Supplementary Materials:

Quasi-planar aromatic B_{36} and B_{36}^- clusters:

all-boron analogues of coronene†

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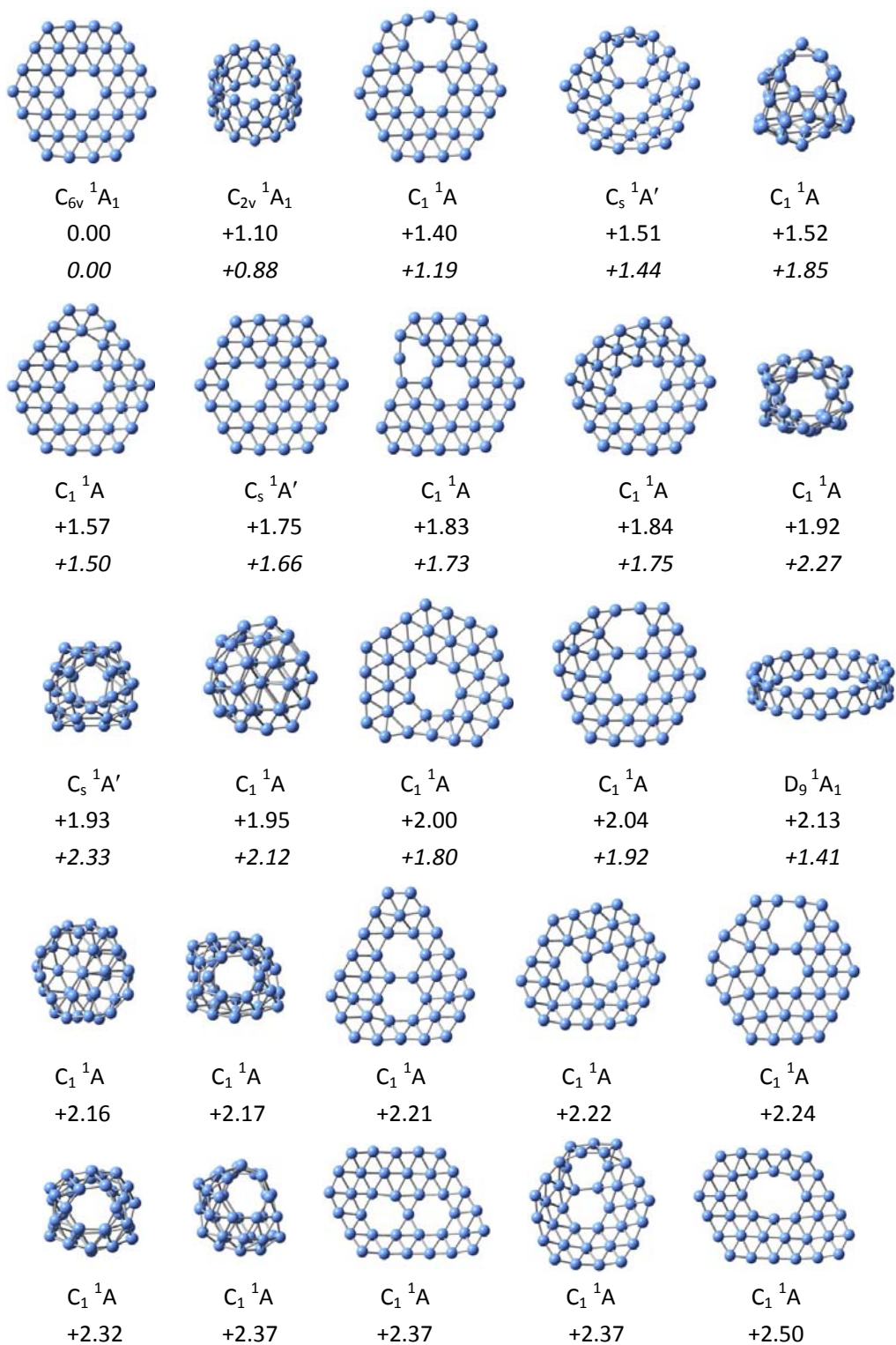
Hua-Jin Zhai,*[ac] and Si-Dian Li*[a]

