Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Planar B_{41}^- and B_{42}^- Clusters with Double-Hexagonal Vacancies

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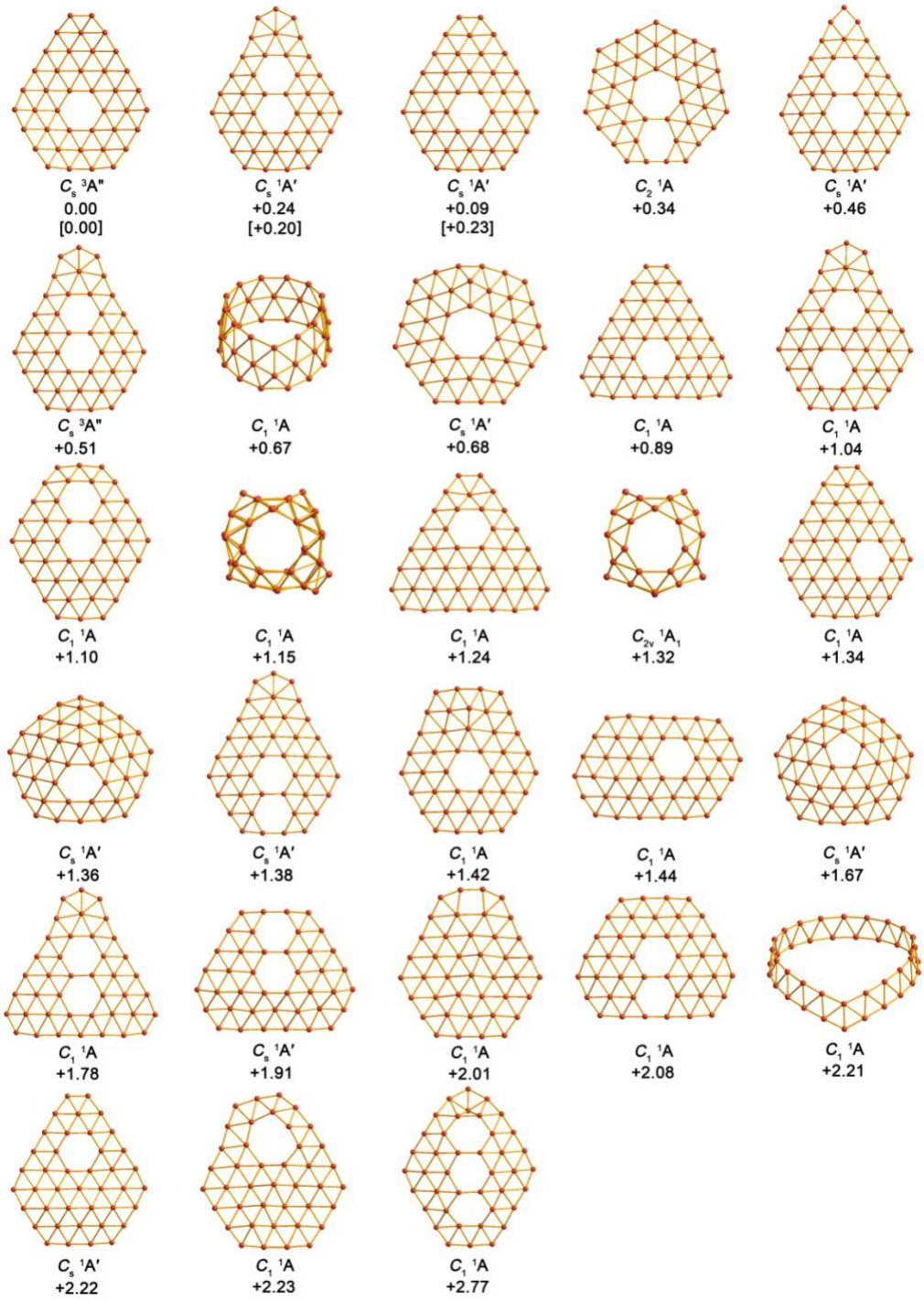

Figure S1 Low-lying isomers of B_{41}^- within 2.8 eV of the global minimum at the PBE0/6-311+G* level. Single-point CCSD(T) energies at the PBE0/6-311+G* geometries for the top three isomers are given in square brackets. The PBE0 energies are corrected for zero-point energies. The point group symmetry and spectroscopic state of each isomer are also given. All energies are given in eV.

