

Supporting Information of
Carbone Stabilized B₂ and B₂²⁺ - Isoelectronic Analogues to
Diborabutyne and Diborabutatriene

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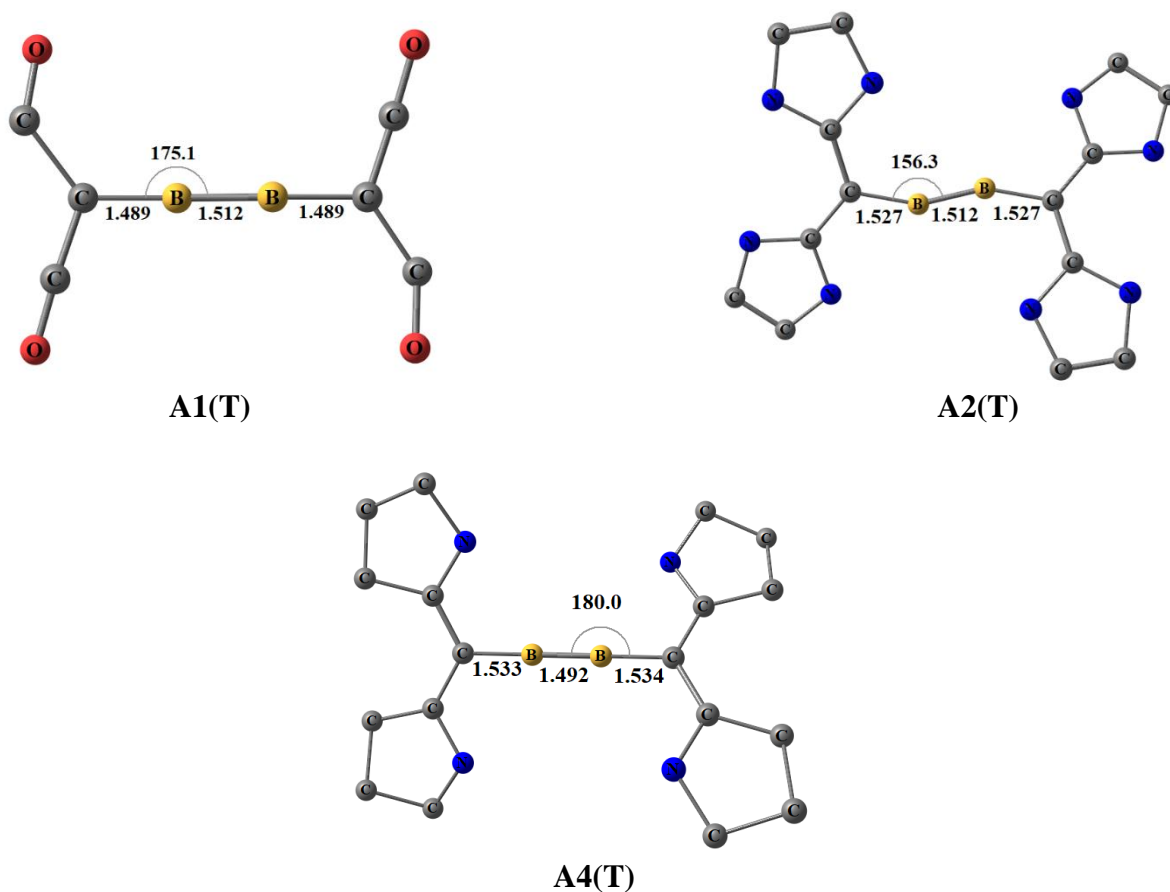
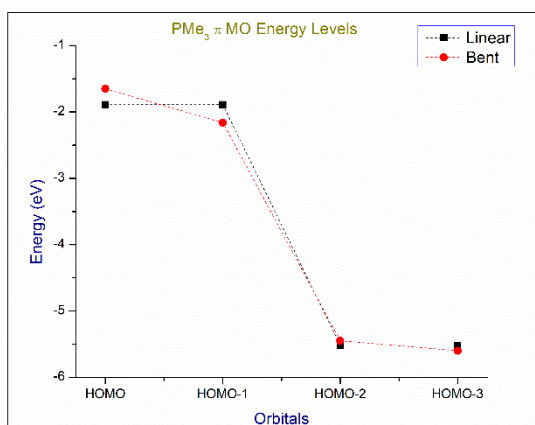
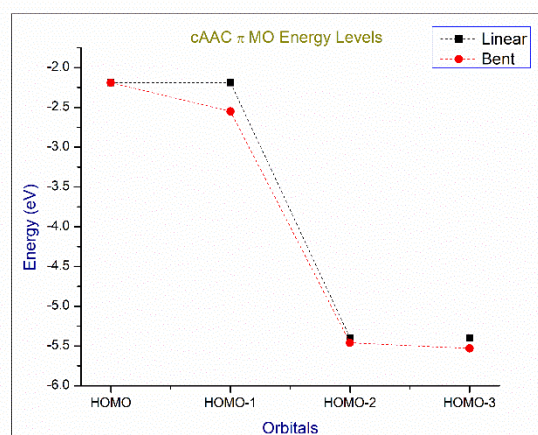


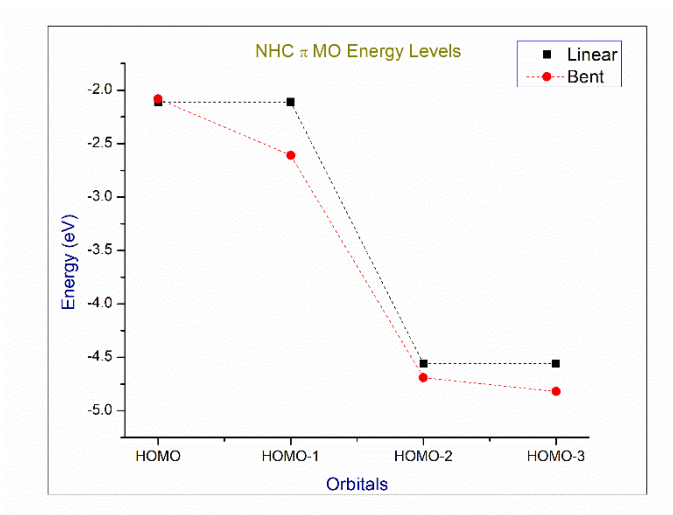
Figure S1: Optimized triplet geometries of **A1(T)**, **A2(T)** and **A4(T)** at BP86/def2-TZVPP level of theory. **A3(T)** was not able to get converged. Hydrogens are omitted for better view.



(a)



(b)



(c)

Figure S2: Energy variation in the π molecular orbitals of **A3** (a), **A4** (b) and **A2** (c) when structure changes from linear to bent. Energies are given in eV. Degenerate orbitals in **A3** are considered as HOMO and HOMO-1, and HOMO-2 and HOMO-3.