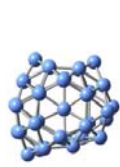[a]*Nanocluster Laboratory, Institute of Molecular Science, Shanxi University, Taiyuan 030006, China*
[b]*Department of Chemistry, Fudan University, Shanghai 200433, China*
[c]*State Key Laboratory of Quantum Optics and Quantum Optics Devices, Shanxi University, Taiyuan 030006, China*
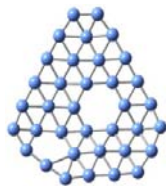
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Fig. S1. Low-lying isomers of B_{36}, with their relative energies indicated in eV at PBE0/6-311+G* and TPSSh/6-311+G*(in *italic*) levels.
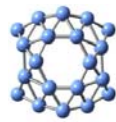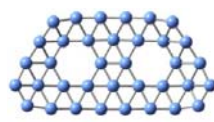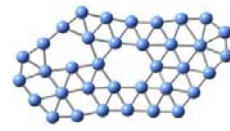

C_{6v} $^1A_1$	C_{2v} $^1A_1$	C_1 ^1A	C_s $^1A'$	C_1 ^1A
0.00	+1.10	+1.40	+1.51	+1.52
0.00	*+0.88*	*+1.19*	*+1.44*	*+1.85*

C_1 ^1A	C_s $^1A'$	C_1 ^1A	C_1 ^1A	C_1 ^1A
+1.57	+1.75	+1.83	+1.84	+1.92
+1.50	*+1.66*	*+1.73*	*+1.75*	*+2.27*

C_s $^1A'$	C_1 ^1A	C_1 ^1A	C_1 ^1A	D_9 $^1A_1$
+1.93	+1.95	+2.00	+2.04	+2.13
+2.33	*+2.12*	*+1.80*	*+1.92*	*+1.41*

C_1 ^1A	C_1 ^1A	C_1 ^1A	C_1 ^1A	C_1 ^1A
+2.16	+2.17	+2.21	+2.22	+2.24

C_1 ^1A	C_1 ^1A	C_1 ^1A	C_1 ^1A	C_1 ^1A
+2.32	+2.37	+2.37	+2.37	+2.50

C₁ ¹A
+2.51

C₁ ¹A
+2.80

