160
H	1.553290322	-2.434899429	2.256734170
C	-0.854487111	-4.920558317	0.544313031
H	-1.519348396	-3.241870465	-0.619147055
C	0.000000000	-5.377999859	1.548758110
H	1.536562992	-4.804726159	2.949068216
H	-1.542569689	-5.610399690	0.059773992
H	-0.012129189	-6.422179656	1.851942129
H	1.334530755	1.680734000	3.120282240
H	0.000000000	0.000000000	6.840717532
H	-1.334530755	-1.680734000	3.120282240

Borole [1]²⁻

C	-0.955638072	0.758912059	0.375628981
C	-0.555786043	0.449998034	-0.974604123
C	0.955638072	-0.758912059	0.375628981
C	0.555786043	-0.449998034	-0.974604123
B	0.000000000	0.000000000	1.307511054
C	0.000000000	0.000000000	2.891400173
C	0.000000000	-1.193828091	3.647108232
C	0.000000000	1.193828091	3.647108232
C	0.000084999	-1.200865090	5.040857340
C	-0.000084999	1.200865090	5.040857340
C	0.000000000	0.000000000	5.755809396
H	0.003194999	-2.151157165	5.574846387

H	-0.003194999	2.151157165	5.574846387
C	-1.198768093	0.970957076	-2.179204215
C	-0.468230036	1.471952112	-3.283468300
C	-2.609008200	1.022747076	-2.294072223
C	-1.097863083	1.961482147	-4.422633387
H	0.616498046	1.474377114	-3.226501295
C	-3.238553249	1.518050113	-3.429960311
H	-3.203328248	0.655879047	-1.461960161
C	-2.493173189	1.990969153	-4.515334399
H	-0.490671037	2.332714175	-5.247734449
H	-4.327257332	1.534683117	-3.470335318
H	-2.985943229	2.379669178	-5.404547464
C	1.198768093	-0.970957076	-2.179204215
C	2.609008200	-1.022747076	-2.294072223
C	0.468230036	-1.471952112	-3.283468300
C	3.238553249	-1.518050113	-3.429960311
H	3.203328248	-0.655879047	-1.461960161
C	1.097863083	-1.961482147	-4.422633387
H	-0.616498046	-1.474377114	-3.226501295
C	2.493173189	-1.990969153	-4.515334399
H	4.327257332	-1.534683117	-3.470335318
H	0.490671037	-2.332714175	-5.247734449
H	2.985943229	-2.379669178	-5.404547464
C	1.930236146	-1.765701133	0.757168012
C	2.116206166	-2.995882231	0.068613960
C	2.752828210	-1.587416122	1.902138099
C	3.036433237	-3.950740301	0.486746993
H	1.501705119	-3.199213244	-0.803472106

C	3.665072281	-2.545994191	2.324741135
H	2.652819203	-0.658292047	2.456214143
C	3.827822295	-3.746331284	1.622216082
H	3.131792242	-4.876981375	-0.080501050
H	4.264769326	-2.351590176	3.214122204
H	4.547300350	-4.495548345	1.947690105
C	-1.930236146	1.765701133	0.757168012
C	-2.752828210	1.587416122	1.902138099
C	-2.116206166	2.995882231	0.068613960
C	-3.665072281	2.545994191	2.324741135
H	-2.652819203	0.658292047	2.456214143
C	-3.036433237	3.950740301	0.486746993
H	-1.501705119	3.199213244	-0.803472106
C	-3.827822295	3.746331284	1.622216082
H	-4.264769326	2.351590176	3.214122204
H	-3.131792242	4.876981375	-0.080501050
H	-4.547300350	4.495548345	1.947690105
H	0.007965000	-2.142295166	3.113681193
H	0.000000000	0.000000000	6.844880463
H	-0.007965000	2.142295166	3.113681193

Borole 2

C	0.575933298	-1.129200177	0.957904316
C	0.336483296	-0.687053482	-0.307447781
C	-0.575933298	1.129200177	0.957904316
C	-0.336483296	0.687053482	-0.307447781
B	0.000000000	0.000000000	1.879716388
C	0.653988667	-1.405306439	-1.554256875

C	-0.306156121	-1.575068141	-2.563068952
C	1.933659283	-1.947706917	-1.746492894
C	0.000000000	-2.285492752	-3.720180043
H	-1.300594898	-1.157808176	-2.434790942
C	2.243425092	-2.639985305	-2.911851979
H	2.684702386	-1.819430346	-0.972493833
C	1.275858958	-2.816173669	-3.900875055
H	-0.759271661	-2.417608541	-4.485854103
H	3.241777309	-3.046617126	-3.046688993
H	1.516403408	-3.361946392	-4.808882126
C	-0.653988667	1.405306439	-1.554256875
C	-1.933659283	1.947706917	-1.746492894
C	0.306156121	1.575068141	-2.563068952
C	-2.243425092	2.639985305	-2.911851979
H	-2.684702386	1.819430346	-0.972493833
C	0.000000000	2.285492752	-3.720180043
H	1.300594898	1.157808176	-2.434790942
C	-1.275858958	2.816173669	-3.900875055
H	-3.241777309	3.046617126	-3.046688993
H	0.759271661	2.417608541	-4.485854103
H	-1.516403408	3.361946392	-4.808882126
C	-1.103492666	2.438248713	1.371877349
C	-0.639117744	3.635226229	0.803034307
C	-2.067802144	2.519187585	2.388282427
C	-1.132931712	4.864878610	1.224895336
H	0.121352023	3.595779002	0.028559245
C	-2.568998881	3.750000790	2.803653457
H	-2.433373419	1.606148885	2.849415462

C	-2.104195256	4.928492753	2.223851413
H	-0.754991490	5.778429395	0.773886304
H	-3.321622149	3.787204946	3.586492518
H	-2.489873261	5.889619906	2.552019440
C	1.103492666	-2.438248713	1.371877349
C	2.067802144	-2.519187585	2.388282427
C	0.639117744	-3.635226229	0.803034307
C	2.568998881	-3.750000790	2.803653457
H	2.433373419	-1.606148885	2.849415462
C	1.132931712	-4.864878610	1.224895336
H	-0.121352023	-3.595779002	0.028559245
C	2.104195256	-4.928492753	2.223851413
H	3.321622149	-3.787204946	3.586492518
H	0.754991490	-5.778429395	0.773886304
H	2.489873261	-5.889619906	2.552019440
Cl	0.000000000	0.000000000	3.628599523

Borole [2]⁻

C	0.517339645	-1.129178068	0.977453833
C	0.300331279	-0.669750730	-0.327239268
C	-0.517339645	1.129178068	0.977453833
C	-0.300331279	0.669750730	-0.327239268
B	0.000000000	0.000000000	1.887182905
C	0.618396703	-1.415146035	-1.557127360
C	-0.312659367	-1.563455241	-2.600862442
C	1.878156617	-2.018960417	-1.722848376
C	0.000000000	-2.281365005	-3.752045531
H	-1.294820797	-1.111162180	-2.497843433

C	2.192068959	-2.735827094	-2.872796465
H	2.611374183	-1.916433008	-0.927864315
C	1.254737245	-2.872962505	-3.897906540
H	-0.743207829	-2.379337215	-4.540241592
H	3.175705947	-3.189997045	-2.969760470
H	1.499055994	-3.433034090	-4.797234612
C	-0.618396703	1.415146035	-1.557127360
C	-1.878156617	2.018960417	-1.722848376
C	0.312659367	1.563455241	-2.600862442
C	-2.192068959	2.735827094	-2.872796465
H	-2.611374183	1.916433008	-0.927864315
C	0.000000000	2.281365005	-3.752045531
H	1.294820797	1.111162180	-2.497843433
C	-1.254737245	2.872962505	-3.897906540
H	-3.175705947	3.189997045	-2.969760470
H	0.743207829	2.379337215	-4.540241592
H	-1.499055994	3.433034090	-4.797234612
C	-0.965631664	2.468027253	1.368032861
C	-0.525702366	3.639267625	0.717873812
C	-1.838788052	2.638612344	2.460743948
C	-0.949626920	4.900941727	1.122283846
H	0.168444309	3.548935904	-0.112385251
C	-2.261547143	3.900767955	2.867958975
H	-2.185409051	1.756238936	2.990144986
C	-1.824834442	5.045047011	2.199904925
H	-0.586817500	5.780798151	0.594727805
H	-2.938831340	3.990351969	3.714922043
H	-2.154766376	6.031520109	2.516816951

C	0.965631664	-2.468027253	1.368032861
C	1.838788052	-2.638612344	2.460743948
C	0.525702366	-3.639267625	0.717873812
C	2.261547143	-3.900767955	2.867958975
H	2.185409051	-1.756238936	2.990144986
C	0.949626920	-4.900941727	1.122283846
H	-0.168444309	-3.548935904	-0.112385251
C	1.824834442	-5.045047011	2.199904925
H	2.938831340	-3.990351969	3.714922043
H	0.586817500	-5.780798151	0.594727805
H	2.154766376	-6.031520109	2.516816951
Cl	0.000000000	0.000000000	3.695318042

Borole [2]²⁻

C	0.475811245	-1.137907820	0.983199173
C	0.264242464	-0.662956205	-0.369087933
C	-0.475811245	1.137907820	0.983199173
C	-0.264242464	0.662956205	-0.369087933
B	0.000000000	0.000000000	1.871017238
C	0.565884835	-1.429794767	-1.575740027
C	-0.314493092	-1.508242342	-2.681313111
C	1.771782343	-2.163607838	-1.689993036
C	0.000000000	-2.237240719	-3.823115200
H	-1.263821678	-0.983580943	-2.623697107
C	2.083231264	-2.897347236	-2.828204122
H	2.465558641	-2.137702849	-0.854277969
C	1.204791601	-2.941613659	-3.916499204
H	-0.709647498	-2.262738908	-4.649592260

H	3.025254140	-3.443480647	-2.868197126
H	1.447583172	-3.517795495	-4.807428275
C	-0.565884835	1.429794767	-1.575740027
C	-1.771782343	2.163607838	-1.689993036
C	0.314493092	1.508242342	-2.681313111
C	-2.083231264	2.897347236	-2.828204122
H	-2.465558641	2.137702849	-0.854277969
C	0.000000000	2.237240719	-3.823115200
H	1.263821678	0.983580943	-2.623697107
C	-1.204791601	2.941613659	-3.916499204
H	-3.025254140	3.443480647	-2.868197126
H	0.709647498	2.262738908	-4.649592260
H	-1.447583172	3.517795495	-4.807428275
C	-0.765053864	2.504270894	1.371435200
C	-0.344263961	3.648331484	0.637370146
C	-1.479865053	2.789580141	2.567227291
C	-0.627490296	4.944975254	1.050960177
H	0.235752534	3.501084131	-0.268206925
C	-1.754052730	4.086330853	2.982863322
H	-1.819680864	1.951221930	3.167149341
C	-1.339511879	5.191997363	2.229443266
H	-0.275696704	5.780438575	0.444942129
H	-2.309240914	4.238980158	3.909009399
H	-1.560171712	6.208258219	2.551360292
C	0.765053864	-2.504270894	1.371435200
C	1.479865053	-2.789580141	2.567227291
C	0.344263961	-3.648331484	0.637370146
C	1.754052730	-4.086330853	2.982863322

H	1.819680864	-1.951221930	3.167149341
C	0.627490296	-4.944975254	1.050960177
H	-0.235752534	-3.501084131	-0.268206925
C	1.339511879	-5.191997363	2.229443266
H	2.309240914	-4.238980158	3.909009399
H	0.275696704	-5.780438575	0.444942129
H	1.560171712	-6.208258219	2.551360292
Cl	0.000000000	0.000000000	3.728249382

Borole 3

C	0.617576150	-1.104659629	0.646938597
C	0.353506808	-0.679544689	-0.618959498
C	-0.617576150	1.104659629	0.646938597
C	-0.353506808	0.679544689	-0.618959498
B	0.000000000	0.000000000	1.562025668
C	0.664417105	-1.406053415	-1.861036595
C	-0.299410363	-1.572750937	-2.867047674
C	1.939128526	-1.960546435	-2.052807610
C	0.000000000	-2.286191155	-4.023685760
H	-1.290298173	-1.147239067	-2.738747660
C	2.240655336	-2.659537330	-3.216214698
H	2.693176397	-1.834629174	-1.281521551
C	1.270609969	-2.829554582	-4.203928775
H	-0.761212069	-2.413547550	-4.788235821
H	3.235058764	-3.075731680	-3.351043711
H	1.505539860	-3.379301575	-5.111000843
C	-0.664417105	1.406053415	-1.861036595
C	-1.939128526	1.960546435	-2.052807610

C	0.299410363	1.572750937	-2.867047674
C	-2.240655336	2.659537330	-3.216214698
H	-2.693176397	1.834629174	-1.281521551
C	0.000000000	2.286191155	-4.023685760
H	1.290298173	1.147239067	-2.738747660
C	-1.270609969	2.829554582	-4.203928775
H	-3.235058764	3.075731680	-3.351043711
H	0.761212069	2.413547550	-4.788235821
H	-1.505539860	3.379301575	-5.111000843
C	-1.178588739	2.398542597	1.066085629
C	-0.664357863	3.612571633	0.586442594
C	-2.236051441	2.440393998	1.986118703
C	-1.196379350	4.827123718	1.007043625
H	0.162244886	3.597497738	-0.118287461
C	-2.771382461	3.656012396	2.403670732
H	-2.644431087	1.508429490	2.367564730
C	-2.253081788	4.854354306	1.916728696
H	-0.780988323	5.756484414	0.626839599
H	-3.594133171	3.665896792	3.113346790
H	-2.666522486	5.803296068	2.246599722
C	1.178588739	-2.398542597	1.066085629
C	2.236051441	-2.440393998	1.986118703
C	0.664357863	-3.612571633	0.586442594
C	2.771382461	-3.656012396	2.403670732
H	2.644431087	-1.508429490	2.367564730
C	1.196379350	-4.827123718	1.007043625
H	-0.162244886	-3.597497738	-0.118287461
C	2.253081788	-4.854354306	1.916728696

H	3.594133171	-3.665896792	3.113346790
H	0.780988323	-5.756484414	0.626839599
H	2.666522486	-5.803296068	2.246599722
Br	0.000000000	0.000000000	3.457904812

Borole [3]⁻

C	0.567903874	-1.102437297	0.659443415
C	0.324278982	-0.660311176	-0.644554685
C	-0.567903874	1.102437297	0.659443415
C	-0.324278982	0.660311176	-0.644554685
B	0.000000000	0.000000000	1.563007482
C	0.634595151	-1.415605149	-1.868723779
C	-0.303214272	-1.564542583	-2.906624862
C	1.888930407	-2.030271914	-2.036366792
C	0.000000000	-2.287950907	-4.056444948
H	-1.281680341	-1.104804042	-2.801577849
C	2.191429347	-2.756407274	-3.183548883
H	2.627671091	-1.928413036	-1.246571733
C	1.249060252	-2.891138505	-4.204301961
H	-0.747300285	-2.383897960	-4.841029009
H	3.170865340	-3.219234993	-3.282100891
H	1.485419165	-3.457057737	-5.102075030
C	-0.634595151	1.415605149	-1.868723779
C	-1.888930407	2.030271914	-2.036366792
C	0.303214272	1.564542583	-2.906624862
C	-2.191429347	2.756407274	-3.183548883
H	-2.627671091	1.928413036	-1.246571733
C	0.000000000	2.287950907	-4.056444948

H	1.281680341	1.104804042	-2.801577849
C	-1.249060252	2.891138505	-4.204301961
H	-3.170865340	3.219234993	-3.282100891
H	0.747300285	2.383897960	-4.841029009
H	-1.485419165	3.457057737	-5.102075030
C	-1.062274595	2.424664141	1.055331446
C	-0.567586167	3.616483195	0.491941402
C	-2.045458830	2.548218614	2.054508523
C	-1.040908074	4.861658746	0.893746432
H	0.202562027	3.553396165	-0.271723657
C	-2.514760959	3.793503875	2.463499554
H	-2.442943574	1.642619490	2.503840556
C	-2.018087386	4.961779039	1.885248508
H	-0.636787099	5.761910756	0.435344398
H	-3.275862917	3.850928989	3.238929616
H	-2.384249244	5.934935524	2.203623533
C	1.062274595	-2.424664141	1.055331446
C	2.045458830	-2.548218614	2.054508523
C	0.567586167	-3.616483195	0.491941402
C	2.514760959	-3.793503875	2.463499554
H	2.442943574	-1.642619490	2.503840556
C	1.040908074	-4.861658746	0.893746432
H	-0.202562027	-3.553396165	-0.271723657
C	2.018087386	-4.961779039	1.885248508
H	3.275862917	-3.850928989	3.238929616
H	0.636787099	-5.761910756	0.435344398
H	2.384249244	-5.934935524	2.203623533
Br	0.000000000	0.000000000	3.522108634

Borole [3]²⁻

C	0.389942145	-1.169135707	0.664547976
C	0.209393730	-0.682925444	-0.686764128
C	-0.389942145	1.169135707	0.664547976
C	-0.209393730	0.682925444	-0.686764128
B	0.000000000	0.000000000	1.544590045
C	0.428022178	-1.481390629	-1.889827219
C	-0.461261438	-1.473063003	-2.991117307
C	1.552053820	-2.335093366	-2.005628230
C	-0.227248392	-2.233209050	-4.131800392
H	-1.351254502	-0.853277512	-2.930312301
C	1.781272317	-3.100737941	-3.142365314
H	2.248625576	-2.378574982	-1.173052164
C	0.898251726	-3.058299677	-4.226912398
H	-0.939046979	-2.188534319	-4.955610457
H	2.662160917	-3.740687969	-3.184324318
H	1.077048774	-3.658935545	-5.116816469
C	-0.428022178	1.481390629	-1.889827219
C	-1.552053820	2.335093366	-2.005628230
C	0.461261438	1.473063003	-2.991117307
C	-1.781272317	3.100737941	-3.142365314
H	-2.248625576	2.378574982	-1.173052164
C	0.227248392	2.233209050	-4.131800392
H	1.351254502	0.853277512	-2.930312301
C	-0.898251726	3.058299677	-4.226912398
H	-2.662160917	3.740687969	-3.184324318
H	0.939046979	2.188534319	-4.955610457

H	-1.077048774	3.658935545	-5.116816469
C	-0.570029664	2.555074963	1.054871009
C	0.000000000	3.654747102	0.359164953
C	-1.328120106	2.895246815	2.206102094
C	-0.188703312	4.970575738	0.767039983
H	0.611928707	3.455117763	-0.515364114
C	-1.505070284	4.209613424	2.620071127
H	-1.787934452	2.087316936	2.766810136
C	-0.941969185	5.274017535	1.905899073
H	0.271984471	5.773980760	0.191715940
H	-2.099715437	4.409119698	3.511966195
H	-1.086010751	6.304610971	2.225729098
C	0.570029664	-2.555074963	1.054871009
C	1.328120106	-2.895246815	2.206102094
C	0.000000000	-3.654747102	0.359164953
C	1.505070284	-4.209613424	2.620071127
H	1.787934452	-2.087316936	2.766810136
C	0.188703312	-4.970575738	0.767039983
H	-0.611928707	-3.455117763	-0.515364114
C	0.941969185	-5.274017535	1.905899073
H	2.099715437	-4.409119698	3.511966195
H	-0.271984471	-5.773980760	0.191715940
H	1.086010751	-6.304610971	2.225729098
Br	0.000000000	0.000000000	3.559891202

Borole 4

6	0.425903066	-1.282849050	-0.384558007
6	1.648159135	-0.720950952	-0.112277980

6	0.339218962	1.243786138	-0.537329092
6	1.585959069	0.804058165	-0.162363028
5	-0.564880055	-0.067850006	-0.715998086
6	2.926523254	-1.452873949	0.096951079
6	4.030152348	-1.232617916	-0.760273976
6	3.076552286	-2.399212990	1.135577186
6	5.225611464	-1.942328916	-0.595600921
1	3.944752327	-0.507743884	-1.575885058
6	4.277683404	-3.099770991	1.307606243
1	2.246150217	-2.576000018	1.825051230
6	5.356727516	-2.878233952	0.440707188
1	6.061649556	-1.760708886	-1.281502961
1	4.369299427	-3.824188017	2.125738326
1	6.295343596	-3.429145955	0.573274229
6	2.755796116	1.652735285	0.187271996
6	3.241841133	2.637150354	-0.703462093
6	3.410819155	1.506802334	1.432589109
6	4.334347180	3.444056471	-0.361493068
1	2.763813109	2.760383316	-1.679717181
6	4.493077198	2.324504450	1.779663131
1	3.057707141	0.754124280	2.144406176
6	4.962721213	3.295401517	0.883149044
1	4.696466188	4.194999523	-1.073860138
1	4.975704222	2.198470485	2.756215219
1	5.815710249	3.929733609	1.151719060
6	-0.050446123	2.674476226	-0.646819146
6	-0.103296181	3.517733322	0.487221917
6	-0.385010149	3.242421222	-1.898881262

6	-0.476020261	4.864307405	0.376136864
1	0.152098838	3.106861326	1.469775008
6	-0.749171228	4.591128308	-2.012635315
1	-0.347108107	2.615281152	-2.796894313
6	-0.800208289	5.409552423	-0.874506251
1	-0.508628305	5.493237466	1.274229917
1	-0.993313248	5.005468304	-2.998439411
1	-1.088125349	6.463761452	-0.962112296
6	0.185381109	-2.744618178	-0.546573983
6	-0.293157915	-3.546540229	0.513851113
6	0.408457174	-3.374300252	-1.792510057
6	-0.534645873	-4.916803349	0.340086133
1	-0.474639964	-3.085890174	1.490973171
6	0.166727212	-4.743692373	-1.968811035
1	0.779215193	-2.777211216	-2.633130131
6	-0.307459811	-5.522842445	-0.903765943
1	-0.900284893	-5.514901400	1.183801209
1	0.353274263	-5.204850428	-2.946302095
1	-0.495790781	-6.594101513	-1.041173928
6	-3.297176272	-1.101897112	2.183297121
6	-2.500841259	0.090187011	2.231723105
6	-3.353056368	1.214177057	1.970546038
6	-4.684400444	0.716852961	1.771490015
6	-4.649777387	-0.714187146	1.901300062
1	-2.939528209	-2.122567173	2.333812165
1	-1.424862179	0.134654063	2.413143137
1	-3.040233380	2.259533147	1.924612008
1	-5.568373544	1.319926966	1.549829964

1	-5.502425411	-1.389754232	1.797627058
26	-3.425632292	-0.098421092	0.391984952
6	-2.983166271	0.945184958	-1.297224198
6	-2.048037156	-0.162234085	-1.144666138
6	-4.313383347	0.432738865	-1.380177214
1	-2.715771287	2.000557051	-1.332256229
6	-2.874724173	-1.362134207	-1.114826119
6	-4.246009288	-0.995191240	-1.265577165
1	-5.224952443	1.026163868	-1.487531254
1	-2.508848102	-2.381222271	-0.993544075
1	-5.097480327	-1.680523324	-1.272489162