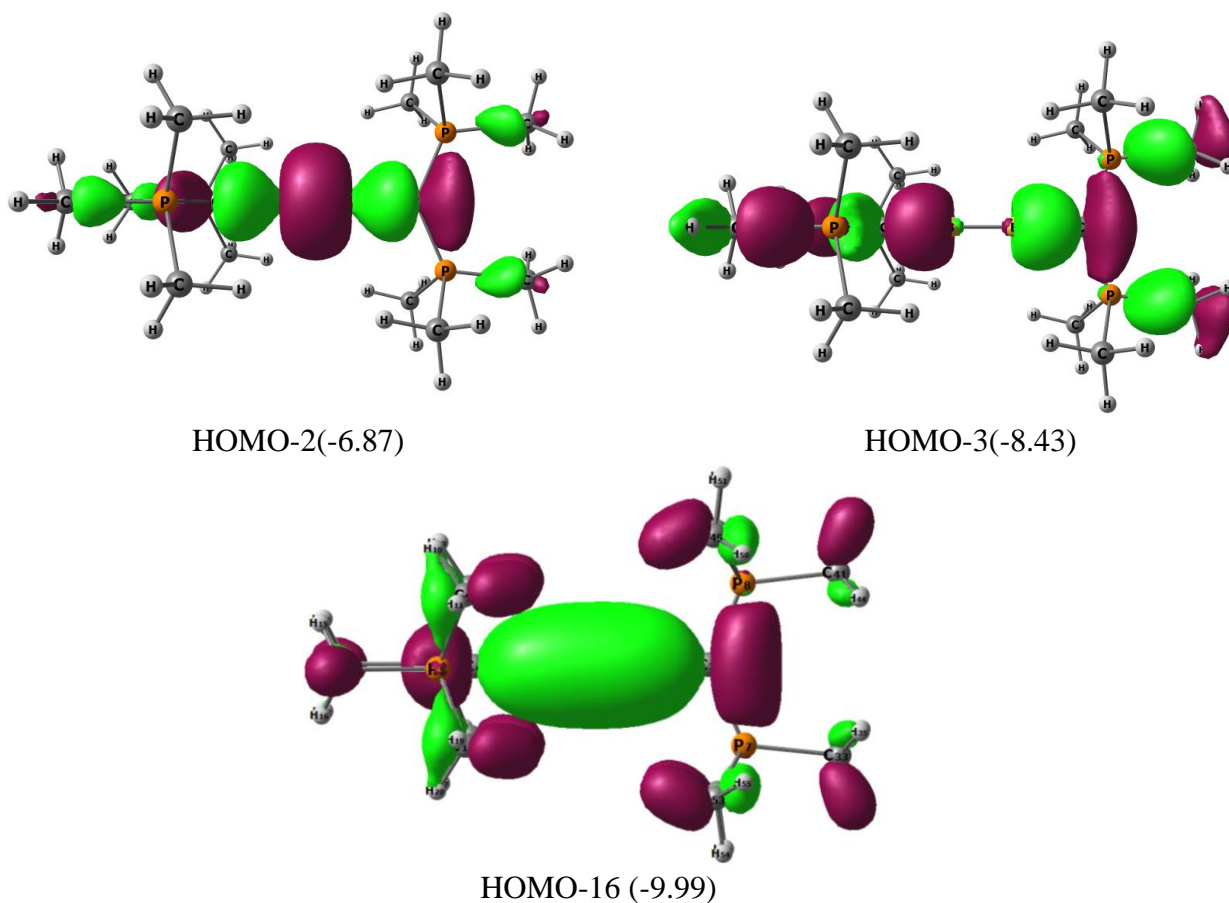
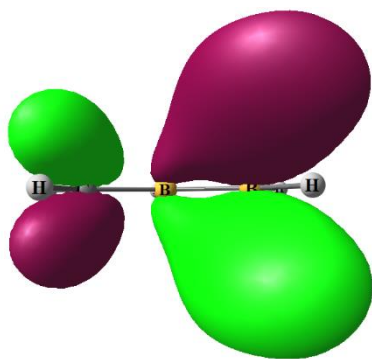
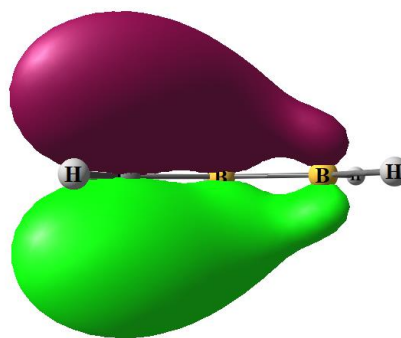


Figure S3: Selected σ MOs of **A3** at M06/def2-TZVPP//BP86/def2-TZVPP level of theory. Eigenvalues are given in eV in parenthesis. Isosurface value is 0.03. Similar orbitals are present for **A1**, **A2** and **A4**.

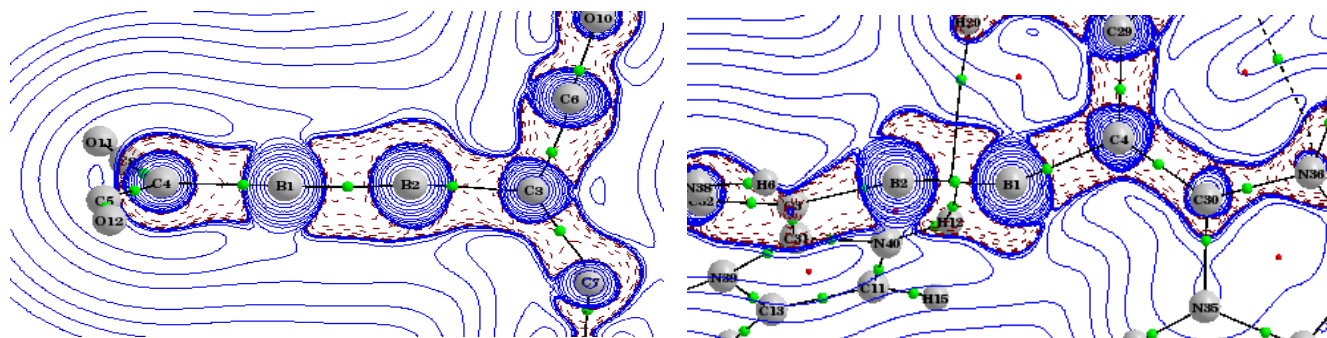


HOMO (11.89)



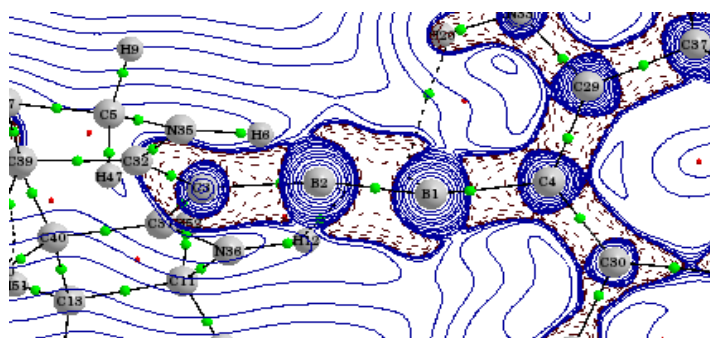
HOMO (9.36)

Figure S4: Allylic type π MOs of B_2CH_5 at M06/def2-TZVPP level of theory. Eigenvalues are given in eV in parenthesis. Isosurface value is 0.03.



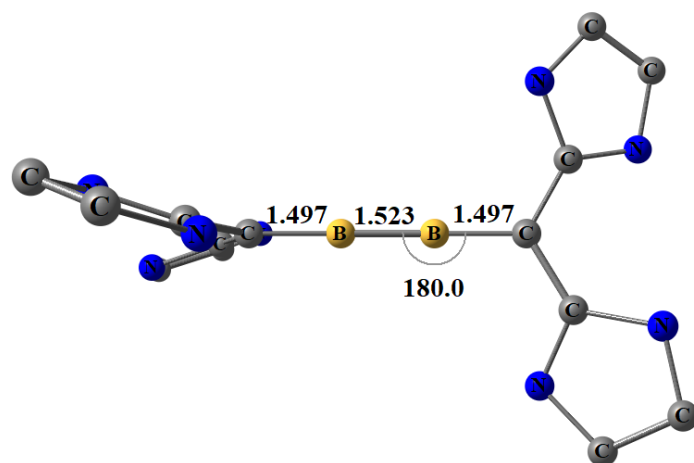
(a)

(b)

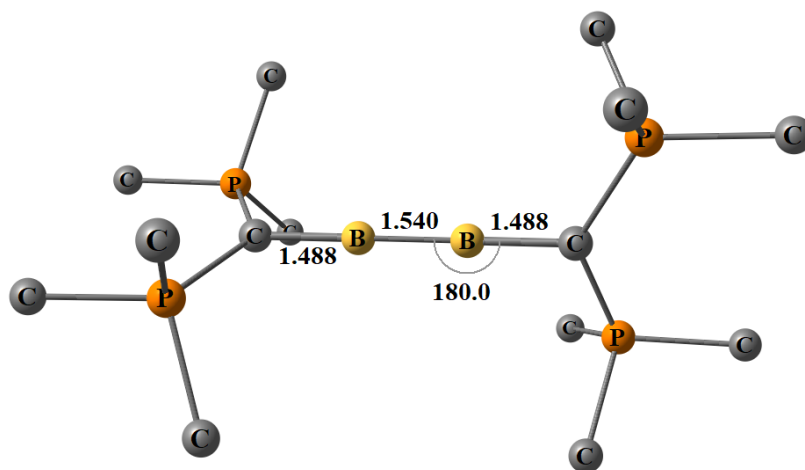


(c)

Figure S5: The Laplacian of the electron density plotted in the plane of B1-B2-C $_x$ ($x=6/29$) of A1 (a), A2 (b) and A4 (c). BCPs are marked by green dots. The wave function was generated at M06/def2-TZVPP//BP86/def2-TZVPP level of theory.