C₂ₕ ¹Ag
+2.84

+3.11

Cₛ ¹A′
+2.98

C₁ ¹A
+3.10
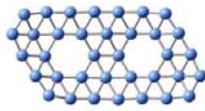
C₁ ¹A
+3.21
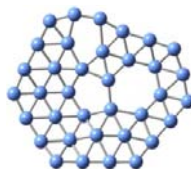
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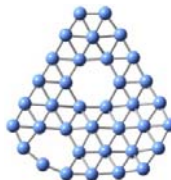
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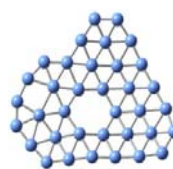
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+3.27
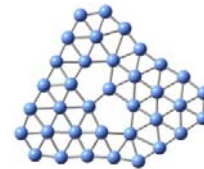
C₁ ¹A
+3.29
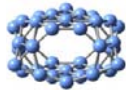
Cᵢ ¹Ag
+3.35
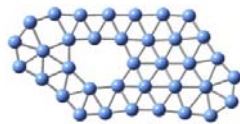
C₁ ¹A
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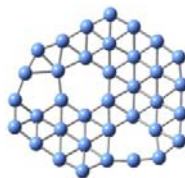
C₁ ¹A
+3.42
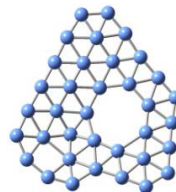
C₁ ¹A
+3.46
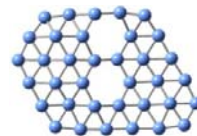
C₁ ¹A
+3.47
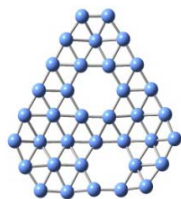
C₁ ¹A
+3.48
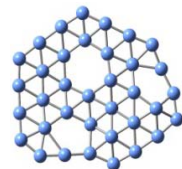
C₁ ¹A
+3.81
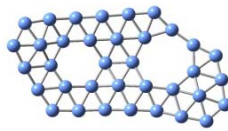
C₁ ¹A
+3.95
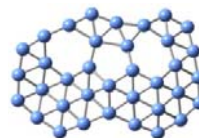
C₁ ¹A
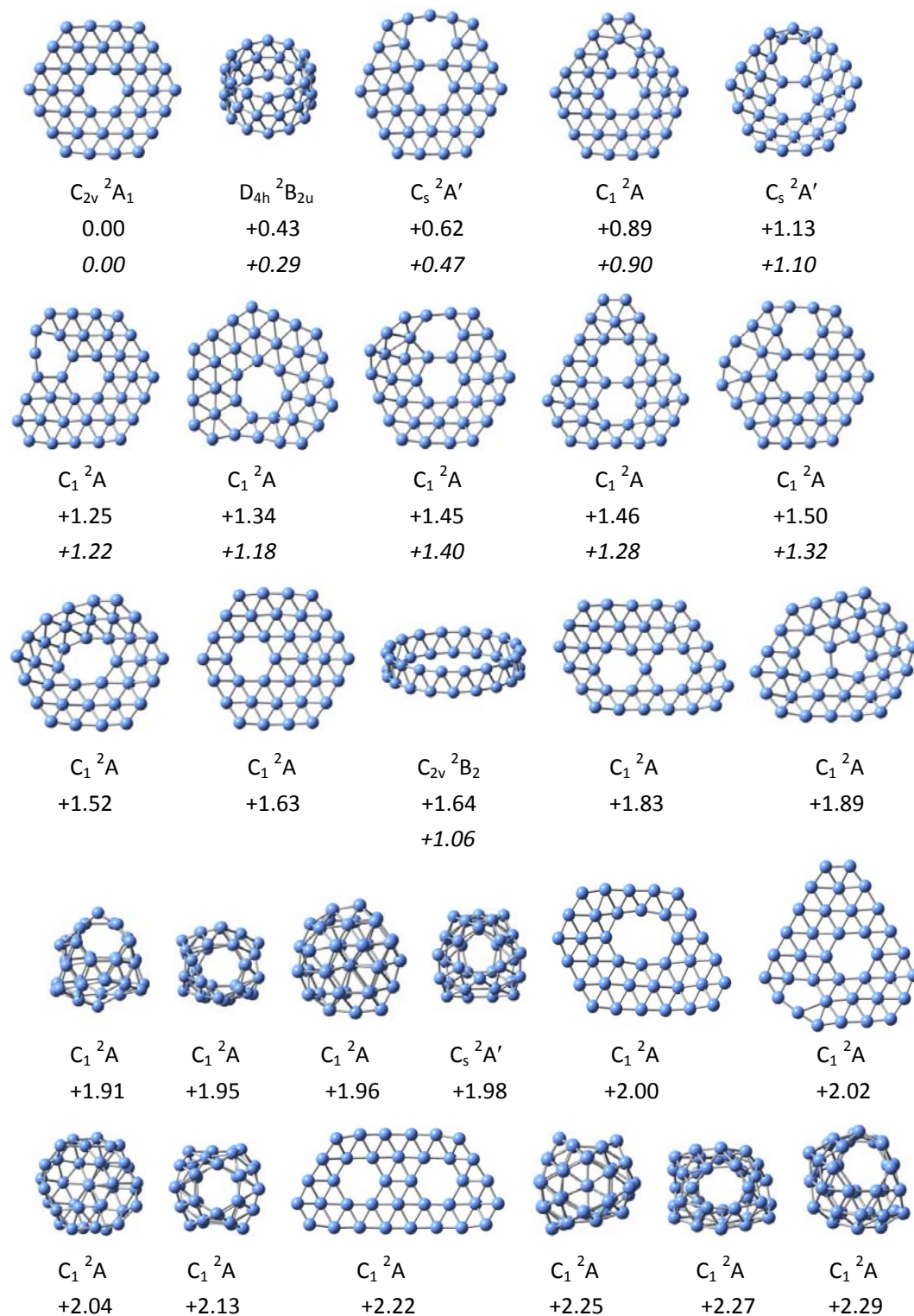+4.92
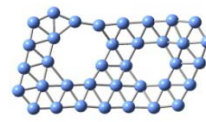
C₁ ¹A
+4.92

Fig. S2. Low-lying isomers of B_{36}^-, with their relative energies indicated in eV at PBE0/6-311+G* and TPSSh/6-311+G*(in *italic*) levels.