Borole [4]⁻

C	0.494892139	-1.240967137	-0.326714997
C	1.771660225	-0.709772045	-0.089235010
C	0.466546054	1.237048050	-0.495223061
C	1.747592175	0.773554065	-0.153200045
B	-0.468449979	-0.026628078	-0.622436029
C	3.011623349	-1.501944063	0.097434001
C	4.173837418	-1.256303022	-0.679576080
C	3.090382402	-2.554102123	1.045658096
C	5.339015530	-2.015971042	-0.520107074
H	4.151443377	-0.461544980	-1.431516154
C	4.255736519	-3.313586143	1.207026105
H	2.220814354	-2.764517153	1.674849163
C	5.392013584	-3.051805100	0.425673020
H	6.215113604	-1.798342009	-1.144968140
H	4.277523561	-4.116474186	1.955532179

H	6.305492686	-3.646358113	0.551996028
C	2.917398238	1.622042174	0.176281944
C	3.332291225	2.687668255	-0.663833147
C	3.671736327	1.414448209	1.361081027
C	4.429852291	3.494625358	-0.340034158
H	2.787628165	2.870155230	-1.594743216
C	4.768036390	2.221935310	1.686322017
H	3.377759341	0.610913152	2.043174102
C	5.158971369	3.269937386	0.838386925
H	4.722430275	4.305611416	-1.019815233
H	5.321841453	2.032101333	2.615110085
H	6.019443437	3.901892467	1.091586919
C	0.098909979	2.672451149	-0.547974091
C	0.127006973	3.497843238	0.605088985
C	-0.312172092	3.288634160	-1.757881190
C	-0.235689100	4.850347328	0.554731959
H	0.435938026	3.055844231	1.558389062
C	-0.673014166	4.642031248	-1.812942215
H	-0.338090090	2.682803095	-2.670772244
C	-0.639719170	5.435183335	-0.655566139
H	-0.203282102	5.454196409	1.471263012
H	-0.980813219	5.082528254	-2.770622292
H	-0.923602226	6.494270426	-0.696439160
C	0.228377162	-2.696049258	-0.464405973
C	-0.514282855	-3.417681319	0.503426127
C	0.691286207	-3.430761322	-1.584699051
C	-0.779871833	-4.787099434	0.362369149
H	-0.882392887	-2.883687272	1.385914189

C	0.426868226	-4.799249439	-1.731203031
H	1.265162222	-2.904637277	-2.355390129
C	-0.312216793	-5.489716479	-0.758537930
H	-1.355406850	-5.310842503	1.137137227
H	0.801002256	-5.331865498	-2.615513095
H	-0.520139776	-6.561113608	-0.871909912
C	-3.882925162	-1.170331224	1.989025252
C	-2.989800127	-0.066720104	2.207792228
C	-3.702749225	1.146130959	1.922206194
C	-5.043736323	0.794105880	1.540152195
C	-5.155733286	-0.637925232	1.581220229
H	-3.638068107	-2.228605293	2.109548275
H	-1.937934040	-0.135225070	2.494715238
H	-3.291000223	2.157263050	1.974163171
H	-5.835422419	1.493543904	1.257196167
H	-6.048895326	-1.220905308	1.339281237
Fe	-3.687859209	-0.068021168	0.277993092
C	-2.902907211	1.038034912	-1.238162058
C	-1.998350101	-0.075581139	-0.996867033
C	-4.207677302	0.552641825	-1.583761057
H	-2.634092223	2.091899002	-1.172967083
C	-2.832419130	-1.256737259	-1.152075006
C	-4.163431247	-0.880647284	-1.527824022
H	-5.080178390	1.164749838	-1.831688071
H	-2.494428070	-2.283515328	-1.015648979
H	-4.995289294	-1.562723367	-1.727821012

Borole [4]²⁻

C	-0.416078006	1.201353082	-0.298071043
C	-1.779798135	0.790518149	-0.065507004
C	-0.617166201	-1.246495092	-0.441351047
C	-1.892105248	-0.656379950	-0.116733003
B	0.427492963	-0.091678077	-0.539424073
C	-2.911740153	1.704618304	0.158373030
C	-4.169768272	1.554128380	-0.500881001
C	-2.815879055	2.818429382	1.046973097
C	-5.238603289	2.429006527	-0.279503968
H	-4.290410350	0.734210324	-1.215191051
C	-3.883669069	3.694327528	1.265759128
H	-1.876489963	2.974518329	1.585855123
C	-5.115103189	3.513317603	0.608436094
H	-6.184045396	2.267909578	-0.817819996
H	-3.756420985	4.531335586	1.967617180
H	-5.953314220	4.202198715	0.779079120
C	-3.126544396	-1.405360923	0.170011040
C	-3.579809518	-2.476223970	-0.658500014
C	-3.943258417	-1.123643837	1.307760138
C	-4.748350657	-3.192703940	-0.380750975
H	-2.998463510	-2.728607037	-1.550334095
C	-5.113988556	-1.837659809	1.582696178
H	-3.628512330	-0.330753799	1.993091185
C	-5.537561669	-2.884449858	0.743237125
H	-5.054615747	-4.003018986	-1.058261019
H	-5.702579562	-1.580104744	2.475312256
H	-6.454621767	-3.448094835	0.961282155

C	-0.389433287	-2.699012217	-0.488292052
C	-0.726134359	-3.579603260	0.583927038
C	0.194592695	-3.327538309	-1.629463149
C	-0.493086443	-4.958330381	0.524379032
H	-1.166606351	-3.150137192	1.489594114
C	0.429499612	-4.706358432	-1.691318154
H	0.455193747	-2.694162281	-2.484427218
C	0.088838542	-5.544468491	-0.614479066
H	-0.764016497	-5.587862401	1.384612106
H	0.879508601	-5.136723503	-2.598111229
H	0.269675477	-6.626830544	-0.662141066
C	-0.044193880	2.602731163	-0.550175071
C	1.057981259	3.234989134	0.099110961
C	-0.750520890	3.429333279	-1.478857134
C	1.423783382	4.562839212	-0.154243066
H	1.625808275	2.653189050	0.829100012
C	-0.387219770	4.755663352	-1.734501160
H	-1.595419991	2.994473302	-2.022268161
C	0.706966369	5.346519316	-1.075861126
H	2.279282486	4.996513181	0.384276961
H	-0.963453782	5.339167457	-2.467722209
H	0.991525460	6.388628390	-1.274692148
C	4.398465402	1.314630748	1.628023030
C	3.321591272	0.534547768	2.182293092
C	3.744353204	-0.835765370	2.218557090
C	5.090227297	-0.905641474	1.710736027
C	5.497806435	0.425050601	1.348238991
H	4.387792479	2.395469834	1.460523016

H	2.334463227	0.901392869	2.473264128
H	3.136275103	-1.681145388	2.552334126
H	5.691507269	-1.814625586	1.608882012
H	6.469412483	0.711381554	0.932524943
Fe	3.827673236	-0.124042324	0.301347940
C	2.776514041	-1.456969353	-0.829149130
C	1.970313063	-0.246076200	-0.874639122
C	4.090748149	-1.224923430	-1.366201193
H	2.423118948	-2.425075401	-0.475241094
C	2.911478200	0.763062808	-1.330637174
C	4.176313253	0.175199671	-1.674343216
H	4.877153156	-1.974909544	-1.506871212
H	2.675543259	1.821038908	-1.450165181
H	5.038983349	0.698144651	-2.102348263

Borole [4]²⁻ (isomer with η^5 -borole coordination)

C	1.249923970	-0.418974153	-0.358356132
C	0.655761040	0.917129002	-0.302726127
C	-1.176358236	-0.619647963	-0.398846135
C	-0.809458085	0.792519116	-0.317639128
B	0.112922790	-1.508225138	-0.502853143
C	1.396473206	2.205447036	-0.406906135
C	1.129971262	3.112893131	-1.464235215
C	2.430037316	2.568193976	0.492444934
C	1.834855419	4.316482162	-1.601897227
H	0.356694181	2.858125174	-2.195024271
C	3.141340473	3.766261010	0.353465923
H	2.671410274	1.887101903	1.311718998

C	2.847163527	4.657620101	-0.691959156
H	1.591351460	4.993232234	-2.432509294
H	3.935373554	4.008500960	1.073053978
H	3.400466649	5.600363102	-0.796716164
C	-1.723678057	1.960522283	-0.446244139
C	-2.649986120	2.031641367	-1.518224223
C	-1.691906959	3.064602368	0.440770930
C	-3.497360093	3.134722524	-1.687738233
H	-2.695572194	1.200767309	-2.228762273
C	-2.533846928	4.171417522	0.270418917
H	-0.991840908	3.036493304	1.279394994
C	-3.448825999	4.216292604	-0.794027165
H	-4.204232147	3.148598588	-2.528656297
H	-2.478413854	5.007026583	0.981689971
H	-4.114858973	5.079775728	-0.923685175
C	-2.586506382	-1.092666880	-0.428775137
C	-3.643238417	-0.535831743	0.338864922
C	-2.937527501	-2.152694928	-1.307731203
C	-4.965513554	-0.990090670	0.223976913
H	-3.422063330	0.268869298	1.044407979
C	-4.258795639	-2.604629851	-1.426593213
H	-2.140312476	-2.623724032	-1.888902249
C	-5.287907670	-2.028204720	-0.663659154
H	-5.751388596	-0.526559565	0.837383959
H	-4.483894729	-3.426571894	-2.120168265
H	-6.322803767	-2.386334658	-0.754777163
C	2.701436060	-0.691634299	-0.461245139
C	3.315482016	-1.738581429	0.278635917

C	3.542525181	0.008830685	-1.367334209
C	4.679278098	-2.028169567	0.156136908
H	2.690910916	-2.337421423	0.943981969
C	4.908174262	-0.284671454	-1.495753219
H	3.110423218	0.790404783	-1.998540255
C	5.495816199	-1.300024583	-0.726666161
H	5.108437058	-2.846522667	0.750615951
H	5.517086373	0.288111539	-2.209783273
H	6.565857259	-1.529995691	-0.822224169
C	1.194519975	-0.321822140	2.935541123
C	0.367447010	0.849859022	3.075826133
C	-1.003825132	0.428262105	3.030145129
C	-1.021677255	-0.997523001	2.852911117
C	0.331304810	-1.469765155	2.808973111
H	2.287542054	-0.342118235	2.934012123
H	0.721692123	1.874745070	3.220390145
H	-1.880818146	1.077006229	3.104823136
H	-1.913315376	-1.617489974	2.734609108
H	0.635714748	-2.506970258	2.654488101
Fe	0.004314899	-0.126198024	1.289653995
C	-0.451877475	-4.111739293	-0.007078105
C	0.273319671	-3.056747272	-0.665878158
C	-0.028204549	-5.364526424	-0.505162143
H	-1.212879520	-3.963598218	0.769403955
C	1.154551683	-3.725916399	-1.585999229
C	0.965972549	-5.123540491	-1.497664221
H	-0.395423661	-6.349828479	-0.180278118
H	1.850576777	-3.222859418	-2.269064280

H	1.494321524	-5.888614575	-2.086263265
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Borole 5

C	0.562203164	-1.267869064	-0.367144985
C	1.775329238	-0.714818983	-0.107861972
C	0.480425061	1.238134129	-0.537647953
C	1.710492177	0.809006131	-0.150305949
B	-0.414925961	-0.061316005	-0.678938977
C	3.039338367	-1.446105994	0.090332015
C	4.198503433	-1.075888908	-0.609685048
C	3.107020428	-2.544961089	0.959629063
C	5.380134560	-1.794727918	-0.460077065
H	4.170007391	-0.225138833	-1.284020088
C	4.294525550	-3.251201104	1.122782045
H	2.221990376	-2.838489153	1.515076110
C	5.434357606	-2.882213015	0.410147983
H	6.263257621	-1.498892854	-1.019437115
H	4.328085590	-4.094462174	1.806985087
H	6.360215699	-3.436760027	0.534824973
C	2.857046240	1.654567238	0.226239079
C	3.238835216	2.750067349	-0.562788969
C	3.584303317	1.388147227	1.396862157
C	4.312416271	3.553267442	-0.192160940
H	2.690919150	2.965760361	-1.474937026
C	4.645490374	2.203923323	1.776363182
H	3.309602338	0.540724140	2.018293193
C	5.016938348	3.286536433	0.981115136
H	4.597852251	4.392111534	-0.820876979

H	5.188706436	1.987536311	2.691969244
H	5.852480395	3.917007505	1.272095158
C	0.077283974	2.654231222	-0.669201936
C	0.054940953	3.518682269	0.433682163
C	-0.303423091	3.166045266	-1.919370021
C	-0.335815130	4.847662357	0.292153180
H	0.341316003	3.138576236	1.410057228
C	-0.686408171	4.497565357	-2.064051002
H	-0.286681077	2.510161234	-2.787073095
C	-0.706810193	5.344059383	-0.956269904
H	-0.352105144	5.497230372	1.163048258
H	-0.968711221	4.873826394	-3.043892069
H	-1.010375256	6.381407449	-1.065278888
C	0.317807200	-2.717221185	-0.552598020
C	-0.359303811	-3.477944284	0.410266050
C	0.739197243	-3.358832200	-1.725788125
C	-0.608544782	-4.833901394	0.207045015
H	-0.686163845	-3.004726275	1.331456134
C	0.489345271	-4.713778306	-1.931164165
H	1.271082249	-2.784748123	-2.480032184
C	-0.187489740	-5.457520382	-0.966331093
H	-1.131270789	-5.403039468	0.971261072
H	0.827579305	-5.189670317	-2.847760243
H	-0.382491717	-6.514275495	-1.125701119
C	-1.901171075	-0.138540062	-1.069182989
C	-2.805679189	0.963758990	-1.306262974
C	-2.715919097	-1.325361182	-1.152485002
C	-4.102359277	0.463863908	-1.533677987

H	-2.528195209	2.009285083	-1.299291963
C	-4.049046214	-0.964681203	-1.437484004
H	-2.353619026	-2.335253247	-1.009616014
H	-4.987398367	1.054192921	-1.733910980
H	-4.883933256	-1.642757283	-1.557081010
Mn	-3.441801176	-0.091550143	0.428403148
C	-3.056110084	-1.338830246	1.653522219
C	-2.889002169	1.235865964	1.504440245
C	-5.117610304	0.035323793	1.030033217
O	-2.827864025	-2.147054311	2.445090261
O	-2.542722167	2.089355030	2.196546306
O	-6.214406412	0.114931752	1.380866261

Borole [5]²⁻

C	-0.474830078	1.164043191	-0.289464025
C	-1.855530189	0.849800204	-0.077302999
C	-0.829599174	-1.246376985	-0.381937045
C	-2.062715247	-0.568712896	-0.113503010
B	0.265704940	-0.171025930	-0.478736054
C	-2.918417243	1.834150311	0.133060031
C	-4.170607346	1.754963344	-0.518693010
C	-2.734227195	2.937125384	0.998490105
C	-5.170797396	2.698398440	-0.307047980
H	-4.344609388	0.931775289	-1.205849067
C	-3.730511240	3.884427480	1.204687131
H	-1.782719114	3.030744359	1.514126136
C	-4.965657348	3.776904511	0.558054092
H	-6.121038484	2.593477462	-0.829359013

H	-3.542108200	4.716788536	1.881540192
H	-5.746116403	4.517831591	0.720367116
C	-3.348850362	-1.226453917	0.117162013
C	-3.798038432	-2.288855980	-0.701824052
C	-4.205407407	-0.856647868	1.180776104
C	-5.014719540	-2.924982994	-0.481456031
H	-3.167840399	-2.603703013	-1.528758125
C	-5.425926543	-1.486948884	1.396515128
H	-3.887176360	-0.059650821	1.846822159
C	-5.849561612	-2.531078949	0.568691057
H	-5.317291587	-3.737836042	-1.140616086
H	-6.051740553	-1.164146846	2.227713195
H	-6.801961648	-3.028656961	0.741005076
C	-0.692547204	-2.699361098	-0.411272058
C	-1.216210257	-3.548276152	0.594312020
C	-0.006673176	-3.350000158	-1.465414148
C	-1.057689285	-4.929285265	0.553582004
H	-1.746532280	-3.092579112	1.425925090
C	0.161481799	-4.730748269	-1.503823161
H	0.391397866	-2.730958118	-2.265837209
C	-0.363762256	-5.542528315	-0.494242086
H	-1.476151329	-5.536735306	1.355390065
H	0.700626820	-5.180335313	-2.337452232
H	-0.238895277	-6.623162393	-0.524224096
C	0.026045996	2.515675282	-0.513934037
C	1.263504108	2.943561280	0.023055998
C	-0.659854036	3.473643385	-1.304137084
C	1.780935183	4.213278363	-0.212540016

H	1.819531133	2.245263205	0.641648036
C	-0.149125964	4.746277468	-1.533970098
H	-1.608023120	3.190531393	-1.752320114
C	1.079998144	5.137305461	-0.993411067
H	2.741696268	4.483274354	0.223648012
H	-0.716187991	5.442355538	-2.151841137
H	1.480611203	6.132441513	-1.176966075
C	1.776858047	-0.449301990	-0.791178091
C	2.502503071	-1.684202106	-0.568801089
C	2.738644137	0.397493053	-1.438931145
C	3.766478163	-1.642283135	-1.224289148
H	2.096767020	-2.548731165	-0.061935052
C	3.923554206	-0.336749035	-1.763991182
H	2.553407150	1.426942137	-1.718716158
H	4.482648194	-2.453087214	-1.287854162
H	4.775343280	0.032995975	-2.321847229
Mn	3.811907215	-0.245292037	0.331217981
C	4.689986328	1.288900055	0.469028995
C	2.898194163	-0.048876008	1.856796108
C	5.109924300	-1.150985150	1.103231025
O	5.275173401	2.295634116	0.524550001
O	2.336602130	0.052757009	2.864723189
O	5.985607368	-1.753036223	1.590845053

Borole 6

C	-0.154487322	-1.259264076	0.015165991
C	-1.416374292	-0.759807712	-0.016990012
C	-0.154759674	1.259347119	-0.015611012

C	-1.416537898	0.759602407	0.016615991
B	0.828951080	0.000148769	-0.000130011
C	-2.665522589	-1.546461449	-0.086386017
C	-3.682701620	-1.368063172	0.862234054
C	-2.851800850	-2.501097476	-1.095798096
C	-4.843024907	-2.135307936	0.813015050
H	-3.559484423	-0.628152149	1.648000117
C	-4.019413135	-3.256170232	-1.154011102
H	-2.071231826	-2.648761688	-1.836561153
C	-5.017645165	-3.079658964	-0.197038026
H	-5.615683948	-1.989095722	1.562787112
H	-4.147212330	-3.987838256	-1.947065163
H	-5.926871392	-3.672828771	-0.239595029
C	-2.665881795	1.545926789	0.086275996
C	-2.852256561	2.500449911	1.095773071
C	-3.683188918	1.367290039	-0.862168076
C	-4.020074458	3.255181268	1.154243077
H	-2.071599461	2.648291721	1.836409131
C	-4.843726808	2.134196394	-0.812694073
H	-3.559910098	0.627469949	-1.648009139
C	-5.018434581	3.078438512	0.197444005
H	-4.147939277	3.986768360	1.947362137
H	-5.616478931	1.987798582	-1.562334131
H	-5.927822482	3.671345794	0.240213008
C	0.190745721	2.688826142	0.056461994
C	-0.329635078	3.623262347	-0.852729078
C	1.056212907	3.155594952	1.057734069
C	-0.004731705	4.973108364	-0.757770068

H	-0.999898219	3.281261494	-1.636748136
C	1.368822282	4.508721974	1.163894080
H	1.477898757	2.445897790	1.764607123
C	0.841745475	5.424163165	0.254703009
H	-0.418348556	5.676780531	-1.475254125
H	2.031997418	4.847440833	1.955602141
H	1.090248768	6.478852211	0.332286015
C	0.191403336	-2.688646275	-0.057009015
C	1.056853280	-3.155066531	-1.058461090
C	-0.328519945	-3.623299209	0.852207055
C	1.369915959	-4.508076717	-1.164743102
H	1.478176496	-2.445190587	-1.765376145
C	-0.003169267	-4.973033401	0.757123048
H	-0.998788910	-3.281577010	1.636344115
C	0.843304680	-5.423744639	-0.255504030
H	2.033081925	-4.846527912	-1.956572160
H	-0.416430480	-5.676884355	1.474637104
H	1.092162431	-6.478343778	-0.333177036
N	2.259181186	0.000344400	0.000153989
Si	3.123660470	0.828119240	-1.324516112
Si	3.123151042	-0.827594884	1.325075093
C	1.931016429	1.038271565	-2.765274226
H	1.130714550	1.747616824	-2.534115205
H	2.476695573	1.427222453	-3.633278291
H	1.473720151	0.086951609	-3.059855246
C	3.875861958	2.500442174	-0.908420078
H	4.494918089	2.823631041	-1.754803146
H	3.108283093	3.260674435	-0.741149065

H	4.517337996	2.464642011	-0.023041012
C	4.519073284	-0.305684205	-1.895579159
H	5.297751293	-0.439562416	-1.137959097
H	4.146212000	-1.295834187	-2.177789179
H	4.996780436	0.137397706	-2.777685226
C	1.930096893	-1.037313596	2.765558203
H	1.129426654	-1.746159443	2.534101187
H	2.475256835	-1.426712765	3.633674269
H	1.473244104	-0.085764404	3.060095223
C	4.518646440	0.305937842	1.896546135
H	4.995848365	-0.137370315	2.778824201
H	5.297674510	0.439667651	1.139261074
H	4.145925667	1.296134014	2.178754155
C	3.875130667	-2.500051208	0.909180061
H	4.494172632	-2.823289393	1.755551122
H	3.107532412	-3.260261068	0.741879044
H	4.516598725	-2.464271370	0.023793991

Borole 7

C	0.041273945	1.257990092	-0.054142989
C	1.309636061	0.764462096	-0.040844988
C	0.047470031	-1.259062104	0.049384019
C	1.313386113	-0.759198021	0.037325018
B	-0.919383085	-0.002884039	-0.002271985
C	-2.477985204	-0.005838093	-0.000246985
C	-3.196528246	-0.490058154	-1.114604071
C	-3.193396279	0.471467919	1.118977102
C	-4.591512353	-0.477537201	-1.096954068

C	-4.588390382	0.447330870	1.110204100
C	-5.308755428	-0.015104190	0.007696016
H	-5.132954380	-0.844887248	-1.967445134
H	-5.127109437	0.802035877	1.987546169
C	2.558742129	1.546692196	-0.096019992
C	3.570815214	1.369940222	0.859012084
C	2.751353112	2.497755277	-1.109025072
C	4.730347275	2.138879316	0.814831076
H	3.442882227	0.633514159	1.647121143
C	3.918759177	3.251858374	-1.162972073
H	1.974072047	2.641102260	-1.854210129
C	4.910578256	3.079318396	-0.197670000
H	5.498419328	1.996191333	1.569875134
H	4.052654161	3.979557436	-1.958573133
H	5.819934301	3.672459474	-0.236692003
C	2.566353233	-1.535055038	0.094846023
C	2.762094283	-2.484571106	1.108697098
C	3.579111305	-1.353678991	-0.858576053
C	3.933245399	-3.232659125	1.165077103
H	1.984255227	-2.631524142	1.852596160
C	4.742470424	-2.116683008	-0.812000046
H	3.448723270	-0.618368937	-1.647324109
C	4.925807470	-3.055601074	0.201361031
H	4.069491432	-3.959232172	1.961309165
H	5.511066452	-1.970514970	-1.565844105
H	5.838110534	-3.644070088	0.242252034
C	-0.354330952	-2.673601226	0.035944018
C	0.302567132	-3.631688277	-0.756324043