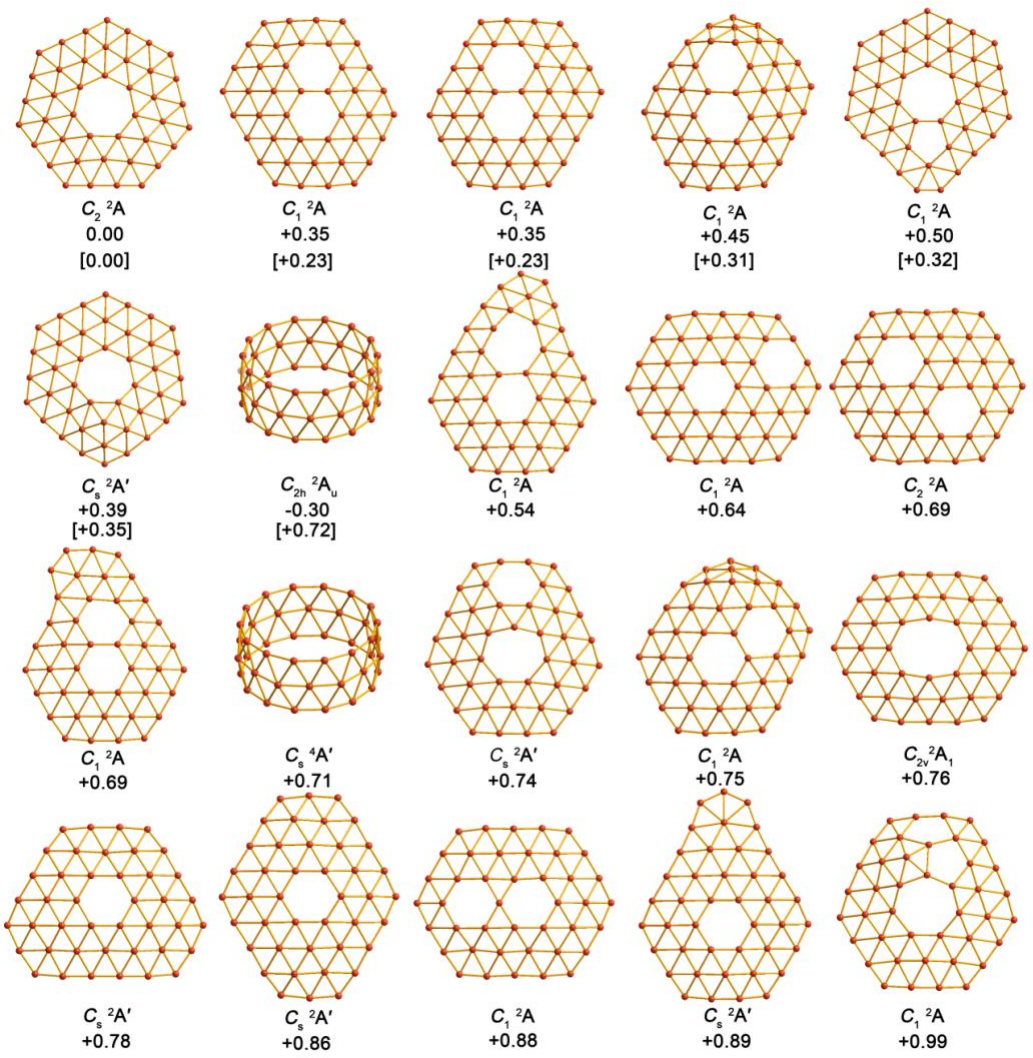
C_2 ^{2}A
0.00
[0.00]
C_1 ^{2}A
+0.35
[+0.23]
C_1 ^{2}A
+0.35
[+0.23]
C_1 ^{2}A
+0.45
[+0.31]
C_1 ^{2}A
+0.50
[+0.32]
C_s ^{2}A′
+0.39
[+0.35]
C_{2h} ^{2}A$_u$
-0.30
[+0.72]
C_1 ^{2}A
+0.54
C_1 ^{2}A
+0.64
C_2 ^{2}A
+0.69
C_1 ^{2}A
+0.69
C_s ^{4}A′
+0.71
C_s ^{2}A′
+0.74
C_1 ^{2}A
+0.75
C_{2v} ^{2}A$_1$
+0.76
C_s ^{2}A′
+0.78
C_s ^{2}A′
+0.86
C_1 ^{2}A
+0.88
C_s ^{2}A′
+0.89
C_1 ^{2}A
+0.99

Figure S2

(**Figure S2** Continued)

