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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1996, 118(27), 6407-6421, DOI:[10.1021/ja960787m](https://doi.org/10.1021/ja960787m)

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Table S11. Bond Distances in *hypho*-12-CH₃-12,11-CN B₉H₁₄⁻ (**4a⁻**), Å

N11-C12	1.463(7)	N11-B5	1.547(9)	N11-B10	1.544(7)
N23-C22	1.475(5)	N23-C25	1.481(6)	N23-C26	1.478(6)
N24-C14	1.469(5)	N24-C27	1.492(7)	N24-C28	1.452(7)
C12-C12a	1.527(8)	C12-B7	1.612(11)	C12-H12	1.185(77)
C13-C14	1.403(6)	C13-C18	1.444(6)	C13-C22	1.436(6)
C14-C15	1.365(6)	C15-C16	1.401(7)	C15-H13	1.022(48)
C16-C17	1.319(8)	C16-H14	0.953(50)	C17-C18	1.428(7)
C17-H15	0.928(43)	C18-C19	1.378(7)	C19-C20	1.364(7)
C19-H16	1.065(44)	C20-C21	1.397(7)	C20-H17	0.918(46)
C21-C22	1.337(7)	C21-H18	0.893(46)	C25-H20	1.019(56)
C25-H21	1.017(52)	C25-H22	1.014(53)	C26-H23	0.955(69)
C26-H24	1.052(51)	C26-H25	0.849(56)	C27-H26	0.919(52)
C27-H27	1.116(88)	C27-H28	0.952(59)	C28-H29	1.019(64)
C28-H30	0.968(51)	C28-H31	0.947(65)	B1-B2	1.803(11)
B1-B3	1.800(9)	B1-B4	1.804(9)	B1-B5	1.770(9)
B1-B7	1.798(12)	B1-H1	1.002(56)	B2-B3	1.727(10)
B2-B7	1.817(11)	B2-B8	1.869(10)	B2-H2	1.044(54)
B2-H2,7	1.288(43)	B3-B4	1.752(9)	B3-B8	1.683(10)
B3-B9	1.706(10)	B3-H3	1.001(60)	B4-B5	1.758(8)
B4-B9	1.754(10)	B4-B10	1.743(9)	B4-H4	1.176(47)
B5-B10	1.912(9)	B5-H5	1.161(47)	B7-H7	1.116(50)
B7-H2,7	1.455(41)	B8-B9	1.865(10)	B8-H8a	1.137(47)
B8-H8b	1.164(59)	B9-B10	1.821(9)	B9-H9	1.052(54)
B9-H9,10	1.384(48)	B10-H10	1.233(50)	B10-H9,10	1.479(48)

Table S11a. Selected (a) Crystallographically Determined and (b) Calculated Bond Distances (Å) for *hypho*-12-CH₃-12,11-CNB₉H₁₄- (**4a**⁻)

(a) *Crystallographically Determined*

B1-B2	1.803(11)	B1-B3	1.800(9)	B1-B4	1.804(9)
B1-B5	1.770(9)	B1-B7	1.798(12)	B1-H1	1.002(56)
B2-B3	1.727(10)	B2-B7	1.817(11)	B2-B8	1.869(10)
B2-H2	1.044(54)	B2-H2,7	1.288(43)	B3-B4	1.752(9)
B3-B8	1.683(10)	B3-B9	1.706(10)	B3-H3	1.001(60)
B4-B5	1.758(8)	B4-B9	1.754(10)	B4-B10	1.743(9)
B4-H4	1.176(47)	B5-B10	1.912(9)	B5-H5	1.161(47)
B7-H7	1.116(50)	B7-H2,7	1.455(41)	B8-B9	1.865(10)
B8-H8a	1.137(47)	B8-H8b	1.164(59)	B9-B10	1.821(9)
B9-H9	1.052(54)	B9-H9,10	1.384(48)	B10-H10	1.233(50)
B10-H9,10	1.479(48)	N11-C12	1.463(7)	N11-B5	1.547(9)
N11-B10	1.544(7)	C12-C12a	1.527(8)	C12-B7	1.612(11)
C12-H12	1.185(77)				

