

Supporting Information

Fully optimized (B3LYP/6-31G*) staggered and eclipsed geometries and absolute energies of complexes **1-17** and BH₃.

Structure of **1**

staggered

Fe	0.000000	0.000000	0.000000
C	-1.214271	0.000000	1.655274
C	-0.375230	-1.154841	1.655274
C	0.982366	-0.713731	1.655274
C	0.982366	0.713731	1.655274
C	-0.375230	1.154841	1.655274
H	-2.296588	0.000000	1.640267
H	-0.709685	-2.184185	1.640267
H	1.857978	-1.349900	1.640267
H	1.857978	1.349900	1.640267
H	-0.709685	2.184185	1.640267
C	1.214271	0.000000	-1.655274
C	0.375230	1.154841	-1.655274
C	0.375230	-1.154841	-1.655274
C	-0.982366	0.713731	-1.655274
C	-0.982366	-0.713731	-1.655274
H	2.296588	0.000000	-1.640267
H	0.709685	2.184185	-1.640267
H	0.709685	-2.184185	-1.640267
H	-1.857978	1.349900	-1.640267
H	-1.857978	-1.349900	-1.640267

E_{tot} = -1650.703029 a.u.

eclipsed

Fe	0.000000	0.000000	0.000000
C	-1.214635	0.000000	1.653913
C	-0.375343	-1.155186	1.653913
C	0.982660	-0.713945	1.653913
C	0.982660	0.713945	1.653913
C	-0.375343	1.155186	1.653913
H	-2.296917	0.000000	1.644699
H	-0.709786	-2.184498	1.644699
H	1.858245	-1.350094	1.644699
H	1.858245	1.350094	1.644699
H	-0.709786	2.184498	1.644699
C	-1.214635	0.000000	-1.653913
C	-0.375343	1.155186	-1.653913
C	0.982660	0.713945	-1.653913
C	0.982660	-0.713945	-1.653913
C	-0.375343	-1.155186	-1.653913
H	-2.296917	0.000000	-1.644699
H	-0.709786	2.184498	-1.644699
H	1.858245	1.350094	-1.644699
H	1.858245	-1.350094	-1.644699
H	-0.709786	-2.184498	-1.644699

E_{tot} = -1650.703273 a.u.

Structure of 2

staggered

Fe	0.000000	0.007658	0.000000
N	-2.003909	0.386714	0.000000
C	-1.656059	-0.371613	1.101735
C	-1.656059	-0.371613	-1.101735
C	-1.073889	-1.610029	0.711904
C	-1.073889	-1.610029	-0.711904
H	-1.840416	-0.004109	2.102525
H	-1.840416	-0.004109	-2.102525
H	-0.701461	-2.386612	1.366327
H	-0.701461	-2.386612	-1.366327
C	1.054796	1.617042	-0.713518
C	1.054796	1.617042	0.713518
C	1.649487	0.397886	-1.154724
C	1.649487	0.397886	1.154724
C	2.016790	-0.357444	0.000000
H	0.641435	2.390477	-1.347605
H	0.641435	2.390477	1.347605
H	1.780422	0.088883	-2.183734
H	1.780422	0.088883	2.183734
H	2.474661	-1.338135	0.000000

$E_{\text{tot}} = -1666.739128$ a.u.

eclipsed

Fe	-0.000796	0.000000	-0.002778
N	1.240720	0.000000	1.613752
C	0.407140	-1.101876	1.644048
C	0.407140	1.101876	1.644048
C	-0.961412	-0.712268	1.683036
C	-0.961412	0.712268	1.683036
H	0.818411	-2.102592	1.649668
H	0.818411	2.102592	1.649668
H	-1.821833	-1.367244	1.705679
H	-1.821833	1.367244	1.705679
C	-0.981507	0.713699	-1.656721
C	-0.981507	-0.713699	-1.656721
C	0.377416	1.155327	-1.654567
C	0.377416	-1.155327	-1.654567
C	1.213924	0.000000	-1.654289
H	-1.857404	1.349362	-1.647859
H	-1.857404	-1.349362	-1.647859
H	0.713596	2.183935	-1.642542
H	0.713596	-2.183935	-1.642542
H	2.294859	0.000000	-1.603054

$E_{\text{tot}} = -1666.739298$ a.u.