C_{2v} $^2A_1$	D_{4h} $^2B_{2u}$	C_s $^2A'$	C_1 ^2A	C_s $^2A'$
0.00	+0.43	+0.62	+0.89	+1.13
0.00	*+0.29*	*+0.47*	*+0.90*	*+1.10*

C_1 ^2A	C_1 ^2A	C_1 ^2A	C_1 ^2A	C_1 ^2A
+1.25	+1.34	+1.45	+1.46	+1.50
+1.22	*+1.18*	*+1.40*	*+1.28*	*+1.32*

C_1 ^2A	C_1 ^2A	C_{2v} $^2B_2$	C_1 ^2A	C_1 ^2A
+1.52	+1.63	+1.64	+1.83	+1.89
		+1.06		

C_1 ^2A	C_1 ^2A	C_1 ^2A	C_s $^2A'$	C_1 ^2A	C_1 ^2A
+1.91	+1.95	+1.96	+1.98	+2.00	+2.02

C_1 ^2A	C_1 ^2A	C_1 ^2A	C_1 ^2A	C_1 ^2A	C_1 ^2A
+2.04	+2.13	+2.22	+2.25	+2.27	+2.29
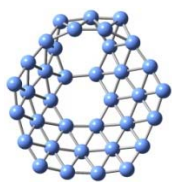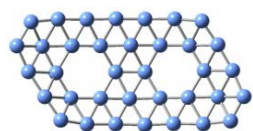
C$_1$ ^{2}A
+2.31

C$_2$ ^{2}A
+2.32
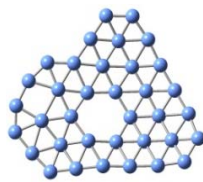
C$_1$ ^{2}A
+2.39
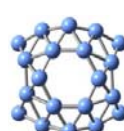
C$_{2v}$ ^{2}B$_1$
+2.41

+2.71
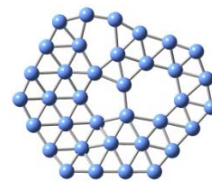
C$_1$ ^{2}A
+2.43
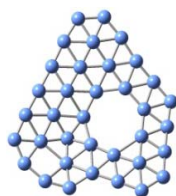
C$_1$ ^{2}A
+2.77
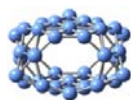
C$_{2h}$ ^{2}B$_g$
+3.63

Fig. S3. Optimized geometries (bond lengths labeled in Å) of (**a**) C_{6v} B_{36} ($^1A_1$) and (**b**) C_{2v} B_{36}^{-} ($^2A_1$) at PBE0/6-311+G* level.

(a)

C_{6v} B_{36} ($^1A_1$)