C	-1.461284020	-3.094505296	0.791466074
C	-0.119211856	-4.956478392	-0.775647046
H	1.145910186	-3.327725225	-1.369143090
C	-1.877031009	-4.423416411	0.779628078
H	-2.000328086	-2.368721258	1.393566123
C	-1.207831926	-5.361789466	-0.002871985
H	0.402627209	-5.676147423	-1.400832092
H	-2.732133066	-4.723204467	1.379472122
H	-1.535512914	-6.397511530	-0.018084986
C	-0.367841135	2.670396185	-0.040296988
C	-1.476239236	3.085822180	-0.796695044
C	0.283155883	3.631519279	0.753144074
C	-1.898919310	4.412539268	-0.784763044
H	-2.010639253	2.357360102	-1.399706093
C	-0.145597196	4.954069366	0.772654077
H	1.127524960	3.331698288	1.366596123
C	-1.235494291	5.354038343	-0.001096985
H	-2.754823388	4.708228258	-1.385514093
H	0.371798820	5.676177427	1.398720124
H	-1.568587355	6.388028409	0.014230017
C	-2.462111236	0.971449983	2.337573197
H	-3.161440302	1.275524983	3.121446255
H	-1.806696162	0.200403946	2.761409226
H	-1.833636221	1.836488073	2.096516174
C	-2.468729169	-0.992015166	-2.334417162
H	-3.170311212	-1.304293218	-3.113018224
H	-1.820808149	-0.218649086	-2.765490199
H	-1.833205095	-1.851648213	-2.092639147

C	-6.811925527	0.010186761	-0.000924985
H	-7.185617588	0.959969822	-0.402927016
H	-7.221764522	-0.791406314	-0.622810030
H	-7.219297550	-0.099470262	1.008598094

Borole [7]⁻

C	0.037649994	1.228323108	-0.090821007
C	1.346097088	0.735114053	-0.053400004
C	0.045647959	-1.229592081	0.087626007
C	1.350858064	-0.727797061	0.050882004
B	-0.906444098	-0.003743972	-0.001706000
C	-2.489449221	-0.007890949	-0.000300000
C	-3.219728282	-0.469292974	-1.117151086
C	-3.218595271	0.445357096	1.120801086
C	-4.617359391	-0.464994953	-1.102343087
C	-4.616058377	0.428868115	1.112552086
C	-5.338028455	-0.018049909	0.005465000
H	-5.157080433	-0.825321972	-1.978693151
H	-5.154790413	0.775852149	1.994878153
C	2.574734194	1.546364096	-0.105128008
C	3.615126273	1.378195069	0.826265061
C	2.743970222	2.533446171	-1.092889082
C	4.765262368	2.161030115	0.775567060
H	3.509800252	0.624777014	1.601754121
C	3.893249320	3.315528213	-1.145727086
H	1.951424160	2.679377196	-1.821532138
C	4.914128395	3.135771184	-0.210941016
H	5.550585409	2.007471090	1.512401114

H	3.992902339	4.070510273	-1.922482149
H	5.812689494	3.746601218	-0.251480019
C	2.584796150	-1.530900140	0.103860008
C	2.759750150	-2.516153219	1.092442086
C	3.624798231	-1.356486139	-0.826790063
C	3.914115229	-3.290590296	1.146764088
H	1.967580084	-2.666863217	1.820520139
C	4.780016312	-2.131726216	-0.774664062
H	3.515119234	-0.604243084	-1.602823123
C	4.934519309	-3.104780294	0.212644016
H	4.018125223	-4.044353354	1.924132150
H	5.564891346	-1.973494217	-1.510987115
H	5.837043342	-3.709662354	0.254297020
C	-0.343338092	-2.641600184	0.053549004
C	0.332373946	-3.608754264	-0.721394053
C	-1.478632186	-3.083719198	0.764020058
C	-0.086711105	-4.934666362	-0.762918057
H	1.194276019	-3.303328254	-1.307090099
C	-1.900333240	-4.409385297	0.720852054
H	-2.033833219	-2.361268135	1.355560105
C	-1.205485199	-5.350830364	-0.039207003
H	0.462298927	-5.648659417	-1.373707107
H	-2.781159312	-4.708063309	1.285544097
H	-1.533639235	-6.386892477	-0.073746005
C	-0.360889017	2.637624222	-0.056186005
C	-1.498706097	3.072279275	-0.767234059
C	0.307498049	3.608963290	0.719872055
C	-1.929713113	4.394915379	-0.723533056

H	-2.048157153	2.346188223	-1.359666103
C	-0.120892965	4.931894394	0.761918060
H	1.171128112	3.309205254	1.305962100
C	-1.242038044	5.340692440	0.037679003
H	-2.812092177	4.687894416	-1.288815101
H	0.422634087	5.649329461	1.373573103
H	-1.577443057	6.374413525	0.072650006
C	-2.492613203	0.945422125	2.342120179
H	-1.975270152	1.888878187	2.132238163
H	-3.184311258	1.112797148	3.175158243
H	-1.724131154	0.233547058	2.665721205
C	-2.495271234	-0.973590024	-2.337640180
H	-1.974476206	-1.914442105	-2.124666166
H	-3.188423288	-1.146839025	-3.168268244
H	-1.729850163	-0.260809979	-2.666410205
C	-6.843190536	0.010926115	-0.004871000
H	-7.223176578	0.970668193	-0.379458029
H	-7.253663591	-0.774910939	-0.648199050
H	-7.252129612	-0.129125889	1.001718075

Borole [7]²⁻

C	0.037142052	1.212142127	-0.137254050
C	1.393251136	0.714654028	-0.073188056
C	0.047973947	-1.213718054	0.136510009
C	1.399543074	-0.704147076	0.072476978
B	-0.886084073	-0.005022921	-0.000664007
C	-2.480764195	-0.010948849	-0.000122984
C	-3.220131287	-0.477057869	-1.112721052

C	-3.221227213	0.445584238	1.116070104
C	-4.618885395	-0.474685805	-1.100423031
C	-4.619700323	0.430193300	1.108077125
C	-5.343105435	-0.022340720	0.003481058
H	-5.157333470	-0.840195822	-1.977259085
H	-5.159023334	0.781873366	1.990075198
C	2.594129265	1.542892037	-0.162438094
C	3.703392355	1.386989990	0.702685960
C	2.697955302	2.575640098	-1.125225188
C	4.839204475	2.182017994	0.594023920
H	3.653843325	0.623835946	1.474106033
C	3.830243429	3.374631104	-1.229705224
H	1.858193236	2.732092135	-1.796657230
C	4.922230517	3.186695053	-0.375333169
H	5.669171544	2.020279958	1.281181967
H	3.862855453	4.155467151	-1.988890296
H	5.808621602	3.813092059	-0.456002198
C	2.607709128	-1.521848192	0.161381980
C	2.721142108	-2.553020263	1.124738069
C	3.714895208	-1.356940247	-0.704681106
C	3.860241159	-3.342346376	1.228687071
H	1.883316042	-2.716269227	1.796972133
C	4.857467265	-2.142321355	-0.596639098
H	3.658216229	-0.594605195	-1.476434175
C	4.949803239	-3.145721425	0.373185988
H	3.900141139	-4.122422424	1.988305142
H	5.685436336	-1.973955390	-1.284612168
H	5.841499279	-3.764604510	0.453393992

C	-0.342047148	-2.607051144	0.050252031
C	0.386796852	-3.601986267	-0.661850018
C	-1.552152253	-3.063720119	0.643258101
C	-0.047013242	-4.919531348	-0.755537998
H	1.304614931	-3.314088295	-1.165054073
C	-1.989339350	-4.377928197	0.538159123
H	-2.148781260	-2.345347022	1.198338142
C	-1.241308345	-5.336016312	-0.157528929
H	0.555575764	-5.633994433	-1.317121040
H	-2.928090429	-4.662301171	1.013812173
H	-1.579171419	-6.367848393	-0.233917913
C	-0.365672915	2.601741252	-0.050253060
C	-1.580495997	3.047072335	-0.642369093
C	0.354203197	3.603489311	0.661474969
C	-2.030176969	4.356960459	-0.536633102
H	-2.170416084	2.323061299	-1.197250117
C	-0.092108777	4.916845435	0.755630964
H	1.275189263	3.324373257	1.163858000
C	-1.290825858	5.322032486	0.158701927
H	-2.971921037	4.632520515	-1.011617129
H	0.504058310	5.636956450	1.316857986
H	-1.638490839	6.350564618	0.235616922
C	-2.496662118	0.950532263	2.334923183
H	-2.014530039	1.913795313	2.130127142
H	-3.182179155	1.077527315	3.182954252
H	-1.692153084	0.261300177	2.617144200
C	-2.494870271	-0.987176962	-2.329035149
H	-2.009304276	-1.947664054	-2.119404122

H	-3.180507347	-1.121030955	-3.175922201
H	-1.693006187	-0.296725948	-2.615696191
C	-6.849193522	0.010890351	-0.009907922
H	-7.233811506	0.970680438	-0.384218961
H	-7.260757582	-0.775901702	-0.653609956
H	-7.260693552	-0.130334625	0.997010165

Borole 8

C	-1.170939090	0.464458035	-0.162375057
C	-0.711342056	0.275556021	-1.429825153
C	1.170939090	-0.464458035	-0.162375057
C	0.711342056	-0.275556021	-1.429825153
B	0.000000000	0.000000000	0.801611016
C	0.000000000	0.000000000	2.362532138
C	0.014537001	-1.222899094	3.063194191
C	-0.014537001	1.222899094	3.063194191
C	0.008857001	-1.222966093	4.466835298
C	-0.008857001	1.222966093	4.466835298
C	0.000000000	0.000000000	5.137483349
C	-1.445466113	0.543723040	-2.680950249
C	-0.892046069	1.339100105	-3.695149330
C	-2.726744211	0.006143000	-2.873941266
C	-1.608865126	1.606356122	-4.858230418
H	0.101796008	1.758043134	-3.566645318
C	-3.433789263	0.258088020	-4.044765356
H	-3.163741244	-0.611497046	-2.094528209
C	-2.879555223	1.063515082	-5.039472430
H	-1.168734088	2.233820170	-5.628244499

H	-4.422481339	-0.171860014	-4.179319366
H	-3.434277265	1.264418098	-5.951722508
C	1.445466113	-0.543723040	-2.680950249
C	2.726744211	-0.006143000	-2.873941266
C	0.892046069	-1.339100105	-3.695149330
C	3.433789263	-0.258088020	-4.044765356
H	3.163741244	0.611497046	-2.094528209
C	1.608865126	-1.606356122	-4.858230418
H	-0.101796008	-1.758043134	-3.566645318
C	2.879555223	-1.063515082	-5.039472430
H	4.422481339	0.171860014	-4.179319366
H	1.168734088	-2.233820170	-5.628244499
H	3.434277265	-1.264418098	-5.951722508
C	2.452998190	-1.055736081	0.249369974
C	3.012907233	-2.168351166	-0.402093076
C	3.133813244	-0.536194039	1.362883061
C	4.212227327	-2.723357207	0.031125957
H	2.494710190	-2.604521200	-1.250865144
C	4.339750334	-1.085389084	1.790166093
H	2.708435208	0.307980024	1.897712103
C	4.886034375	-2.181557170	1.126212040
H	4.621375354	-3.586738274	-0.486883083
H	4.849240374	-0.658473052	2.649896160
H	5.823523445	-2.615830200	1.462306068
C	-2.452998190	1.055736081	0.249369974
C	-3.133813244	0.536194039	1.362883061
C	-3.012907233	2.168351166	-0.402093076
C	-4.339750334	1.085389084	1.790166093

H	-2.708435208	-0.307980024	1.897712103
C	-4.212227327	2.723357207	0.031125957
H	-2.494710190	2.604521200	-1.250865144
C	-4.886034375	2.181557170	1.126212040
H	-4.849240374	0.658473052	2.649896160
H	-4.621375354	3.586738274	-0.486883083
H	-5.823523445	2.615830200	1.462306068
C	0.000000000	2.534573197	2.322637132
H	0.879519068	3.134791243	2.588081155
H	0.017676002	2.396672183	1.237232051
H	-0.883612069	3.140356240	2.556528152
C	0.000000000	-2.534573197	2.322637132
H	-0.879519068	-3.134791243	2.588081155
H	-0.017676002	-2.396672183	1.237232051
H	0.883612069	-3.140356240	2.556528152
H	0.000000000	0.000000000	6.226621410
C	-0.014773001	2.510922191	5.242281357
H	0.866114066	3.124870238	5.017616341
H	-0.893865068	3.122146240	5.005115338
H	-0.021412001	2.320089180	6.318919448
C	0.014773001	-2.510922191	5.242281357
H	-0.866114066	-3.124870238	5.017616341
H	0.893865068	-3.122146240	5.005115338
H	0.021412001	-2.320089180	6.318919448

Borole 9

C	-0.697484100	1.251426040	0.168280044
C	-1.974879185	0.788230981	0.084850991

C	-0.751933047	-1.247877144	-0.133305069
C	-2.007550154	-0.722768131	-0.106689079
B	0.243122002	-0.021809038	0.038881011
C	1.804134123	-0.061510012	0.074366050
C	2.478772160	-0.680801083	1.147987128
C	2.560518191	0.519138085	-0.969179993
C	3.874868269	-0.700227058	1.163640159
C	3.952953299	0.463415105	-0.925926955
C	4.632166337	-0.139481966	0.135809119
H	4.394758298	-1.165018115	1.999701217
H	4.525052358	0.899787181	-1.742466993
C	-3.209214297	1.592913014	0.157829996
C	-4.196689350	1.497850025	-0.833945106
C	-3.412831357	2.482206044	1.223247102
C	-5.342888472	2.285270064	-0.772530102
H	-4.060474305	0.809901006	-1.663361190
C	-4.567087463	3.255284077	1.292888109
H	-2.654694316	2.562387033	1.997062184
C	-5.534456510	3.163498087	0.292342007
H	-6.091777469	2.205759070	-1.555630180
H	-4.709819505	3.934407097	2.128870193
H	-6.433590570	3.771052117	0.344521011
C	-3.274990235	-1.465907204	-0.238008145
C	-3.472278208	-2.342746238	-1.314863263
C	-4.301782337	-1.323315251	0.707078909
C	-4.659108280	-3.056953312	-1.441475328
H	-2.683543128	-2.459682207	-2.052553308
C	-5.481544395	-2.052615323	0.589249847

H	-4.170152359	-0.644189225	1.544476997
C	-5.666542380	-2.918504356	-0.486854273
H	-4.796132257	-3.726907336	-2.285770422
H	-6.261334485	-1.937167358	1.336910888
H	-6.591380430	-3.480325412	-0.583306324
C	-0.386234990	-2.671043247	-0.209253117
C	-1.072802042	-3.657900358	0.519254887
C	0.711450119	-3.075467229	-0.986272164
C	-0.689597983	-4.993151450	0.455695844
H	-1.910258128	-3.369299374	1.147531924
C	1.088073177	-4.414196318	-1.059909210
H	1.275359166	-2.328521138	-1.536475170
C	0.389312125	-5.380605422	-0.339489206
H	-1.234124023	-5.735294517	1.033445850
H	1.936460266	-4.699803301	-1.676092248
H	0.686687169	-6.424340499	-0.389609240
C	-0.265520094	2.654673149	0.262759112
C	0.816436965	3.003449169	1.087379214
C	-0.869366141	3.674643246	-0.492811924
C	1.256163970	4.321575276	1.180376279
H	1.317923003	2.228780096	1.659394240
C	-0.422937135	4.989018348	-0.409444860
H	-1.691397186	3.428434233	-1.158340004
C	0.638265922	5.321897387	0.432865242
H	2.090432012	4.564166288	1.833166359
H	-0.903807171	5.757591400	-1.008735892
H	0.984941923	6.349443450	0.498296293
C	1.868844156	1.143257162	-2.170820079

H	0.792128070	1.183167138	-1.947254085
C	1.705395083	-1.268240186	2.317568175
H	0.638448006	-1.252512197	2.048664131
C	6.146414438	-0.186595942	0.178320156
H	6.423343476	-0.715775011	1.100381215
C	2.038968217	0.277867144	-3.424865202
H	3.095243308	0.204658168	-3.707896199
H	1.665302202	-0.739146950	-3.268284237
H	1.493926187	0.712545199	-4.270317262
C	2.325833172	2.579242292	-2.437135039
H	2.186115127	3.210547305	-1.555184952
H	3.384251261	2.614524323	-2.719450032
H	1.751076140	3.014211343	-3.262121100
C	1.866746047	-0.413302163	3.579915306
H	2.912619122	-0.393860154	3.907011358
H	1.551422009	0.621301917	3.410591323
H	1.265673994	-0.820519234	4.400702345
C	2.076665132	-2.725922304	2.598347157
H	1.944234160	-3.347284320	1.708237062
H	3.118318209	-2.815445299	2.926885201
H	1.444501074	-3.132550373	3.395312187
C	6.724132534	-0.977276950	-0.999368946
H	6.498797537	-0.487008881	-1.953143007
H	7.813896612	-1.055162935	-0.915283920
H	6.310027524	-1.989719035	-1.038307999
C	6.756762450	1.216398173	0.248933227
H	6.368602418	1.774964180	1.106428304
H	7.847135558	1.159154191	0.341420258

H	6.529252481	1.792730248	-0.654853829
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Borole 10

C	3.939046843	-0.752978579	-1.007268092
C	5.206357953	-0.455493247	-0.611882060
C	3.939057755	0.752652537	1.007253063
C	5.206366843	0.455143824	0.611864036
B	2.976343223	-0.000140181	-0.000012014
C	6.452852146	-0.920098993	-1.248388112
C	7.467563703	-0.018258712	-1.602244139
C	6.641703017	-2.282640995	-1.524176133
C	8.626645820	-0.464215337	-2.230827186
H	7.342867529	1.039888244	-1.391611120
C	7.808796084	-2.729239996	-2.134887176
H	5.864140604	-2.990565423	-1.252665108
C	8.803955918	-1.821058794	-2.495063204
H	9.396631526	0.250655453	-2.507290210
H	7.939731152	-3.789260244	-2.333966192
H	9.713267591	-2.169538650	-2.976730242
C	6.452865798	0.919742153	1.248364083
C	6.641703017	2.282281366	1.524188103
C	7.467594448	0.017909290	1.602192111
C	7.808796137	2.728881431	2.134894151
H	5.864132296	2.990205043	1.252700082
C	8.626676512	0.463865734	2.230776158
H	7.342911556	-1.040236919	1.391547095
C	8.803972428	1.820705489	2.495039179
H	7.939719087	3.788899350	2.333995165

H	9.396671902	-0.251002588	2.507219178
H	9.713282937	2.169185689	2.976707213
C	3.561783809	1.561263367	2.179487156
C	4.097735046	1.310591104	3.452833252
C	2.623155537	2.597348658	2.051173145
C	3.718316990	2.074438037	4.552196335
H	4.815905150	0.504809218	3.575805260
C	2.251551858	3.369102218	3.148902230
H	2.186472015	2.799302239	1.076701068
C	2.796883734	3.110875516	4.405204326
H	4.143597848	1.858372987	5.528632385
H	1.529351582	4.171275295	3.022586219
H	2.502042819	3.707683448	5.263781390
C	3.561743729	-1.561598876	-2.179482181
C	2.622974865	-2.597558741	-2.051151174
C	4.097795568	-1.311084102	-3.452817281
C	2.251337483	-3.369345296	-3.148845254
H	2.186210326	-2.799388187	-1.076690098
C	3.718342560	-2.074961287	-4.552146365
H	4.816066570	-0.505396868	-3.575813288
C	2.796774682	-3.111275966	-4.405134353
H	1.529032652	-4.171421342	-3.022513245
H	4.143699768	-1.859014307	-5.528575446
H	-2.501908551	3.708108124	-5.263686418
C	-3.939046843	0.752978579	-1.007268092
C	-5.206357953	0.455493247	-0.611882060
C	-3.939057755	-0.752652537	1.007253063
C	-5.206366843	-0.455143824	0.611864036

B	-2.976343223	0.000140181	-0.000012014
C	-6.452852146	0.920098993	-1.248388112
C	-7.467563703	0.018258712	-1.602244139
C	-6.641703017	2.282640995	-1.524176133
C	-8.626645820	0.464215337	-2.230827186
H	-7.342867529	-1.039888244	-1.391611120
C	-7.808796084	2.729239996	-2.134887176
H	-5.864140604	2.990565423	-1.252665108
C	-8.803955918	1.821058794	-2.495063204
H	-9.396631526	-0.250655453	-2.507290210
H	-7.939731152	3.789260244	-2.333966192
H	-9.713267591	2.169538650	-2.976730242
C	-6.452865798	-0.919742153	1.248364083
C	-6.641703017	-2.282281366	1.524188103
C	-7.467594448	-0.017909290	1.602192111
C	-7.808796137	-2.728881431	2.134894151
H	-5.864132296	-2.990205043	1.252700082
C	-8.626676512	-0.463865734	2.230776158
H	-7.342911556	1.040236919	1.391547095
C	-8.803972428	-1.820705489	2.495039179
H	-7.939719087	-3.788899350	2.333995165
H	-9.396671902	0.251002588	2.507219178
H	-9.713282937	-2.169185689	2.976707213
C	-3.561783809	-1.561263367	2.179487156
C	-4.097735046	-1.310591104	3.452833252
C	-2.623155537	-2.597348658	2.051173145
C	-3.718316990	-2.074438037	4.552196335
H	-4.815905150	-0.504809218	3.575805260

C	-2.251551858	-3.369102218	3.148902230
H	-2.186472015	-2.799302239	1.076701068
C	-2.796883734	-3.110875516	4.405204326
H	-4.143597848	-1.858372987	5.528632385
H	-1.529351582	-4.171275295	3.022586219
H	-2.502042819	-3.707683448	5.263781390
C	-3.561743729	1.561598876	-2.179482181
C	-2.622974865	2.597558741	-2.051151174
C	-4.097795568	1.311084102	-3.452817281
C	-2.251337483	3.369345296	-3.148845254
H	-2.186210326	2.799388187	-1.076690098
C	-3.718342560	2.074961287	-4.552146365
H	-4.816066570	0.505396868	-3.575813288
C	-2.796774682	3.111275966	-4.405134353
H	-1.529032652	4.171421342	-3.022513245
H	-4.143699768	1.859014307	-5.528575446
H	2.501908551	-3.708108124	-5.263686418
C	-1.426528108	0.000074187	-0.000020014
C	-0.694082003	0.022359691	-1.204711108
C	-0.694085104	-0.022286312	1.204671076
C	0.694082003	-0.022359691	-1.204711108
H	-1.222613709	0.050685587	-2.153518179
C	0.694085104	0.022286312	1.204671076
H	-1.222620477	-0.050549420	2.153477152
C	1.426528108	-0.000074187	-0.000020014
H	1.222613709	-0.050685587	-2.153518179
H	1.222620477	0.050549420	2.153477152

