Electron Deficient Bonding in $\blacklozenge$ Rhomboid Rings

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Supplementary Information

Total Energies and Optimized geometries of molecules and extended Structures:

1) $\text{B}_4(\text{BH}_2)_2\text{F}_2$ (D_{2h})

B3LYP / 6-311+G**

Total Energy = -351.32097 Hartrees

5	-1.378462	0.000000	0.000000
5	0.000000	0.810507	0.000000
5	1.378462	0.000000	0.000000
5	0.000000	-0.810507	0.000000
5	0.000000	2.433946	0.000000
1	0.000000	3.028565	1.030740
1	0.000000	3.028565	-1.030740
5	0.000000	-2.433946	0.000000
1	0.000000	-3.028565	-1.030740
1	0.000000	-3.028565	1.030740
9	-2.682205	0.000000	0.000000
9	2.682205	0.000000	0.000000

2) $\text{B}_4\text{H}_4\text{F}_4$ (C_{2v})

B3LYP / 6-31G*

Total Energy = -501.37059 Hartrees

5	0.844740	0.000000	-0.320004
5	-0.844740	0.000000	-0.320004
5	0.000000	1.650015	0.020948
5	0.000000	-1.650015	0.020948
1	1.358159	0.000000	-1.394725
1	1.563198	0.000000	0.642758
1	-1.358159	0.000000	-1.394725

1	-1.563198	0.000000	0.642758
9	0.000000	2.140691	1.241861
9	0.000000	2.491243	-0.992166
9	0.000000	-2.140691	1.241861
9	0.000000	-2.491243	-0.992166

3) B₄H₄F₄ (*D*_{2h})

B3LYP / 6-31G*

Total Energy = -501.36868 Hartrees

5	0.000000	0.000000	0.849317
5	0.000000	0.000000	-0.849317
5	-1.680968	0.000000	0.000000
5	1.680968	0.000000	0.000000
1	0.000000	1.025581	1.464956
1	0.000000	-1.025581	1.464956
1	0.000000	1.025581	-1.464956
1	0.000000	-1.025581	-1.464956
9	-2.355027	-1.130028	0.000000
9	-2.355027	1.130028	0.000000
9	2.355027	-1.130028	0.000000
9	2.355027	1.130028	0.000000

4) B₁₄H₁₂²⁻ (*C*₂)

B3LYP / 6-31G*

Total Energy = -355.24308 Hartrees

5	-0.632764	1.919412	1.183626
1	0.446558	-1.844696	2.368951
5	-1.634074	2.953954	0.130024
5	-0.001166	3.006902	-0.055534
5	-0.686728	0.446847	-0.071522
5	-2.022975	1.356707	0.188707
5	0.632764	1.441991	-0.211596
1	0.770314	3.923151	-0.155064
1	1.802039	1.501301	-0.439502
5	0.686728	-0.446847	-0.071522
1	-3.096557	0.839345	0.326144
1	-2.389474	3.885809	0.229722
1	-0.446558	1.844696	2.368951
1	2.389474	-3.885809	0.229722
5	0.632764	-1.919412	1.183626
1	1.085401	-1.947087	-2.353952

5	0.001166	-3.006902	-0.055534
1	3.096557	-0.839345	0.326144
5	-0.934230	1.931084	-1.158966
1	-1.085401	1.947087	-2.353952
5	2.022975	-1.356707	0.188707
5	1.634074	-2.953954	0.130024
5	-0.632764	-1.441991	-0.211596
5	0.934230	-1.931084	-1.158966
1	-1.802039	-1.501301	-0.439502
1	-0.770314	-3.923151	-0.155064

5) B₂₁H₁₆³⁻ (C₁)