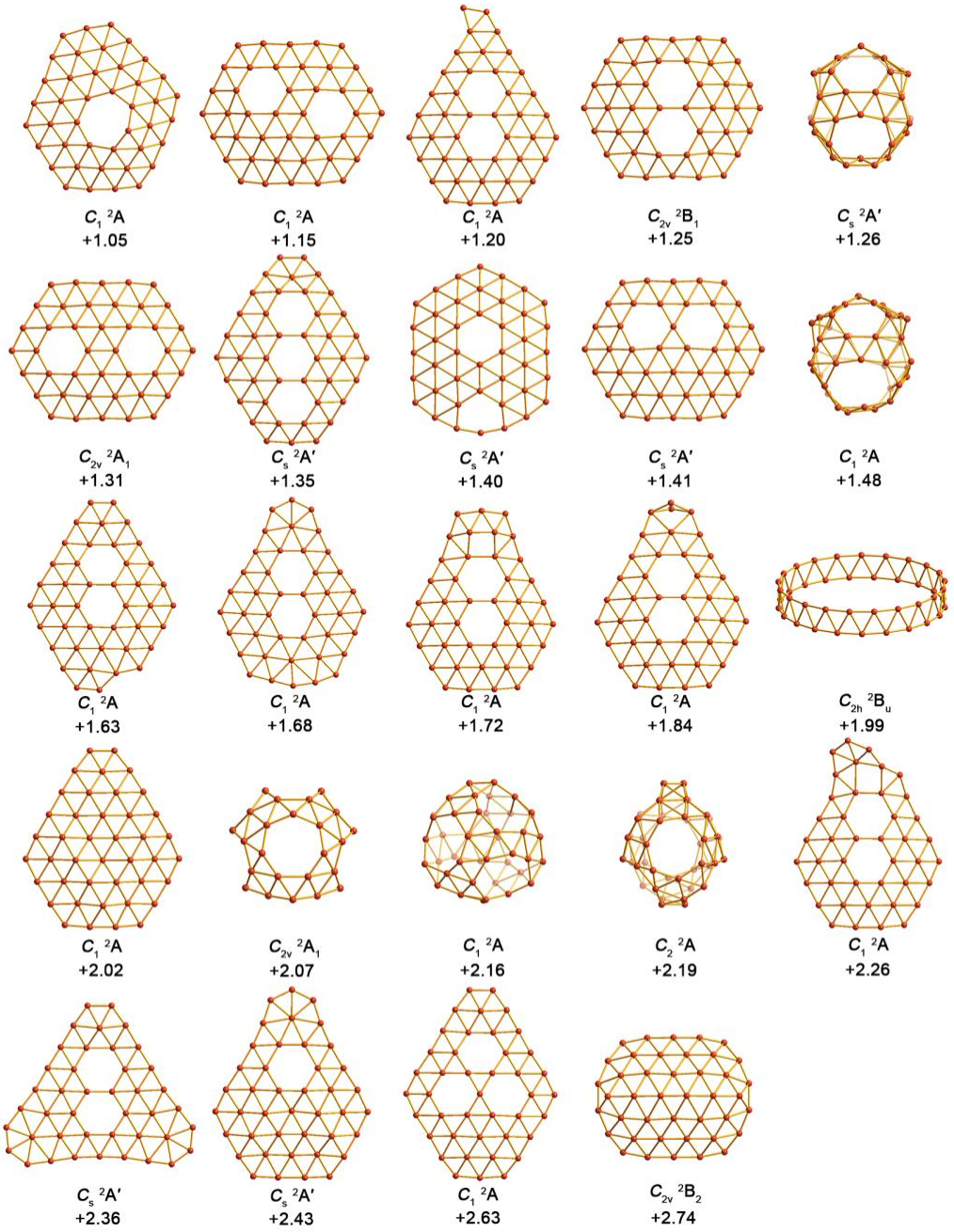

Figure S2 Low-lying isomers of B_{42}^- within 2.8 eV of the global minimum at the PBE0/6-311+G* level. Single-point CCSD energies at the PBE0/6-311+G* geometries for the top seven isomers are given in square brackets. The PBE0 energies are corrected for zero-point energies. The point group symmetry and spectroscopic state of each isomer are also given. All energies are given in eV.