Structure of 3

staggered

Fe	-0.004122	0.161115	0.000000
P	-0.131585	-2.156558	0.000000
C	0.812828	-1.287723	1.245867
C	0.812828	-1.287723	-1.245867
C	1.824690	-0.451313	0.712582
C	1.824690	-0.451313	-0.712582
H	0.629717	-1.378740	2.310984
H	0.629717	-1.378740	-2.310984
H	2.491207	0.159058	1.312499
H	2.491207	0.159058	-1.312499
C	-1.795890	0.866161	-0.714544
C	-1.795890	0.866161	0.714544
C	-0.731410	1.704934	-1.154744
C	-0.731410	1.704934	1.154744
C	-0.069983	2.220795	0.000000
H	-2.470070	0.306598	-1.349261
H	-2.470070	0.306598	1.349261
H	-0.456399	1.898582	-2.183546
H	-0.456399	1.898582	2.183546
H	0.789329	2.878920	0.000000

$E_{\text{tot}} = -1953.351304$ a.u.

eclipsed

Fe	0.000000	0.000000	0.000000
P	1.561586	0.000000	1.719693
C	0.280718	-1.246468	1.638552
C	0.280718	1.246468	1.638552
C	-1.032920	-0.712618	1.627313
C	-1.032920	0.712618	1.627313
H	0.481528	-2.311475	1.599635
H	0.481528	2.311475	1.599635
H	-1.934533	-1.313696	1.578754
H	-1.934533	1.313696	1.578754
C	0.322823	1.154966	-1.669768
C	0.322823	-1.154966	-1.669768
C	-1.033765	0.714147	-1.622429
C	-1.033765	-0.714147	-1.622429
C	1.160031	0.000000	-1.703764
H	0.658629	2.183637	-1.667470
H	0.658629	-2.183637	-1.667470
H	-1.908454	1.350345	-1.582477
H	-1.908454	-1.350345	-1.582477
H	2.241491	0.000000	-1.722196

$E_{\text{tot}} = -1953.351563$ a.u.

Structure of 4

staggered

Fe	0.000000	0.254969	0.000000
N	0.786440	-1.598039	0.000000
C	1.223000	-0.905497	1.120177
C	1.223000	-0.905497	-1.120177
C	1.946446	0.241099	0.712622
C	1.946446	0.241099	-0.712622
B	0.008626	-3.007513	0.000000
H	1.013573	-1.291213	2.106421
H	1.013573	-1.291213	-2.106421
H	2.397346	0.974726	1.365927
H	2.397346	0.974726	-1.365927
C	-1.924710	0.242265	-0.713297
C	-1.924710	0.242265	0.713297
C	-1.243979	1.414864	-1.154024
C	-1.243979	1.414864	1.154024
C	-0.819374	2.140157	0.000000
H	-2.325575	-0.540837	-1.342968
H	-2.325575	-0.540837	1.342968
H	-1.055409	1.692561	-2.183047
H	-1.055409	1.692561	2.183047
H	-0.258500	3.065741	0.000000
H	0.876238	-3.857124	0.000000
H	-0.659330	-3.019076	-1.014454
H	-0.659330	-3.019076	1.014454

E_{tot} = -1693.404681 a.u.

eclipsed

Fe	-0.219357	0.000000	-0.143220
N	0.885911	0.000000	1.538423
C	0.067377	-1.120544	1.517359
C	0.067377	1.120544	1.517359
C	-1.288172	-0.712984	1.483606
C	-1.288172	0.712984	1.483606
B	2.490139	0.000000	1.685963
H	0.503532	-2.106961	1.560977
H	0.503532	2.106961	1.560977
H	-2.149559	-1.365267	1.456475
H	-2.149559	1.365267	1.456475
C	-1.079545	0.713470	-1.864396
C	-1.079545	-0.713470	-1.864396
C	0.276646	1.154208	-1.767429
C	0.276646	-1.154208	-1.767429
C	1.110202	0.000000	-1.706395
H	-1.954675	1.348344	-1.914139
H	-1.954675	-1.348344	-1.914139
H	0.611428	2.182131	-1.722962
H	0.611428	-2.182131	-1.722962
H	2.181878	0.000000	-1.556116
H	2.705457	0.000000	2.880992
H	2.874917	1.014589	1.140038
H	2.874917	-1.014589	1.140038

E_{tot} = -1693.404705 a.u.