B2(T)



B3(T)

Figure S6: Optimized triplet geometries of **B2(T)** and **B3(T)** at BP86/def2-TZVPP level of theory. Hydrogens are omitted for better view. Geometries for **B1(T)** and **B4(T)** are already given in the manuscript.

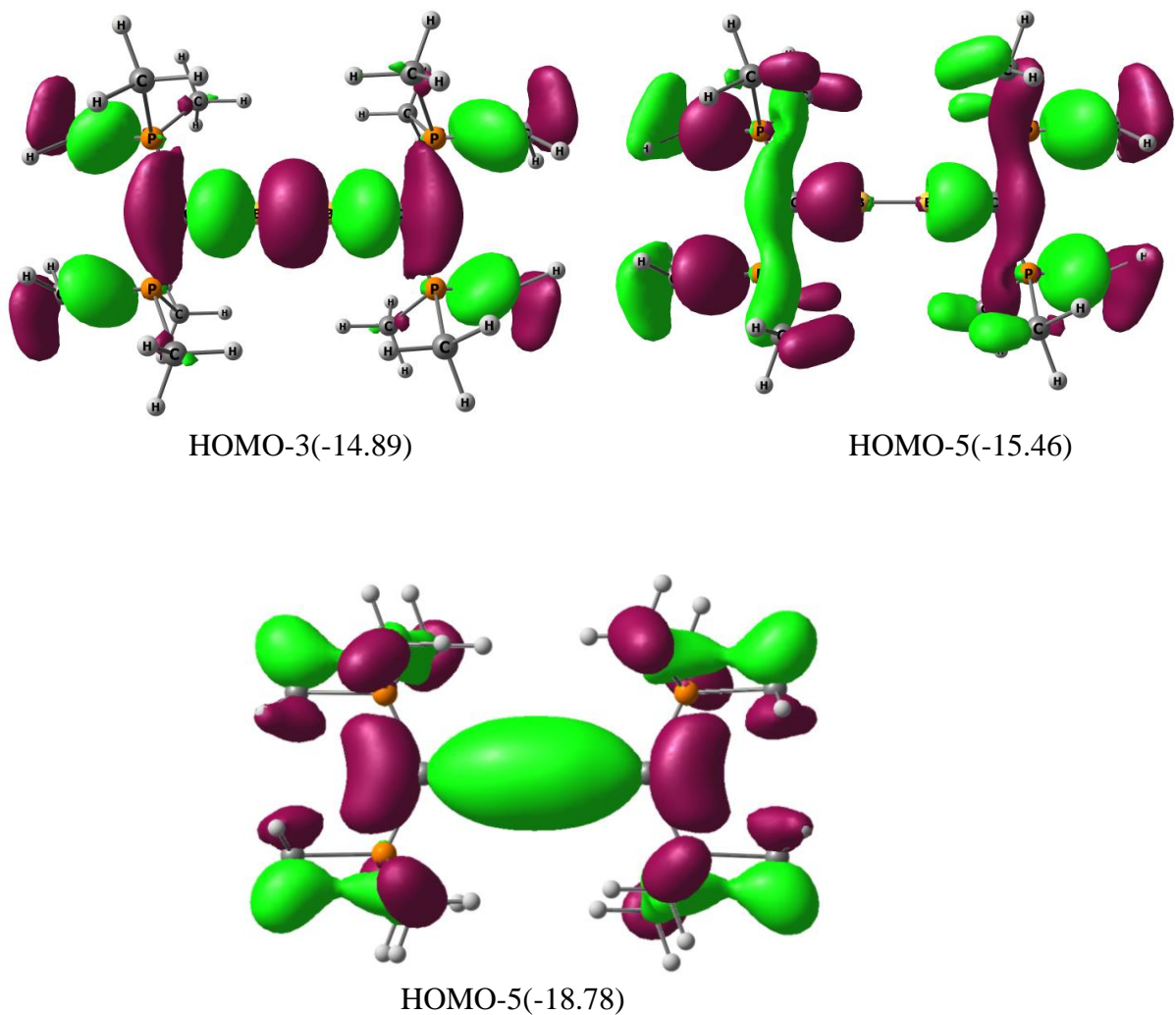
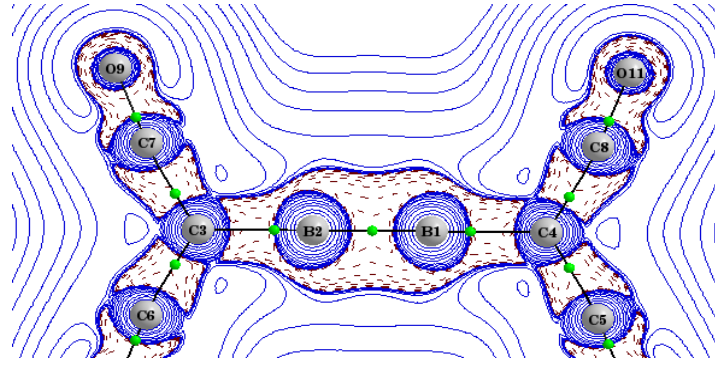
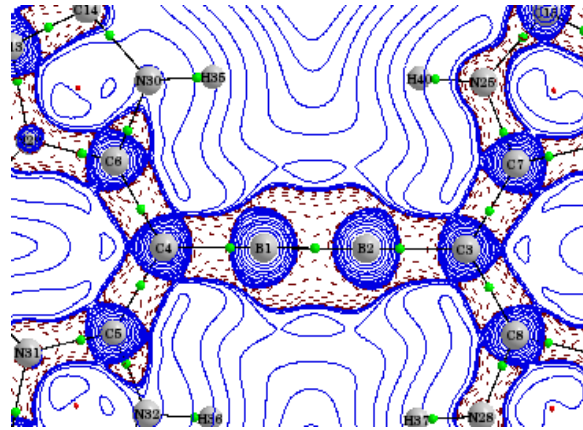


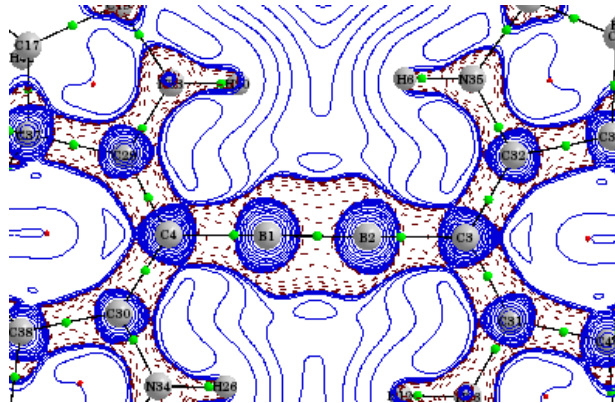
Figure S7: Selected σ MOs of **B3** at M06/def2-TZVPP//BP86/def2-TZVPP level of theory. Eigenvalues are given in eV in parenthesis. Isosurface value is 0.03. Similar orbitals are present for **B1**, **B2** and **B4**.