Borole 11

C	-0.733801159	3.916854573	1.279469031
C	-0.434259117	4.802232855	0.290868957
C	0.765138887	2.881057811	-0.453314101
C	0.476401682	4.174394181	-0.759211123
B	0.007994035	2.569445443	0.902121006
C	-0.900455659	6.198411447	0.197920950
C	0.000000000	7.252919779	-0.014943067
C	-2.263633398	6.499366350	0.335595960
C	-0.448310439	8.569743390	-0.067118071
H	1.058665760	7.039878575	-0.130603076
C	-2.712497273	7.813941063	0.264882954
H	-2.969949312	5.690526121	0.498137973
C	-1.805707918	8.855066873	0.068376940
H	0.265407323	9.374111277	-0.222046083
H	-3.773040352	8.026361860	0.367608963
H	-2.155594480	9.882389888	0.018392936
C	0.952024479	4.919989293	-1.939800216
C	2.317493645	4.941192398	-2.260535239
C	0.057668771	5.609333927	-2.772218280
C	2.774548168	5.630482178	-3.378963325
H	3.019273860	4.411541404	-1.622900192
C	0.514181335	6.282857024	-3.901637367
H	-1.002936628	5.608623824	-2.538090262
C	1.873969666	6.300260975	-4.206613392
H	3.836730406	5.640823042	-3.607285343
H	-0.194829100	6.802179299	-4.540422417
H	2.230485539	6.834401378	-5.082929455

C	1.579148987	1.955504715	-1.260056164
C	1.335255013	1.756075145	-2.627888265
C	2.613721534	1.219894437	-0.660126118
C	2.105358742	0.865435619	-3.369208324
H	0.526356565	2.300378714	-3.106582306
C	3.391732986	0.336672805	-1.404139175
H	2.810862285	1.351250480	0.400628965
C	3.140481676	0.154465424	-2.762930277
H	1.893328589	0.723358661	-4.425610406
H	4.193732529	-0.213938094	-0.919393135
H	3.741704719	-0.540022271	-3.343155324
C	-1.548030613	4.188136618	2.476395127
C	-2.576370558	3.305243023	2.843498154
C	-1.312033731	5.302816419	3.297215188
C	-3.354166915	3.538736251	3.974639242
H	-2.767976543	2.430327634	2.227921104
C	-2.082184583	5.530765181	4.433582276
H	-0.513255658	5.992080105	3.038171166
C	-3.110155999	4.652541090	4.776051303
H	-4.149799218	2.844874031	4.232710260
H	-1.877637177	6.398244864	5.055433321
H	-3.741704719	0.540022271	-3.343155324
C	-0.765138887	-2.881057811	-0.453314101
C	-0.476401682	-4.174394181	-0.759211123
C	0.733801159	-3.916854573	1.279469031
C	0.434259117	-4.802232855	0.290868957
B	-0.007994035	-2.569445443	0.902121006
C	-0.952024479	-4.919989293	-1.939800216

C	-0.057668771	-5.609333927	-2.772218280
C	-2.317493645	-4.941192398	-2.260535239
C	-0.514181335	-6.282857024	-3.901637367
H	1.002936628	-5.608623824	-2.538090262
C	-2.774548168	-5.630482178	-3.378963325
H	-3.019273860	-4.411541404	-1.622900192
C	-1.873969666	-6.300260975	-4.206613392
H	0.194829100	-6.802179299	-4.540422417
H	-3.836730406	-5.640823042	-3.607285343
H	-2.230485539	-6.834401378	-5.082929455
C	0.900455659	-6.198411447	0.197920950
C	2.263633398	-6.499366350	0.335595960
C	0.000000000	-7.252919779	-0.014943067
C	2.712497273	-7.813941063	0.264882954
H	2.969949312	-5.690526121	0.498137973
C	0.448310439	-8.569743390	-0.067118071
H	-1.058665760	-7.039878575	-0.130603076
C	1.805707918	-8.855066873	0.068376940
H	3.773040352	-8.026361860	0.367608963
H	-0.265407323	-9.374111277	-0.222046083
H	2.155594480	-9.882389888	0.018392936
C	1.548030613	-4.188136618	2.476395127
C	1.312033731	-5.302816419	3.297215188
C	2.576370558	-3.305243023	2.843498154
C	2.082184583	-5.530765181	4.433582276
H	0.513255658	-5.992080105	3.038171166
C	3.354166915	-3.538736251	3.974639242
H	2.767976543	-2.430327634	2.227921104

C	3.110155999	-4.652541090	4.776051303
H	1.877637177	-6.398244864	5.055433321
H	4.149799218	-2.844874031	4.232710260
H	3.711853635	-4.832568386	5.662528358
C	-1.579148987	-1.955504715	-1.260056164
C	-2.613721534	-1.219894437	-0.660126118
C	-1.335255013	-1.756075145	-2.627888265
C	-3.391732986	-0.336672805	-1.404139175
H	-2.810862285	-1.351250480	0.400628965
C	-2.105358742	-0.865435619	-3.369208324
H	-0.526356565	-2.300378714	-3.106582306
C	-3.140481676	-0.154465424	-2.762930277
H	-4.193732529	0.213938094	-0.919393135
H	-1.893328589	-0.723358661	-4.425610406
H	-3.711853635	4.832568386	5.662528358
C	-0.000296489	-1.234216571	1.684907065
C	0.000000000	0.000000000	1.009688014
C	0.028882412	-1.204589964	3.094453172
C	0.000296489	1.234216571	1.684907065
H	0.000000000	0.000000000	-0.076592072
C	0.000000000	0.000000000	3.791170224
H	0.061494351	-2.138781889	3.648786216
C	-0.028882412	1.204589964	3.094453172
H	0.000000000	0.000000000	4.877784311
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C	0.720075058	3.914190303	-1.125593077
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C	1.367199105	4.636529356	-2.079365148
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B	0.950276072	2.392855185	-1.497155105
C	1.445546109	6.107191450	-2.160645154
C	2.678758207	6.761541502	-2.297958168
C	0.279517022	6.883594542	-2.088505150
C	2.744187211	8.151290607	-2.341399169
H	3.592253274	6.177396496	-2.361079171
C	0.344656027	8.271705631	-2.151152154
H	-0.680836051	6.387224483	-1.983647144
C	1.577950120	8.911214696	-2.272778163
H	3.709388288	8.640779668	-2.437451180
H	-0.570003041	8.855894665	-2.100004151
H	1.629181124	9.995578785	-2.316131167
C	2.811187216	4.256782326	-4.243170316
C	4.104953314	3.778598291	-4.499009339
C	2.276318173	5.231816401	-5.098241384
C	4.840485375	4.258919329	-5.577326429
H	4.529750346	3.024837233	-3.842463285
C	3.006186232	5.697835435	-6.188109478
H	1.278549099	5.618844406	-4.913084366
C	4.291762329	5.216833403	-6.429435470
H	5.843284459	3.880652298	-5.755577457
H	2.571004198	6.445151505	-6.845804512
H	4.864105376	5.588114448	-7.274963557
C	2.267222172	1.260504097	-3.616600270
C	2.049279157	1.189309092	-5.001839376

C	2.902424226	0.174532014	-2.992698219
C	2.461658186	0.081446006	-5.735255410
H	1.543477122	2.010622155	-5.501245399
C	3.324889258	-0.929919073	-3.728316276
H	3.071523234	0.205411015	-1.919561138
C	3.105299237	-0.982374075	-5.103552382
H	2.275943177	0.047066003	-6.805477502
H	3.823184294	-1.753917134	-3.224115235
H	3.427470262	-1.846840140	-5.677413427
C	0.000000000	4.448525342	0.042117014
C	-1.285984098	3.976032306	0.350666037
C	0.571794047	5.407754437	0.893032080
C	-1.984738154	4.462007344	1.452729119
H	-1.740675135	3.224380247	-0.289421013
C	-0.121641010	5.885020457	2.000622166
H	1.573505121	5.771820447	0.683802063
C	-1.405000109	5.418528433	2.284161183
H	-2.983037231	4.088238314	1.665119138
H	0.344391026	6.622988505	2.648180212
H	-3.427470262	1.846840140	-5.677413427
C	-1.819304138	-2.415073184	-2.819809206
C	-2.036555158	-3.727299287	-3.105101229
C	-0.720075058	-3.914190303	-1.125593077
C	-1.367199105	-4.636529356	-2.079365148
B	-0.950276072	-2.392855185	-1.497155105
C	-2.811187216	-4.256782326	-4.243170316
C	-2.276318173	-5.231816401	-5.098241384
C	-4.104953314	-3.778598291	-4.499009339

C	-3.006186232	-5.697835435	-6.188109478
H	-1.278549099	-5.618844406	-4.913084366
C	-4.840485375	-4.258919329	-5.577326429
H	-4.529750346	-3.024837233	-3.842463285
C	-4.291762329	-5.216833403	-6.429435470
H	-2.571004198	-6.445151505	-6.845804512
H	-5.843284459	-3.880652298	-5.755577457
H	-4.864105376	-5.588114448	-7.274963557
C	-1.445546109	-6.107191450	-2.160645154
C	-0.279517022	-6.883594542	-2.088505150
C	-2.678758207	-6.761541502	-2.297958168
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H	0.680836051	-6.387224483	-1.983647144
C	-2.744187211	-8.151290607	-2.341399169
H	-3.592253274	-6.177396496	-2.361079171
C	-1.577950120	-8.911214696	-2.272778163
H	0.570003041	-8.855894665	-2.100004151
H	-3.709388288	-8.640779668	-2.437451180
H	-1.629181124	-9.995578785	-2.316131167
C	0.000000000	-4.448525342	0.042117014
C	-0.571794047	-5.407754437	0.893032080
C	1.285984098	-3.976032306	0.350666037
C	0.121641010	-5.885020457	2.000622166
H	-1.573505121	-5.771820447	0.683802063
C	1.984738154	-4.462007344	1.452729119
H	1.740675135	-3.224380247	-0.289421013
C	1.405000109	-5.418528433	2.284161183
H	-0.344391026	-6.622988505	2.648180212

H	2.983037231	-4.088238314	1.665119138
H	1.945638152	-5.793141422	3.148902251
C	-2.267222172	-1.260504097	-3.616600270
C	-2.902424226	-0.174532014	-2.992698219
C	-2.049279157	-1.189309092	-5.001839376
C	-3.324889258	0.929919073	-3.728316276
H	-3.071523234	-0.205411015	-1.919561138
C	-2.461658186	-0.081446006	-5.735255410
H	-1.543477122	-2.010622155	-5.501245399
C	-3.105299237	0.982374075	-5.103552382
H	-3.823184294	1.753917134	-3.224115235
H	-2.275943177	-0.047066003	-6.805477502
H	-1.945638152	5.793141422	3.148902251
C	-0.448603035	-1.148787090	-0.725089049
C	0.000000000	0.000000000	-1.402098096
C	-0.432706034	-1.122481086	0.681356063
C	0.448603035	1.148787090	-0.725089049
H	0.000000000	0.000000000	-2.489020180
C	0.000000000	0.000000000	1.411514117
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C	0.432706034	1.122481086	0.681356063
H	0.769373062	2.001645155	1.224370101
H	-5.346623405	-3.575302272	2.461400197
C	-1.062279083	-0.672988051	3.921223312
C	-0.643913047	-0.408504031	5.188196410
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B	0.000000000	0.000000000	2.959326238

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C	-0.591673045	-1.495765115	7.446035608
C	-2.675325206	-0.599655044	6.627176520
C	-1.232817093	-1.923969148	8.604945690
H	0.470492036	-1.682893128	7.318059594
C	-3.310767253	-1.011387075	7.794040612
H	-3.237974250	-0.088051006	5.851731450
C	-2.592952200	-1.679607128	8.785512662
H	-0.665281050	-2.443281189	9.372183749
H	-4.370749336	-0.813671061	7.927571611
H	-3.090635238	-2.005693155	9.694537732
C	1.305961100	0.835728063	6.435093486
C	2.675325206	0.599655044	6.627176520
C	0.591673045	1.495765115	7.446035608
C	3.310767253	1.011387075	7.794040612
H	3.237974250	0.088051006	5.851731450
C	1.232817093	1.923969148	8.604945690
H	-0.470492036	1.682893128	7.318059594
C	2.592952200	1.679607128	8.785512662
H	4.370749336	0.813671061	7.927571611
H	0.665281050	2.443281189	9.372183749
H	3.090635238	2.005693155	9.694537732
C	2.237544171	1.474141112	3.539476284
C	2.468373192	2.750451209	4.076542322
C	3.149746242	0.982132077	2.592077211
C	3.575848277	3.499114268	3.691196296
H	1.764045137	3.157265242	4.796401380
C	4.263846329	1.726997131	2.213647182

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C	4.481693347	2.990037230	2.761097223
H	3.730157289	4.487162346	4.116698329
H	4.961197383	1.320970101	1.485441126
H	5.346623405	3.575302272	2.461400197
C	-2.237544171	-1.474141112	3.539476284
C	-3.149746242	-0.982132077	2.592077211
C	-2.468373192	-2.750451209	4.076542322
C	-4.263846329	-1.726997131	2.213647182
H	-2.982357227	-0.000339000	2.156796178
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H	-4.961197383	-1.320970101	1.485441126
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C	2.581255684	2.851651421	-1.665212136
C	3.752867221	3.003386139	-2.487590195
C	3.404453650	0.666835979	-2.345862187
C	4.244758636	1.699505282	-2.892674225
B	2.277596877	1.338016414	-1.519129126
C	4.365569368	4.263151578	-2.861905219
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C	4.137852820	6.603276652	-3.605446272

H	2.495384145	5.278854173	-3.217715249
C	5.531523810	6.785732470	-3.635405271
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C	6.339115497	0.437437401	-3.444975266
C	5.716319226	2.262536074	-4.880873373
C	7.471192588	0.219067667	-4.215457319
H	6.139047444	-0.196848894	-2.586217197
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H	8.143455132	-0.596647983	-3.943466299
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H	8.647332523	0.841026180	-5.943731455
C	3.448648735	-0.728825723	-2.757661223
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H	2.766426033	-1.476783294	-0.856058079
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H	-2.495384145	-5.278854173	-3.217715249
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H	-5.971175910	-7.741897496	-3.920691293
C	-1.987413955	-3.922278751	-0.877606071
C	-2.723665590	-5.003959292	-0.322720026
C	-0.599637353	-3.915827059	-0.578628053
C	-2.119647634	-6.007055927	0.429186032
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H	-2.738436150	-6.808743161	0.838220064
H	1.065230770	-4.844442123	0.394598019
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C	-3.079439678	1.761639603	-1.856446152
C	-3.812811669	1.161484593	-4.061557319
C	-3.100523349	3.102377427	-2.217217181
H	-2.766426033	1.476783294	-0.856058079
C	-3.841725210	2.506009590	-4.418764350
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C	-3.494157788	3.501804426	-3.501516283

H	-2.787345262	3.850067038	-1.490130128
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C	-1.075880113	-0.632050481	-0.712345074
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H	1.850275612	1.084702487	1.246574072
H	-5.469391522	3.329197602	2.516516166
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C	-1.484865984	0.187994325	7.717777597
C	-1.592890720	2.347737390	6.666422474
C	-2.077663547	0.714892772	8.857750648
H	-1.241495372	-0.869957258	7.683669584
C	-2.186723157	2.870481177	7.805434592
H	-1.410272736	2.988948871	5.808777445
C	-2.436780442	2.070455253	8.934172680
H	-2.272555696	0.052936775	9.704212733
H	-2.465987301	3.925592443	7.816274576

H	-2.914214449	2.481122961	9.824290724
C	1.192667473	-0.982008424	6.570473484
C	1.592890720	-2.347737390	6.666422474
C	1.484865984	-0.187994325	7.717777597
C	2.186723157	-2.870481177	7.805434592
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C	2.077663547	-0.714892772	8.857750648
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C	3.376647074	-1.380017207	4.389805326
C	2.229673553	-2.240596709	2.465089176
C	4.533141710	-2.048582394	4.000070299
H	3.403333017	-0.754822307	5.277421399
C	3.386971047	-2.900283746	2.073200148
H	1.336195023	-2.306927738	1.850847123
C	4.557877281	-2.827461549	2.839706207
H	5.436983596	-1.940624758	4.603668348
H	3.383156907	-3.466883252	1.143347074
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H	-1.336195023	2.306927738	1.850847123

C	-4.533141710	2.048582394	4.000070299
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C	-7.316604568	1.052512498	0.746363239
C	-8.559615996	0.579658811	0.459273175
C	-7.205468561	-0.968318640	-0.745064035
C	-8.492618875	-0.642318986	-0.448003992
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C	-3.945436145	-0.969532753	-0.096648974
C	-4.087551485	1.425237673	0.066662228
C	-2.562764083	-0.896422884	-0.086328962
C	-2.702798708	1.504503255	0.034451237
C	-1.906877220	0.347435403	-0.028317857
H	-1.986772973	-1.815324111	-0.142132037
H	-2.218332110	2.477534282	0.075582320
C	-9.838522734	1.139479958	0.935907254
C	-10.875475664	1.445936531	0.042140203
C	-10.036316913	1.388576929	2.302125375
C	-12.066037583	2.003104007	0.500007279
H	-10.743514574	1.255376496	-1.018993892
C	-11.233603564	1.928287769	2.760448447
H	-9.241034047	1.153336242	3.003489413
C	-12.251433562	2.242257653	1.860467402

H	-12.853747499	2.243735063	-0.208526760
H	-11.370546857	2.108005052	3.823184543
H	-13.184566784	2.668605608	2.217959458
C	-9.702457717	-1.344904370	-0.915326090
C	-9.877104359	-1.621382237	-2.279513218
C	-10.694689083	-1.761587405	-0.015220056
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C	-11.816477963	-2.452053424	-0.464936150
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H	-11.128284697	-2.493591160	-3.791085408
H	-12.569093320	-2.776371639	0.248369876
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C	-6.770802316	-2.116934357	-1.559333188
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H	-5.479431337	-0.937926843	-2.817177185
C	-5.896356439	-4.297498589	-3.116264477
H	-7.161280673	-5.494772503	-1.847054478
H	-4.726145226	-2.844277135	-4.194711444
H	-5.559935072	-5.138456617	-3.716173589
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C	-7.318793774	4.604704345	2.066339625
H	-8.348434956	3.560008107	0.494461415
C	-6.394573379	4.516168567	3.107003701
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C	4.754466036	-0.185791184	-0.008687873
C	3.945436114	0.969532896	-0.096648791
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C	2.562764051	0.896423027	-0.086328801
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H	2.218332073	-2.477534165	0.075583941
C	9.838522681	-1.139479979	0.935907142
C	10.875474500	-1.445937213	0.042140054
C	10.036317707	-1.388578326	2.302124227
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H	9.241034788	-1.153337750	3.003489296
C	12.251433298	-2.242258807	1.860466137
H	12.853747288	-2.243735883	-0.208528022
H	11.370546645	-2.108006517	3.823184294
H	13.184566572	-2.668606814	2.217957130
C	9.702458510	1.344903486	-0.915325804
C	9.877104518	1.621383713	-2.279512885
C	10.694689030	1.761587537	-0.015219697
C	11.007782623	2.294697197	-2.729789864
H	9.116684961	1.301254809	-2.985841966
C	11.816477751	2.452052646	-0.464935672
H	10.581043718	1.551294446	1.044313367
C	11.979713057	2.717172061	-1.823395757
H	11.128284697	2.493591896	-3.791083926
H	12.569093108	2.776370745	0.248370411
H	12.860550443	3.247522835	-2.174376738
C	6.770803268	2.116934558	-1.559332802
C	7.229200309	3.418837535	-1.301633679
C	5.855184649	1.936038289	-2.608182900
C	6.795419747	4.495741574	-2.068760653
H	7.929647838	3.581562513	-0.487341598
C	5.429005137	3.011744472	-3.382921878
H	5.479431337	0.937927419	-2.817176999
C	5.896357391	4.297499034	-3.116263752
H	7.161280673	5.494772926	-1.847052552
H	4.726146205	2.844277754	-4.194710957
H	5.559935072	5.138457337	-3.716172732

C	7.013812415	-2.245360891	1.556619091
C	6.074961433	-2.176091642	2.598239173
C	7.626344924	-3.483065349	1.302529978
C	5.774964342	-3.295656602	3.369999142
H	5.581065172	-1.230194401	2.804089266
C	7.318792769	-4.604704371	2.066339942
H	8.348433897	-3.560007880	0.494460910
C	6.394573273	-4.516168932	3.107004029
H	5.051112102	-3.214077245	4.176505206
H	7.803541090	-5.552487431	1.847779853
H	6.156668623	-5.391648928	3.704685003
H	4.416919464	1.945584361	-0.165271717
H	4.665366552	-2.341987964	0.139622966
C	-0.456204632	0.496941580	-0.029678840
H	-0.109288425	1.529060577	-0.022038755
C	0.456204596	-0.496941447	-0.029678915
H	0.109288566	-1.529059460	-0.022037998

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C	0.012717001	1.261994096	-0.769006067
C	0.023159002	0.699806055	-2.048302168
C	-0.023159002	-0.699806055	-2.048302168
C	-0.012717001	-1.261994096	-0.769006067
S	0.000000000	0.000000000	0.412528022
H	0.044486004	1.304669103	-2.947498237
H	-0.044486004	-1.304669103	-2.947498237
C	-0.499465038	3.441513267	0.924966064
C	-0.293660022	4.776332365	0.761156051

C	0.498489039	3.943960302	-1.327590114
C	0.292054023	5.082075390	-0.612528058
B	0.000000000	2.755292212	-0.407635041
C	-0.561459040	5.829794460	1.757011128
C	0.406287032	6.799420539	2.061576151
C	-1.789785138	5.875535431	2.433722179
C	0.159307013	7.772173579	3.025799224
H	1.362325107	6.784734547	1.546667108
C	-2.042467158	6.860187550	3.383070249
H	-2.547939193	5.131878393	2.207077161
C	-1.067476080	7.809987580	3.685972274
H	0.925415071	8.507557655	3.255205240
H	-3.002700230	6.883144529	3.890829292
H	-1.263706095	8.575974664	4.431033330
C	0.558722046	6.458397500	-1.069745091
C	1.799106141	6.795219507	-1.631473133
C	-0.423463032	7.455314572	-0.968225082
C	2.049600161	8.088596597	-2.078120169
H	2.568631198	6.033180455	-1.712641139
C	-0.178199013	8.743922664	-1.433302117
H	-1.388367105	7.215680571	-0.530778047
C	1.060175085	9.066870702	-1.985350163
H	3.019176232	8.332014639	-2.503654201
H	-0.954866071	9.499720705	-1.356083112
H	1.254308098	10.075625787	-2.338927187
C	1.006438077	3.878945299	-2.710661218
C	0.385657030	4.584766354	-3.752729297
C	2.122323164	3.086779234	-3.022261240

C	0.865870068	4.504992349	-5.056691397
H	-0.482596036	5.199170403	-3.531136281
C	2.609524201	3.014499231	-4.324945341
H	2.612251199	2.527071194	-2.229711183
C	1.981900155	3.721893286	-5.349018409
H	0.365837029	5.057136388	-5.847955453
H	3.479471267	2.399842182	-4.540474361
H	2.357097181	3.660915282	-6.366718494
C	-1.007384077	2.793904213	2.149462157
C	-2.152049167	1.984492150	2.102083151
C	-0.360714027	2.955103229	3.383739250
C	-2.644766204	1.372421105	3.251568242
H	-2.663070207	1.843843140	1.152958081
C	-0.845731063	2.334238179	4.530588340
H	0.531560039	3.572877275	3.436685255
C	-1.991979151	1.542891122	4.470731334
H	-3.536786270	0.754544060	3.192236238
H	-0.325402025	2.468276188	5.475178392
H	2.370080185	-1.058447083	5.366678429
C	0.499465038	-3.441513267	0.924966064
C	0.293660022	-4.776332365	0.761156051
C	-0.498489039	-3.943960302	-1.327590114
C	-0.292054023	-5.082075390	-0.612528058
B	0.000000000	-2.755292212	-0.407635041
C	0.561459040	-5.829794460	1.757011128
C	-0.406287032	-6.799420539	2.061576151
C	1.789785138	-5.875535431	2.433722179
C	-0.159307013	-7.772173579	3.025799224