B3LYP / 6-31G*

Total Energy = -531.54428 Hartrees

5	-2.912933	-1.208310	1.097042
1	0.214099	1.789274	2.364467
5	-3.797832	-2.011862	-0.247556
5	-4.329799	-0.528934	0.194856
5	-1.635067	-0.374267	0.028221
5	-2.164681	-1.873612	-0.436643
5	-3.015325	0.512596	0.407129
1	-5.430546	-0.103360	0.450033
1	-3.381012	1.565447	0.851199
5	-1.272127	1.296061	0.134326
1	-1.377164	-2.712945	-0.768614
1	-4.443420	-3.015660	-0.435393
1	-2.798955	-1.541151	2.252726
1	1.553387	3.844914	-0.120956
5	0.091478	1.840126	1.169322
1	-0.214940	1.781613	-2.365826
5	1.271404	1.296445	-0.133680
1	-1.555539	3.844715	0.113031
5	-3.189891	-0.594554	-1.155142
1	-3.278725	-0.218517	-2.297954
5	-0.836725	2.881991	0.057973
5	0.834436	2.882474	-0.062880
5	0.000000	0.279663	0.001260
5	-0.092351	1.836495	-1.170904
5	3.187872	-0.601153	1.157751
5	1.636360	-0.372759	-0.025273
5	2.163818	-1.876047	0.428184
1	3.275033	-0.232613	2.303173
5	3.017242	0.515978	-0.396916

5	2.915982	-1.201601	-1.098633
1	4.443483	-3.017377	0.427176
1	1.375226	-2.717172	0.752797
5	4.330399	-0.528008	-0.190753
1	5.431644	-0.101048	-0.441454
1	2.803243	-1.526147	-2.256755
5	3.797591	-2.013140	0.243025
1	3.385004	1.572120	-0.831190

6) B₂₁H₁₆³⁻ (C_i)

B3LYP / 6-31G*

Total Energy = -707.79186 Hartrees

5	1.611490	-4.396678	1.133567
1	-1.624648	-1.406507	2.219398
5	2.546121	-5.214453	-0.169879
5	1.045376	-5.793738	0.128726
5	0.836220	-3.082857	0.054123
5	2.378220	-3.575887	-0.315343
5	-0.039775	-4.504231	0.309859
1	0.625352	-6.914972	0.311455
1	-1.110636	-4.906377	0.674619
5	-0.840485	-2.742985	-0.019430
1	3.233507	-2.770054	-0.550977
1	3.585058	-5.825370	-0.296940
1	1.856391	-4.326263	2.317270
1	-3.443401	-0.001700	-0.412639
5	-1.524494	-1.435161	1.017822
1	-1.058728	-1.534512	-2.488863
5	-0.904388	-0.124025	-0.124538
1	-3.356697	-3.092464	-0.347346
5	1.192331	-4.603377	-1.168417
1	0.912291	-4.663951	-2.341864
5	-2.408592	-2.354729	-0.251182
5	-2.465754	-0.683765	-0.284409
5	0.133476	-1.448434	0.034697
5	-1.251949	-1.479118	-1.300954
5	1.251949	1.479118	1.300954
5	0.904388	0.124025	0.124538
5	2.465754	0.683765	0.284409
1	1.058728	1.534512	2.488863
5	-0.133476	1.448434	-0.034697
5	1.524494	1.435161	-1.017822
1	3.356697	3.092464	0.347346
1	3.443401	0.001700	0.412639

5	0.840485	2.742985	0.019430
5	-0.836220	3.082857	-0.054123
1	1.624648	1.406507	-2.219398
5	2.408592	2.354729	0.251182
5	-1.045376	5.793738	-0.128726
5	-2.378220	3.575887	0.315343
1	-0.912291	4.663951	2.341864
1	1.110636	4.906377	-0.674619
5	-1.192331	4.603377	1.168417
1	-0.625352	6.914972	-0.311455
1	-3.233507	2.770054	0.550977
5	-1.611490	4.396678	-1.133567
1	-1.856391	4.326263	-2.317270
5	0.039775	4.504231	-0.309859
5	-2.546121	5.214453	0.169879
1	-3.585058	5.825370	0.296940

7) $\text{Si}_4\text{H}_8\text{F}_2^{2+} (C_{2v})$

B3LYP / 6-311++G**

Total Energy = -1361.94594 Hartrees

9	-2.663339	0.000000	1.400795
9	2.663339	0.000000	1.400795
14	-2.680574	0.000000	-0.181143
14	2.680574	0.000000	-0.181143
14	0.000000	1.125411	-0.525499
14	0.000000	-1.125411	-0.525499
1	-3.003002	1.291220	-0.806384
1	3.003002	1.291220	-0.806384
1	-3.003002	-1.291220	-0.806384
1	3.003002	-1.291220	-0.806384
1	0.000000	1.778987	-1.846379
1	0.000000	-1.778987	-1.846379
1	0.000000	1.874236	0.744985
1	0.000000	-1.874236	0.744985