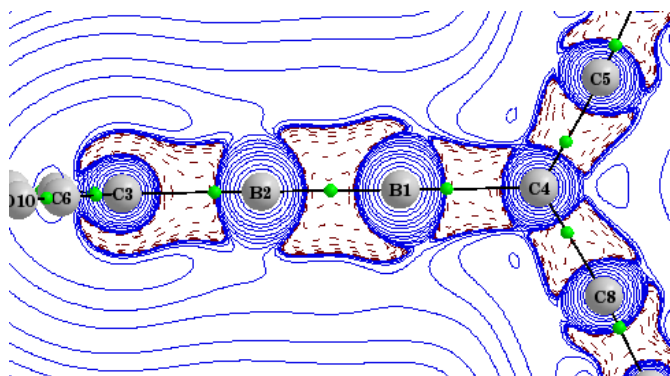
(a)



(b)



(c)



(d)

Figure S8: The Laplacian of the electron density plotted in the plane of B1-B2-C_x ($x=5/7/8/32$) of **B1** (a), **B2** (b), **B4** (c) and **B1 (T)** (d). BCPs are marked by green dots. The wave function was generated at M06/def2-TZVPP//BP86/def2-TZVPP level of theory.

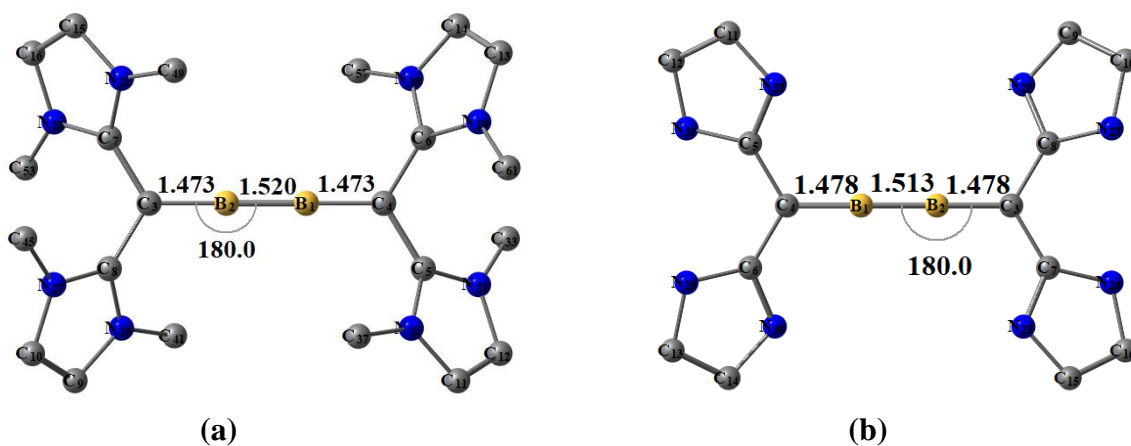


Figure S9: The optimized structures of the (a) **B2** and (b) **B2-NHC^{Me}** at BP86/def2-TZVPP level of theory.

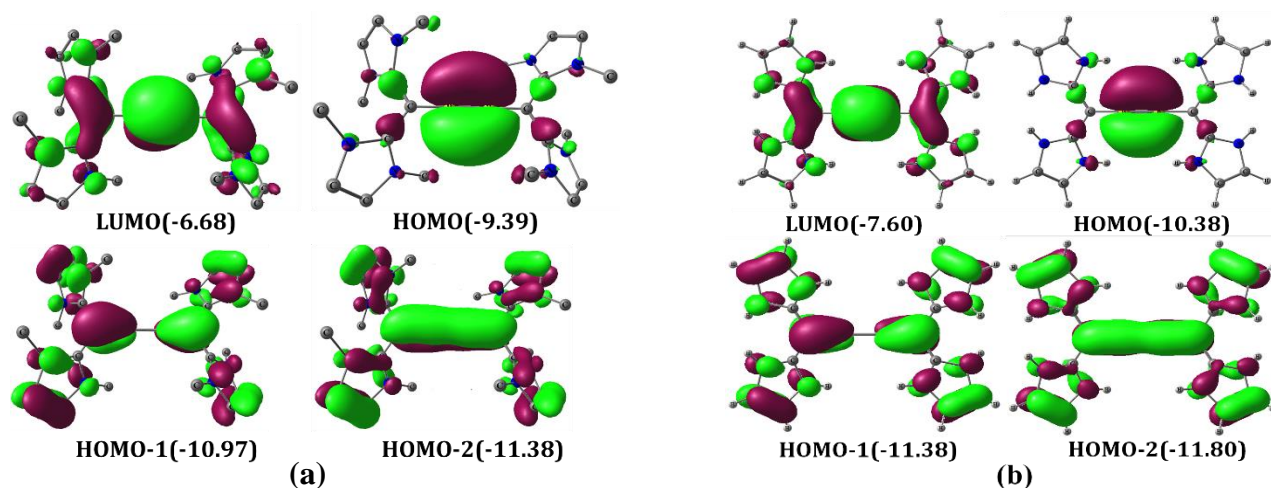


Figure S10: The frontier molecular orbitals of (a) **B2** and (b) **B2-NHC^{Me}** calculated at M06/def2-TZVPP level of theory.

Table S1: HOMO-LUMO gap of the **AX** and **BX** at M06/def2-TZVPP level of theory.

Molecule	HOMO-LUMO Gap (eV)
B₂-CO	2.58
B₂²⁺-CO	2.89
B₂-NHC	2.19
B₂²⁺-NHC	2.78
B₂-PMe₃	2.38
B₂²⁺-PMe₃	2.98
B₂-cAAC	1.70
B₂²⁺-cAAC	2.56

Table S2: The variation in dissociation energy of B-B bond and complexation energies in **B₂²⁺-NHC** and **B₂²⁺-NHC^{Me}** calculated at M06/def2-TZVPP//BP86/def2-TZVPP level of theory

	De(B-B) (kcal/mol)	Complexation Energy/ (kcal/mol)
B2	69.9	-578.7
B2-NHC^{Me}	62.9	-577.5

Table S3: Cartesian coordinates of optimized geometries at BP86/def2-TZVPP level of theory, E_{M06}^{el} (the electronic energy obtained at M06/def2-TZVPP level of theory), ZPE_{BP86} (the zero point energy obtained from the geometry optimized at BP86/def2-TZVPP level of theory) and E_{total} (the sum of ZPE_{BP86} and E_{M06}^{el}) of carbene stabilized B_2 and B_2^{2+} . T in parenthesis indicates triplet geometry. All others are singlet geometries. Energies are in a.u.

A4(T)

$E_{M06}^{el} = -970.9469022$

$ZPE_{BP86} = 0.434818$

$E_{total} = -970.5120842$

B	0.0000000	0.0000000	-0.7446240
B	0.0000000	0.0000000	0.7477380
C	0.0000000	0.0000000	2.2816000
C	0.0000000	0.0000000	-2.2771610
C	-0.2497090	3.5927330	3.0435910
H	-0.0459050	2.3339110	1.2310720
C	0.1325570	3.1259400	4.4613460
H	-1.1447380	1.3641290	4.7827210
H	-1.3255960	3.8512340	2.9850350
H	1.2012520	3.3183200	4.6339490
C	0.2497090	-3.5927330	3.0435910
H	0.0459050	-2.3339110	1.2310720
C	-0.1325570	-3.1259400	4.4613460
H	-0.5706140	-1.0459770	5.0664740
H	1.3255960	-3.8512340	2.9850350
H	0.4358440	-3.6428600	5.2454910
C	-1.3827190	2.8005810	-4.4675450
H	-0.0240890	1.1680560	-5.0759970
C	-1.9201090	3.0473240	-3.0452850
H	-1.1357040	2.0488630	-1.2337110
H	-2.1386560	2.9777370	-5.2436360
H	-2.9887580	2.7643950	-2.9671260
C	1.3827190	-2.8005810	-4.4675450