(b)
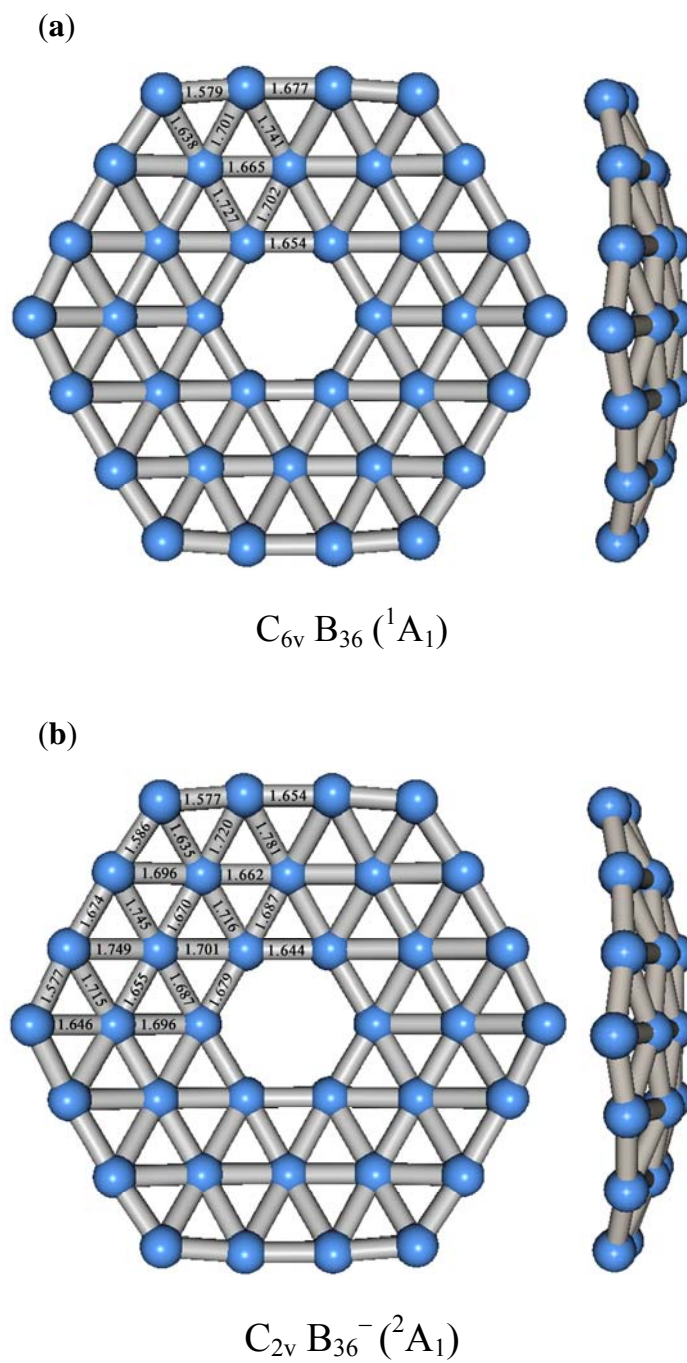
C_{2v} B_{36}^{-} ($^2A_1$)

Fig. S4. Optimized geometries (bond lengths labeled in Å) of (**a**) C_{6v} $B_{36}H_6$ ($^1A_1$) and (**b**) C_{2v} $B_{36}H_6^-$ ($^2A_1$) at PBE0/6-311+G* level.

(**a**)

C_{6v} $B_{36}H_6$ ($^1A_1$)

(**b**)

