Supporting Information for

$B_{12}F_n^{0/-}$ (n = 1– 6) Series: When Do Boron Double Chain Nanoribbons Become Global Minima?

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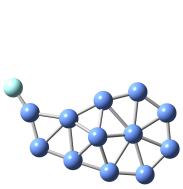
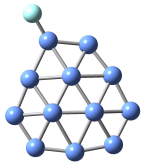
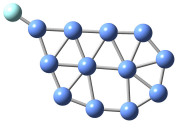
Figure S1 Low-lying isomers of $B_{12}F$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



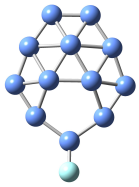
1. C_1 $B_{12}F$ (^2A)
0.00 (*0.00*)



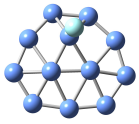
1.1 C_1 $B_{12}F$ (^2A)
+0.09 (*+0.11*)



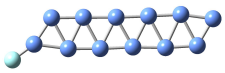
1.2 C_1 $B_{12}F$ (^2A)
+0.26 (*+0.04*)



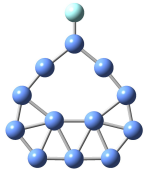
1.3 C_s $B_{12}F$ ($^2A'$)
+0.40 (*+0.47*)



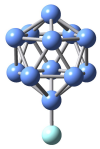
1.4 C_1 $B_{12}F$ (^2A)
+0.42 (*+0.54*)



1.5 C_s $B_{12}F$ ($^2A'$)
+0.58 (*+0.13*)

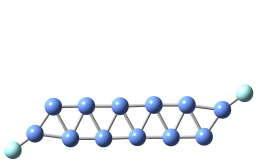


1.6 C_{2v} $B_{12}F$ ($^2B_2$)
+0.95 (*+0.58*)

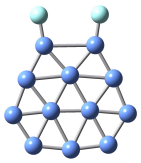


1.7 C_1 $B_{12}F$ (^2A)
+1.87 (*+2.88*)

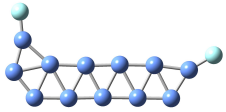
Figure S2 Low-lying isomers of $B_{12}F_2$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



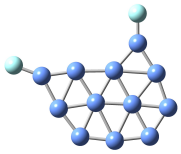
2. C_{2h} $B_{12}F_2$ (^1A_g)
0.00 (*0.00*)



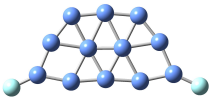
2.1 C_{2v} $B_{12}F_2$ ($^1A_1$)
+0.15 (*+0.59*)



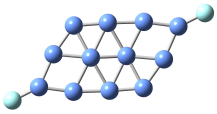
2.2 C_s $B_{12}F_2$ ($^1A'$)
+0.23 (*+0.24*)



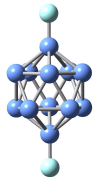
2.3 C_1 $B_{12}F_2$ (^1A)
+0.30 (*+0.70*)



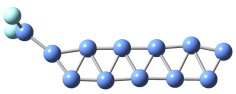
2.4 C_2 $B_{12}F_2$ (^1A)
+0.31 (*+0.69*)



2.5 C_i $B_{12}F_2$ (^1A_g)
+0.46 (*+0.81*)

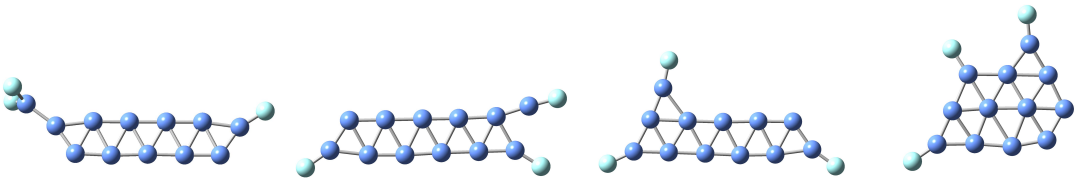


2.6 D_{5d} $B_{12}F_2$ ($^1A_{1g}$)
+1.04 (*+2.72*)



2.7 C_s $B_{12}F_2$ ($^1A'$)
+1.51 (*+1.67*)

Figure S3 Low-lying isomers of $B_{12}F_3$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.