H	0.0240890	-1.1680560	-5.0759970
C	1.9201090	-3.0473240	-3.0452850
H	1.1357040	-2.0488630	-1.2337110
H	2.1386560	-2.9777370	-5.2436360
H	1.8252490	-4.0953230	-2.7250600
C	-0.5819390	1.0998820	-2.9540880
C	0.5819390	-1.0998820	-2.9540880
C	0.0000000	-1.2439200	2.9570620
C	0.0000000	1.2439200	2.9570620
N	-1.0705790	2.1712650	-2.2533140
N	1.0705790	-2.1712650	-2.2533140
N	0.0668080	2.4141530	2.2514660
N	-0.0668080	-2.4141530	2.2514660
C	-0.8883100	1.3353690	-4.4195130
C	0.8883100	-1.3353690	-4.4195130
C	-0.1261430	1.6009510	4.4242360
C	0.1261430	-1.6009510	4.4242360
H	-1.8252490	4.0953230	-2.7250600
H	-0.5344880	3.4732520	-4.6600950
H	-1.6798830	0.6398030	-4.7540380
H	1.6798830	-0.6398030	-4.7540380
H	0.5344880	-3.4732520	-4.6600950
H	2.9887580	-2.7643950	-2.9671260
H	0.3259840	4.4675440	2.7079220
H	-0.4358440	3.6428600	5.2454910
H	0.5706140	1.0459770	5.0664740
H	1.1447380	-1.3641290	4.7827210
H	-1.2012520	-3.3183200	4.6339490
H	-0.3259840	-4.4675440	2.7079220

A4

$E_{M06}^{el} = -970.9525183$

$ZPE_{BP86} = 0.434505$

$E_{total} = -970.5180133$

B	-0.1600920	0.7201250	0.0905390
B	0.1600920	-0.7201250	0.0905390
C	0.0135550	-2.2509790	0.0051170
C	-0.0135550	2.2509790	0.0051170
C	-3.2657340	-2.4200790	-1.6185010
H	-1.7621120	-0.8430730	-0.9285750
C	-2.8938980	-3.9041990	-1.8254700
H	-0.9711740	-4.8390330	-1.2530750
H	-3.5927630	-1.9245420	-2.5443180
H	-3.7390620	-4.5818700	-1.6456880
C	2.7983190	-3.5147070	2.0179870
H	1.9900610	-1.5401980	1.3540110
C	2.4483880	-4.8531290	1.3360630
H	0.8804670	-5.1555640	-0.1938350
H	2.4918940	-3.5061810	3.0808240
H	2.4911410	-5.7036650	2.0288480
C	2.8938980	3.9041990	-1.8254700
H	0.9711740	4.8390330	-1.2530750
C	3.2657340	2.4200790	-1.6185010
H	1.7621120	0.8430730	-0.9285750
H	3.7390620	4.5818700	-1.6456880
H	4.0709290	2.2974160	-0.8709580
C	-2.4483880	4.8531290	1.3360630
H	-0.2492640	4.9626350	1.4450220
C	-2.7983190	3.5147070	2.0179870
H	-1.9900610	1.5401980	1.3540110

H	-3.1604340	5.0460930	0.5209970
H	-2.4918940	3.5061810	3.0808240
C	1.1487680	2.7446020	-0.6392330
C	-0.9560000	3.1110780	0.5922230
C	0.9560000	-3.1110780	0.5922230
C	-1.1487680	-2.7446020	-0.6392330
N	2.0172090	1.8522940	-1.1312810
N	-2.0172090	2.5678140	1.2353040
N	-2.0172090	-1.8522940	-1.1312810
N	2.0172090	-2.5678140	1.2353040
C	1.7115700	4.1343420	-0.8519770
C	-1.0350060	4.6155620	0.7500220
C	-1.7115700	-4.1343420	-0.8519770
C	1.0350060	-4.6155620	0.7500220
H	3.5927630	1.9245420	-2.5443180
H	2.5561240	4.0574760	-2.8604090
H	2.0539650	4.5503000	0.1125020
H	-0.8804670	5.1555640	-0.1938350
H	-2.4911410	5.7036650	2.0288480
H	-3.8719630	3.2796230	1.9764140
H	-4.0709290	-2.2974160	-0.8709580
H	-2.5561240	-4.0574760	-2.8604090
H	-2.0539650	-4.5503000	0.1125020
H	0.2492640	-4.9626350	1.4450220
H	3.1604340	-5.0460930	0.5209970
H	3.8719630	-3.2796230	1.9764140

A1(T)

$E_{M06}^{el} = -578.8846907$

$ZPE_{BP86} = 0.046003$

E_{total} = -578.8386877

B	-0.0250600	0.7539670	0.0514050
B	0.0250600	-0.7539670	-0.0514050
C	0.0927120	-2.2413390	-0.0255160
C	-0.0927120	2.2413390	0.0255160
C	-1.3256050	3.0420900	-0.1394360
C	1.3256050	-3.0420900	0.1394360
C	-1.1621470	-2.7245260	0.0036590
C	1.1621470	2.7245260	-0.0036590
O	-2.2657250	-3.0951450	-0.0147730
O	2.4772820	-2.8753680	-0.0515260
O	2.2657250	3.0951450	0.0147730
O	-2.4772820	2.8753680	0.0515260

A1

E^{el}_{M06} = -578.8847128

ZPE_{BP86} = 0.045575

E_{total} = -578.8391378

B	0.0710650	-0.7524770	-0.0097960
B	-0.0710650	0.7524770	-0.0097960
C	-0.0710650	2.2347070	0.0073370
C	0.0710650	-2.2347070	0.0073370
C	-0.7898410	-2.9815650	0.9029850
C	-0.9607480	2.6182980	-0.9208170
C	0.7898410	2.9815650	0.9029850
C	0.9607480	-2.6182980	-0.9208170
O	1.5918310	2.9506440	1.7539810
O	-1.7496130	2.8971820	-1.7399880
O	1.7496130	-2.8971820	-1.7399880
O	-1.5918310	-2.9506440	1.7539810

A2(T)

$E_{M06}^{el} = -1030.260092$

$ZPE_{BP86} = 0.292376$

$E_{total} = -1029.967716$

B	0.2068890	0.7273930	0.0513490
B	-0.2068890	-0.7273930	0.0513490
C	-0.0006150	-2.2402890	0.0123050
C	0.0006150	2.2402890	0.0123050
C	-1.3306990	2.6857000	-0.2228910
C	1.0910920	3.1163540	0.2212950
C	1.3306990	-2.6857000	-0.2228910
C	-1.0910920	-3.1163540	0.2212950
C	-3.2500330	-3.7056220	0.6286970
C	-2.5335260	-4.8537540	0.4906170
C	-3.5546200	2.4639340	-0.5888150
C	-3.2819210	3.7988230	-0.5607960
C	2.5335260	4.8537540	0.4906170
C	3.2500330	3.7056220	0.6286970
C	3.5546200	-2.4639340	-0.5888150
C	3.2819210	-3.7988230	-0.5607960
H	-4.4882590	1.9352730	-0.7416060
H	-3.9217750	4.6646620	-0.6831250
H	2.8295940	5.8949510	0.5481680
H	4.3009720	3.5434750	0.8361930
H	4.4882590	-1.9352730	-0.7416060
H	3.9217750	-4.6646620	-0.6831250
H	-2.8295940	-5.8949510	0.5481680
H	-4.3009720	-3.5434750	0.8361930
N	2.3584050	-1.8019840	-0.3863110

N	1.9119790	-3.9271590	-0.3395620
N	-1.2112220	-4.4860140	0.2500140
N	-2.3584050	-2.6566970	0.4655580
N	1.2112220	4.4860140	0.2500140
N	2.3584050	2.6566970	0.4655580
N	-1.9119790	3.9271590	-0.3395620
N	-2.3584050	1.8019840	-0.3863110
H	-1.4194310	4.8411130	-0.2514090
H	0.4478940	5.1667370	0.0422340
H	2.5156660	1.6381300	0.4865970
H	-2.1171890	0.7838490	-0.3041650
H	-2.5156660	-1.6381300	0.4865970
H	-0.4478940	-5.1667370	0.0422340
H	1.4194310	-4.8411130	-0.2514090
H	2.1171890	-0.7838490	-0.3041650