Structure of 5

staggered

Fe	0.000000	0.417074	0.000000
P	0.518827	-1.793639	0.000000
C	1.174361	-0.752861	1.264053
C	1.174361	-0.752861	-1.264053
C	1.926073	0.317692	0.712854
C	1.926073	0.317692	-0.712854
B	-0.585504	-3.445648	0.000000
H	1.019489	-0.899803	2.325521
H	1.019489	-0.899803	-2.325521
H	2.411002	1.081384	1.310211
H	2.411002	1.081384	-1.310211
C	-1.914604	0.613959	-0.714386
C	-1.914604	0.613959	0.714386
C	-1.115682	1.709643	-1.154269
C	-1.115682	1.709643	1.154269
C	-0.619518	2.385602	0.000000
H	-2.412517	-0.108905	-1.346886
H	-2.412517	-0.108905	1.346886
H	-0.902338	1.968446	-2.183290
H	-0.902338	1.968446	2.183290
H	0.033031	3.249151	0.000000
H	0.213477	-4.349444	0.000000
H	-1.228669	-3.333925	-1.017236
H	-1.228669	-3.333925	1.017236

$E_{\text{tot}} = -1979.992098$ a.u.

eclipsed

Fe	-0.119164	0.403008	0.000000
P	0.993455	-1.574448	0.000000
C	1.335257	-0.392680	1.264304
C	1.335257	-0.392680	-1.264304
C	1.756350	0.846325	0.713102
C	1.756350	0.846325	-0.713102
B	0.434737	-3.480919	0.000000
H	1.232273	-0.578719	2.325902
H	1.232273	-0.578719	-2.325902
H	2.013297	1.713335	1.310822
H	2.013297	1.713335	-1.310822
C	-1.338340	1.895958	-0.714236
C	-1.338340	1.895958	0.714236
C	-1.807056	0.622287	-1.154076
C	-1.807056	0.622287	1.154076
C	-2.098627	-0.164731	0.000000
H	-1.028333	2.714409	-1.350943
H	-1.028333	2.714409	1.350943
H	-1.906638	0.300554	-2.182379
H	-1.906638	0.300554	2.182379
H	-2.449312	-1.188158	0.000000
H	1.468881	-4.102251	0.000000
H	-0.212144	-3.568577	-1.017176
H	-0.212144	-3.568577	1.017176

$E_{\text{tot}} = -1979.992349$ a.u.

Structure of **6**

staggered

Fe	0.000000	0.003821	0.000000
C	-0.502828	1.989106	0.000000
H	0.224174	2.790393	0.000000
C	0.573354	-2.002392	0.000000
H	-0.065172	-2.874199	0.000000
C	-1.036972	1.342304	1.153417
C	-1.036972	1.342304	-1.153417
H	-0.794592	1.577254	-2.181828
H	-0.794592	1.577254	2.181828
C	-1.899768	0.294558	0.713842
C	-1.899768	0.294558	-0.713842
H	-2.443100	-0.392495	1.349697
H	-2.443100	-0.392495	-1.349697
C	1.094691	-1.303115	1.114975
C	1.094691	-1.303115	-1.114975
N	1.861107	-0.235865	0.693097
N	1.861107	-0.235865	-0.693097
H	0.971150	-1.504099	2.170444
H	0.971150	-1.504099	-2.170444

$$E_{\text{tot}} = -1682.760752 \text{ a.u.}$$

eclipsed

Fe	0.000000	0.002179	0.000000
C	0.675526	-1.969394	0.000000
C	1.611221	1.264363	0.000000
H	2.649947	0.959952	0.000000
H	1.695923	-2.324765	0.000000
C	0.802925	1.490755	1.155427
C	0.802925	1.490755	-1.155427
H	1.120586	1.386030	2.184733
H	1.120586	1.386030	-2.184733
C	-0.503254	1.857666	0.712073
C	-0.503254	1.857666	-0.712073
H	-1.359927	2.046299	1.345531
H	-1.359927	2.046299	-1.345531
C	-0.152031	-1.693783	1.115340
C	-0.152031	-1.693783	-1.115340
N	-1.391755	-1.256914	0.693558
N	-1.391755	-1.256914	-0.693558
H	0.062610	-1.792582	2.170609
H	0.062610	-1.792582	-2.170609