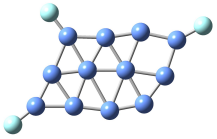


3. C_s $B_{12}F_3$ (^{2}A')
0.00 (*0.00*)

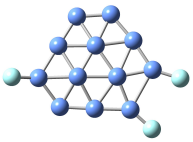
3.1 C_s $B_{12}F_3$ (^{2}A')
+0.31 (*+0.20*)

3.2 C_1 $B_{12}F_3$ (^{2}A)
+0.56 (*+0.55*)

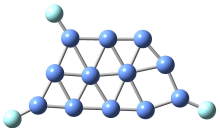
3.3 C_1 $B_{12}F_3$ (^{2}A)
+0.65 (*+0.94*)



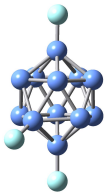
3.4 C_1 $B_{12}F_3$ (^{2}A)
+0.71 (*+0.99*)



3.5 C_1 $B_{12}F_3$ (^{2}A)
+0.79 (*+1.19*)

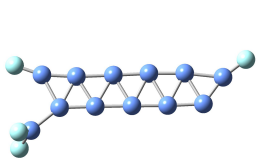


3.6 C_s $B_{12}F_3$ (^{2}A')
+0.80 (*+1.08*)

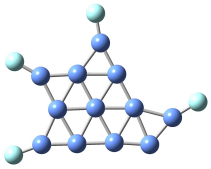


3.7 C_s $B_{12}F_3$ (^{2}A')
+1.29 (*+2.17*)

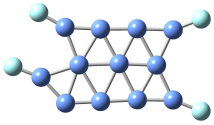
Figure S4 Low-lying isomers of $B_{12}F_4$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



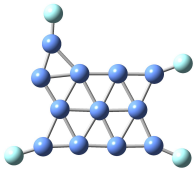
4. C_1 $B_{12}F_4$ (^1A)
0.00 (*0.00*)



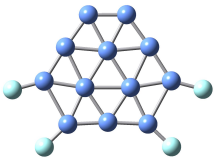
4.1 C_1 $B_{12}F_4$ (^1A)
+0.33 (*+0.49*)



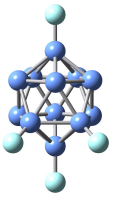
4.2 C_s $B_{12}F_4$ ($^1A'$)
+0.48 (*+0.71*)



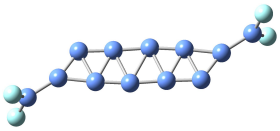
4.3 C_s $B_{12}F_4$ ($^1A'$)
+0.49 (*+0.67*)



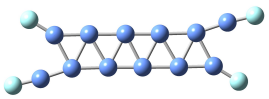
4.4 C_{2v} $B_{12}F_4$ ($^1A_1$)
+0.58 (*+0.86*)



4.5 C_s $B_{12}F_4$ ($^1A'$)
+0.65 (*+2.13*)

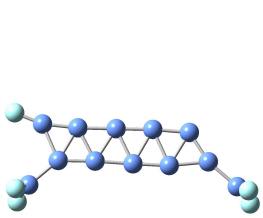


4.6 C_{2h} $B_{12}F_4$ (^1A_g)
+0.67 (*+0.66*)

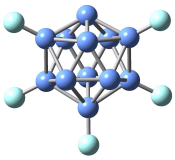


4.7 C_{2h} $B_{12}F_4$ (^1A_g)
+0.96 (*+0.79*)

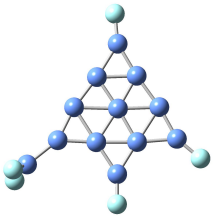
Figure S5 Low-lying isomers of $B_{12}F_5$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