(b) *Calculated, HF/6-31G**

B1-B2	1.818	B1-B3	1.856	B1-B4	1.860
B1-B5	1.771	B1-B7	1.810	B1-H1	1.196
B2-B3	1.741	B2-B7	1.838	B2-B8	1.985
B2-H2	1.193	B2-H2,7	1.260	B3-B4	1.801
B3-B8	1.739	B3-B9	1.748	B3-H3	1.191
B4-B5	1.768	B4-B9	1.795	B4-B10	1.772
B4-H4	1.192	B5-B10	1.933	B5-H5	1.194
B7-H7	1.201	B7-H2,7	1.397	B8-B9	1.931

B8-H8a	1.197	B8-H8b	1.202	B9-B10	1.856
B9-H9	1.192	B9-H9,10	1.293	B10-H10	1.193
B10-H9,10	1.378	N11-C12	1.486	N11-B5	1.560
N11-B10	1.566	C12-C12a	1.527	C12-B7	1.643
C12-H12	1.089				

Table S12. Bond Angles in *hypho*-12-CH₃-12,11-CNB₉H₁₄⁻ (**4a**⁻), °

C12-N11-B5	108.3(5)	C12-N11-B10	127.2(5)	B5-N11-B10	76.4(4)
C22-N23-C25	112.1(4)	C22-N23-C26	112.9(4)	C25-N23-C26	110.7(5)
C14-N24-C27	112.0(4)	C14-N24-C28	112.4(4)	C27-N24-C28	111.3(6)
N11-C12-C12a	108.9(6)	N11-C12-B7	102.0(6)	N11-C12-H12	93.2(38)
C12a-C12-B7	114.3(6)	C12a-C12-H12	122.2(40)	B7-C12-H12	111.9(39)
C14-C13-C18	117.7(4)	C14-C13-C22	126.7(4)	C18-C13-C22	115.6(4)
N24-C14-C13	118.2(4)	N24-C14-C15	119.8(5)	C13-C14-C15	122.0(5)
C14-C15-C16	119.7(6)	C14-C15-H13	117.6(25)	C16-C15-H13	121.7(26)
C15-C16-C17	120.7(6)	C15-C16-H14	129.0(31)	C17-C16-H14	110.2(31)
C16-C17-C18	122.5(5)	C16-C17-H15	127.2(27)	C18-C17-H15	110.3(27)
C13-C18-C17	117.3(5)	C13-C18-C19	120.3(4)	C17-C18-C19	122.4(5)
C18-C19-C20	121.5(5)	C18-C19-H16	123.8(23)	C20-C19-H16	114.1(23)
C19-C20-C21	119.6(6)	C19-C20-H17	122.8(28)	C21-C20-H17	117.4(28)
C20-C21-C22	121.0(5)	C20-C21-H18	115.6(31)	C22-C21-H18	123.0(32)
N23-C22-C13	116.6(4)	N23-C22-C21	121.3(4)	C13-C22-C21	122.1(4)
N23-C25-H20	107.8(32)	N23-C25-H21	114.2(31)	N23-C25-H22	104.8(30)
H20-C25-H21	94.2(41)	H20-C25-H22	121.4(46)	H21-C25-H22	114.5(41)
N23-C26-H23	109.9(41)	N23-C26-H24	115.1(27)	N23-C26-H25	112.7(41)
H23-C26-H24	104.0(47)	H23-C26-H25	116.0(60)	H24-C26-H25	98.6(47)
N24-C27-H26	103.4(34)	N24-C27-H27	108.1(48)	N24-C27-H28	111.3(37)
H26-C27-H27	97.0(56)	H26-C27-H28	119.0(52)	H27-C27-H28	116.4(57)
N24-C28-H29	107.8(35)	N24-C28-H30	113.5(31)	N24-C28-H31	114.0(40)
H29-C28-H30	107.3(45)	H29-C28-H31	111.6(55)	H30-C28-H31	102.6(50)
B2-B1-B3	57.3(4)	B2-B1-B4	109.9(5)	B2-B1-B5	128.4(6)
B2-B1-B7	60.6(5)	B2-B1-H1	111.2(33)	B3-B1-B4	58.2(4)