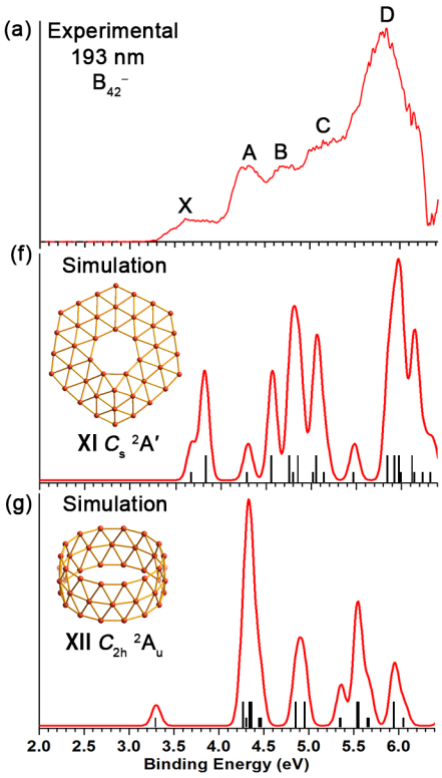

Figure S3 Photoelectron spectrum of B_{42}^- at 193 nm (6.424 eV) (a), compared with simulated spectra of isomers **XI** (f), and **XII** (g). The simulated spectra were obtained by fitting a unit-area Gaussian functions of 0.1 eV half-width for each of the calculated VDEs (vertical bars) at the TDDFT-PBE0/6-311+G* level with. The longer bars are for triplet final states and the shorter bars for the singlet final states. See Fig. 2.