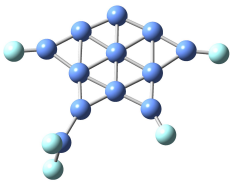
5. C_s $B_{12}F_5$ (^{2}A')
0.00 (*0.00*)



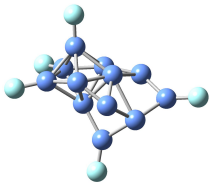
5.1 C_s $B_{12}F_5$ (^{2}A')
+0.28 (*+1.65*)



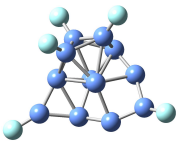
5.2 C_s $B_{12}F_5$ (^{2}A')
+0.55 (*+0.79*)



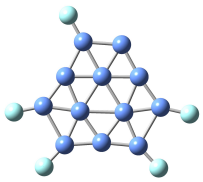
5.3 C_s $B_{12}F_5$ (^{2}A')
+0.69 (*+0.95*)



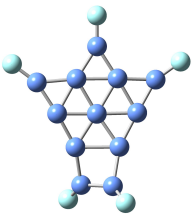
5.4 C_1 $B_{12}F_5$ (^{2}A)
+0.79 (*+1.84*)



5.5 C_1 $B_{12}F_5$ (^{2}A)
+0.94 (*+2.06*)

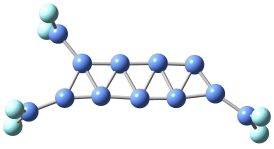


5.6 C_1 $B_{12}F_5$ (^{2}A)
+1.31 (*+1.60*)

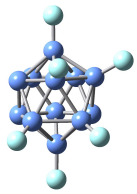


5.7 C_1 $B_{12}F_5$ (^{2}A)
+1.50 (*+1.73*)

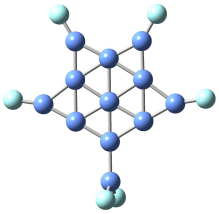
Figure S6 Low-lying isomers of $B_{12}F_6$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



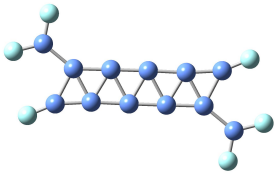
6. C_1 $B_{12}F_6$ (^{1}A)
0.00 (*0.00*)



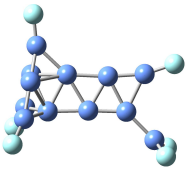
6.1 C_2 $B_{12}F_6$ (^{1}A)
+0.14 (*+1.54*)



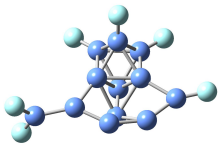
6.2 C_{2v} $B_{12}F_6$ ($^1A_1$)
+0.23 (*+0.41*)



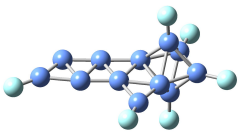
6.3 C_2 $B_{12}F_6$ (^{1}A)
+0.27 (*+0.24*)



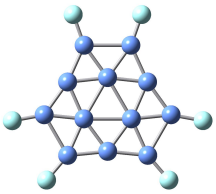
6.4 C_s $B_{12}F_6$ (^{1}A′)
+0.32 (*+0.83*)



6.5 C_1 $B_{12}F_6$ (^{1}A)
+0.41 (*+1.32*)

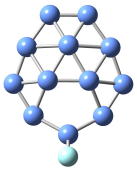


6.6 C_s $B_{12}F_6$ (^{1}A′)
+0.47 (*+1.00*)

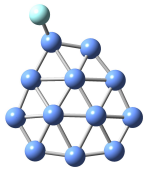


6.7 D_{3h} $B_{12}F_6$ (^{1}A')
+0.74 (*+0.91*)

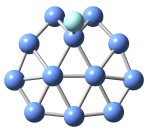
Figure S7 Low-lying isomers of $B_{12}F^-$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



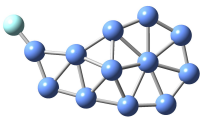
7. C_s $B_{12}F^-$ ($^1A'$)
0.00 (*0.00*)