B3-B1-B5	110.6(5)	B3-B1-B7	106.1(5)	B3-B1-H1	107.8(31)
B4-B1-B5	58.9(3)	B4-B1-B7	118.3(5)	B4-B1-H1	111.4(33)
B5-B1-B7	80.5(5)	B5-B1-H1	119.7(33)	B7-B1-H1	129.3(33)
B1-B2-B3	61.3(4)	B1-B2-B7	59.6(4)	B1-B2-B8	107.1(5)
B1-B2-H2	112.9(30)	B1-B2-H2,7	110.1(20)	B3-B2-B7	108.5(5)
B3-B2-B8	55.6(4)	B3-B2-H2	112.7(29)	B3-B2-H2,7	127.6(20)
B7-B2-B8	111.4(6)	B7-B2-H2	124.7(27)	B7-B2-H2,7	52.6(19)
B8-B2-H2	121.9(27)	B8-B2-H2,7	84.2(19)	H2-B2-H2,7	117.2(36)
B1-B3-B2	61.5(4)	B1-B3-B4	61.0(4)	B1-B3-B8	116.0(5)
B1-B3-B9	109.1(5)	B1-B3-H3	116.7(34)	B2-B3-B4	116.2(5)
B2-B3-B8	66.5(5)	B2-B3-B9	118.2(6)	B2-B3-H3	110.5(36)
B4-B3-B8	120.1(6)	B4-B3-B9	61.0(4)	B4-B3-H3	118.0(36)
B8-B3-B9	66.8(5)	B8-B3-H3	114.5(35)	B9-B3-H3	124.4(34)
B1-B4-B3	60.8(4)	B1-B4-B5	59.6(4)	B1-B4-B9	106.8(5)
B1-B4-B10	108.9(5)	B1-B4-H4	119.9(23)	B3-B4-B5	113.5(5)
B3-B4-B9	58.2(4)	B3-B4-B10	110.3(5)	B3-B4-H4	125.6(23)
B5-B4-B9	117.3(5)	B5-B4-B10	66.2(4)	B5-B4-H4	107.9(22)
B9-B4-B10	62.7(4)	B9-B4-H4	126.7(22)	B10-B4-H4	117.9(24)
N11-B5-B1	114.9(6)	N11-B5-B4	104.1(5)	N11-B5-B10	51.7(3)
N11-B5-H5	117.8(24)	B1-B5-B4	61.5(4)	B1-B5-B10	103.1(4)
B1-B5-H5	121.0(24)	B4-B5-B10	56.5(3)	B4-B5-H5	124.7(24)
B10-B5-H5	129.7(24)	C12-B7-B1	117.9(5)	C12-B7-B2	122.4(6)
C12-B7-H7	114.9(28)	C12-B7-H2,7	92.9(19)	B1-B7-B2	59.9(4)
B1-B7-H7	113.4(28)	B1-B7-H2,7	102.8(19)	B2-B7-H7	116.6(28)
B2-B7-H2,7	44.7(17)	H7-B7-H2,7	112.0(32)	B2-B8-B3	57.9(4)
B2-B8-B9	104.2(5)	B2-B8-H8a	114.4(24)	B2-B8-H8b	93.5(28)
B3-B8-B9	57.2(4)	B3-B8-H8a	109.7(24)	B3-B8-H8b	132.5(29)