A2

$E_{M06}^{el} = -1030.303585$

$ZPE_{BP86} = 0.296388$

$E_{total} = -1030.007197$

B	-0.7188010	0.1828600	0.2899030
B	0.7188590	-0.1833950	0.2900310
C	2.2293360	0.0741210	0.0837930
C	-2.2293460	-0.0744050	0.0837810
C	4.1191880	-2.4484730	1.8234710
H	1.9902950	-1.8975660	1.8081060
C	5.1433430	-1.8737260	1.1419210
H	4.9996440	-0.5226160	-0.4804160
H	4.1280020	-3.2723650	2.5265870
H	6.2005710	-2.1090010	1.1319030

C	2.0656660	3.2075030	-1.6438050
H	0.5644630	1.6495360	-0.8542380
C	3.4221420	3.1614230	-1.4984080
H	4.5856450	1.7292680	-0.4098640
H	1.4427290	3.9696790	-2.0962970
H	4.1969380	3.8608490	-1.7922130
C	-3.4231610	-3.1616980	-1.4976580
H	-4.5859970	-1.7294180	-0.4087010
C	-2.0667440	-3.2081010	-1.6433480
H	-0.5650770	-1.6505550	-0.8545820
H	-4.1981620	-3.8609830	-1.7912510
H	-1.4440710	-3.9704540	-2.0959030
C	-5.1424240	1.8747130	1.1421930
H	-4.9998150	0.5227060	-0.4796200
C	-4.1178970	2.4491410	1.8234810
H	-1.9891750	1.8972800	1.8076550
H	-6.1995520	2.1104420	1.1322780
H	-4.1262280	3.2731560	2.5264560
C	-2.5406880	-1.2604830	-0.6228010
C	-3.2212700	0.7438070	0.6136470
C	2.5402650	1.2601840	-0.6230970
C	3.2215980	-0.7437030	0.6135330
N	-3.7204090	-1.9296020	-0.8985880
N	-1.5439270	-2.0398020	-1.1222560
N	-2.9578890	1.7649400	1.4990690
N	-4.6152500	0.7765180	0.4258650
N	4.6156300	-0.7757800	0.4255080
N	2.9588060	-1.7648630	1.4991390
N	3.7197430	1.9295290	-0.8991610
N	1.5432160	2.0391870	-1.1224040

A3

$E_{M06}^{el} = -1969.858558$

$ZPE_{BP86} = 0.457448$

$E_{total} = -1969.40111$

B	0.0000000	0.0000000	0.7433200
B	0.0000000	0.0000000	-0.7433200
C	0.0000000	0.0000000	2.2698970
C	0.0000000	0.0000000	-2.2698970
P	1.5704600	0.0000000	-2.9470410
P	-1.5704600	0.0000000	-2.9470410
P	0.0000000	1.5704600	2.9470410
P	0.0000000	-1.5704600	2.9470410
C	2.5400700	-1.4545210	-2.4098440
H	2.2116980	-2.3398250	-2.9733800
H	3.6201080	-1.3084020	-2.5464770
H	2.3047870	-1.5833980	-1.3423910
C	1.7715480	0.0000000	-4.7899730
H	2.8350520	0.0000000	-5.0673530
H	1.2980660	-0.8941050	-5.2160600
H	1.2980660	0.8941050	-5.2160600
C	2.5400700	1.4545210	-2.4098440
H	2.3047870	1.5833980	-1.3423910
H	3.6201080	1.3084020	-2.5464770
H	2.2116980	2.3398250	-2.9733800
C	-1.7715480	0.0000000	-4.7899730
H	-1.2980660	0.8941050	-5.2160600
H	-1.2980660	-0.8941050	-5.2160600
H	-2.8350520	0.0000000	-5.0673530
C	-2.5400700	1.4545210	-2.4098440

H	-2.3047870	1.5833980	-1.3423910
H	-2.2116980	2.3398250	-2.9733800
H	-3.6201080	1.3084020	-2.5464770
C	-2.5400700	-1.4545210	-2.4098440
H	-2.2116980	-2.3398250	-2.9733800
H	-2.3047870	-1.5833980	-1.3423910
H	-3.6201080	-1.3084020	-2.5464770
C	0.0000000	1.7715480	4.7899730
H	-0.8941050	1.2980660	5.2160600
H	0.8941050	1.2980660	5.2160600
H	0.0000000	2.8350520	5.0673530
C	-1.4545210	2.5400700	2.4098440
H	-1.5833980	2.3047870	1.3423910
H	-2.3398250	2.2116980	2.9733800
H	-1.3084020	3.6201080	2.5464770
C	0.0000000	-1.7715480	4.7899730
H	-0.8941050	-1.2980660	5.2160600
H	0.0000000	-2.8350520	5.0673530
H	0.8941050	-1.2980660	5.2160600
C	-1.4545210	-2.5400700	2.4098440
H	-1.5833980	-2.3047870	1.3423910
H	-1.3084020	-3.6201080	2.5464770
H	-2.3398250	-2.2116980	2.9733800
C	1.4545210	-2.5400700	2.4098440
H	2.3398250	-2.2116980	2.9733800
H	1.3084020	-3.6201080	2.5464770
H	1.5833980	-2.3047870	1.3423910
C	1.4545210	2.5400700	2.4098440
H	1.3084020	3.6201080	2.5464770
H	2.3398250	2.2116980	2.9733800

H 1.5833980 2.3047870 1.3423910

B4(T)

$E_{M06}^{el} = -970.5642123$

$ZPE_{BP86} = 0.443093$

$E_{total} = -970.1211193$

B 0.0000000 0.0000000 0.7640720

B 0.0000000 0.0000000 -0.7640720

C 0.0000000 0.0000000 -2.2733190

C 0.0000000 0.0000000 2.2733190

C -3.6180080 0.0000000 -3.1674690

H -2.4557590 0.0738140 -1.3031390

C -3.0512870 -0.4340980 -4.5292040

H -1.3554080 0.9339980 -4.8725720

H -4.0448680 1.0151250 -3.1823070

H -3.1647070 -1.5186330 -4.6555020

C 3.6180080 0.0000000 -3.1674690

H 2.4557590 -0.0738140 -1.3031390

C 3.0512870 0.4340980 -4.5292040

H 0.9155130 0.7746150 -4.9928370

H 4.0448680 -1.0151250 -3.1823070

H 3.5599320 -0.0556810 -5.3661850

C -0.4340980 3.0512870 4.5292040

H -0.7746150 0.9155130 4.9928370

C 0.0000000 3.6180080 3.1674690

H 0.0738140 2.4557590 1.3031390

H 0.0556810 3.5599320 5.3661850

H 1.0151250 4.0448680 3.1823070

C 0.4340980 -3.0512870 4.5292040

H 0.7746150 -0.9155130 4.9928370

C	0.0000000	-3.6180080	3.1674690
H	-0.0738140	-2.4557590	1.3031390
H	-0.0556810	-3.5599320	5.3661850
H	0.6857120	-4.3732130	2.7635150
C	-0.0290870	1.2512200	2.9669010
C	0.0290870	-1.2512200	2.9669010
C	1.2512200	0.0290870	-2.9669010
C	-1.2512200	-0.0290870	-2.9669010
N	-0.0107210	2.4129190	2.3196140
N	0.0107210	-2.4129190	2.3196140
N	-2.4129190	-0.0107210	-2.3196140
N	2.4129190	0.0107210	-2.3196140
C	-0.0665780	1.5514810	4.4510920
C	0.0665780	-1.5514810	4.4510920
C	-1.5514810	-0.0665780	-4.4510920
C	1.5514810	0.0665780	-4.4510920
H	-0.6857120	4.3732130	2.7635150
H	-1.5186330	3.1647070	4.6555020
H	0.9339980	1.3554080	4.8725720
H	-0.9339980	-1.3554080	4.8725720
H	1.5186330	-3.1647070	4.6555020
H	-1.0151250	-4.0448680	3.1823070
H	-4.3732130	-0.6857120	-2.7635150
H	-3.5599320	0.0556810	-5.3661850
H	-0.9155130	-0.7746150	-4.9928370
H	1.3554080	-0.9339980	-4.8725720
H	3.1647070	1.5186330	-4.6555020
H	4.3732130	0.6857120	-2.7635150