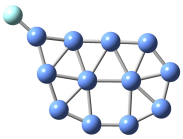
7.1 C_1 $B_{12}F^-$ (^1A)
+0.03 (*+0.06*)



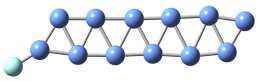
7.2 C_s $B_{12}F^-$ ($^1A'$)
+0.16 (*+0.28*)



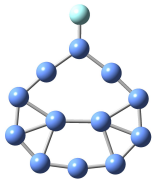
7.3 C_1 $B_{12}F^-$ (^1A)
+0.20 (*+0.18*)



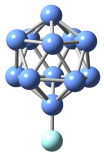
7.4 C_1 $B_{12}F^-$ (^1A)
+0.59 (*+0.34*)



7.5 C_s $B_{12}F^-$ ($^1A'$)
+0.75 (*+0.36*)

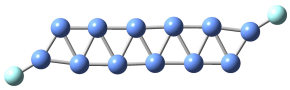


7.6 C_{2v} $B_{12}F^-$ ($^1A_1$)
+0.97 (*+0.57*)

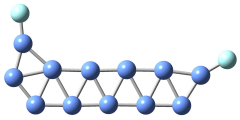


7.7 C_s $B_{12}F^-$ ($^1A'$)
+2.68 (*+4.65*)

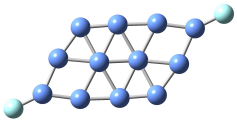
Figure S8 Low-lying isomers of $B_{12}F_2^-$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



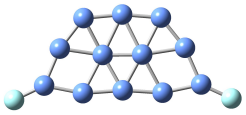
8. C_{2h} $B_{12}F_2^-$ (^2A_g)
0.00 (*0.00*)



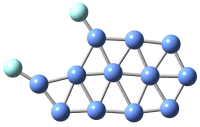
8.1 C_s $B_{12}F_2^-$ ($^2A'$)
+0.41 (*+0.45*)



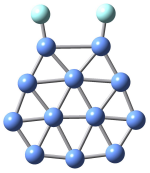
8.2 C_i $B_{12}F_2^-$ (^2A_u)
+0.48 (*+0.84*)



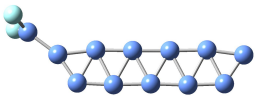
8.3 C_2 $B_{12}F_2^-$ (^2A)
+0.51 (*+0.92*)



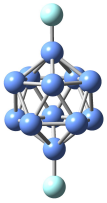
8.4 C_s $B_{12}F_2^-$ ($^2A'$)
+0.52 (*+0.92*)



8.5 C_{2v} $B_{12}F_2^-$ ($^2A_2$)
+0.82 (*+1.30*)

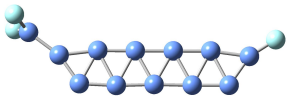


8.6 C_s $B_{12}F_2^-$ ($^2A'$)
+0.91 (*+1.01*)

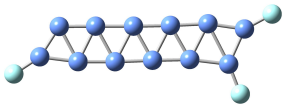


8.7 C_s $B_{12}F_2^-$ ($^2A'$)
+1.56 (*+3.63*)

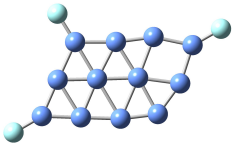
Figure S9 Low-lying isomers of $B_{12}F_3^-$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



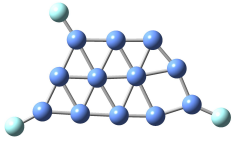
9. C_s $B_{12}F_3^-$ ($^1A'$)
0.00 (*0.00*)



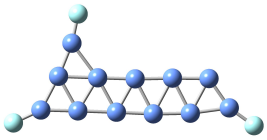
9.1 C_s $B_{12}F_3^-$ ($^1A'$)
+0.74 (*+0.63*)



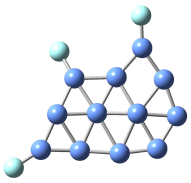
9.2 C_s $B_{12}F_3^-$ ($^1A'$)
+0.89 (*+1.15*)