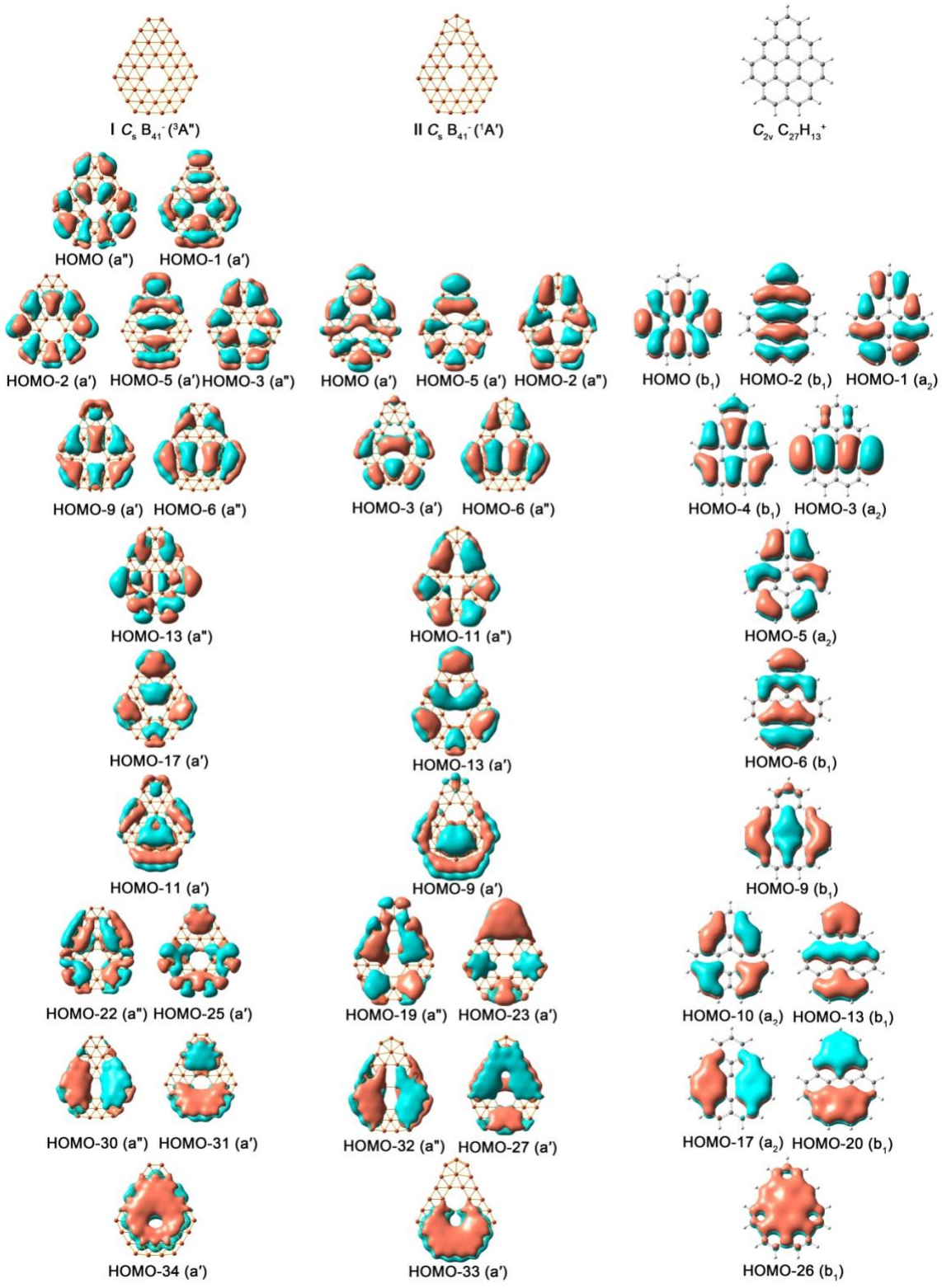

Figure S4 Comparison of the π-MOs of (a) C_s B_{41}^- (**I**), (b) C_s B_{41}^- (**II**), and (c) C_{2v} $C_{27}H_{13}^+$.

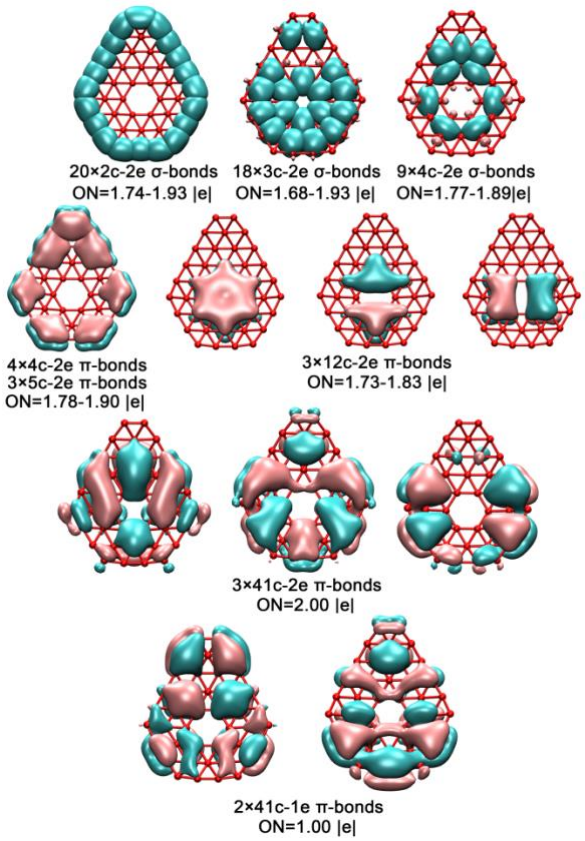

Figure S5 The AdNDP bonding analysis for the triplet C_s isomer **I** of B_{41}^-. Occupation numbers (ONs) are shown.