$$E_{\text{tot}} = -1682.760838 \text{ a.u.}$$

Structure of 7

staggered

Fe	0.000000	0.005888	0.000000
C	0.620674	1.958296	0.000000
H	1.651873	2.287665	0.000000
C	-0.552343	-1.912834	0.000000
H	-1.567907	-2.283815	0.000000
C	-0.172984	1.687031	1.154476
C	-0.172984	1.687031	-1.154476
H	0.151965	1.762186	-2.184016
H	0.151965	1.762186	2.184016
C	-1.459874	1.255178	0.712485
C	-1.459874	1.255178	-0.712485
H	-2.276231	0.942502	1.350596
H	-2.276231	0.942502	-1.350596
N	0.153721	-1.680720	1.156855
N	0.153721	-1.680720	-1.156855
C	1.399650	-1.292396	0.709625
C	1.399650	-1.292396	-0.709625
H	2.200488	-1.053375	-1.395702
H	2.200488	-1.053375	1.395702

$E_{\text{tot}} = -1682.783631$ a.u.

eclipsed

Fe	0.000000	0.007825	0.000000
C	-0.351136	-1.955790	0.000000
C	2.025772	0.302733	0.000000
H	2.774219	-0.478885	0.000000
H	0.394005	-2.738973	0.000000
C	1.435439	0.901471	1.153298
C	1.435439	0.901471	-1.153298
H	1.637678	0.633295	2.182124
H	1.637678	0.633295	-2.182124
C	0.480749	1.865514	0.714908
C	0.480749	1.865514	-0.714908
H	-0.142876	2.477486	1.353492
H	-0.142876	2.477486	-1.353492
N	-0.882998	-1.436361	1.157110
N	-0.882998	-1.436361	-1.157110
C	-1.829009	-0.536683	0.709828
C	-1.829009	-0.536683	-0.709828
H	-2.444914	0.028302	1.395591
H	-2.444914	0.028302	-1.395591

$E_{\text{tot}} = -1682.783854$ a.u.

Structure of 8

staggered

Fe	0.000000	0.004842	0.000000
C	1.965918	-0.582989	0.000000
H	2.313824	-1.607984	0.000000
N	-1.878716	0.595739	0.000000
C	1.680557	0.206932	1.154103
C	1.680557	0.206932	-1.154103
H	1.757915	-0.119883	-2.182915
H	1.757915	-0.119883	2.182915
C	1.222224	1.483293	0.712434
C	1.222224	1.483293	-0.712434
H	0.874743	2.287338	1.347634
H	0.874743	2.287338	-1.347634
N	-1.658662	-0.166122	1.130729
N	-1.658662	-0.166122	-1.130729
C	-1.304083	-1.420980	0.704318
C	-1.304083	-1.420980	-0.704318
H	-1.093371	-2.215140	-1.405229
H	-1.093371	-2.215140	1.405229

$E_{\text{tot}} = -1698.782058 \text{ a.u.}$

eclipsed

Fe	0.000000	0.002935	0.000000
N	1.952011	0.271218	0.000000
C	-0.843973	1.872088	0.000000
H	-0.267488	2.787572	0.000000
C	-1.253283	1.141526	1.153301
C	-1.253283	1.141526	-1.153301
H	-1.045664	1.409473	2.180895
H	-1.045664	1.409473	-2.180895
C	-1.916608	-0.043224	0.714523
C	-1.916608	-0.043224	-0.714523
H	-2.329820	-0.814308	1.351762
H	-2.329820	-0.814308	-1.351762
N	1.607306	-0.442148	1.130603
N	1.607306	-0.442148	-1.130603
C	1.045059	-1.619487	0.704932
C	1.045059	-1.619487	-0.704932
H	0.706962	-2.370487	1.403792
H	0.706962	-2.370487	-1.403792