H	-1.362325107	-6.784734547	1.546667108
C	2.042467158	-6.860187550	3.383070249
H	2.547939193	-5.131878393	2.207077161
C	1.067476080	-7.809987580	3.685972274
H	-0.925415071	-8.507557655	3.255205240
H	3.002700230	-6.883144529	3.890829292
H	1.263706095	-8.575974664	4.431033330
C	-0.558722046	-6.458397500	-1.069745091
C	-1.799106141	-6.795219507	-1.631473133
C	0.423463032	-7.455314572	-0.968225082
C	-2.049600161	-8.088596597	-2.078120169
H	-2.568631198	-6.033180455	-1.712641139
C	0.178199013	-8.743922664	-1.433302117
H	1.388367105	-7.215680571	-0.530778047
C	-1.060175085	-9.066870702	-1.985350163
H	-3.019176232	-8.332014639	-2.503654201
H	0.954866071	-9.499720705	-1.356083112
H	-1.254308098	-10.075625787	-2.338927187
C	-1.006438077	-3.878945299	-2.710661218
C	-0.385657030	-4.584766354	-3.752729297
C	-2.122323164	-3.086779234	-3.022261240
C	-0.865870068	-4.504992349	-5.056691397
H	0.482596036	-5.199170403	-3.531136281
C	-2.609524201	-3.014499231	-4.324945341
H	-2.612251199	-2.527071194	-2.229711183
C	-1.981900155	-3.721893286	-5.349018409
H	-0.365837029	-5.057136388	-5.847955453
H	-3.479471267	-2.399842182	-4.540474361

H	-2.357097181	-3.660915282	-6.366718494
C	1.007384077	-2.793904213	2.149462157
C	2.152049167	-1.984492150	2.102083151
C	0.360714027	-2.955103229	3.383739250
C	2.644766204	-1.372421105	3.251568242
H	2.663070207	-1.843843140	1.152958081
C	0.845731063	-2.334238179	4.530588340
H	-0.531560039	-3.572877275	3.436685255
C	1.991979151	-1.542891122	4.470731334
H	3.536786270	-0.754544060	3.192236238
H	0.325402025	-2.468276188	5.475178392
H	-2.370080185	1.058447083	5.366678429

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C	1.283041533	-0.696190717	-0.036063771
C	0.707624078	-1.957515863	-0.007496844
C	-0.707623427	-1.957516964	0.007498205
C	-1.283041068	-0.696191918	0.036064329
S	0.000000000	0.480362273	0.000000000
H	1.309185631	-2.862082896	-0.005711155
H	-1.309184408	-2.862083071	0.005712825
C	3.543253043	0.716818062	-0.963085718
C	4.904929522	0.606631970	-0.669532375
C	3.938841380	-1.031334009	0.726629405
C	5.141216895	-0.432968666	0.339962355
B	2.803110780	-0.338109564	-0.087153765
C	5.982005417	1.408358448	-1.274284327
C	6.961137583	2.051461113	-0.494121229

C	6.069785339	1.563540258	-2.670892029
C	7.973912562	2.807745568	-1.077745071
H	6.915588810	1.954737487	0.586944830
C	7.081409729	2.318315712	-3.255775719
H	5.323252080	1.079089525	-3.293628498
C	8.044615670	2.947217371	-2.464171233
H	8.712947803	3.292491291	-0.442885657
H	7.117212856	2.417266338	-4.338828830
H	8.835388464	3.538265722	-2.920645773
C	6.476546745	-0.779586897	0.852685267
C	6.710641530	-0.904250680	2.235757600
C	7.568623010	-1.009932361	-0.005860523
C	7.965650201	-1.239606908	2.733091888
H	5.883109068	-0.732590105	2.918090619
C	8.825362196	-1.344883589	0.490382201
H	7.418073194	-0.928126755	-1.078440638
C	9.036268487	-1.462458365	1.864768285
H	8.108997226	-1.327549515	3.808182029
H	9.646033557	-1.516187155	-0.203480058
H	10.017801477	-1.724699544	2.253298825
C	3.812819945	-2.170644625	1.640765147
C	4.669124055	-3.290233625	1.589203905
C	2.783802457	-2.204398238	2.604097324
C	4.519881830	-4.365554213	2.460139046
H	5.458162857	-3.310125155	0.842686347
C	2.632539881	-3.279216822	3.474718271
H	2.094062930	-1.366804243	2.650684242
C	3.502127631	-4.369944817	3.415093690

H	5.201253335	-5.211484194	2.386729752
H	1.823111282	-3.266847288	4.201815506
H	3.381774484	-5.212163276	4.092888184
C	2.953026234	1.698775621	-1.880505275
C	1.941102881	1.312725038	-2.781382450
C	3.333182386	3.055620759	-1.893771934
C	1.357228045	2.222989569	-3.656993898
H	1.612277880	0.277343936	-2.775959055
C	2.751556602	3.967130290	-2.769479476
H	4.091034339	3.393086431	-1.192413749
C	1.760552874	3.558799699	-3.662990958
H	0.571853897	1.887933876	-4.331127396
H	3.066991958	5.008639373	-2.745396894
H	-1.297846796	4.273075017	4.340252237
C	-3.543253657	0.716816522	0.963087438
C	-4.904929681	0.606630595	0.669533074
C	-3.938841332	-1.031333681	-0.726630564
C	-5.141215588	-0.432968929	-0.339963297
B	-2.803111696	-0.338111016	0.087155190
C	-5.982006158	1.408356241	1.274284602
C	-6.961137053	2.051460674	0.494121772
C	-6.069786556	1.563536459	2.670893378
C	-7.973912986	2.807744335	1.077746034
H	-6.915587381	1.954737281	-0.586943957
C	-7.081412375	2.318311118	3.255776153
H	-5.323254567	1.079085112	3.293629758
C	-8.044617046	2.947214556	2.464171916
H	-8.712947485	3.292490688	0.442885374

H	-7.117216401	2.417260506	4.338828936
H	-8.835390369	3.538261293	2.920645794
C	-6.476546322	-0.779585749	-0.852687040
C	-6.710640155	-0.904247986	-2.235759076
C	-7.568623433	-1.009932324	0.005858049
C	-7.965649248	-1.239603812	-2.733095079
H	-5.883107745	-0.732587533	-2.918091900
C	-8.825362143	-1.344883145	-0.490385954
H	-7.418073617	-0.928127914	1.078438256
C	-9.036267535	-1.462456386	-1.864771735
H	-8.108995374	-1.327545213	-3.808184887
H	-9.646033504	-1.516185604	0.203476112
H	-10.017800948	-1.724696252	-2.253303911
C	-3.812819294	-2.170643239	-1.640766264
C	-4.669123727	-3.290232408	-1.589207630
C	-2.783800467	-2.204396630	-2.604098938
C	-4.519881365	-4.365551990	-2.460143993
H	-5.458162539	-3.310124885	-0.842690093
C	-2.632537754	-3.279213207	-3.474721113
H	-2.094061480	-1.366802497	-2.650684009
C	-3.502126266	-4.369941383	-3.415098204
H	-5.201252758	-5.211482141	-2.386735663
H	-1.823109589	-3.266842742	-4.201817432
H	-3.381773013	-5.212159053	-4.092893656
C	-2.953026970	1.698772113	1.880508117
C	-1.941104002	1.312720635	2.781385752
C	-3.333182392	3.055618187	1.893776749
C	-1.357229289	2.222984245	3.656998238

H	-1.612279774	0.277339579	2.775960743
C	-2.751556724	3.967125792	2.769485328
H	-4.091035286	3.393084563	1.192418511
C	-1.760554287	3.558794318	3.662996811
H	-0.571855532	1.887927886	4.331132249
H	-3.066993112	5.008635870	2.745403493
H	1.297844859	4.273081113	-4.340244675

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C	-0.569322434	1.170960003	-0.615968033
C	-0.310901475	0.643003535	-1.863743131
C	0.310901475	-0.643003535	-1.863743131
C	0.569322434	-1.170960003	-0.615968033
S	0.000000000	0.000000000	0.556200056
H	-0.559282899	1.187222245	-2.772889198
H	0.559282899	-1.187222245	-2.772889198
C	-2.625992361	2.879085155	0.301325037
C	-2.777380579	4.311193950	0.353136041
C	-0.610461346	3.971735408	-0.529339029
C	-1.591206031	4.957849438	-0.146436998
B	-1.224507026	2.582981749	-0.266105007
C	-3.955889931	5.020004766	0.831192077
C	-3.890084792	6.154186411	1.683342145
C	-5.265307484	4.598348905	0.475220050
C	-5.028720951	6.825626243	2.112743178
H	-2.911866928	6.494326836	2.010575170
C	-6.402300848	5.267091451	0.908652085
H	-5.360937226	3.723008639	-0.161034998

C	-6.307589234	6.399216486	1.730665149
H	-4.917637947	7.693604569	2.763980229
H	-7.382190002	4.899248709	0.602340062
H	-7.200307231	6.920247157	2.074631176
C	-1.417122703	6.398548188	-0.245193005
C	-0.189384620	7.018264330	0.115644023
C	-2.426248534	7.278716906	-0.721307040
C	0.000000000	8.391114318	0.035345017
H	0.615176347	6.380096359	0.469998050
C	-2.236583095	8.653418643	-0.796541048
H	-3.371216382	6.851539736	-1.044301064
C	-1.021814846	9.239377934	-0.415666018
H	0.962856965	8.810236087	0.329600040
H	-3.049159304	9.279985938	-1.167091077
H	-0.870704626	10.316162776	-0.482264023
C	0.585879020	4.238678818	-1.310411089
C	0.697737491	5.280890764	-2.272299162
C	1.735268155	3.412075015	-1.181218078
C	1.856922798	5.490074256	-3.013582220
H	-0.160537255	5.923213983	-2.445763173
C	2.888169032	3.617538908	-1.926630137
H	1.693747501	2.589331527	-0.473426023
C	2.975583552	4.666529234	-2.853204207
H	1.881694183	6.306602794	-3.737771271
H	3.732818511	2.944013235	-1.785024125
H	3.881680706	4.827064080	-3.436487252
C	-3.529233916	1.914338625	0.909201085
C	-3.658784560	0.609137778	0.363247042

C	-4.301260061	2.160261617	2.077107175
C	-4.495140164	-0.350814762	0.916582087
H	-3.063635101	0.365169757	-0.512345026
C	-5.147159662	1.200472473	2.625097215
H	-4.209958570	3.123509782	2.570102210
C	-5.265458495	-0.069558173	2.053004173
H	-4.537021014	-1.339654598	0.461513050
H	-5.712213922	1.445852460	3.526101287
H	5.915952983	0.825615909	2.490694206
C	2.625992361	-2.879085155	0.301325037
C	2.777380579	-4.311193950	0.353136041
C	0.610461346	-3.971735408	-0.529339029
C	1.591206031	-4.957849438	-0.146436998
B	1.224507026	-2.582981749	-0.266105007
C	3.955889931	-5.020004766	0.831192077
C	3.890084792	-6.154186411	1.683342145
C	5.265307484	-4.598348905	0.475220050
C	5.028720951	-6.825626243	2.112743178
H	2.911866928	-6.494326836	2.010575170
C	6.402300848	-5.267091451	0.908652085
H	5.360937226	-3.723008639	-0.161034998
C	6.307589234	-6.399216486	1.730665149
H	4.917637947	-7.693604569	2.763980229
H	7.382190002	-4.899248709	0.602340062
H	7.200307231	-6.920247157	2.074631176
C	1.417122703	-6.398548188	-0.245193005
C	0.189384620	-7.018264330	0.115644023
C	2.426248534	-7.278716906	-0.721307040

C	0.000000000	-8.391114318	0.035345017
H	-0.615176347	-6.380096359	0.469998050
C	2.236583095	-8.653418643	-0.796541048
H	3.371216382	-6.851539736	-1.044301064
C	1.021814846	-9.239377934	-0.415666018
H	-0.962856965	-8.810236087	0.329600040
H	3.049159304	-9.279985938	-1.167091077
H	0.870704626	-10.316162776	-0.482264023
C	-0.585879020	-4.238678818	-1.310411089
C	-0.697737491	-5.280890764	-2.272299162
C	-1.735268155	-3.412075015	-1.181218078
C	-1.856922798	-5.490074256	-3.013582220
H	0.160537255	-5.923213983	-2.445763173
C	-2.888169032	-3.617538908	-1.926630137
H	-1.693747501	-2.589331527	-0.473426023
C	-2.975583552	-4.666529234	-2.853204207
H	-1.881694183	-6.306602794	-3.737771271
H	-3.732818511	-2.944013235	-1.785024125
H	-3.881680706	-4.827064080	-3.436487252
C	3.529233916	-1.914338625	0.909201085
C	3.658784560	-0.609137778	0.363247042
C	4.301260061	-2.160261617	2.077107175
C	4.495140164	0.350814762	0.916582087
H	3.063635101	-0.365169757	-0.512345026
C	5.147159662	-1.200472473	2.625097215
H	4.209958570	-3.123509782	2.570102210
C	5.265458495	0.069558173	2.053004173
H	4.537021014	1.339654598	0.461513050

H	5.712213922	-1.445852460	3.526101287
H	-5.915952983	-0.825615909	2.490694206

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C	-1.708178889	-0.600075147	2.054970167
C	-1.530089075	0.813923008	2.131582173
C	-1.520441528	1.374308342	0.785703070
C	-1.665162557	0.231887383	-0.108129000
C	-1.799018509	-0.956150151	0.668633060
H	-1.749928323	-1.290660167	2.899932230
H	-1.414669664	1.381188286	3.054450246
H	-1.674659479	0.275648522	-1.196739085
H	-1.915762688	-1.968963126	0.277069030
Fe	0.000000000	0.000000000	1.071219088
C	1.530089075	-0.813923008	2.131582173
C	1.520441528	-1.374308342	0.785703070
C	1.708178889	0.600075147	2.054970167
H	1.414669664	-1.381188286	3.054450246
C	1.665162557	-0.231887383	-0.108129000
C	1.799018509	0.956150151	0.668633060
H	1.749928323	1.290660167	2.899932230
H	1.674659479	-0.275648522	-1.196739085
H	1.915762688	1.968963126	0.277069030
C	0.966310169	-3.381615837	-1.116588078
C	0.414196750	-4.630075822	-0.988671067
C	0.713416796	-4.040110675	1.321377112
C	0.254978073	-5.025428918	0.477847045
B	1.135357620	-2.818602957	0.376230038

C	0.131838389	-5.594568294	-2.093059155
C	1.032620984	-6.648717844	-2.360765173
C	-1.025047913	-5.491174098	-2.894207215
C	0.791221187	-7.555940219	-3.400469253
H	1.937135575	-6.751862798	-1.751730124
C	-1.270830266	-6.403679461	-3.929827295
H	-1.747402486	-4.692176206	-2.696296199
C	-0.362204735	-7.438376878	-4.189139313
H	1.510572674	-8.360393039	-3.594873268
H	-2.177672702	-6.302489182	-4.537974342
H	-0.551769302	-8.150432387	-5.000890376
C	-0.279086593	-6.355691181	0.874867076
C	0.496976279	-7.240437388	1.658320137
C	-1.571622668	-6.776024819	0.485563046
C	0.000000000	-8.493666911	2.037002165
H	1.505131478	-6.943145927	1.962623159
C	-2.073365506	-8.023265591	0.877548078
H	-2.198463754	-6.111325435	-0.116602001
C	-1.288745138	-8.889946533	1.652016133
H	0.625059880	-9.164820299	2.638050209
H	-3.083354537	-8.320994311	0.571634055
H	-1.678747855	-9.869878444	1.951436157
C	0.721269151	-4.127444438	2.803189225
C	-0.459947812	-4.341146081	3.552388283
C	1.934846773	-4.002308692	3.521474277
C	-0.429833233	-4.422255920	4.951016389
H	-1.415284563	-4.442082958	3.027325239
C	1.967700398	-4.094954579	4.919193389

H	2.868134842	-3.842710030	2.969629234
C	0.784064171	-4.301776792	5.643021456
H	-1.362981425	-4.584301260	5.504186407
H	2.925360223	-4.004777960	5.446205409
H	0.807893149	-4.368955526	6.736997521
C	1.435532028	-2.779216707	-2.390785176
C	0.560641419	-2.381547768	-3.426636253
C	2.822996018	-2.583569681	-2.596969190
C	1.049646288	-1.827486244	-4.618274344
H	-0.519168749	-2.491284492	-3.290598244
C	3.312923788	-2.037838069	-3.789943285
H	3.526837431	-2.877447293	-1.810100131
C	2.427526434	-1.656622219	-4.809211359
H	0.344312263	-1.526462465	-5.401754414
H	4.393985578	-1.910638067	-3.924090294
H	2.809157143	-1.227350597	-5.743111417
C	-0.966310169	3.381615837	-1.116588078
C	-0.414196750	4.630075822	-0.988671067
C	-0.713416796	4.040110675	1.321377112
C	-0.254978073	5.025428918	0.477847045
B	-1.135357620	2.818602957	0.376230038
C	-0.131838389	5.594568294	-2.093059155
C	-1.032620984	6.648717844	-2.360765173
C	1.025047913	5.491174098	-2.894207215
C	-0.791221187	7.555940219	-3.400469253
H	-1.937135575	6.751862798	-1.751730124
C	1.270830266	6.403679461	-3.929827295
H	1.747402486	4.692176206	-2.696296199

C	0.362204735	7.438376878	-4.189139313
H	-1.510572674	8.360393039	-3.594873268
H	2.177672702	6.302489182	-4.537974342
H	0.551769302	8.150432387	-5.000890376
C	0.279086593	6.355691181	0.874867076
C	-0.496976279	7.240437388	1.658320137
C	1.571622668	6.776024819	0.485563046
C	0.000000000	8.493666911	2.037002165
H	-1.505131478	6.943145927	1.962623159
C	2.073365506	8.023265591	0.877548078
H	2.198463754	6.111325435	-0.116602001
C	1.288745138	8.889946533	1.652016133
H	-0.625059880	9.164820299	2.638050209
H	3.083354537	8.320994311	0.571634055
H	1.678747855	9.869878444	1.951436157
C	-0.721269151	4.127444438	2.803189225
C	0.459947812	4.341146081	3.552388283
C	-1.934846773	4.002308692	3.521474277
C	0.429833233	4.422255920	4.951016389
H	1.415284563	4.442082958	3.027325239
C	-1.967700398	4.094954579	4.919193389
H	-2.868134842	3.842710030	2.969629234
C	-0.784064171	4.301776792	5.643021456
H	1.362981425	4.584301260	5.504186407
H	-2.925360223	4.004777960	5.446205409
H	-0.807893149	4.368955526	6.736997521
C	-1.435532028	2.779216707	-2.390785176
C	-0.560641419	2.381547768	-3.426636253

C	-2.822996018	2.583569681	-2.596969190
C	-1.049646288	1.827486244	-4.618274344
H	0.519168749	2.491284492	-3.290598244
C	-3.312923788	2.037838069	-3.789943285
H	-3.526837431	2.877447293	-1.810100131
C	-2.427526434	1.656622219	-4.809211359
H	-0.344312263	1.526462465	-5.401754414
H	-4.393985578	1.910638067	-3.924090294
H	-2.809157143	1.227350597	-5.743111417

Borole [15]²⁻

C	0.140313011	1.822456140	1.422912187
C	1.330870102	1.055828084	1.647750202
C	1.989516154	0.761309057	0.383790104
C	1.098534085	1.321349103	-0.622628972
C	0.000000000	1.990223155	0.006172076
H	-0.549037044	2.188194169	2.188895245
H	1.685721131	0.744470060	2.629496276
H	1.257913097	1.272543096	-1.699727055
H	-0.818797063	2.509179192	-0.498831963
Fe	0.000000000	0.000000000	0.523587115
C	-1.330870102	-1.055828084	1.647750202
C	-1.989516154	-0.761309057	0.383790104
C	-0.140313011	-1.822456140	1.422912187
H	-1.685721131	-0.744470060	2.629496276
C	-1.098534085	-1.321349103	-0.622628972
C	0.000000000	-1.990223155	0.006172076
H	0.549037044	-2.188194169	2.188895245

H	-1.257913097	-1.272543096	-1.699727055
H	0.818797063	-2.509179192	-0.498831963
C	-4.069163311	0.383750029	-1.190196014
C	-5.310547434	0.960906074	-0.861996993
C	-4.413946340	0.398486030	1.267145171
C	-5.503059419	0.997018076	0.606762122
B	-3.366239258	-0.029219003	0.164353088
C	-6.338387508	1.402174107	-1.832818065
C	-7.696149594	0.996219077	-1.726193056
C	-6.014882458	2.242742173	-2.931258152
C	-8.663014690	1.403379107	-2.653195130
H	-7.988169603	0.334878025	-0.904912993
C	-6.980956541	2.649984204	-3.858643223
H	-4.983143385	2.588150197	-3.043576161
C	-8.316799629	2.235498170	-3.729920212
H	-9.700182731	1.061283081	-2.535800121
H	-6.687031494	3.303811255	-4.690643286
H	-9.074583725	2.554776195	-4.456926269
C	-6.662180536	1.641440123	1.265929174
C	-7.405163545	0.986976076	2.284558251
C	-7.079544538	2.956280225	0.924447148
C	-8.490135658	1.603851124	2.918351297
H	-7.126229560	-0.031824003	2.568352274
C	-8.164236611	3.573948277	1.558187196
H	-6.525432510	3.503825269	0.155877087
C	-8.882626688	2.904548222	2.562103273
H	-9.039421696	1.059525080	3.698328362
H	-8.448743626	4.594228355	1.267679174

H	-9.733004738	3.388576259	3.059387311
C	-4.289710328	0.339679026	2.742463284
C	-4.191945323	1.508001116	3.541628347
C	-4.258110328	-0.900839069	3.431216340
C	-4.072287314	1.442408109	4.936169453
H	-4.201669326	2.484458190	3.045754308
C	-4.142170319	-0.970310077	4.825944447
H	-4.329596333	-1.824460139	2.846109294
C	-4.048510311	0.201947015	5.592464497
H	-3.991607305	2.371194182	5.516714520
H	-4.122583315	-1.951190153	5.319761468
H	-3.952221304	0.149077011	6.684429582
C	-3.672315284	0.065982004	-2.583707124
C	-2.528353195	0.642504049	-3.191503168
C	-4.418350338	-0.843564067	-3.378166183
C	-2.158034167	0.339940026	-4.509162271
H	-1.922922150	1.345102102	-2.611081125
C	-4.049740310	-1.152086087	-4.693969286
H	-5.301650430	-1.319966104	-2.939392152
C	-2.916384224	-0.560503045	-5.273501333
H	-1.265135096	0.811010061	-4.939166306
H	-4.652590356	-1.865629145	-5.272104332
H	-2.624741201	-0.801249059	-6.303833398
C	4.069163311	-0.383750029	-1.190196014
C	5.310547434	-0.960906074	-0.861996993
C	4.413946340	-0.398486030	1.267145171
C	5.503059419	-0.997018076	0.606762122
B	3.366239258	0.029219003	0.164353088