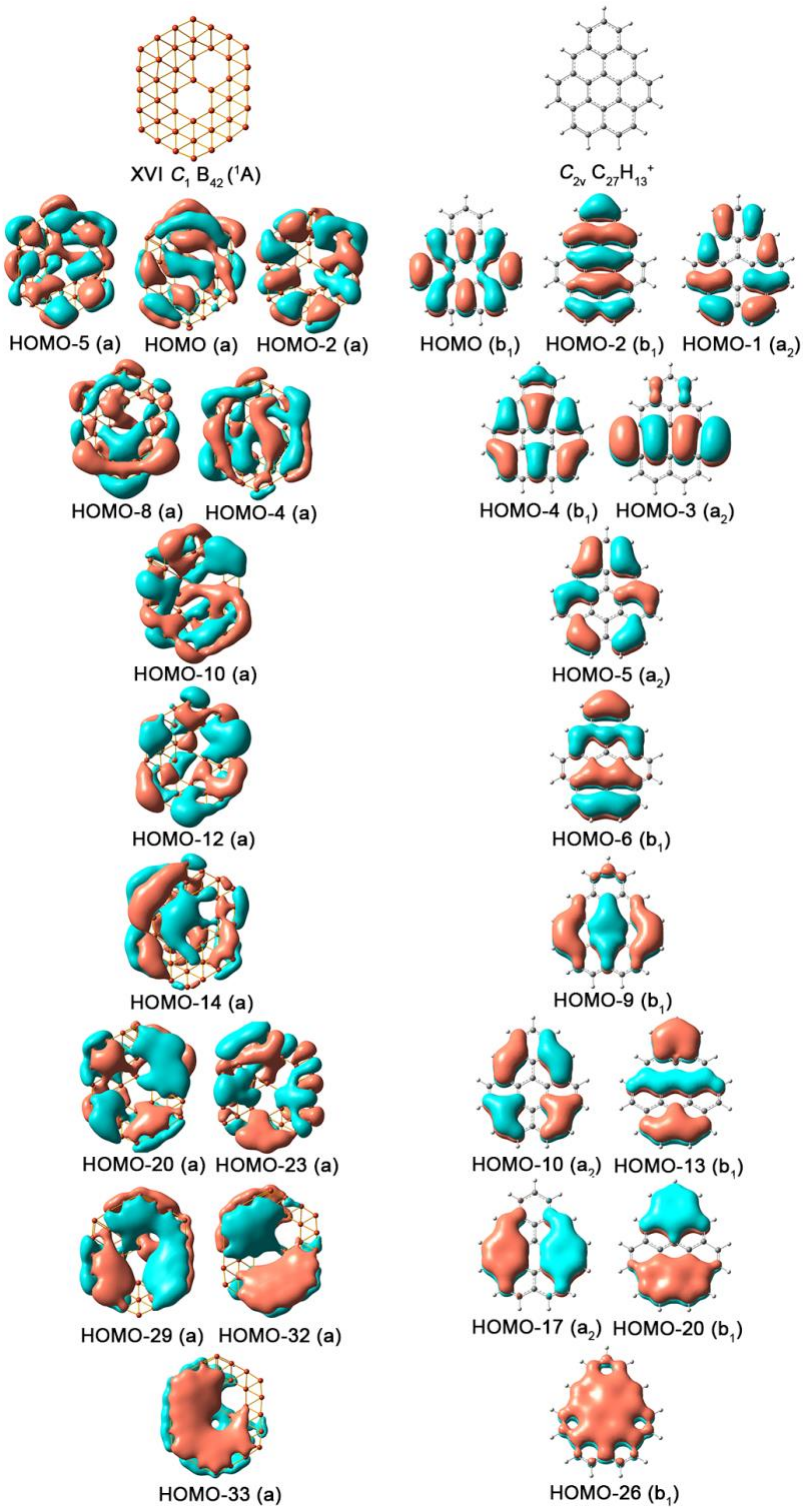

Figure S6 Comparison of the π-MOs of (a) the C_s B_{42} neutral (**XVI**), and (b) C_{2v} $C_{27}H_{13+}$.

Table S1 Vertical detachment energies (VDE) measured from the photoelectron spectrum of B_{41}^- compared with the calculated VDEs at the TDDFT-PBE0/6-311+G* level. All energies are in eV.

Feature	VDE_{exptl}[a]	Final states and electronic configurations	VDE_{theob}	ADE_{theoc}
II C_s B_{41}^- ($^1A'$)				
X	3.89(6)	$^2A'$ (...24a"^{2}32a'^{2}25a"^{2}33a'^{2}26a"^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1})	3.790	3.727
A	4.40(3)	$^2A'$ (...24a"^{2}32a'^{2}25a"^{2}33a'^{2}26a"^{2}34a'^{2}27a"^{2}35a'^{1}36a'^{2})	4.513	
		$^2A''$ (...24a"^{2}32a'^{2}25a"^{2}33a'^{2}26a"^{2}34a'^{2}27a"^{1}35a'^{2}36a'^{2})	4.872	
		$^2A'$ (...24a"^{2}32a'^{2}25a"^{2}33a'^{2}26a"^{2}34a'^{1}27a"^{2}35a'^{2}36a'^{2})	4.977	
B	~5.1	$^2A''$ (...24a"^{2}32a'^{2}25a"^{2}33a'^{2}26a"^{1}34a'^{2}27a"^{2}35a'^{2}36a'^{2})	5.176	
		$^2A'$ (...24a"^{2}32a'^{2}25a"^{2}33a'^{1}26a"^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{2})	5.289	
C	~5.4	$^2A''$ (...24a"^{2}32a'^{2}25a"^{1}33a'^{2}26a"^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{2})	5.415	
D	5.80	$^2A'$ (...24a"^{2}32a'^{1}25a"^{2}33a'^{2}26a"^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{2})	5.885	
E	~ 6.1	$^2A''$ (...24a"^{1}32a'^{2}25a"^{2}33a'^{2}26a"^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{2})	6.454	
I C_s B_{41}^- ($^3A''$)				
		$^2A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{0})	3.528	3.426
		$^2A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{0}28a"^{1})	3.553	
		$^4A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{1}36a'^{1}28a"^{1})	4.367	
		$^2A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{1}36a'^{1}28a"^{1})	4.658	
		$^4A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{1}35a'^{2}36a'^{1}28a"^{1})	4.800	
		$^2A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{1}35a'^{2}36a'^{1}28a"^{1})	4.814	
		$^2A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{1}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.041	
		$^4A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{1}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.081	
		$^4A''$(...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{1}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.138	
		$^4A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{1}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.413	
		$^2A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{1}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.504	
		$^4A''$ (...30a'^{2}24a"^{2}31a'^{1}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.689	
		$^2A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{1}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.814	
		$^4A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{1}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.947	
		$^2A'$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{2}25a"^{1}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	5.972	
		$^4A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{1}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	6.008	
		$^2A''$ (...30a'^{2}24a"^{2}31a'^{2}32a'^{1}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	6.047	
		$^2A''$ (...30a'^{2}24a"^{2}31a'^{1}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	6.187	
		$^4A'$ (...30a'^{1}24a"^{2}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	6.337	
		$^2A'$ (...30a'^{2}24a"^{1}31a'^{2}32a'^{2}25a"^{2}26a"^{2}33a'^{2}34a'^{2}27a"^{2}35a'^{2}36a'^{1}28a"^{1})	6.366	