B9-B8-H8a	120.7(24)	B9-B8-H8b	103.0(29)	H8a-B8-H8b	117.0(38)
B3-B9-B4	60.8(4)	B3-B9-B8	56.0(4)	B3-B9-B10	108.8(4)
B3-B9-H9	130.3(30)	B3-B9-H9,10	117.7(19)	B4-B9-B8	110.6(5)
B4-B9-B10	58.3(4)	B4-B9-H9	118.3(31)	B4-B9-H9,10	104.3(20)
B8-B9-B10	121.0(5)	B8-B9-H9	122.8(30)	B8-B9-H9,10	82.6(21)
B10-B9-H9	109.3(30)	B10-B9-H9,10	52.9(20)	H9-B9-H9,10	110.5(36)
N11-B10-B4	105.0(5)	N11-B10-B5	51.9(3)	N11-B10-B9	124.0(5)
N11-B10-H10	110.7(22)	N11-B10-H9,10	93.0(19)	B4-B10-B5	57.3(4)
B4-B10-B9	58.9(4)	B4-B10-H10	124.1(24)	B4-B10-H9,10	100.8(19)
B5-B10-B9	106.9(4)	B5-B10-H10	120.7(23)	B5-B10-H9,10	118.8(18)
B9-B10-H10	122.4(22)	B9-B10-H9,10	48.2(19)	H10-B10-H9,10	118.2(29)

Table S13. Cartesian coordinates (Å) of the optimized geometry of 1⁻ at the HF/6-31G* level (E = -411.6166615 a.u.).

B	0.000000	1.492557	0.000000
B	-1.675989	0.841999	0.000000
B	-0.989261	-1.879149	0.000000
B	0.816125	-1.321633	0.000000
B	-1.905024	-0.689022	0.894386
B	-1.905024	-0.689022	-0.894386
B	-0.653633	0.476431	1.427496
B	-0.653633	0.476431	-1.427496
C	-0.303610	-1.085359	1.290834
C	-0.303610	-1.085359	-1.290834
C	1.471138	1.034467	0.000000
C	2.557409	2.085307	0.000000
N	1.846572	-0.209499	0.000000
H	-0.100425	2.694858	0.000000
H	-2.478726	1.723623	0.000000
H	-1.156569	-3.055205	0.000000
H	-2.822001	-1.012121	1.583029
H	-2.822001	-1.012121	-1.583029
H	-0.778435	0.973310	2.510603
H	-0.778435	0.973310	-2.510603
H	-0.173891	-1.669351	2.187842
H	-0.173891	-1.669351	-2.187842
H	3.557878	1.656942	0.000000
H	2.450289	2.720368	-0.872213
H	2.450289	2.720368	0.872213
H	1.385318	-2.388815	0.000000
H	2.818838	-0.426610	0.000000

Table S14. Cartesian coordinates (Å) of the optimized geometry of *arachno*-7-CH₃-5,7,11,12-C₃NB₈H₁₁⁻ at the HF/6-31G* level (E = -411.5263384 a.u.).

B	0.831799	1.268508	-0.017137
B	-0.914826	1.657473	-0.073143
B	-2.014559	-0.956859	0.047827
B	-0.320064	0.910710	1.435369
B	-0.224753	0.710884	-1.432615
B	-1.982695	0.534318	0.859532
B	-1.921800	0.448913	-0.938299
B	-0.827350	-0.742752	1.409813
C	-0.087271	-1.450520	0.068492
C	-0.763540	-0.792908	-1.182875
C	1.761966	0.039527	0.023768
C	3.257395	0.237339	0.006487
N	1.345526	-1.192379	0.046267
H	1.457070	2.298575	-0.085726
H	-1.107162	2.830452	-0.190530
H	-2.760940	-1.875335	-0.061599
H	-0.193081	-2.527864	0.039999
H	-0.179513	1.581372	2.421508
H	-0.037924	1.099899	-2.548963
H	-2.945471	0.871811	1.481110
H	-2.770055	0.609080	-1.759965
H	-1.008374	-1.432331	2.381481
H	-0.891353	-1.432953	-2.041792
H	1.977698	-1.959751	0.079970
H	3.812928	-0.698145	0.026497
H	3.539187	0.791370	-0.881197
H	3.548242	0.833866	0.863377

Table S15. Cartesian coordinates (Å) of the optimized geometry of **2a⁻** at the HF/6-31G* level (E = -386.3710536 a.u.).