C	6.338387508	-1.402174107	-1.832818065
C	7.696149594	-0.996219077	-1.726193056
C	6.014882458	-2.242742173	-2.931258152
C	8.663014690	-1.403379107	-2.653195130
H	7.988169603	-0.334878025	-0.904912993
C	6.980956541	-2.649984204	-3.858643223
H	4.983143385	-2.588150197	-3.043576161
C	8.316799629	-2.235498170	-3.729920212
H	9.700182731	-1.061283081	-2.535800121
H	6.687031494	-3.303811255	-4.690643286
H	9.074583725	-2.554776195	-4.456926269
C	6.662180536	-1.641440123	1.265929174
C	7.405163545	-0.986976076	2.284558251
C	7.079544538	-2.956280225	0.924447148
C	8.490135658	-1.603851124	2.918351297
H	7.126229560	0.031824003	2.568352274
C	8.164236611	-3.573948277	1.558187196
H	6.525432510	-3.503825269	0.155877087
C	8.882626688	-2.904548222	2.562103273
H	9.039421696	-1.059525080	3.698328362
H	8.448743626	-4.594228355	1.267679174
H	9.733004738	-3.388576259	3.059387311
C	4.289710328	-0.339679026	2.742463284
C	4.191945323	-1.508001116	3.541628347
C	4.258110328	0.900839069	3.431216340
C	4.072287314	-1.442408109	4.936169453
H	4.201669326	-2.484458190	3.045754308
C	4.142170319	0.970310077	4.825944447

H	4.329596333	1.824460139	2.846109294
C	4.048510311	-0.201947015	5.592464497
H	3.991607305	-2.371194182	5.516714520
H	4.122583315	1.951190153	5.319761468
H	3.952221304	-0.149077011	6.684429582
C	3.672315284	-0.065982004	-2.583707124
C	2.528353195	-0.642504049	-3.191503168
C	4.418350338	0.843564067	-3.378166183
C	2.158034167	-0.339940026	-4.509162271
H	1.922922150	-1.345102102	-2.611081125
C	4.049740310	1.152086087	-4.693969286
H	5.301650430	1.319966104	-2.939392152
C	2.916384224	0.560503045	-5.273501333
H	1.265135096	-0.811010061	-4.939166306
H	4.652590356	1.865629145	-5.272104332
H	2.624741201	0.801249059	-6.303833398

Borole [15]⁴⁻

C	1.781623135	0.093339007	1.266803089
C	1.186671091	-1.200685091	1.461247105
C	1.055725080	-1.907161145	0.198556007
C	1.497592115	-0.934347070	-0.787981067
C	1.976741153	0.259577020	-0.144201020
H	2.013948156	0.827995064	2.044191149
H	0.895168067	-1.603232124	2.432186178
H	1.527036119	-1.106200085	-1.865789152
H	2.398650184	1.141296089	-0.634524057
Fe	0.000000000	0.000000000	0.316882016

C	-1.186671091	1.200685091	1.461247105
C	-1.055725080	1.907161145	0.198556007
C	-1.781623135	-0.093339007	1.266803089
H	-0.895168067	1.603232124	2.432186178
C	-1.497592115	0.934347070	-0.787981067
C	-1.976741153	-0.259577020	-0.144201020
H	-2.013948156	-0.827995064	2.044191149
H	-1.527036119	1.106200085	-1.865789152
H	-2.398650184	-1.141296089	-0.634524057
C	-0.074055006	4.267314330	-1.166446100
C	0.093809006	5.642864449	-0.734602063
C	-0.951668073	4.562787352	1.111160080
C	-0.414007033	5.814742437	0.617628041
B	-0.689398054	3.462944268	0.026353994
C	0.689077050	6.714175535	-1.541136126
C	0.151593010	8.040162644	-1.623417135
C	1.865783141	6.492264526	-2.329013188
C	0.745375054	9.045841674	-2.392274191
H	-0.770244061	8.263461631	-1.078652092
C	2.457175187	7.497950595	-3.097073245
H	2.321354179	5.497610428	-2.305405184
C	1.912859146	8.798630701	-3.142214250
H	0.280490019	10.043832764	-2.417736194
H	3.367177257	7.266326538	-3.671340291
H	2.376068180	9.588208719	-3.750974296
C	-0.366654030	7.074268535	1.369015098
C	-1.499934116	7.581922557	2.084416150
C	0.814323060	7.882251602	1.459856104

C	-1.463028115	8.784022657	2.795634209
H	-2.432739190	7.011152559	2.049807148
C	0.849444062	9.084397687	2.171864156
H	1.723986133	7.528449567	0.965289069
C	-0.288780024	9.564148723	2.852304208
H	-2.371605184	9.126253703	3.314825249
H	1.789400135	9.656648747	2.208555164
H	-0.258507022	10.506362785	3.417781255
C	-1.489602115	4.398358339	2.467001183
C	-0.833861067	4.868498373	3.648936270
C	-2.744890212	3.750989288	2.694936198
C	-1.383524107	4.717370362	4.926971368
H	0.144514010	5.347760395	3.544878263
C	-3.295009254	3.598364277	3.971613295
H	-3.289165253	3.373127257	1.823434133
C	-2.626567201	4.084058311	5.112528387
H	-0.825744065	5.092111390	5.799035451
H	-4.265796326	3.091800237	4.080730305
H	-3.057683238	3.964047304	6.116457449
C	0.000000000	3.870212298	-2.578047209
C	0.524441040	2.607872199	-2.995497238
C	-0.483359038	4.697282359	-3.645234289
C	0.585564043	2.220399172	-4.338398344
H	0.886130069	1.921161148	-2.228090181
C	-0.422438034	4.311065334	-4.988445392
H	-0.938463074	5.660056413	-3.394895270
C	0.120678009	3.068187237	-5.362550423
H	1.001281075	1.234486097	-4.588051359

H	-0.817584062	4.991356386	-5.759593436
H	0.168168013	2.761780211	-6.416993508
C	0.074055006	-4.267314330	-1.166446100
C	-0.093809006	-5.642864449	-0.734602063
C	0.951668073	-4.562787352	1.111160080
C	0.414007033	-5.814742437	0.617628041
B	0.689398054	-3.462944268	0.026353994
C	-0.689077050	-6.714175535	-1.541136126
C	-0.151593010	-8.040162644	-1.623417135
C	-1.865783141	-6.492264526	-2.329013188
C	-0.745375054	-9.045841674	-2.392274191
H	0.770244061	-8.263461631	-1.078652092
C	-2.457175187	-7.497950595	-3.097073245
H	-2.321354179	-5.497610428	-2.305405184
C	-1.912859146	-8.798630701	-3.142214250
H	-0.280490019	-10.043832764	-2.417736194
H	-3.367177257	-7.266326538	-3.671340291
H	-2.376068180	-9.588208719	-3.750974296
C	0.366654030	-7.074268535	1.369015098
C	1.499934116	-7.581922557	2.084416150
C	-0.814323060	-7.882251602	1.459856104
C	1.463028115	-8.784022657	2.795634209
H	2.432739190	-7.011152559	2.049807148
C	-0.849444062	-9.084397687	2.171864156
H	-1.723986133	-7.528449567	0.965289069
C	0.288780024	-9.564148723	2.852304208
H	2.371605184	-9.126253703	3.314825249
H	-1.789400135	-9.656648747	2.208555164

H	0.258507022	-10.506362785	3.417781255
C	1.489602115	-4.398358339	2.467001183
C	0.833861067	-4.868498373	3.648936270
C	2.744890212	-3.750989288	2.694936198
C	1.383524107	-4.717370362	4.926971368
H	-0.144514010	-5.347760395	3.544878263
C	3.295009254	-3.598364277	3.971613295
H	3.289165253	-3.373127257	1.823434133
C	2.626567201	-4.084058311	5.112528387
H	0.825744065	-5.092111390	5.799035451
H	4.265796326	-3.091800237	4.080730305
H	3.057683238	-3.964047304	6.116457449
C	0.000000000	-3.870212298	-2.578047209
C	-0.524441040	-2.607872199	-2.995497238
C	0.483359038	-4.697282359	-3.645234289
C	-0.585564043	-2.220399172	-4.338398344
H	-0.886130069	-1.921161148	-2.228090181
C	0.422438034	-4.311065334	-4.988445392
H	0.938463074	-5.660056413	-3.394895270
C	-0.120678009	-3.068187237	-5.362550423
H	-1.001281075	-1.234486097	-4.588051359
H	0.817584062	-4.991356386	-5.759593436
H	-0.168168013	-2.761780211	-6.416993508

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B	-3.022624849	0.154591203	-1.600419039
C	-4.147935980	2.461034980	-1.702872787
B	-3.022719529	-0.154690826	1.600481841

Br	-3.524531064	-1.407977932	-2.690387422
Fe	-0.228986977	-0.000048378	0.000093839
Br	-3.524677398	1.407905049	2.690409160
C	-3.877723667	-2.652731126	3.079630706
C	-4.240410265	4.897284345	-1.456038514
C	-5.287195911	-0.655792653	0.353554486
C	-6.551397755	1.460957375	-0.233824093
C	-7.106107913	1.763915922	1.029242447
C	-4.212204536	-1.078420381	1.123534842
C	-5.287144819	0.655751589	-0.353617899
C	-8.443163610	-2.617079741	1.274250883
C	-8.969231520	-2.927495866	0.011834226
C	-8.294477239	-2.497528641	-1.139320850
C	-3.877517849	2.652594371	-3.079647359
C	-4.240482302	-4.897396398	1.455951792
C	-3.987068181	5.067086349	-2.825340342
C	-3.987225352	-5.067223358	2.825266267
C	-7.106187077	-1.763916192	-1.029307594
C	-8.969042762	2.927681697	-0.011887698
C	-4.319089460	-3.614255993	0.901314561
C	-4.148063575	-2.461141392	1.702834987
C	-3.805286991	3.936763486	-3.634626206
C	-7.247610438	-1.897068301	1.383362919
C	-6.551493166	-1.460921306	0.233756094
C	-7.247444594	1.897222826	-1.383425690
C	-8.294355951	2.497599784	1.139265604
C	-3.805508515	-3.936913756	3.634589544
C	-4.212113030	1.078334130	-1.123551950

C	-4.319032124	3.614152396	-0.901384492
C	-8.442951622	2.617309843	-1.274304706
H	-6.591412604	1.433507316	1.935609455
H	-8.697126885	2.729972256	2.132296012
H	-9.902707013	3.496121850	0.073630963
H	-8.967357915	2.936597054	-2.182750835
H	-6.854435658	1.656154146	-2.375324575
H	-6.854620341	-1.655954196	2.375267471
H	-8.967624355	-2.936272917	2.182703019
H	-9.902932443	-3.495877820	-0.073680495
H	-8.697232403	-2.729933192	-2.132346189
H	-6.591445308	-1.433596419	-1.935673824
H	-3.746056065	-1.784012217	3.733473240
H	-3.607110084	-4.052742232	4.706662687
H	-3.930651579	-6.073005647	3.257879601
H	-4.381885930	-5.772995379	0.811198316
H	-4.509059896	-3.501639539	-0.168989213
H	-4.509072718	3.501552632	0.168906450
H	-4.381866662	5.772895894	-0.811312068
H	-3.930479945	6.072860547	-3.257969143
H	-3.606824387	4.052574493	-4.706683421
H	-3.745800424	1.783874244	-3.733454571
C	-0.799598068	-1.631430275	1.029476745
C	0.635697047	-1.487565085	1.210804542
C	-1.491889881	-0.465252003	1.562454212
H	-1.291232007	-2.506966803	0.607595089
C	0.810060495	-0.169200591	1.787982755
C	-0.453263869	0.439960831	2.000572492

H	1.767818059	0.299361704	2.007588514
H	-0.615701762	1.436530691	2.410487964
C	0.635752134	1.487462313	-1.210596501
C	0.810144714	0.169095433	-1.787747028
C	-0.799548971	1.631323905	-1.029328549
C	-0.453168119	-0.440066994	-2.000391799
H	1.767907295	-0.299466446	-2.007296006
C	-1.491812266	0.465142802	-1.562324055
H	-1.291194107	2.506855104	-0.607482125
H	-0.615584252	-1.436634664	-2.410297195
C	1.859111300	3.747273061	0.079305904
C	3.127341417	4.261161453	-0.050041010
C	3.269460201	2.369902355	-1.519269141
C	3.953909485	3.468742362	-1.065396688
B	1.806598380	2.456166168	-0.865269166
C	3.702046388	5.407800211	0.699357599
C	4.914742320	5.270656418	1.415553930
C	3.055950384	6.665271037	0.728641008
C	5.446492170	6.339390246	2.146922419
H	5.438613779	4.309622098	1.413283220
C	3.598119273	7.738450436	1.446247375
H	2.125429271	6.804050681	0.170901812
C	4.793035167	7.580208446	2.162954886
H	6.380680306	6.202386362	2.704416022
H	3.081617840	8.705691513	1.445655739
H	5.214602858	8.419782231	2.728099016
C	5.275616010	3.945540658	-1.549507647
C	6.425875642	3.126455865	-1.488297482

C	5.412409874	5.237973151	-2.108920983
C	7.661278136	3.579388780	-1.968859159
H	6.353086412	2.129815976	-1.044158726
C	6.643813376	5.682901735	-2.603907207
H	4.539207997	5.894750968	-2.173036226
C	7.775613972	4.857483770	-2.533024253
H	8.540127033	2.927098327	-1.902124319
H	6.720118619	6.683897018	-3.044853442
H	8.741745152	5.210138062	-2.912736933
C	3.731870214	1.485180575	-2.627611257
C	3.474660522	1.833919389	-3.973122773
C	4.403532925	0.265776566	-2.385372063
C	3.874174549	1.002688258	-5.028445509
H	2.954404328	2.773076833	-4.191729805
C	4.804713951	-0.567027128	-3.440214639
H	4.608658093	-0.038948970	-1.353405793
C	4.541119264	-0.202856093	-4.768238038
H	3.662928373	1.301283649	-6.062387388
H	5.326406136	-1.506556489	-3.220573595
H	4.852985282	-0.853303733	-5.593736004
C	0.862214787	4.255870729	1.060346999
C	-0.315605663	4.913891446	0.639223288
C	1.079712780	4.126131189	2.451919965
C	-1.225329076	5.436771448	1.568697736
H	-0.508429075	5.039224929	-0.432129449
C	0.164631347	4.638557438	3.381289837
H	1.982811541	3.618332283	2.807281205
C	-0.990825073	5.302318463	2.944639696

H	-2.122954822	5.955696523	1.213042279
H	0.360115773	4.523058349	4.454241039
H	-1.703283396	5.710958131	3.670725720
C	3.269468382	-2.369966496	1.519382682
C	3.953906204	-3.468796577	1.065457052
C	1.859098071	-3.747270029	-0.079237012
C	3.127329150	-4.261170661	0.050080947
B	1.806581981	-2.456218625	0.865418680
C	5.275641887	-3.945580261	1.549488845
C	5.412518038	-5.238064344	2.108756795
C	6.425853417	-3.126424929	1.488347484
C	6.643953714	-5.682979524	2.603669759
H	4.539356781	-5.894898714	2.172812177
C	7.661289143	-3.579339788	1.968834134
H	6.352998621	-2.129740092	1.044319490
C	7.775708271	-4.857490655	2.532856943
H	6.720322511	-6.684019893	3.044501639
H	8.540101368	-2.926992989	1.902151964
H	8.741868292	-5.210134443	2.912511032
C	3.702047266	-5.407735599	-0.699413803
C	3.055981166	-6.665217643	-0.728790109
C	4.914733520	-5.270506126	-1.415604811
C	3.598166364	-7.738325550	-1.446490696
H	2.125470139	-6.804065445	-0.171050975
C	5.446501748	-6.339167463	-2.147063413
H	5.438582134	-4.309463795	-1.413254464
C	4.793071654	-7.579997411	-2.163197381
H	3.081685718	-8.705578375	-1.445972753

H	6.380682741	-6.202095050	-2.704551957
H	5.214653029	-8.419514838	-2.728415125
C	0.862209431	-4.255766528	-1.060338394
C	1.079740472	-4.125926641	-2.451896708
C	-0.315669302	-4.913733857	-0.639290584
C	0.164644762	-4.638217553	-3.381325027
H	1.982871846	-3.618150362	-2.807198225
C	-1.225411030	-5.436476961	-1.568826003
H	-0.508533919	-5.039122422	0.432052519
C	-0.990865999	-5.301932799	-2.944751929
H	0.360156366	-4.522641580	-4.454259935
H	-2.123085423	-5.955361924	-1.213229867
H	-1.703338785	-5.710462715	-3.670884426
C	3.731925445	-1.485274054	2.627734476
C	4.403409833	-0.265766903	2.385494917
C	3.474972091	-1.834159212	3.973261259
C	4.804641871	0.567003204	3.440346568
H	4.608348699	0.039066526	1.353521990
C	3.874538131	-1.002958594	5.028593821
H	2.954872211	-2.773406860	4.191873985
C	4.541288521	0.202692432	4.768382276
H	5.326187744	1.506613423	3.220703402
H	3.663487274	-1.301666218	6.062545506
H	4.853198546	0.853112832	5.593886978

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C	-3.844630314	1.365225099	-0.510411066
C	-4.953724406	0.580823049	-0.563671086

C	-3.387162302	-0.926424090	0.417660977
C	-4.699399402	-0.773899067	0.096933950
B	-2.683323233	0.429994011	0.013474966
C	-6.223509478	0.903537090	-1.233213135
C	-6.856481563	-0.045816966	-2.052272215
C	-6.816918526	2.168007190	-1.094964113
C	-8.030550615	0.268104076	-2.728780268
H	-6.418153517	-1.032603045	-2.167633231
C	-8.002687634	2.472393235	-1.754862160
H	-6.346867468	2.910242238	-0.458249051
C	-8.611142673	1.526319174	-2.578715242
H	-8.497966688	-0.476073969	-3.367412328
H	-8.451510640	3.453474308	-1.627110141
H	-9.534810713	1.767080206	-3.097496280
C	-5.792497466	-1.707534134	0.414255958
C	-5.642145509	-3.088550237	0.214527926
C	-7.003461602	-1.238001093	0.948235004
C	-6.667549569	-3.970056302	0.538955937
H	-4.714668420	-3.466905271	-0.203364107
C	-8.020423644	-2.123179162	1.291392014
H	-7.143790572	-0.173128014	1.108040029
C	-7.858862655	-3.491755265	1.083179981
H	-6.534079583	-5.034864381	0.369662909
H	-8.944777763	-1.740986127	1.715297048
H	-8.657619728	-4.181579312	1.340861990
C	-2.863289272	-2.033175192	1.249688031
C	-3.241136306	-2.120190215	2.597949131
C	-2.004746213	-3.013479269	0.736897978

C	-2.788639285	-3.160079306	3.404612181
H	-3.900887353	-1.361504158	3.010416168
C	-1.562701189	-4.061359364	1.542264031
H	-1.699997184	-2.969130257	-0.306259099
C	-1.951671222	-4.140731385	2.877077128
H	-3.094144313	-3.204876324	4.446449258
H	-0.908429143	-4.822546419	1.127116991
H	-1.598157203	-4.955486455	3.502395167
C	-3.709604293	2.709552211	-1.116212098
C	-3.681833283	3.855858285	-0.309148018
C	-3.576892275	2.871056239	-2.501244201
C	-3.533426259	5.123232388	-0.868176042
H	-3.790407294	3.747983265	0.768270061
C	-3.423104248	4.137297342	-3.061543226
H	-3.599234281	1.992723179	-3.140967260
C	-3.400977242	5.268486416	-2.248263148
H	-3.521933254	5.998445472	-0.223851984
H	-3.323113239	4.239536361	-4.138810308
H	-3.282480226	6.255645512	-2.685935168
C	-1.185737114	0.824132027	0.004077976
C	-0.039569033	0.012299961	-0.254278050
C	-0.674266067	2.156857124	0.232591012
C	1.161631064	0.805429014	-0.214488033
H	-0.065449042	-1.048175117	-0.469174081
C	0.723116043	2.140180113	0.124057009
H	-1.277467106	3.024505195	0.463496039
H	1.375489100	2.990570170	0.270444033
Mn	0.157705982	0.814155999	1.694764108

C	1.359182075	1.564083030	2.794610209
C	-1.156747123	1.145559019	2.860958199
C	0.489407992	-0.809766140	2.386940142
O	2.115326134	2.045483051	3.518918272
O	-2.017243189	1.377170032	3.594659258
O	0.745427003	-1.842430226	2.828237164
C	3.937765282	1.183184019	-0.164138014
C	4.974381353	0.318713946	-0.324547034
C	3.128355204	-1.103965142	-0.820727094
C	4.485581307	-1.050059147	-0.782461086
B	2.616484173	0.330913966	-0.386187047
C	6.400685482	0.601299954	-0.083626007
C	7.183804521	-0.282279131	0.674954045
C	7.004567530	1.760145042	-0.594220028
C	8.522435632	-0.004069124	0.933045071
H	6.736522478	-1.189131204	1.071626062
C	8.348107607	2.027076049	-0.352016002
H	6.413713508	2.450332111	-1.188544066
C	9.111083672	1.149044969	0.416764048
H	9.109033640	-0.695164187	1.531842112
H	8.799672651	2.925985123	-0.762502023
H	10.159091750	1.360721975	0.609613069
C	5.408577361	-2.112944233	-1.219337133
C	5.221103345	-3.438801339	-0.801217118
C	6.480326446	-1.829944209	-2.080735193
C	6.074554390	-4.449223417	-1.231975162
H	4.403324281	-3.671565360	-0.126667072
C	7.322425518	-2.844391289	-2.525168235

H	6.648458494	-0.809604127	-2.412292204
C	7.125991483	-4.156964395	-2.099423220
H	5.916377384	-5.468241514	-0.890005149
H	8.139754596	-2.606385269	-3.200197281
H	7.790506554	-4.946662456	-2.438722253
C	2.367535138	-2.217326213	-1.434497163
C	2.387566143	-2.374465207	-2.828431271
C	1.622968070	-3.130958290	-0.676946117
C	1.695004085	-3.411816273	-3.446650334
H	2.963418196	-1.674368151	-3.427992306
C	0.941307015	-4.178167357	-1.295491180
H	1.594117067	-3.032871292	0.405636968
C	0.971079019	-4.323088347	-2.680799291
H	1.728814092	-3.512492271	-4.528145420
H	0.389359962	-4.892077415	-0.690783144
H	0.437491973	-5.140440402	-3.157702337
C	4.077953299	2.592241118	0.261702037
C	3.668442283	3.628092216	-0.592374020
C	4.622591340	2.938558126	1.505580141
C	3.803304301	4.963212311	-0.219090971
H	3.249934253	3.378147212	-1.564947097
C	4.750210361	4.272445222	1.883858184
H	4.941545360	2.151096055	2.182245180
C	4.343681343	5.290883319	1.023787132
H	3.485700287	5.748006359	-0.900652015
H	5.166953394	4.515739224	2.857373266
H	4.444704354	6.331197365	1.319919166