B4

$E_{M06}^{el} = -970.5584108$

$ZPE_{BP86} = 0.442913$

$E_{total} = -970.1154978$

B	0.0000000	0.0000000	0.7627750
B	0.0000000	0.0000000	-0.7627750
C	0.0000000	0.0000000	-2.2590880
C	0.0000000	0.0000000	2.2590880
C	0.4338820	3.5925170	-3.1591930
H	0.3089050	2.3772460	-1.3003440
C	0.7119760	2.9970090	-4.5506330
H	0.7956660	0.8371200	-5.0244560
H	1.2354540	4.2435230	-2.7882330
H	0.2301410	3.5682000	-5.3509960
C	-0.4338820	-3.5925170	-3.1591930
H	-0.3089050	-2.3772460	-1.3003440
C	-0.7119760	-2.9970090	-4.5506330
H	0.8486960	-1.4575460	-4.8360150
H	-1.2354540	-4.2435230	-2.7882330
H	-1.7916820	-2.9897740	-4.7474910
C	-0.7119760	2.9970090	4.5506330
H	-0.7956660	0.8371200	5.0244560
C	-0.4338820	3.5925170	3.1591930
H	-0.3089050	2.3772460	1.3003440
H	-0.2301410	3.5682000	5.3509960
H	0.5152850	4.1488950	3.1093020
C	0.7119760	-2.9970090	4.5506330
H	0.7956660	-0.8371200	5.0244560
C	0.4338820	-3.5925170	3.1591930
H	0.3089050	-2.3772460	1.3003440

H	0.2301410	-3.5682000	5.3509960
H	1.2354540	-4.2435230	2.7882330
C	-0.1698560	1.2442710	2.9728850
C	0.1698560	-1.2442710	2.9728850
C	-0.1698560	-1.2442710	-2.9728850
C	0.1698560	1.2442710	-2.9728850
N	-0.3332230	2.3834250	2.3261890
N	0.3332230	-2.3834250	2.3261890
N	0.3332230	2.3834250	-2.3261890
N	-0.3332230	-2.3834250	-2.3261890
C	-0.1836680	1.5458270	4.4564490
C	0.1836680	-1.5458270	4.4564490
C	0.1836680	1.5458270	-4.4564490
C	-0.1836680	-1.5458270	-4.4564490
H	-1.2354540	4.2435230	2.7882330
H	-1.7916820	2.9897740	4.7474910
H	0.8486960	1.4575460	4.8360150
H	-0.8486960	-1.4575460	4.8360150
H	1.7916820	-2.9897740	4.7474910
H	-0.5152850	-4.1488950	3.1093020
H	-0.5152850	4.1488950	-3.1093020
H	1.7916820	2.9897740	-4.7474910
H	-0.8486960	1.4575460	-4.8360150
H	-0.7956660	-0.8371200	-5.0244560
H	-0.2301410	-3.5682000	-5.3509960
H	0.5152850	-4.1488950	-3.1093020

B1(T)

$E_{M06}^{el} = -578.2779957$

$ZPE_{BP86} = 0.051248$

$$E_{\text{total}} = -578.2267477$$

B	0.0000000	0.0000000	0.7635720
B	0.0000000	0.0000000	-0.7635720
C	0.0000000	0.0000000	-2.2888550
C	0.0000000	0.0000000	2.2888550
C	0.0000000	1.1965250	2.9822770
C	-1.1965250	0.0000000	-2.9822770
C	1.1965250	0.0000000	-2.9822770
C	0.0000000	-1.1965250	2.9822770
O	2.2249290	0.0000000	-3.4669870
O	-2.2249290	0.0000000	-3.4669870
O	0.0000000	-2.2249290	3.4669870
O	0.0000000	2.2249290	3.4669870

B1

$$E^{\text{el}}_{\text{M06}} = -578.2764926$$

$$\text{ZPE}_{\text{BP86}} = 0.051264$$

$$E_{\text{total}} = -578.2252286$$

B	0.0000000	0.0000000	0.7651450
B	0.0000000	0.0000000	-0.7651450
C	0.0000000	0.0000000	-2.2533010
C	0.0000000	0.0000000	2.2533010
C	0.0000000	1.2253850	2.9153590
C	0.0000000	-1.2253850	-2.9153590
C	0.0000000	1.2253850	-2.9153590
C	0.0000000	-1.2253850	2.9153590
O	0.0000000	2.2860680	-3.3232650
O	0.0000000	-2.2860680	-3.3232650
O	0.0000000	-2.2860680	3.3232650
O	0.0000000	2.2860680	3.3232650

B2(T)

$E_{M06}^{el} = -1029.945003$

$ZPE_{BP86} = 0.307834$

$E_{total} = -1029.637169$

B	0.0000000	0.0000000	0.7613010
B	0.0000000	0.0000000	-0.7613010
C	0.0000000	0.0000000	-2.2582920
C	0.0000000	0.0000000	2.2582920
C	-3.4484770	0.3281350	-3.4060100
H	-2.6338120	-0.3458450	-1.5286320
C	-2.7949090	0.7183410	-4.5328060
H	-0.7016880	0.9976510	-4.8526780
H	-4.5074400	0.2452700	-3.1954640
H	-3.1699580	1.0495200	-5.4934070
C	3.4484770	-0.3281350	-3.4060100
H	2.6338120	0.3458450	-1.5286320
C	2.7949090	-0.7183410	-4.5328060
H	0.7016880	-0.9976510	-4.8526780
H	4.5074400	-0.2452700	-3.1954640
H	3.1699580	-1.0495200	-5.4934070
C	0.7183410	2.7949090	4.5328060
H	0.9976510	0.7016880	4.8526780
C	0.3281350	3.4484770	3.4060100
H	-0.3458450	2.6338120	1.5286320
H	1.0495200	3.1699580	5.4934070
H	0.2452700	4.5074400	3.1954640
C	-0.7183410	-2.7949090	4.5328060
H	-0.9976510	-0.7016880	4.8526780
C	-0.3281350	-3.4484770	3.4060100

H	0.3458450	-2.6338120	1.5286320
H	-1.0495200	-3.1699580	5.4934070
H	-0.2452700	-4.5074400	3.1954640
C	0.1830000	1.2242890	2.9773540
C	-0.1830000	-1.2242890	2.9773540
C	1.2242890	-0.1830000	-2.9773540
C	-1.2242890	0.1830000	-2.9773540
N	0.6132850	1.4316390	4.2613520
N	0.0000000	2.4749410	2.4717720
N	0.0000000	-2.4749410	2.4717720
N	-0.6132850	-1.4316390	4.2613520
N	-1.4316390	0.6132850	-4.2613520
N	-2.4749410	0.0000000	-2.4717720
N	1.4316390	-0.6132850	-4.2613520
N	2.4749410	0.0000000	-2.4717720

B2

$E_{M06}^{el} = -1029.954739$

$ZPE_{BP86} = 0.308825$

$E_{total} = -1029.645914$

B	0.0000130	0.7567460	0.0001020
B	-0.0000130	-0.7567460	0.0001020
C	-0.0000130	-2.2348940	0.0000430
C	0.0000130	2.2348940	0.0000430
C	-1.2398800	2.9682850	-0.0517590
C	1.2399010	2.9682950	0.0517850
C	1.2398800	-2.9682850	-0.0517590
C	-1.2399010	-2.9682950	0.0517850
C	-3.4377480	-3.3989360	0.3813260
C	-2.8886810	-4.5118810	-0.1795690