7) $\text{Na}_3\text{B}_{20}^{-1} (Cmmm)$

LDA

Total Energy = -150.42 eV

Primitive cell vectors

9.395	2.834	0.000
-9.395	2.834	0.000
0.000	0.000	4.122

Atomic Positions

B	0.0325560506474596	0.2637798576025527	0.5000000000000000
B	0.2637798576025527	0.0325560506474596	0.5000000000000000
B	0.0293408225721796	0.4318438947926461	0.5000000000000000
B	0.4318438947926461	0.0293408225721796	0.5000000000000000
B	0.2985497937809503	0.3914937019721166	0.5000000000000000
B	0.3914937019721166	0.2985497937809503	0.5000000000000000
B	0.5000000000000000	0.5000000000000000	0.7962954330696984
B	0.5000000000000000	0.5000000000000000	0.2037045669303016
B	0.2548082341938791	0.7451917658061210	0.5000000000000000
B	0.7451917658061210	0.2548082341938791	0.5000000000000000
B	0.1745873682280064	0.8254126317719937	0.7891647743818321
B	0.8254126317719937	0.1745873682280064	0.7891647743818321
B	0.1745873682280064	0.8254126317719937	0.2108352256181678
B	0.8254126317719937	0.1745873682280064	0.2108352256181678
B	0.7014502062190497	0.6085062980278835	0.5000000000000000
B	0.6085062980278835	0.7014502062190497	0.5000000000000000
B	0.5681561052073539	0.9706591774278204	0.5000000000000000
B	0.9706591774278204	0.5681561052073539	0.5000000000000000
B	0.9674439493525405	0.7362201423974472	0.5000000000000000
B	0.7362201423974472	0.9674439493525405	0.5000000000000000
Na	0.0000000000000000	0.0000000000000000	0.0000000000000000
Na	0.6337492085464404	0.3662507914535596	0.0000000000000000
Na	0.3662507914535596	0.6337492085464404	0.0000000000000000

9) β -SiB₃ (*Imma*)

LDA

Total Energy = -228.19 eV

Primitive cell vectors

B	0.1491791413304063	0.7230847193733561	0.4260944219570503
B	0.1528084934449871	0.8296120576365555	0.6738173767374372
B	0.1528084934449871	0.4789911167075427	0.3231964358084315
B	0.1148968746634163	0.6133627917569693	0.7231983303297945
B	0.1148968746634163	0.3916985443336218	0.5015340829064541
B	0.2969238485921392	0.7278390181315499	0.5690848304605819
B	0.6557946808991113	0.8296120576365555	0.1768035641915684
B	0.3442053191008888	0.5210088832924571	0.1738173767374372
B	0.3412458123290323	0.2721609818684501	0.0690848304605822
B	0.6098355385728253	0.3866372082430306	0.0015340829064539
B	0.7969902974163059	0.7230847193733561	0.0739055780429497
B	0.6098355385728253	0.6083014556663782	0.2231983303297945
B	0.8851031253365836	0.6083014556663782	0.4984659170935462

B	0.8471915065550130	0.5210088832924571	0.6768035641915685
B	0.8508208586695938	0.2769152806266440	0.5739055780429499
B	0.8471915065550130	0.1703879423634445	0.3261826232625629
B	0.8851031253365836	0.3866372082430306	0.2768016696702054
B	0.7030761514078608	0.2721609818684501	0.4309151695394178
B	0.3901644614271749	0.6133627917569693	0.9984659170935458
B	0.2030097025836943	0.2769152806266440	0.9260944219570501
B	0.3442053191008888	0.1703879423634445	0.8231964358084316
B	0.6557946808991113	0.4789911167075427	0.8261826232625628
B	0.6587541876709677	0.7278390181315499	0.9309151695394181
B	0.3901644614271749	0.3916985443336218	0.7768016696702055
Si	0.1516570748014461	0.9974840955579245	0.1541729792435216
Si	0.3433111163144029	0.9974840955579245	0.3458270207564784
Si	0.3129290019683671	0.7948425181094789	0.9819135161411122
Si	0.6870709980316327	0.2051574818905207	0.0180864838588879
Si	0.6870709980316327	0.6689845141727381	0.4819135161411122
Si	0.3129290019683671	0.3310154858272620	0.5180864838588878
Si	0.6566888836855972	0.0025159044420755	0.6541729792435218
Si	0.8483429251985539	0.0025159044420755	0.8458270207564782