Borole [17]⁴⁻

C	-3.475830284	1.505946178	-0.400632970
C	-4.850541399	1.118126164	-0.622933974
C	-3.807344326	-0.837728999	0.198295062
C	-5.044465424	-0.255042942	-0.252442956
B	-2.736717234	0.269860073	0.172761056
C	-5.894857491	1.990085247	-1.135379998
C	-6.886851575	1.569082231	-2.061955063
C	-5.970593445	3.355021351	-0.742847957
C	-7.882444645	2.422353308	-2.522262079
H	-6.850989550	0.546662154	-2.426485098
C	-6.962284521	4.207412428	-1.208317975
H	-5.219845395	3.724428368	-0.049860909
C	-7.944961646	3.757554409	-2.101782038
H	-8.618886705	2.041226291	-3.231025131
H	-6.969780529	5.244629507	-0.871139943
H	-8.719643694	4.428607470	-2.470870051
C	-6.328100514	-0.945269981	-0.302717950
C	-6.443014582	-2.258688077	-0.828220001
C	-7.532597628	-0.368569928	0.176322103
C	-7.659601650	-2.924648115	-0.895029994
H	-5.540118495	-2.742383119	-1.190051041
C	-8.751307703	-1.033798964	0.104651106
H	-7.487034568	0.624318143	0.614657144
C	-8.839319722	-2.322683059	-0.435663944
H	-7.690473692	-3.932251191	-1.310398034
H	-9.647730788	-0.540909924	0.482960148

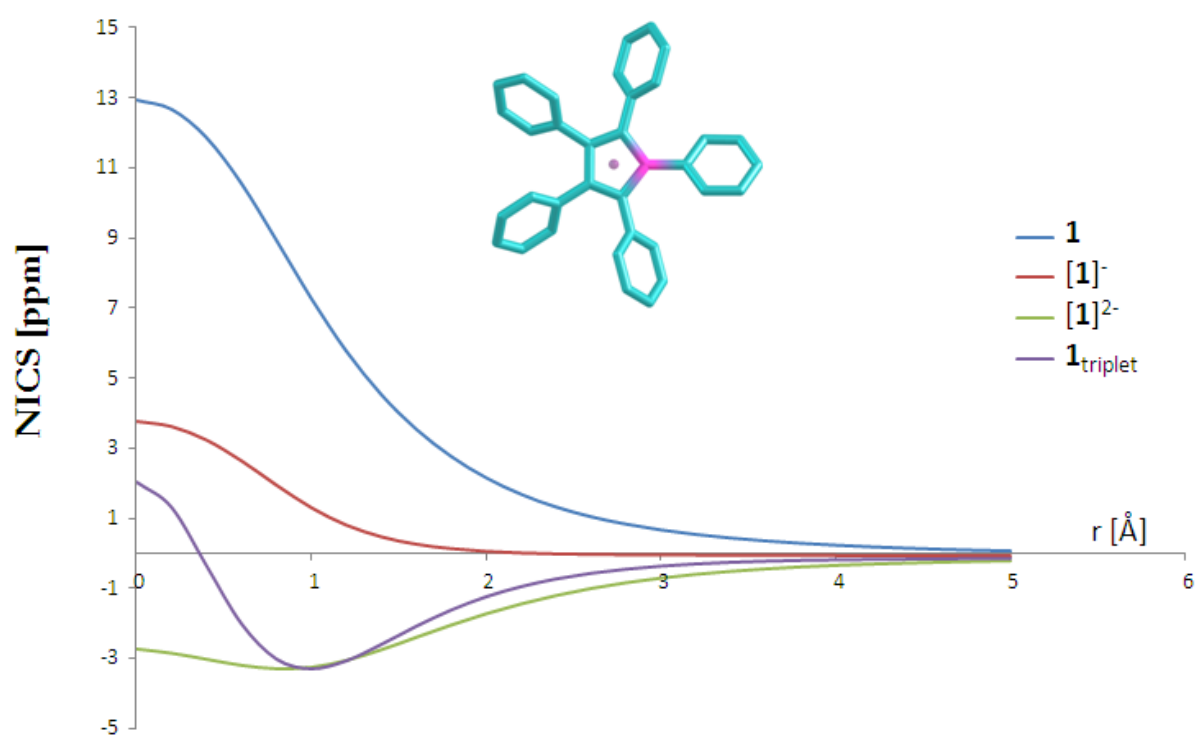
H	-9.792722814	-2.847430089	-0.484570942
C	-3.726116327	-2.166409106	0.793653101
C	-4.711125398	-2.693344147	1.669000172
C	-2.629017254	-3.021732185	0.531159060
C	-4.623449401	-3.973325247	2.202899201
H	-5.552084463	-2.062348088	1.941126207
C	-2.535289258	-4.301110287	1.069230091
H	-1.846379201	-2.659911157	-0.128999998
C	-3.536714328	-4.802410320	1.905890162
H	-5.408410458	-4.323350274	2.874896256
H	-1.658324196	-4.905194338	0.844753059
H	-3.459391329	-5.801385421	2.333185185
C	-2.888151236	2.678891268	-1.039134018
C	-1.823889141	3.419852311	-0.462133978
C	-3.312062277	3.149974317	-2.314202110
C	-1.249945090	4.522865395	-1.083243022
H	-1.439923103	3.106998277	0.500999089
C	-2.748336230	4.260512402	-2.930819152
H	-4.092468351	2.601556289	-2.832737144
C	-1.708166136	4.973830443	-2.326025115
H	-0.424732018	5.034585425	-0.588374990
H	-3.117565264	4.563544436	-3.911772222
H	-1.253295099	5.833657507	-2.815478150
C	-1.197513112	0.280611055	0.635161075
C	-0.036145034	-0.340746000	0.067252015
C	-0.651317052	1.171772111	1.629271153
C	1.206325072	0.198519027	0.579303045
H	-0.082789054	-1.083391048	-0.720526049

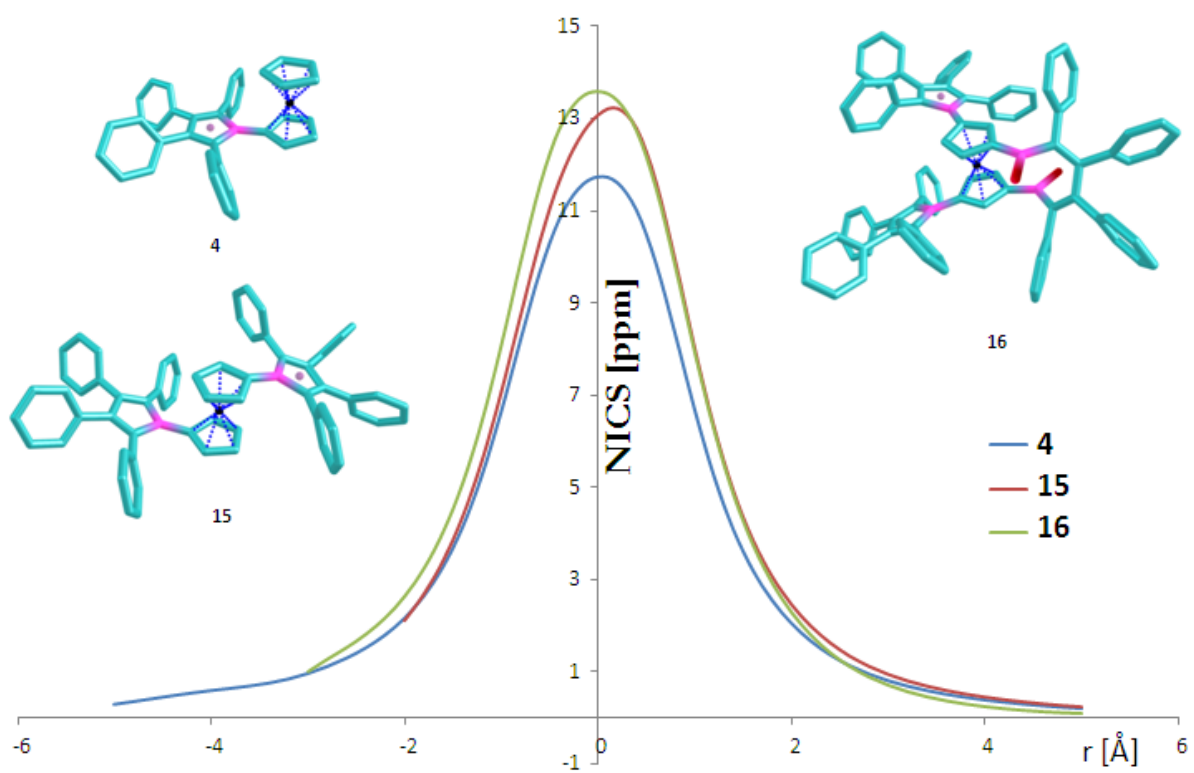
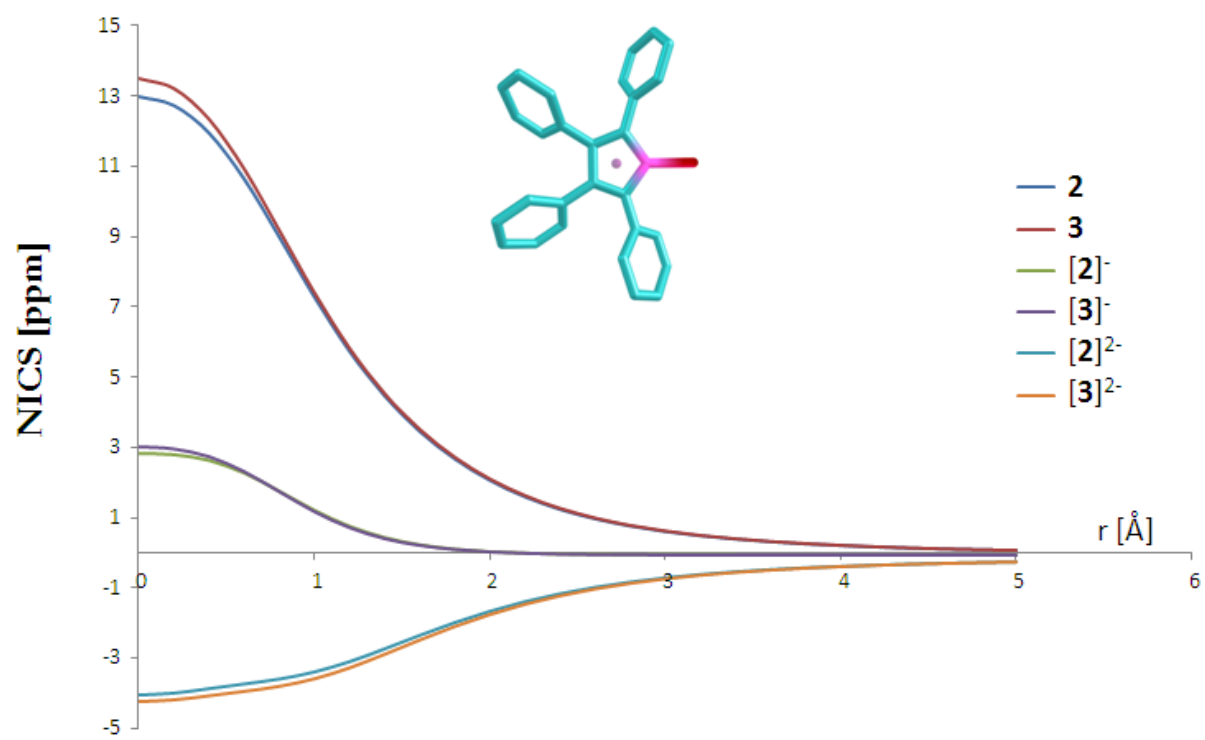
C	0.768355057	1.120201094	1.593426136
H	-1.247304082	1.798490162	2.283465215
H	1.427072124	1.704260125	2.221882180
MN	-0.001729013	-0.739934048	2.204632177
C	1.069683088	-0.643784060	3.594140273
C	-1.418195112	-0.977528060	3.238799269
C	0.329249994	-2.478968183	2.080995152
O	1.761147150	-0.580973071	4.535236337
O	-2.303904173	-1.089611061	3.985716334
O	0.575311001	-3.618934275	2.085151140
C	3.845863281	1.059861066	0.337159005
C	5.065619364	0.521021018	-0.200224053
C	3.410799216	-1.070605084	-0.753965087
C	4.803516327	-0.727158069	-0.866193109
B	2.717053182	0.032799001	0.077058990
C	6.383599460	1.123506049	-0.065613052
C	7.536168569	0.372410979	0.289484957
C	6.598880513	2.513927156	-0.263097060
C	8.793097677	0.953225008	0.406098958
H	7.416414541	-0.690477105	0.479436965
C	7.854812597	3.094001186	-0.141109061
H	5.746572448	3.131302213	-0.531484065
C	8.979178676	2.325330115	0.190580949
H	9.643036721	0.325927951	0.677771967
H	7.960828602	4.166247269	-0.309178066
H	9.963039781	2.782231139	0.289867949
C	5.807446406	-1.516077134	-1.564629178
C	5.810052392	-2.935368246	-1.492326188

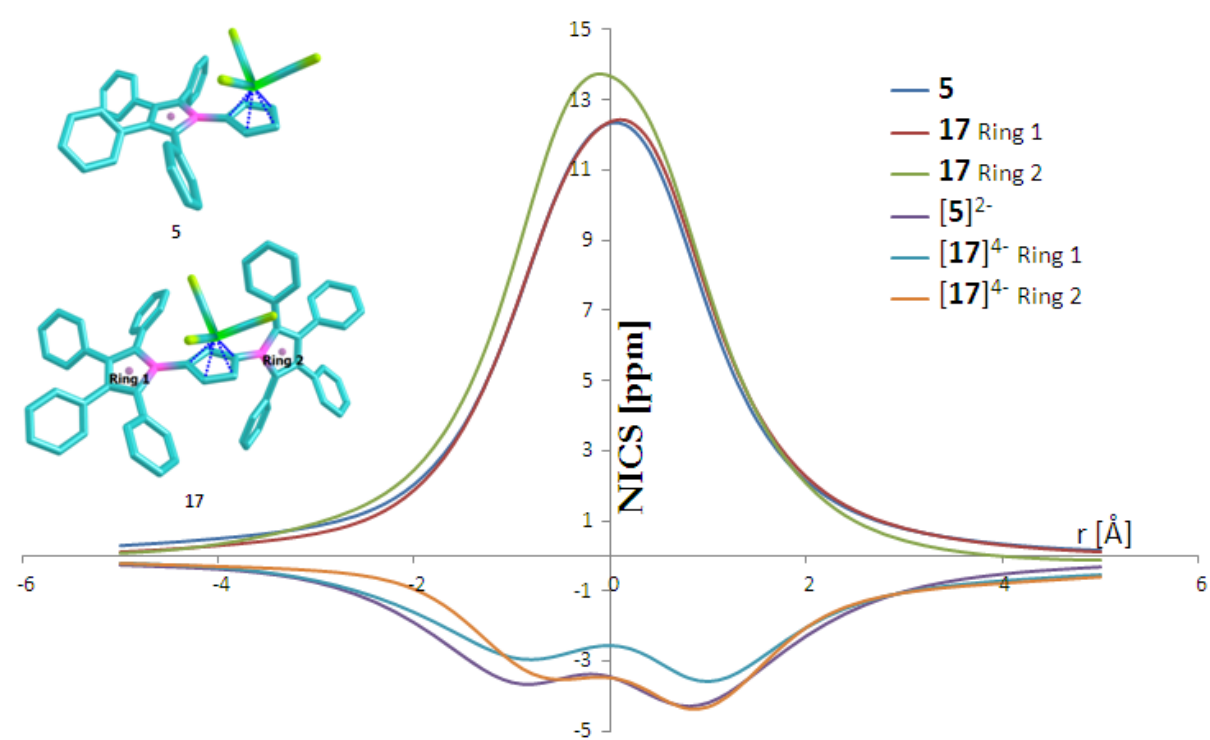
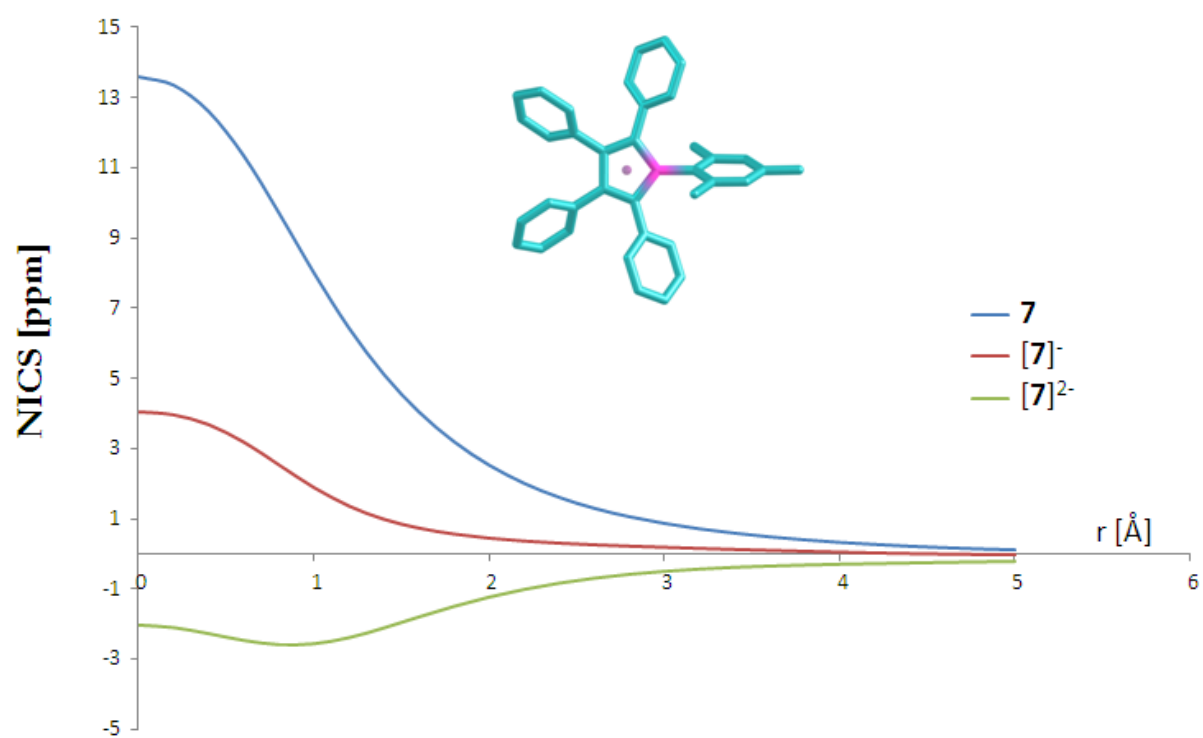
C	6.829854475	-0.945072096	-2.368603251
C	6.763448446	-3.708894312	-2.140177250
H	5.036812314	-3.415026278	-0.899082137
C	7.787711546	-1.720650163	-3.011126314
H	6.850606479	0.134433987	-2.486047252
C	7.777151496	-3.117485268	-2.907056316
H	6.716629436	-4.794294392	-2.046653252
H	8.551938587	-1.226579125	-3.612508364
H	8.522274551	-3.725464323	-3.418731371
C	2.794104146	-2.084246147	-1.604757154
C	3.152314159	-2.260655156	-2.967599268
C	1.773789068	-2.942468206	-1.133484115
C	2.546786094	-3.214900217	-3.777263330
H	3.913302222	-1.610166113	-3.389332299
C	1.159373001	-3.891866268	-1.942498178
H	1.479516055	-2.857733207	-0.095477032
C	1.539343015	-4.048024278	-3.279565285
H	2.855638110	-3.299421222	-4.820091413
H	0.372345939	-4.515186314	-1.519913139
H	1.052344965	-4.783520322	-3.918042332
C	3.815745300	2.289206158	1.124426072
C	2.866919232	3.308168246	0.857896071
C	4.719990382	2.559976160	2.182863148
C	2.821074252	4.491635333	1.586654138
H	2.155891169	3.140099245	0.052669016
C	4.681322400	3.746343249	2.908026213
H	5.455609418	1.801333093	2.435756156
C	3.731994333	4.732810335	2.622178210

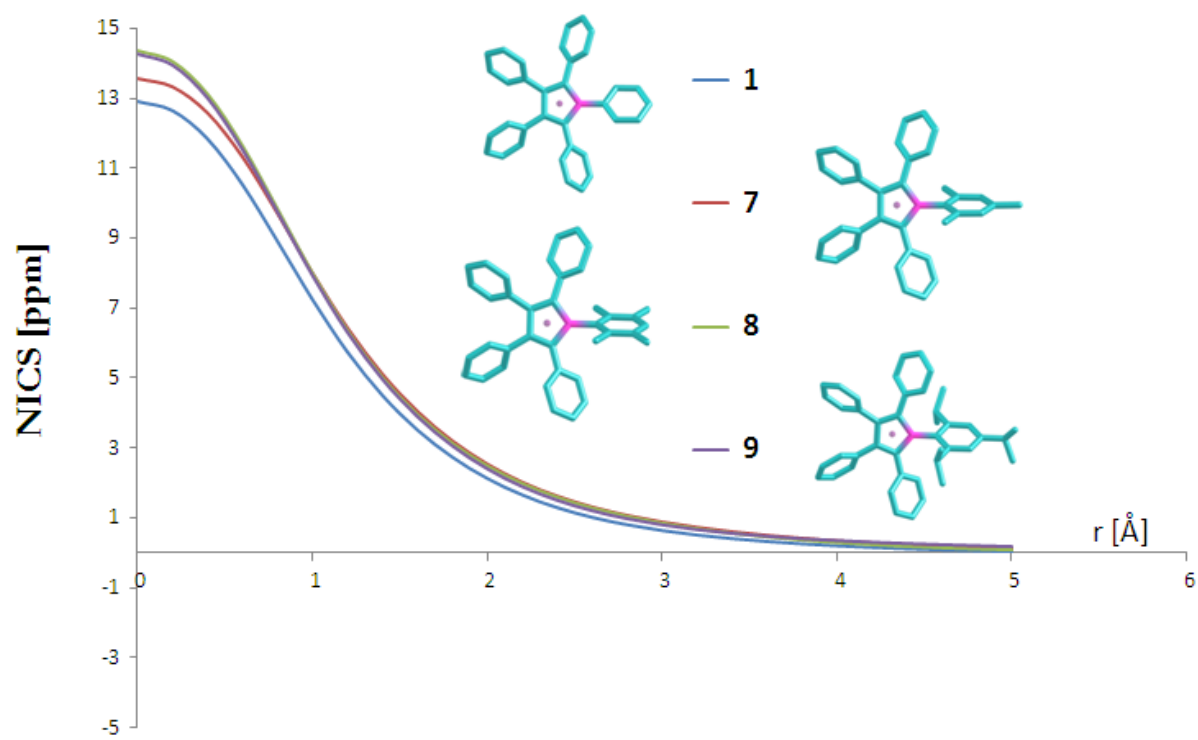
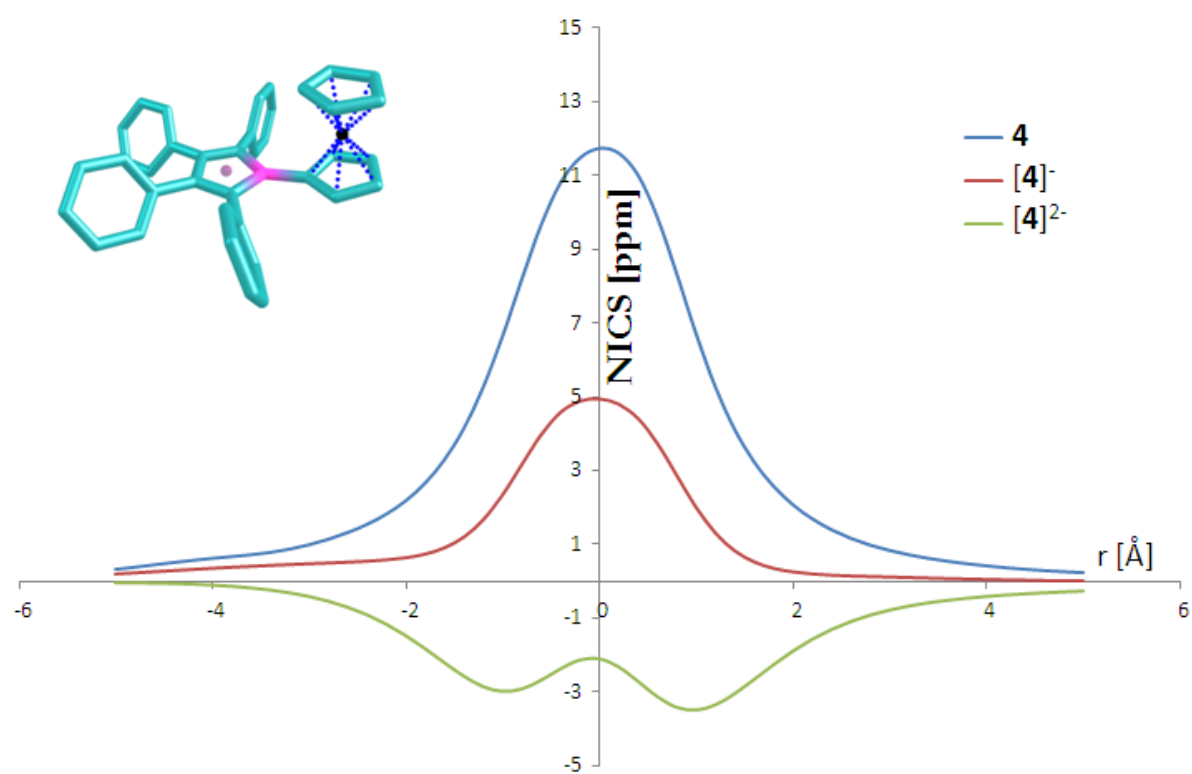
H	2.064069195	5.236285398	1.341751130
H	5.397160468	3.899435243	3.716563270
H	3.695783348	5.658719394	3.194648259