III C_s B_{41}^- ($^1A'$)			
	$^2A''$ (...31a'^{2}25a''^{2}32a'^{2}26a''^{2}33a'^{2}34a'^{2}27a''^{2}35a'^{2}28a''^{1})	3.548	3.331
	$^2A'$ (...31a'^{2}25a''^{2}32a'^{2}26a''^{2}33a'^{2}34a'^{2}27a''^{2}35a'^{1}28a''^{2})	4.404	
	$^2A''$ (...31a'^{2}25a''^{2}32a'^{2}26a''^{2}33a'^{2}34a'^{2}27a''^{1}35a'^{2}28a''^{2})	4.957	
	$^2A'$ (...31a'^{2}25a''^{2}32a'^{2}26a''^{2}33a'^{2}34a'^{1}27a''^{2}35a'^{2}28a''^{2})	4.998	
	$^2A'$ (...31a'^{2}25a''^{2}32a'^{2}26a''^{2}33a'^{1}34a'^{2}27a''^{2}35a'^{2}28a''^{2})	5.233	
	$^2A''$ (...31a'^{2}25a''^{2}32a'^{2}26a''^{1}33a'^{2}34a'^{2}27a''^{2}35a'^{2}28a''^{2})	5.493	
	$^2A'$ (...31a'^{2}25a''^{2}32a'^{1}26a''^{2}33a'^{2}34a'^{2}27a''^{2}35a'^{2}28a''^{2})	5.804	
	$^2A''$ (...31a'^{2}25a''^{1}32a'^{2}26a''^{2}33a'^{2}34a'^{2}27a''^{2}35a'^{2}28a''^{2})	5.956	
	$^2A'$ (...31a'^{1}25a''^{2}32a'^{2}26a''^{2}33a'^{2}34a'^{2}27a''^{2}35a'^{2}28a''^{2})	5.990	

a The number in the parenthesis represents the uncertainty in the last digit.

b Ground-state VDEs were calculated at the PBE0/6-311+G* level and higher VDEs at the TDDFT-PBE0/6-311+G* level.

c The ADE for band X was measured to be 3.71 eV.

Table S2 Vertical detachment energies (VDE) measured from the photoelectron spectrum of B_{42}^- compared with the calculated VDEs at the TDDFT-PBE0/6-311+G* level. All energies are in eV.

Feature	VDE_{exptla}	Final states and their elecronic configurations	VDE_{theob}	ADE_{theoc}
VIII C_1 B_{42}^- (^{2}A)				
X	3.61(4)	^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_0$)	3.730	3.633
A	4.31(6)	^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_1$64a$_1$)	4.101	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_1$63a$_2$64a$_1$)	4.278	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_1$64a$_1$)	4.339	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_1$63a$_2$64a$_1$)	4.489	
B	4.66(4)	^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_1$62a$_2$63a$_2$64a$_1$)	4.740	
C	~5.2	^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_1$62a$_2$63a$_2$64a$_1$)	4.986	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_1$61a$_2$62a$_2$63a$_2$64a$_1$)	5.061	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_1$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.198	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_1$61a$_2$62a$_2$63a$_2$64a$_1$)	5.229	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_1$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.425	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_1$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.505	
D	5.84	^{1}A (...55a$_2$56a$_2$57a$_2$58a$_1$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.695	
		^{3}A (...55a$_2$56a$_2$57a$_1$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.884	
		^{1}A (...55a$_2$56a$_2$57a$_1$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.940	
		^{3}A (...55a$_2$56a$_1$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.985	
		^{3}A (...55a$_1$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.265	
		^{1}A (...55a$_2$56a$_1$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.266	
		^{1}A (...55a$_1$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.399	
IX C_1 B_{42}^- (^{2}A)				
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_0$)	3.762	3.639
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_1$64a$_1$)	4.172	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_1$63a$_2$64a$_1$)	4.358	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_1$64a$_1$)	4.384	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_1$62a$_2$63a$_2$64a$_1$)	4.563	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_1$63a$_2$64a$_1$)	4.770	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_1$61a$_2$62a$_2$63a$_2$64a$_1$)	4.778	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_1$62a$_2$63a$_2$64a$_1$)	4.828	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_2$60a$_1$61a$_2$62a$_2$63a$_2$64a$_1$)	5.047	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_1$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.083	
		^{3}A (...55a$_2$56a$_2$57a$_1$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.289	
		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_1$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.382	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_2$59a$_1$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.430	