B	0.000000	1.529917	0.000000
B	-1.643290	0.851340	0.000000
B	-0.869662	-1.830231	0.000000
B	0.868493	-1.512851	0.000000
B	-1.891752	-0.663512	0.910930
B	-1.891752	-0.663512	-0.910930
B	-0.788393	0.599052	1.521418
B	-0.788393	0.599052	-1.521418
B	-0.330615	-1.201385	1.536403
B	-0.330615	-1.201385	-1.536403
C	1.456450	0.977368	0.000000
C	2.598617	1.968093	0.000000
N	1.774455	-0.285282	0.000000
H	-0.037658	2.731127	0.000000
H	-2.455331	1.722197	0.000000
H	-1.082682	-3.002415	0.000000
H	-2.925817	-0.935553	1.438727
H	-2.925817	-0.935553	-1.438727
H	-1.017938	1.204699	2.521130
H	-1.017938	1.204699	-2.521130
H	-0.251664	-1.848810	2.533965
H	-0.251664	-1.848810	-2.533965
H	0.310563	-0.097570	1.736157
H	0.310563	-0.097570	-1.736157
H	3.573331	1.484658	0.000000
H	2.531341	2.609619	-0.872010
H	2.531341	2.609619	0.872010
H	1.538703	-2.507334	0.000000
H	2.748971	-0.501228	0.000000

Table S16. Cartesian coordinates (Å) of the optimized geometry of **3a** at the HF/6-31G* level (E = -362.7605063 a.u.).

B	-0.783430	1.524700	-0.375388
B	1.888740	0.575184	0.312919
B	1.614622	-1.191881	0.308212
B	1.034420	1.596251	-0.852785
B	0.607703	1.656199	0.885237
B	1.673048	-0.218873	-1.221709
B	0.980072	-0.118654	1.625866
B	0.414604	-1.519833	-0.997600
B	-0.057264	-1.451912	0.937129
C	-1.656317	0.152096	-0.545830
C	-2.909980	0.179199	0.331661
N	-0.941029	-1.148429	-0.315965
H	-1.421161	2.507323	-0.573563
H	2.960162	1.008875	0.561005
H	2.507540	-1.930889	0.551961
H	-1.601033	-1.889615	-0.453124
H	1.575717	2.538886	-1.319159
H	0.887353	2.635649	1.486434
H	2.579704	-0.403759	-1.956655
H	1.446946	-0.240043	2.704673
H	0.430082	-2.552388	-1.577392
H	-0.325141	-2.443038	1.527079
H	0.019793	1.385950	-1.532847
H	-0.613877	1.480656	1.028149
H	0.622855	-0.561330	-1.904141
H	-0.269003	-0.432134	1.772679
H	-1.976534	0.117585	-1.584254
H	-2.663836	0.215344	1.388666
H	-3.532834	-0.696749	0.167589
H	-3.504326	1.055009	0.100273

Table S17. Cartesian coordinates (Å) of the two optimized geometries of **3a⁻** at the HF/6-31G* level.

Structure from Figure 13a (E = -362.2289829 a.u.)