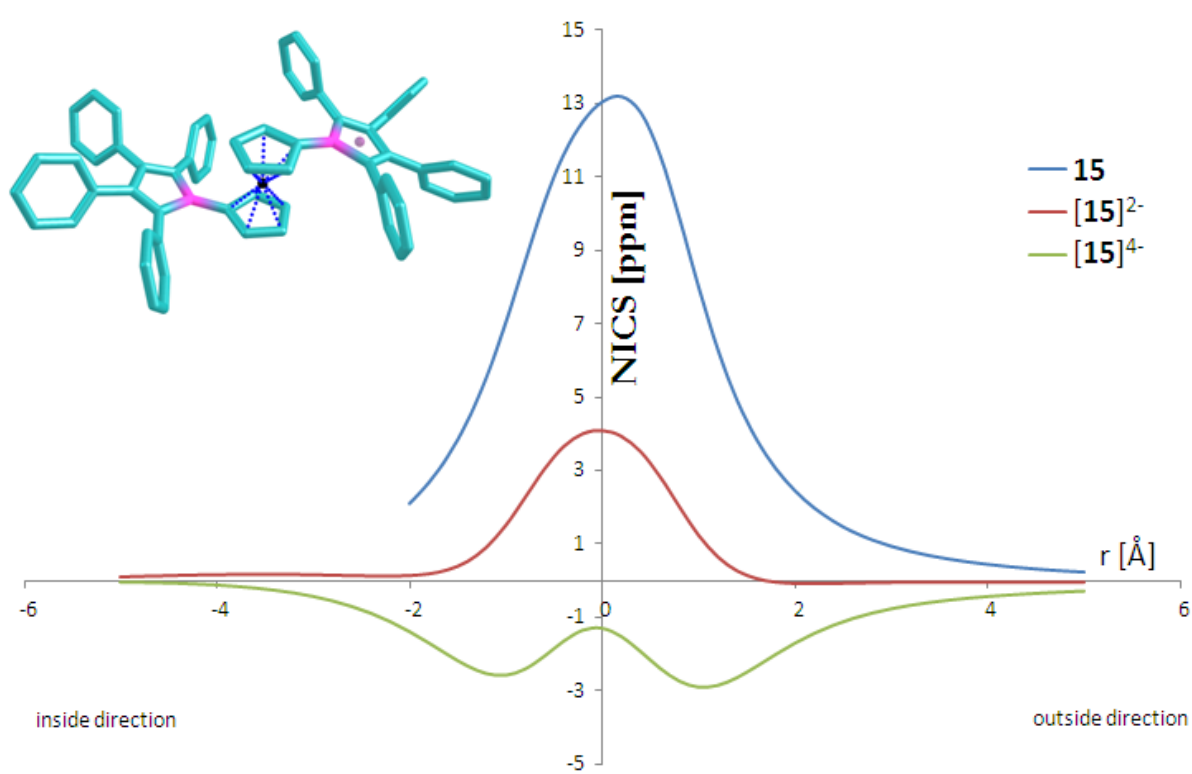
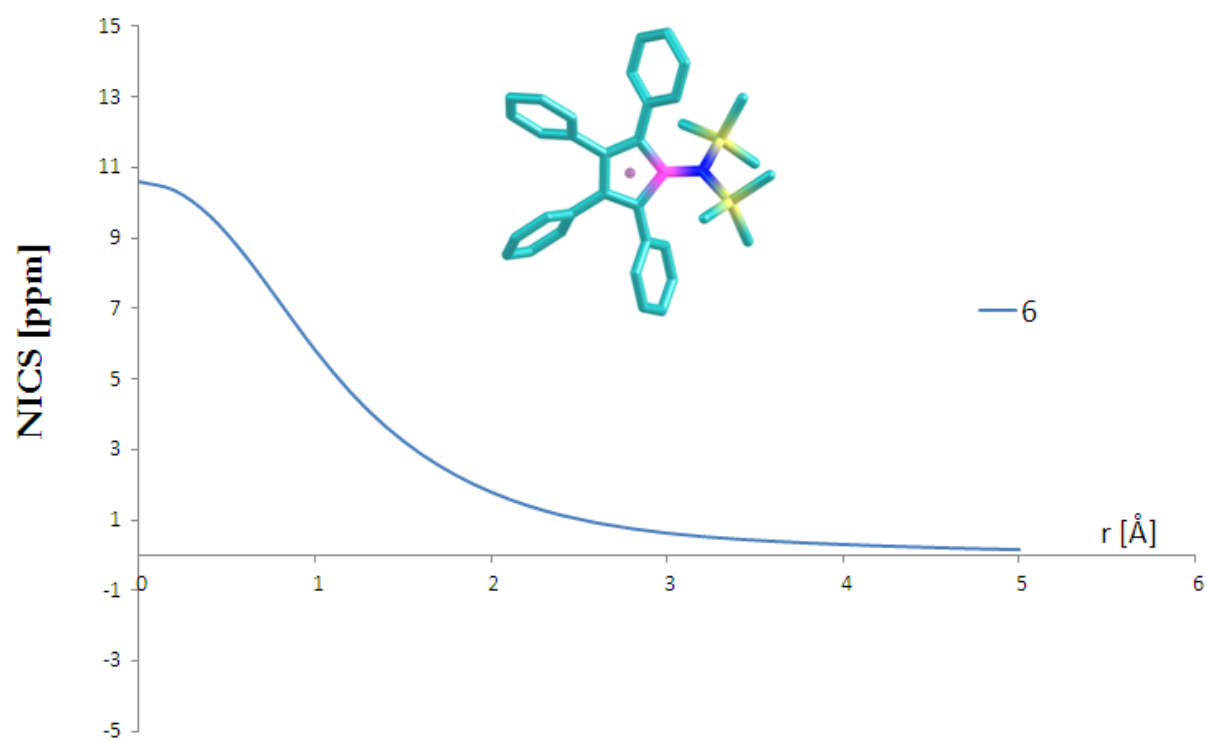
B) Complete list of NICS profiles

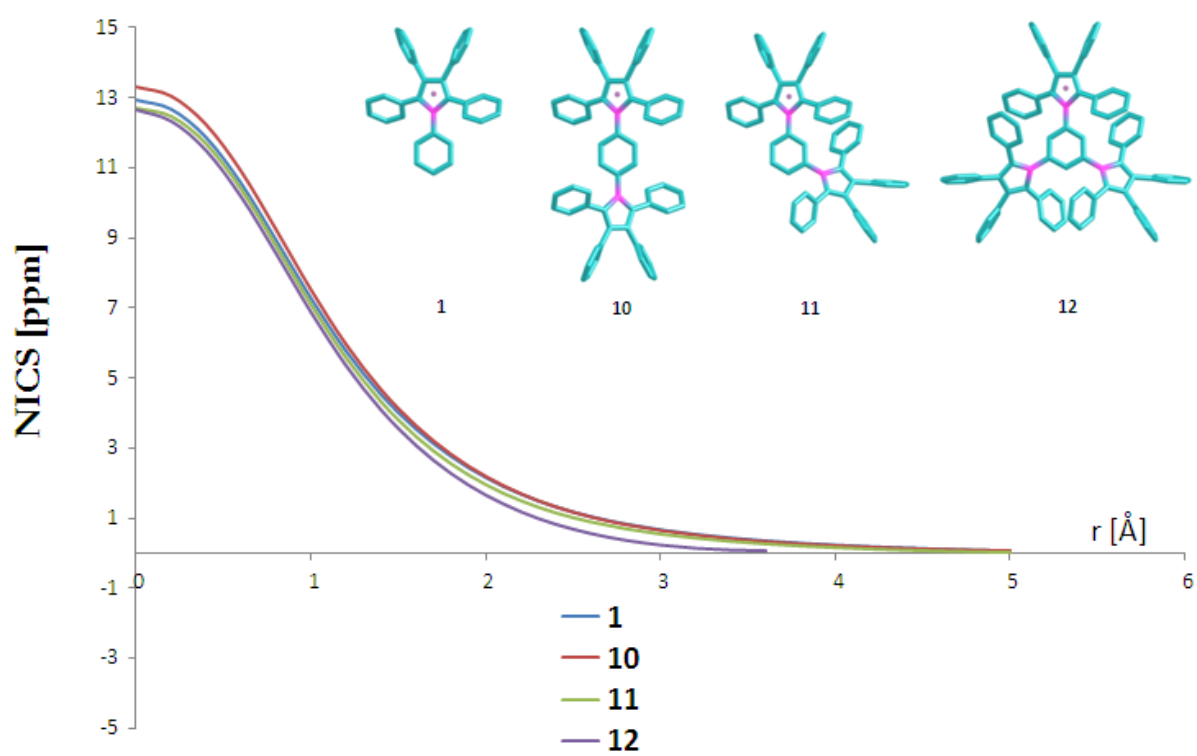
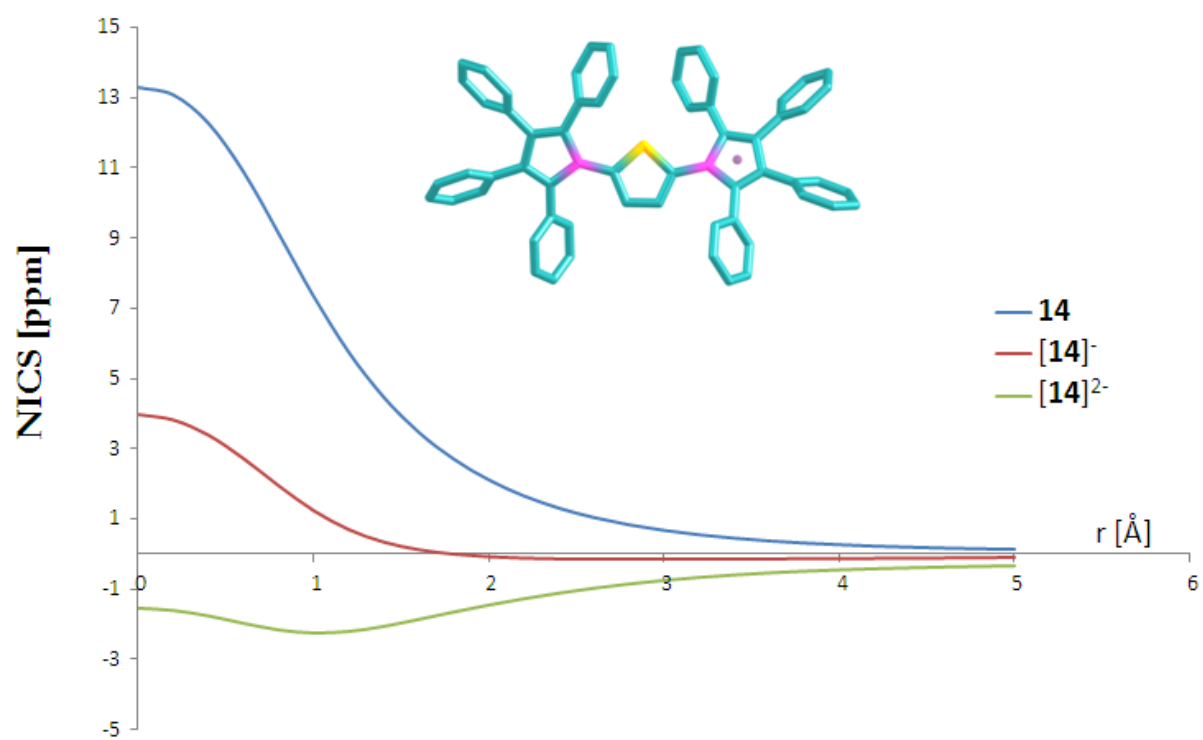


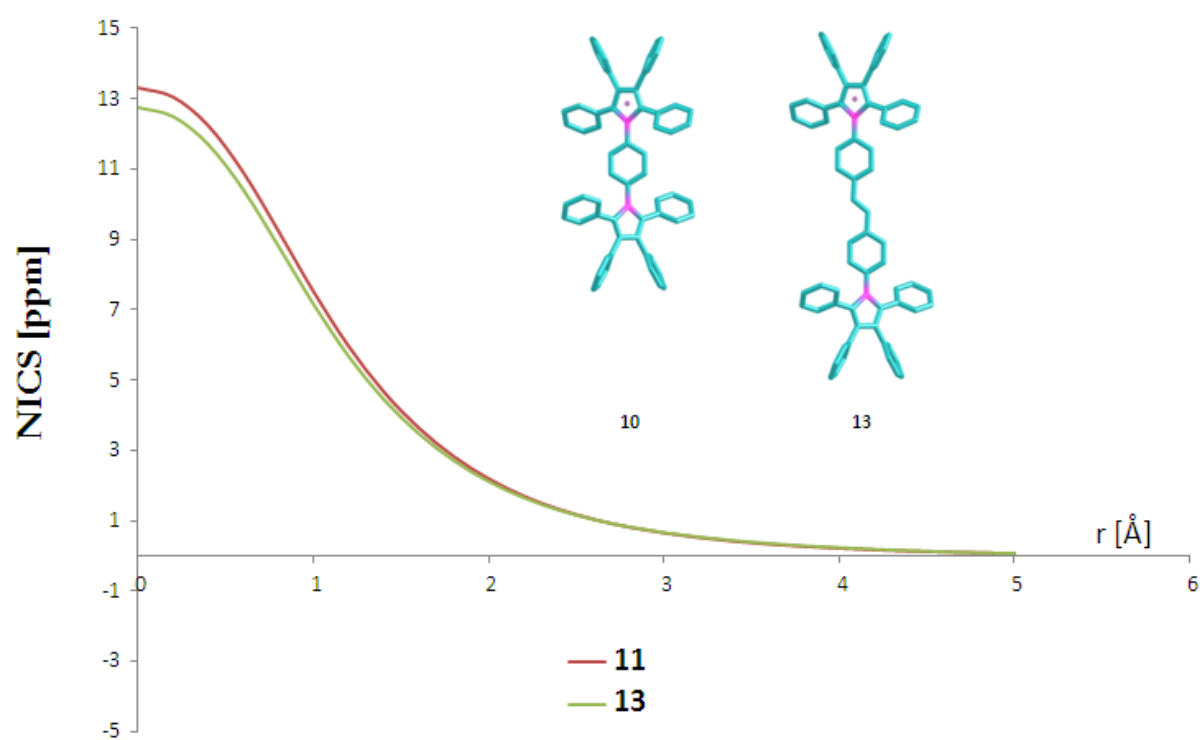
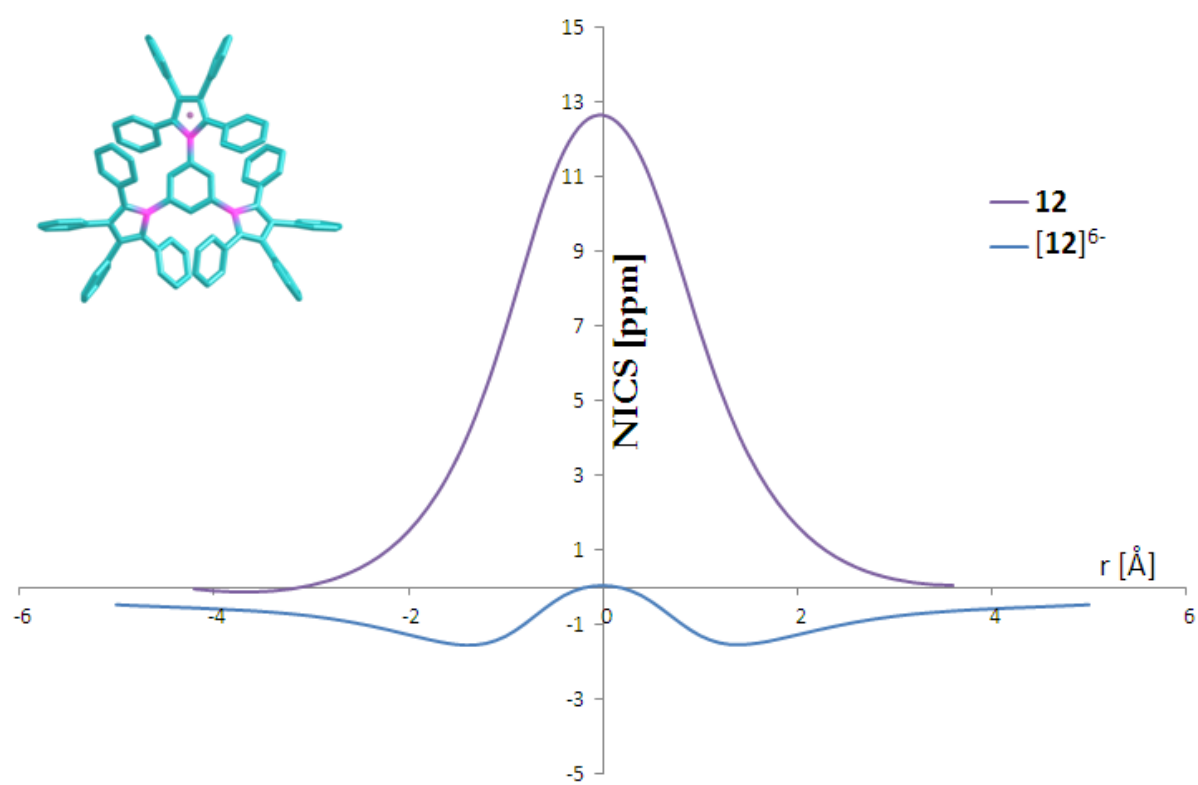


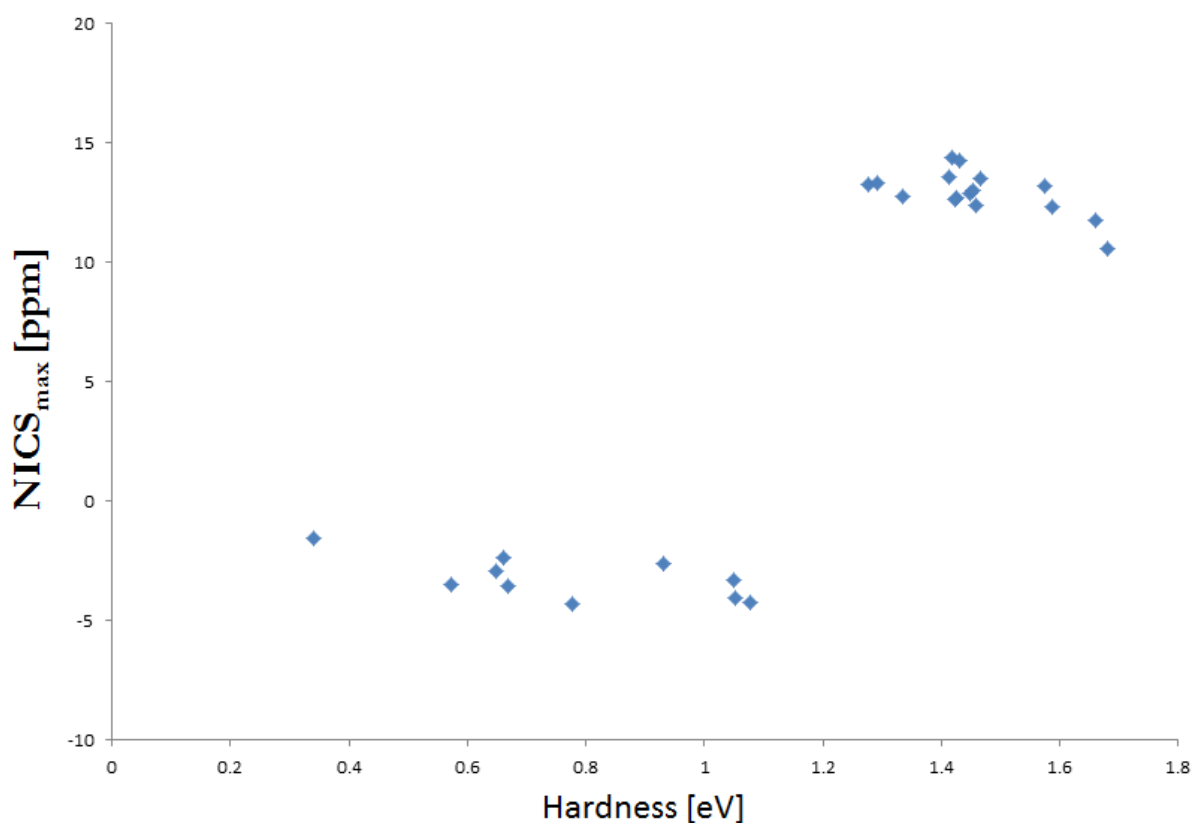












Plot of NICS maxima values vs calculated hardness of the singlet (closed-shell) species studied here: all the antiaromatic neutral boroles possess high hardness values (>1.2 eV) and all the aromatic anionic boroles have low hardness values (<1.2 eV)

Within DFT, we can rigorously define hardness, η , as:

$$\eta = \frac{1}{2} \left(\frac{\delta\mu}{\delta N} \right)_v = \frac{1}{2} \left(\frac{\delta^2 E}{\delta N^2} \right) = \frac{(I - A)}{2}$$

And using Koopmans' theorem, we took the orbital energies of the frontier orbitals as:

$$-\varepsilon_{HOMO} = I, \quad -\varepsilon_{LUMO} = A$$