$E_{\text{tot}} = -1698.782052 \text{ a.u.}$

Structure of 9

staggered

Fe	0.000000	0.006548	0.000000
C	0.344310	2.019942	0.000000
H	1.333998	2.456856	0.000000
N	-0.318589	-2.043758	0.000000
C	-0.407948	1.647339	1.153763
C	-0.407948	1.647339	-1.153763
H	-0.088773	1.761447	-2.181639
H	-0.088773	1.761447	2.181639
C	-1.619693	1.038820	0.714098
C	-1.619693	1.038820	-0.714098
H	-2.388605	0.616053	1.347686
H	-2.388605	0.616053	-1.347686
C	0.443498	-1.643698	1.063787
C	0.443498	-1.643698	-1.063787
N	1.601390	-1.002395	0.692401
N	1.601390	-1.002395	-0.692401
H	0.187646	-1.835729	2.096138
H	0.187646	-1.835729	-2.096138

$E_{\text{tot}} = -1698.801200 \text{ a.u.}$

eclipsed

Fe	0.000000	0.006468	0.000000
N	0.101760	-2.064142	0.000000
C	1.912066	0.730356	0.000000
H	2.795054	0.104473	0.000000
C	1.209479	1.185108	1.155649
C	1.209479	1.185108	-1.155649
H	1.480457	0.986681	2.184365
H	1.480457	0.986681	-2.184365
C	0.071110	1.924998	0.711932
C	0.071110	1.924998	-0.711932
H	-0.691940	2.359048	1.344540
H	-0.691940	2.359048	-1.344540
C	-0.614156	-1.585473	1.064208
C	-0.614156	-1.585473	-1.064208
N	-1.699207	-0.826953	0.692594
N	-1.699207	-0.826953	-0.692594
H	-0.382547	-1.807739	2.096100
H	-0.382547	-1.807739	-2.096100

$E_{\text{tot}} = -1698.801354 \text{ a.u.}$

Structure of 10

staggered

Fe	0.000000	0.004649	0.000000
C	-1.095641	1.730356	0.000000
H	-0.647817	2.715442	0.000000
C	1.188359	-1.643815	0.000000
H	0.885245	-2.680061	0.000000
C	-1.398974	0.949856	1.153845
C	-1.398974	0.949856	-1.153845
H	-1.226595	1.240534	-2.181713
H	-1.226595	1.240534	2.181713
C	-1.896088	-0.312970	0.712765
C	-1.896088	-0.312970	-0.712765
H	-2.178411	-1.140984	1.350066
H	-2.178411	-1.140984	-1.350066
N	1.419514	-0.917778	1.131761
N	1.419514	-0.917778	-1.131761
N	1.834559	0.309406	0.689698
N	1.834559	0.309406	-0.689698

$E_{\text{tot}} = -1714.804736 \text{ a.u.}$

eclipsed

Fe	0.000000	0.003625	0.000000
C	-1.118624	-1.690859	0.000000
C	1.992994	-0.451741	0.000000
H	2.404690	-1.452577	0.000000
H	-0.777876	-2.715277	0.000000
C	1.659297	0.320411	1.153831
C	1.659297	0.320411	-1.153831
H	1.745572	-0.003847	2.182653
H	1.745572	-0.003847	-2.182653
C	1.120410	1.563921	0.713113
C	1.120410	1.563921	-0.713113
H	0.721479	2.343189	1.348872
H	0.721479	2.343189	-1.348872
N	-1.380397	-0.974857	1.132081
N	-1.380397	-0.974857	-1.132081
N	-1.845575	0.234754	0.689718
N	-1.845575	0.234754	-0.689718

$E_{\text{tot}} = -1714.804709 \text{ a.u.}$

Structure of 11

staggered

Fe	0.000000	0.000115	0.000000
C	-1.918829	0.707990	0.000000
H	-2.163781	1.762017	0.000000
N	1.895531	-0.657428	0.000000
C	-1.686130	-0.097267	1.153687
C	-1.686130	-0.097267	-1.153687
H	-1.723928	0.239468	-2.181404
H	-1.723928	0.239468	2.181404
C	-1.309273	-1.400087	0.713041
C	-1.309273	-1.400087	-0.713041
H	-1.010988	-2.223855	1.348196
H	-1.010988	-2.223855	-1.348196
N	1.673390	0.111202	1.101273
N	1.673390	0.111202	-1.101273
N	1.313947	1.354945	0.680638
N	1.313947	1.354945	-0.680638