C_{2v} $B_{36}H_6^-$ ($^2A_1$)
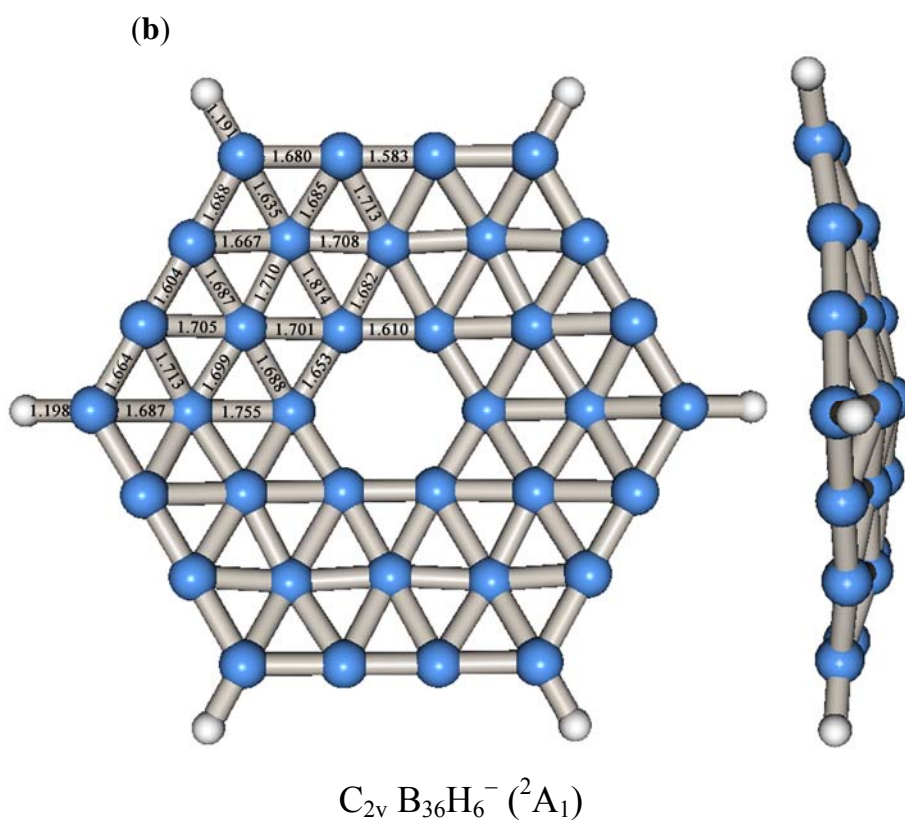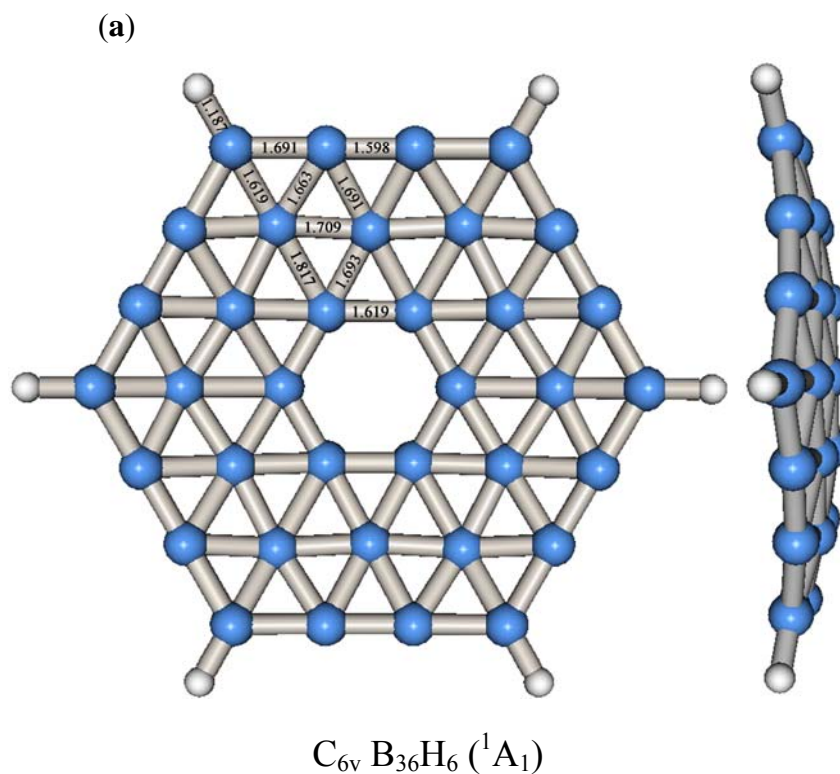
Fig. S5. Comparison of the π molecular orbitals of (**a**) C_{6v} B_{36}, (**b**) C_{6v} $B_{36}H_6$, and (**c**) D_{6h} $C_{24}H_{12}$.

(a)

HOMO' (e_2)   HOMO (e_2)

HOMO-1' (e_1)   HOMO-1 (e_1)

HOMO-6 (b_2)

HOMO-3 (b_1)

HOMO-5 (a_1)

HOMO-10' (e_2)   HOMO-10 (e_2)

HOMO-17' (e_1)   HOMO-17 (e_1)

HOMO-18 (a_1)

C_{6v} B_{36}

(b)

HOMO' (e_2)   HOMO (e_2)

HOMO-2' (e_1)   HOMO-2 (e_1)

HOMO-5 (b_2)

HOMO-3 (b_1)

HOMO-6 (a_1)

HOMO-11' (e_2)   HOMO-11 (e_2)

HOMO-15' (e_1)   HOMO-15 (e_1)

HOMO-18 (a_1)

C_{6v} $B_{36}H_6$

(c)

HOMO' (e_{2u})   HOMO (e_{2u})

HOMO-1' (e_{1g})   HOMO-1 (e_{1g})

HOMO-2 (b_{1g})

HOMO-3 (b_{2g})

HOMO-5 (a_{2u})

HOMO-6' (e_{2u})   HOMO-6 (e_{2u})

HOMO-11' (e_{1g})   HOMO-11 (e_{1g})

HOMO-16 (a_{2u})

D_{6h} $C_{24}H_{12}$