B	-0.808193	1.530029	-0.401750
B	1.881243	0.660970	0.461459
B	1.679970	-1.092315	0.293120
B	1.011887	1.572086	-0.810471
B	0.410024	1.580726	0.886003
B	1.729636	-0.090521	-1.184528
B	0.808938	-0.182472	1.634906
B	0.492630	-1.499769	-0.946699
B	0.005248	-1.501047	0.881137
C	-1.658782	0.132706	-0.562678
C	-2.877241	0.126180	0.363361
N	-0.908796	-1.152376	-0.352761
H	2.973431	1.080745	0.683901
H	2.585553	-1.797569	0.615577
H	-1.534843	-1.910985	-0.533504
H	1.516200	2.595314	-1.161251
H	0.551841	2.512504	1.619722
H	2.655905	-0.268671	-1.913820
H	1.209251	-0.194258	2.759284
H	0.545758	-2.491573	-1.608114
H	-0.223592	-2.579870	1.346258
H	-0.102012	1.547855	-1.522424
H	-1.497555	2.506418	-0.546995
H	0.687059	-0.440970	-1.828950
H	-0.249914	0.610578	1.480810
H	-2.025890	0.066656	-1.586911
H	-2.579244	0.176489	1.405531
H	-3.483589	-0.772207	0.236291
H	-3.507566	0.984416	0.153954

Structure from **Figure 13b** (E = -362.2297343 a.u.)

B	-0.696514	1.551511	-0.273278
B	1.916731	0.608550	0.383386
B	1.535862	-1.200701	0.362367
B	1.154293	1.558085	-0.844466
B	0.587711	1.600913	0.869102
B	1.710513	-0.250144	-1.169835
B	0.834937	-0.076221	1.626621
B	0.400891	-1.503815	-0.978498
B	-0.146693	-1.435713	0.918164
C	-1.633348	0.226349	-0.562880
C	-2.891393	0.276268	0.307014
N	-0.983444	-1.114012	-0.366191
H	3.049846	0.855026	0.664367
H	2.387848	-1.985435	0.649681
H	-1.656992	-1.832235	-0.544783
H	1.744389	2.474227	-1.336893
H	0.840418	2.558485	1.549654
H	2.633525	-0.563203	-1.855331
H	1.247225	-0.258583	2.732114
H	0.407924	-2.539250	-1.571604
H	-0.451169	-2.438747	1.487932
H	0.043664	1.505083	-1.476789
H	-1.342911	2.552976	-0.478766
H	0.658644	-0.521264	-1.874655
H	-0.419387	-0.407259	1.707701
H	-1.954114	0.222936	-1.604075
H	-2.642503	0.314828	1.362738
H	-3.541267	-0.586424	0.146491
H	-3.461240	1.168902	0.072934

Table S18. Cartesian coordinates (Å) of the optimized geometry of **4a⁻** at the HF/6-31G* level (E = -362.2432284 a.u.).

B	-1.764127	-1.038173	-1.363303
B	-2.028448	-0.415289	0.238169
B	0.391871	1.012084	1.191654
B	-1.317861	1.153519	0.764355
B	-0.607206	-0.430652	1.432123
B	-1.775590	0.846534	-0.944343
B	-0.971500	-1.797848	0.290072
B	-0.215468	1.743528	-0.491544
B	0.759367	-1.247762	0.571082
C	1.568969	-0.321005	-0.518042
C	3.084424	-0.435174	-0.367422
N	1.156506	1.062302	-0.167064
H	-2.777930	-1.523936	-1.787524
H	-0.828941	-1.141042	-2.102895
H	-3.144249	-0.605898	0.607985
H	0.846082	1.647671	2.095244
H	-2.012571	1.821065	1.466651
H	-0.852786	-0.665001	2.578747
H	-2.608584	1.568873	-1.396695
H	-1.364425	-2.794029	0.816765
H	-0.109013	2.896098	-0.781378
H	1.442633	-1.983050	1.230571
H	-0.680880	1.065335	-1.596924
H	0.092797	-2.100766	-0.311870
H	1.900386	1.726428	-0.240067
H	1.312559	-0.516372	-1.554090
H	3.393689	-0.224802	0.652732
H	3.617154	0.246170	-1.032634
H	3.403004	-1.445492	-0.603714

Table S19. Cartesian coordinates (Å) of the two optimized geometries of **5a** at the HF/6-31G* level (E = -337.4927448 a.u.).

Structure from Figure 20a (E = -337.4927448 a.u.)