$E_{\text{tot}} = -1730.812172$ a.u.

eclipsed

Fe	0.000000	0.000394	0.000000
N	0.506425	-1.941533	0.000000
C	1.715779	1.113649	0.000000
H	2.707392	0.680566	0.000000
C	0.931256	1.409085	1.153841
C	0.931256	1.409085	-1.153841
H	1.224015	1.239153	2.181592
H	1.224015	1.239153	-2.181592
C	-0.338114	1.887139	0.713103
C	-0.338114	1.887139	-0.713103
H	-1.175862	2.143283	1.348267
H	-1.175862	2.143283	-1.348267
N	-0.242483	-1.659867	1.101596
N	-0.242483	-1.659867	-1.101596
N	-1.454736	-1.204528	0.680748
N	-1.454736	-1.204528	-0.680748

$E_{\text{tot}} = -1730.812070$ a.u.

Structure of 12

staggered

Fe	0.000000	0.000000	0.000000
P	1.363122	-1.085481	1.593677
P	1.363122	1.085481	1.593677
C	-1.164550	0.000000	1.700782
C	-0.414912	-1.198669	1.638075
C	-0.414912	1.198669	1.638075
H	-2.251509	0.000000	1.692719
H	-0.909962	-2.164429	1.591378
H	-0.909962	2.164429	1.591378
C	0.164689	1.154564	-1.700304
C	0.164689	-1.154564	-1.700304
C	0.997346	0.000000	-1.798298
C	-1.180266	0.713500	-1.536435
C	-1.180266	-0.713500	-1.536435
H	0.501273	2.182614	-1.716861
H	0.501273	-2.182614	-1.716861
H	2.074265	0.000000	-1.899149
H	-2.047092	1.349266	-1.410664
H	-2.047092	-1.349266	-1.410664

$E_{\text{tot}} = -2256.009681$ a.u.

eclipsed

Fe	0.000000	0.000000	0.000000
P	1.509445	-1.085832	1.456924
P	1.509445	1.085832	1.456924
C	-0.997787	0.000000	1.802217
C	-0.257181	-1.198922	1.667778
C	-0.257181	1.198922	1.667778
H	-2.079633	0.000000	1.905981
H	-0.753835	-2.164909	1.674572
H	-0.753835	2.164909	1.674572
C	0.608903	0.712746	-1.841754
C	0.608903	-0.712746	-1.841754
C	-1.533886	0.000000	-1.363332
C	-0.714161	1.154788	-1.543408
C	-0.714161	-1.154788	-1.543408
H	1.468171	1.347689	-2.009457
H	1.468171	-1.347689	-2.009457
H	-2.588470	0.000000	-1.119575
H	-1.035290	2.184534	-1.456931
H	-1.035290	-2.184534	-1.456931

$E_{\text{tot}} = -2256.009744$ a.u.

Structure of 13

staggered

Fe	-0.009708	0.236031	0.000000
P	-0.031313	-1.504639	1.541775
P	-0.031313	-1.504639	-1.541775
C	-0.893592	-1.671143	0.000000
C	1.475345	-1.046607	0.704836
C	1.475345	-1.046607	-0.704836
H	-1.961648	-1.873312	0.000000
H	2.348715	-0.726925	1.267853
H	2.348715	-0.726925	-1.267853
C	-1.353264	1.627448	-0.711240
C	-1.353264	1.627448	0.711240
C	0.781655	2.145938	0.000000
C	-0.031313	1.944356	-1.152466
C	-0.031313	1.944356	1.152466
H	-2.196637	1.398299	-1.349046
H	-2.196637	1.398299	1.349046
H	1.838314	2.380494	0.000000
H	0.296677	2.000643	-2.181849
H	0.296677	2.000643	2.181849

$E_{\text{tot}} = -2255.995500$ a.u.