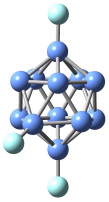
9.3 C_s $B_{12}F_3^-$ ($^1A'$)
+0.90 (*+1.16*)



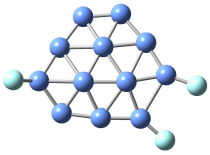
9.4 C_s $B_{12}F_3^-$ ($^1A'$)
+1.13 (*+1.08*)



9.5 C_1 $B_{12}F_3^-$ (^1A)
+1.23 (*+1.40*)

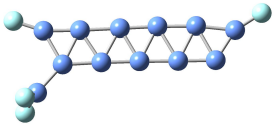


9.6 C_s $B_{12}F_3^-$ ($^1A'$)
+1.27 (*+3.11*)

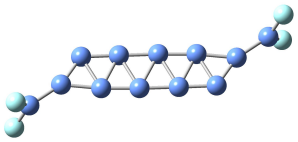


9.7 C_1 $B_{12}F_3^-$ (^1A)
+1.35 (*+1.83*)

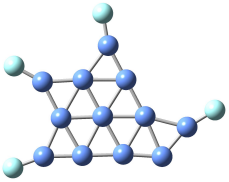
Figure S10 Low-lying isomers of $B_{12}F_4^-$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



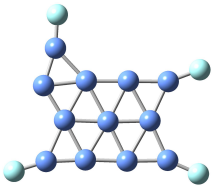
10. C_s $B_{12}F_4^-$ ($^2A'$)
0.00 (*0.00*)



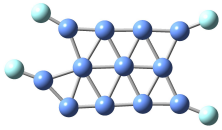
10.1 C_{2h} $B_{12}F_4^-$ (^2A_g)
+0.09 (*+0.12*)



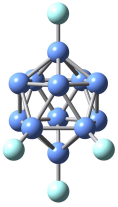
10.2 C_1 $B_{12}F_4^-$ (^2A)
+0.77 (*+0.99*)



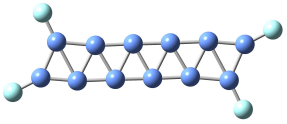
10.3 C_s $B_{12}F_4^-$ ($^2A'$)
+0.81 (*+1.04*)



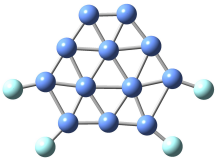
10.4 C_s $B_{12}F_4^-$ ($^2A'$)
+0.96 (*+1.23*)



10.5 C_1 $B_{12}F_4^-$ (^2A)
+1.00 (*+2.53*)

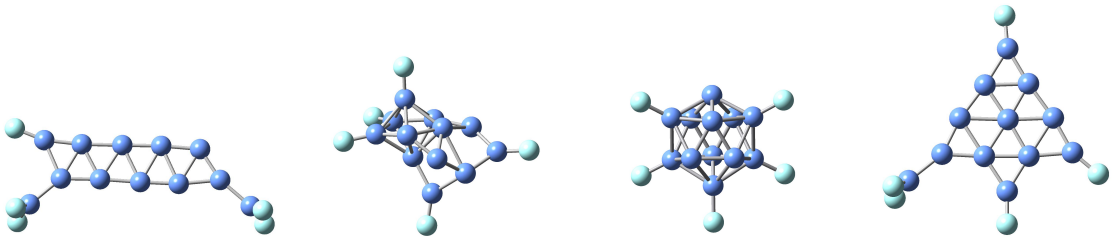


10.6 C_2 $B_{12}F_4^-$ (^2A)
+1.53 (*+1.34*)



10.7 C_s $B_{12}F_4^-$ ($^2A'$)
+1.58 (*+1.92*)

Figure S11 Low-lying isomers of $B_{12}F_5^-$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.