C	-3.4377320	3.3988790	-0.3813220
C	-2.8886660	4.5118850	0.1794530
C	2.8886810	4.5118810	-0.1795690
C	3.4377480	3.3989360	0.3813260
C	3.4377320	-3.3988790	-0.3813220
C	2.8886660	-4.5118850	0.1794530
H	-4.4522670	3.1968140	-0.7015610
H	-3.3296690	5.4624110	0.4540840
H	3.3296820	5.4623800	-0.4542940
H	4.4522810	3.1969090	0.7015970
H	4.4522670	-3.1968140	-0.7015610
H	3.3296690	-5.4624110	0.4540840
H	-3.3296820	-5.4623800	-0.4542940
H	-4.4522810	-3.1969090	0.7015970
N	2.4125320	-2.4767950	-0.5207890
N	1.5360100	-4.2357520	0.3640570
N	-1.5360290	-4.2357210	-0.3641590
N	-2.4125520	-2.4768590	0.5208760
N	1.5360290	4.2357210	-0.3641590
N	2.4125520	2.4768590	0.5208760
N	-1.5360100	4.2357520	0.3640570
N	-2.4125320	2.4767950	-0.5207890
H	-0.8999210	4.8232590	0.8942870
H	0.8999430	4.8231680	-0.8944580
H	2.4683680	1.5269760	0.8886280
H	-2.4683430	1.5268700	-0.8884370
H	-2.4683680	-1.5269760	0.8886280
H	-0.8999430	-4.8231680	-0.8944580
H	0.8999210	-4.8232590	0.8942870
H	2.4683430	-1.5268700	-0.8884370

B3(T)

B	0.0000000	0.0000000	0.7698240
B	0.0000000	0.0000000	-0.7698240
C	0.0000000	0.0000000	2.2579110
C	0.0000000	0.0000000	-2.2579110
P	-1.1263970	1.1264670	-2.9999770
P	1.1263970	-1.1264670	-2.9999770
P	-1.1263970	-1.1264670	2.9999770
P	1.1263970	1.1264670	2.9999770
C	-0.7782300	2.8310710	-2.4760150
H	0.2069150	3.1388710	-2.8494120
H	-1.5456000	3.5154000	-2.8625830
H	-0.7734740	2.8717090	-1.3792670
C	-1.1681070	1.1689380	-4.8164580
H	-1.9167200	1.9156090	-5.1163290
H	-0.1988810	1.4705050	-5.2306260
H	-1.4664300	0.1991410	-5.2315710
C	-2.8310710	0.7780350	-2.4764940
H	-2.8721520	0.7740510	-1.3797490
H	-3.5156240	1.5448240	-2.8637970
H	-3.1383150	-0.2075800	-2.8491140
C	1.1681070	-1.1689380	-4.8164580
H	0.1988810	-1.4705050	-5.2306260
H	1.4664300	-0.1991410	-5.2315710
H	1.9167200	-1.9156090	-5.1163290
C	0.7782300	-2.8310710	-2.4760150
H	0.7734740	-2.8717090	-1.3792670
H	-0.2069150	-3.1388710	-2.8494120
H	1.5456000	-3.5154000	-2.8625830

C	2.8310710	-0.7780350	-2.4764940
H	3.1383150	0.2075800	-2.8491140
H	2.8721520	-0.7740510	-1.3797490
H	3.5156240	-1.5448240	-2.8637970
C	-1.1681070	-1.1689380	4.8164580
H	-0.1988810	-1.4705050	5.2306260
H	-1.4664300	-0.1991410	5.2315710
H	-1.9167200	-1.9156090	5.1163290
C	-0.7782300	-2.8310710	2.4760150
H	-0.7734740	-2.8717090	1.3792670
H	0.2069150	-3.1388710	2.8494120
H	-1.5456000	-3.5154000	2.8625830
C	1.1681070	1.1689380	4.8164580
H	1.4664300	0.1991410	5.2315710
H	1.9167200	1.9156090	5.1163290
H	0.1988810	1.4705050	5.2306260
C	2.8310710	0.7780350	2.4764940
H	2.8721520	0.7740510	1.3797490
H	3.5156240	1.5448240	2.8637970
H	3.1383150	-0.2075800	2.8491140
C	0.7782300	2.8310710	2.4760150
H	-0.2069150	3.1388710	2.8494120
H	1.5456000	3.5154000	2.8625830
H	0.7734740	2.8717090	1.3792670
C	-2.8310710	-0.7780350	2.4764940
H	-3.5156240	-1.5448240	2.8637970
H	-3.1383150	0.2075800	2.8491140
H	-2.8721520	-0.7740510	1.3797490

B3

$E_{M06}^{el} = -1969.533922$

$ZPE_{BP86} = 0.465129$

$E_{total} = -1969.068793$

B	0.0000000	0.0000000	0.7642070
B	0.0000000	0.0000000	-0.7642070
C	0.0000000	0.0000000	2.2282470
C	0.0000000	0.0000000	-2.2282470
P	-0.0035580	1.5975570	-2.9991020
P	0.0035580	-1.5975570	-2.9991020
P	-0.0035580	-1.5975570	2.9991020
P	0.0035580	1.5975570	2.9991020
C	1.2659470	2.6472490	-2.2434110
H	2.2609500	2.2508160	-2.4842910
H	1.1802250	3.6756770	-2.6192480
H	1.1262760	2.6294950	-1.1553960
C	0.3306400	1.6474640	-4.7881380
H	0.3809600	2.7001130	-5.0995820
H	1.2941200	1.1745650	-5.0172580
H	-0.4679530	1.1598990	-5.3589400
C	-1.6006140	2.4280090	-2.7639210
H	-1.8360400	2.4444680	-1.6922880
H	-1.5634660	3.4558580	-3.1495770
H	-2.3887450	1.8729460	-3.2893920
C	-0.3306400	-1.6474640	-4.7881380
H	-1.2941200	-1.1745650	-5.0172580
H	0.4679530	-1.1598990	-5.3589400
H	-0.3809600	-2.7001130	-5.0995820
C	-1.2659470	-2.6472490	-2.2434110
H	-1.1262760	-2.6294950	-1.1553960

H	-2.2609500	-2.2508160	-2.4842910
H	-1.1802250	-3.6756770	-2.6192480
C	1.6006140	-2.4280090	-2.7639210
H	2.3887450	-1.8729460	-3.2893920
H	1.8360400	-2.4444680	-1.6922880
H	1.5634660	-3.4558580	-3.1495770
C	0.3306400	-1.6474640	4.7881380
H	1.2941200	-1.1745650	5.0172580
H	-0.4679530	-1.1598990	5.3589400
H	0.3809600	-2.7001130	5.0995820
C	1.2659470	-2.6472490	2.2434110
H	1.1262760	-2.6294950	1.1553960
H	2.2609500	-2.2508160	2.4842910
H	1.1802250	-3.6756770	2.6192480
C	-0.3306400	1.6474640	4.7881380
H	0.4679530	1.1598990	5.3589400
H	-0.3809600	2.7001130	5.0995820
H	-1.2941200	1.1745650	5.0172580
C	1.6006140	2.4280090	2.7639210
H	1.8360400	2.4444680	1.6922880
H	1.5634660	3.4558580	3.1495770
H	2.3887450	1.8729460	3.2893920
C	-1.2659470	2.6472490	2.2434110
H	-2.2609500	2.2508160	2.4842910
H	-1.1802250	3.6756770	2.6192480
H	-1.1262760	2.6294950	1.1553960
C	-1.6006140	-2.4280090	2.7639210
H	-1.5634660	-3.4558580	3.1495770
H	-2.3887450	-1.8729460	3.2893920
H	-1.8360400	-2.4444680	1.6922880