eclipsed

Fe	0.000000	0.000000	0.000000
P	0.280047	-1.542588	1.717929
P	0.280047	1.542588	1.717929
C	1.157992	0.000000	1.749520
C	-1.277578	-0.705299	1.485828
C	-1.277578	0.705299	1.485828
H	2.243906	0.000000	1.796984
H	-2.190133	-1.267551	1.304870
H	-2.190133	1.267551	1.304870
C	0.521767	1.153499	-1.627952
C	0.521767	-1.153499	-1.627952
C	1.356730	0.000000	-1.551127
C	-0.831704	0.712966	-1.740277
C	-0.831704	-0.712966	-1.740277
H	0.853850	2.181838	-1.583920
H	0.853850	-2.181838	-1.583920
H	2.432976	0.000000	-1.440183
H	-1.704345	1.350031	-1.801368
H	-1.704345	-1.350031	-1.801368

$E_{\text{tot}} = -2255.995841$ a.u.

Structure of 14

staggered

Fe	0.000000	0.000000	0.000000
P	-0.192331	-1.656949	1.671976
P	-0.192331	1.656949	1.671976
P	1.104470	0.000000	2.140129
C	-1.593008	-0.703401	1.134442
C	-1.593008	0.703401	1.134442
H	-2.447547	-1.235447	0.719782
H	-2.447547	1.235447	0.719782
C	1.411399	0.711962	-1.327989
C	1.411399	-0.711962	-1.327989
C	-0.692563	0.000000	-1.951650
C	0.109974	1.152780	-1.712565
C	0.109974	-1.152780	-1.712565
H	2.241304	1.347460	-1.049952
H	2.241304	-1.347460	-1.049952
H	-1.736760	0.000000	-2.236360
H	-0.215165	2.182146	-1.782761
H	-0.215165	-2.182146	-1.782761

$$E_{\text{tot}} = -2558.664486 \text{ a.u.}$$

eclipsed

Fe	0.004118	0.345886	0.000000
P	0.322728	-1.306976	1.658041
P	0.322728	-1.306976	-1.658041
P	-0.936811	-1.868241	0.000000
C	1.677032	-0.660841	0.703772
C	1.677032	-0.660841	-0.703772
H	2.501029	-0.188396	1.235518
H	2.501029	-0.188396	-1.235518
C	-0.949028	1.772775	-1.153142
C	-0.949028	1.772775	1.153142
C	-1.732185	1.477003	0.000000
C	0.322728	2.248422	-0.713072
C	0.322728	2.248422	0.713072
H	-1.255860	1.636585	-2.181144
H	-1.255860	1.636585	2.181144
H	-2.735275	1.072767	0.000000
H	1.146264	2.542204	-1.350764
H	1.146264	2.542204	1.350764

$$E_{\text{tot}} = -2558.664653 \text{ a.u.}$$

Structure of 15

staggered

Fe	0.000000	0.000000	0.000000
P	-0.882237	-1.080419	1.913047
P	-0.882237	1.080419	1.913047
P	1.991095	0.000000	1.210033
C	0.808363	-1.296368	1.432146
C	0.808363	1.296368	1.432146
H	1.139685	-2.314445	1.231984
H	1.139685	2.314445	1.231984
C	0.583433	0.714544	-1.850287
C	0.583433	-0.714544	-1.850287
C	-1.551982	0.000000	-1.363305
C	-0.736294	1.154550	-1.553767
C	-0.736294	-1.154550	-1.553767
H	1.444057	1.347984	-2.018890
H	1.444057	-1.347984	-2.018890
H	-2.599472	0.000000	-1.094102
H	-1.059269	2.182292	-1.454640
H	-1.059269	-2.182292	-1.454640

$E_{\text{tot}} = -2558.651174$ a.u.

eclipsed

Fe	0.000000	0.000000	0.000000
P	-0.903754	-1.080699	1.903463
P	-0.903754	1.080699	1.903463
P	1.978596	0.000000	1.234162
C	0.791810	-1.296413	1.437402
C	0.791810	1.296413	1.437402
H	1.127335	-2.315076	1.248349
H	1.127335	2.315076	1.248349
C	0.010135	1.154329	-1.707118
C	0.010135	-1.154329	-1.707118
C	0.828560	0.000000	-1.890481
C	-1.316155	0.713288	-1.427383
C	-1.316155	-0.713288	-1.427383
H	0.340552	2.183333	-1.758544
H	0.340552	-2.183333	-1.758544
H	1.888640	0.000000	-2.104634
H	-2.167790	1.348275	-1.224938
H	-2.167790	-1.348275	-1.224938

$E_{\text{tot}} = -2558.651461$ a.u.