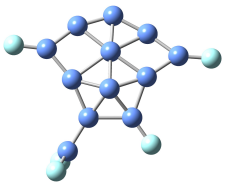


11. C_s $B_{12}F_5^-$ (^{1}A')
0.00 (*0.00*)

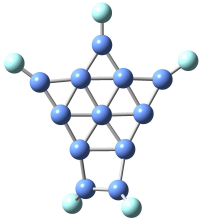
11.1 C_1 $B_{12}F_5^-$ (^{1}A)
+0.34 (*+1.37*)

11.2 C_s $B_{12}F_5^-$ (^{1}A')
+0.36 (*+2.02*)

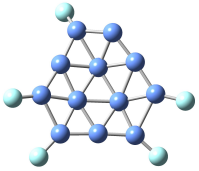
11.3 C_s $B_{12}F_5^-$ (^{1}A')
+0.39 (*+0.54*)



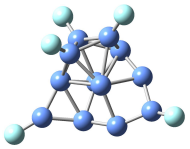
11.4 C_1 $B_{12}F_5^-$ (^{1}A)
+0.49 (+0.79)



11.5 C_1 $B_{12}F_5^-$ (^{1}A)
+1.14 (*+1.28*)

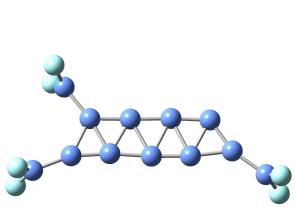


11.6 C_1 $B_{12}F_5^-$ (^{1}A)
+1.58 (*+1.88*)

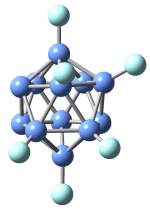


11.7 C_1 $B_{12}F_5^-$ (^{1}A)
+3.21 (*+1.29*)

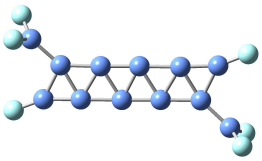
Figure S12 Low-lying isomers of $B_{12}F_6^-$, with their relative energies indicated in eV at CCSD(T)//B3LYP and B3LYP/6-311++G(d,p) (in *italic*) levels.



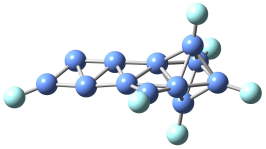
12. C_1 $B_{12}F_6^-$ (^{2}A)
0.00 (*0.00*)



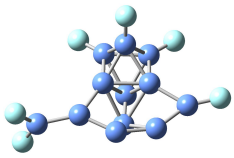
12.1 C_1 $B_{12}F_6^-$ (^{2}A)
+0.10 (*+1.68*)



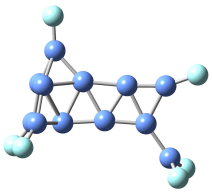
12.2 C_2 $B_{12}F_6^-$ (^{2}A)
+0.29 (*+0.25*)



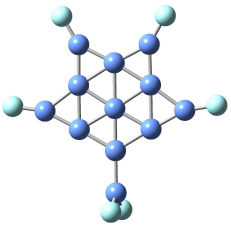
12.3 C_1 $B_{12}F_6^-$ (^{2}A)
+0.80 (*+1.28*)



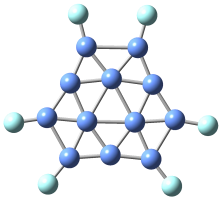
12.4 C_1 $B_{12}F_6^-$ (^{2}A)
+0.52 (*+1.46*)



12.5 C_1 $B_{12}F_6^-$ (^{2}A)
+1.27 (*+1.71*)



12.6 C_{2v} $B_{12}F_6^-$ (^{2}B$_1$)
+1.67 (*+1.84*)



12.7 C_{2v} $B_{12}F_6^-$ (^{2}A$_2$)
+2.05 (*+2.20*)

Figure S13 Simulated photoelectron spectra based on the global minimum C_s $B_{12}F^-$ (**7**, ^{1}A') (**a**) and its low-lying isomer C_1 $B_{12}F^-$ (**7.1**, ^{1}A) (**b**). The simulations were done by fitting the distribution of the calculated VDEs with unit-area Gaussian functions of 0.1 eV halfwidth.