B	0.904929	0.972979	1.011110
B	1.646933	-0.644778	0.549077
B	0.801555	2.075796	-0.366674
B	-0.741310	1.344921	0.270897
B	2.036372	0.745365	-0.385817
B	0.043432	-0.545665	1.361681
B	1.683988	-1.105084	-1.223524
B	0.367463	-1.811904	-0.028856
C	-1.466300	0.083395	-0.466857
C	-2.989084	0.131128	-0.402595
N	-0.956981	-1.078413	0.323193
H	1.306214	1.480601	2.006257
H	2.576449	-1.012798	1.184792
H	1.213812	3.178828	-0.271957
H	-1.427099	2.085755	0.901239
H	3.150142	1.098006	-0.550762
H	-0.050523	-0.920707	2.480221
H	2.543086	-1.914433	-1.336977
H	0.422510	-2.941188	0.322134
H	1.343844	1.457297	-1.349796
H	1.463057	-0.463066	-2.207052
H	-1.673286	-1.696771	0.648127
H	-1.171618	-0.057862	-1.501510
H	-0.369922	2.129882	-0.828267
H	0.515920	-1.783471	-1.310745
H	-3.336174	0.235145	0.620646
H	-3.439943	-0.760084	-0.832701
H	-3.352112	0.988463	-0.958756

Structure from **Figure 20b** (E = -337.4917664 a.u.)

B	0.974541	0.913969	0.912806
B	1.706141	-0.727487	0.609196
B	0.671890	2.197847	-0.406242
B	-0.785560	1.261110	0.442740
B	2.011401	0.641732	-0.459070
B	0.049852	-0.526264	1.340413
B	1.732274	-1.007577	-1.125850
B	0.430473	-1.799337	-0.118355
C	-1.466086	0.078798	-0.447702
C	-2.987658	0.035652	-0.421446
N	-0.895533	-1.118588	0.263571
H	1.429246	1.463637	1.859613
H	2.591832	-1.100472	1.301194
H	1.081496	3.212765	0.049157
H	-1.453344	1.727778	1.313689
H	3.042681	1.136374	-0.740322
H	-0.121117	-0.821226	2.473185
H	2.573305	-1.632387	-1.669365
H	0.479181	-2.973278	0.020267
H	0.763616	2.090755	-1.595948
H	1.530142	0.114163	-1.684975
H	-1.587811	-1.771899	0.573018
H	-1.134087	0.042332	-1.480128
H	-0.624620	2.311586	-0.327146
H	0.592417	-1.543124	-1.446541
H	-3.363168	0.025693	0.596833
H	-3.381435	-0.832109	-0.945815
H	-3.382197	0.922862	-0.905014

Table S20. Cartesian coordinates (Å) of the optimized geometry of **5a⁻** at the HF/6-31G* level (E = -336.9599729 a.u.).

B	0.919966	0.877545	1.028454
B	1.621413	-0.759189	0.530293
B	0.884079	2.034300	-0.284736
B	-0.682621	1.329787	0.294688
B	2.076156	0.641162	-0.439117
B	0.065324	-0.724498	1.302480
B	1.575441	-0.984691	-1.248665
B	0.434157	-1.818076	-0.119357
C	-1.461444	0.122123	-0.485538
C	-2.977562	0.187434	-0.305257
N	-0.935977	-1.097026	0.169254
H	1.311092	1.383777	2.040048
H	2.611802	-1.149698	1.068248
H	1.286688	3.134155	-0.074851
H	-1.364967	2.087051	0.928518
H	3.194694	1.054094	-0.430523
H	-0.169522	-1.060780	2.423469
H	2.499679	-1.628052	-1.677910
H	0.371433	-2.999243	0.064456
H	1.428501	1.480840	-1.308527
H	0.816463	-0.557337	-2.079286
H	-1.647240	-1.755147	0.412274
H	-1.248417	0.067020	-1.547123
H	-0.276426	2.144756	-0.797582
H	-3.246608	0.216139	0.747448
H	-3.479969	-0.665992	-0.761897
H	-3.370903	1.088555	-0.766972