Structure of 16

staggered

Fe	0.000000	0.000000	0.000000
P	-1.164870	-1.071303	1.814420
P	-1.164870	1.071303	1.814420
P	0.890901	-1.606501	1.498750
P	0.890901	1.606501	1.498750
C	1.602977	0.000000	1.327842
H	2.650918	0.000000	1.023348
C	0.758074	0.711207	-1.796714
C	0.758074	-0.711207	-1.796714
C	-1.418272	0.000000	-1.515492
C	-0.587537	1.151466	-1.620091
C	-0.587537	-1.151466	-1.620091
H	1.627042	1.349692	-1.883510
H	1.627042	-1.349692	-1.883510
H	-2.486483	0.000000	-1.345941
H	-0.915067	2.179492	-1.545611
H	-0.915067	-2.179492	-1.545611

$E_{\text{tot}} = -2861.318349 \text{ a.u.}$

eclipsed

Fe	0.000000	0.000000	0.000000
P	-1.113014	-1.071961	1.845890
P	-1.113014	1.071961	1.845890
P	0.934081	-1.606963	1.473745
P	0.934081	1.606963	1.473745
C	1.640059	0.000000	1.280416
H	2.681621	0.000000	0.955187
C	0.100069	1.153275	-1.716710
C	0.100069	-1.153275	-1.716710
C	0.929462	0.000000	-1.840747
C	-1.238966	0.712174	-1.503604
C	-1.238966	-0.712174	-1.503604
H	0.431561	2.182116	-1.750933
H	0.431561	-2.182116	-1.750933
H	2.001310	0.000000	-1.988862
H	-2.099761	1.347268	-1.345391
H	-2.099761	-1.347268	-1.345391

$E_{\text{tot}} = -2861.318426 \text{ a.u.}$

Structure of 17

staggered

Fe	0.000000	0.000000	0.000000
P	1.817575	0.000000	1.577620
P	0.561662	-1.728617	1.577620
P	-1.470449	-1.068344	1.577620
P	-1.470449	1.068344	1.577620
P	0.561662	1.728617	1.577620
C	-1.211190	0.000000	-1.694736
C	-0.374278	1.151910	-1.694736
C	0.979873	0.711920	-1.694736
C	0.979873	-0.711920	-1.694736
C	-0.374278	-1.151910	-1.694736
H	-2.292259	0.000000	-1.663960
H	-0.708347	2.180068	-1.663960
H	1.854477	1.347356	-1.663960
H	1.854477	-1.347356	-1.663960
H	-0.708347	-2.180068	-1.663960

$E_{\text{tot}} = -3163.983826$ a.u.

eclipsed

Fe	0.000000	0.000000	0.000000
P	1.818325	0.000000	1.578399
P	0.561893	-1.729330	1.578399
P	-1.471056	-1.068785	1.578399
P	-1.471056	1.068785	1.578399
P	0.561893	1.729330	1.578399
C	1.211994	0.000000	-1.688642
C	0.374527	1.152674	-1.688642
C	-0.980523	0.712392	-1.688642
C	-0.980523	-0.712392	-1.688642
C	0.374527	-1.152674	-1.688642
H	2.293221	0.000000	-1.668725
H	0.708644	2.180983	-1.668725
H	-1.855255	1.347921	-1.668725
H	-1.855255	-1.347921	-1.668725
H	0.708644	-2.180983	-1.668725

$E_{\text{tot}} = -3163.983739$ a.u.

Structure of BH₃

B	0.000000	0.000000	0.000000
H	0.000000	1.193883	0.000000
H	1.033933	-0.596941	0.000000
H	-1.033933	-0.596941	0.000000

$E_{\text{tot}} = -26.613000$ a.u.