		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{1}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.533	
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{1}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.549	
		^{3}A (...55a$_{2}$56a$_{1}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.741	
		^{1}A (...55a$_{2}$56a$_{1}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	6.134	
		^{3}A (...55a$_{1}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	6.251	
		^{1}A (...55a$_{1}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	6.346	
VII C_2 B$_{42}$- ($_{2}$A)				
		^{1}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{0}$)	3.366	3.287
		^{3}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{1}$33a$_{1}$)	4.148	
		^{3}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{1}$31b$_{2}$33a$_{1}$)	4.200	
		^{1}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{1}$33a$_{1}$)	4.383	
		^{1}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{1}$31b$_{2}$33a$_{1}$)	4.408	
		^{3}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{1}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	4.958	
		^{3}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{1}$32a$_{2}$31b$_{2}$33a$_{1}$)	4.986	
		^{1}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{1}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.381	
		^{1}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{1}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.402	
		^{3}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{1}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.663	
		^{3}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{1}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.820	
		^{1}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{1}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.844	
		^{3}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{1}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.911	
		^{1}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{1}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.979	
		^{1}A (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{1}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	5.999	
		^{1}B (...26b$_{2}$27b$_{2}$28a$_{2}$28b$_{1}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	6.012	
		^{3}B (...26b$_{1}$27b$_{2}$28a$_{2}$28b$_{2}$29a$_{2}$29b$_{2}$30a$_{2}$30b$_{2}$31a$_{2}$32a$_{2}$31b$_{2}$33a$_{1}$)	6.333	
X C_1 B$_{42}$- ($_{2}$A)				
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{0}$)	3.715	3.665
		^{3}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{1}$64a$_{1}$)	4.052	
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{1}$64a$_{1}$)	4.259	
		^{3}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{1}$63a$_{2}$64a$_{1}$)	4.934	
		^{3}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{1}$62a$_{2}$63a$_{2}$64a$_{1}$)	4.995	
		^{3}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{1}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.037	
		^{3}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{1}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.067	
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{1}$63a$_{2}$64a$_{1}$)	5.075	
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{1}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.149	
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{2}$60a$_{1}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.218	
		^{1}A (...55a$_{2}$56a$_{2}$57a$_{2}$58a$_{2}$59a$_{1}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.333	
		^{3}A (...55a$_{2}$56a$_{2}$57a$_{1}$58a$_{2}$59a$_{2}$60a$_{2}$61a$_{2}$62a$_{2}$63a$_{2}$64a$_{1}$)	5.603	

		^{3}A (...55a$_2$56a$_2$57a$_2$58a$_1$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.677	
		^{1}A (...55a$_2$56a$_2$57a$_2$58a$_1$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	5.999	
		^{3}A (...55a$_2$56a$_1$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.002	
		^{1}A (...55a$_2$56a$_1$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.091	
		^{3}A (...55a$_1$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.181	
		^{1}A (...55a$_1$56a$_2$57a$_2$58a$_2$59a$_2$60a$_2$61a$_2$62a$_2$63a$_2$64a$_1$)	6.182	

a The number in the parenthesis represents the uncertainty in the last digit.

b Ground-state VDEs were calculated at the PBE0/6-311+G* level and higher VDEs at the TDDFT-PBE0/6-311+G* level.

c The ADE for band X was estimated to be 3.4 eV.

Table S3 The coordinates of the top low-lying isomers of B_{41}^- (**I**–**III**) and B_{42}^- (**VII**–**XII**) at the PBE0/6-311+G* level.

I C_s B_{41}^- ($^3A''$)

B	-0.44975600	2.10339000	1.72114700
B	-0.02215300	2.09383600	3.34567900
B	0.19646500	0.68144300	4.18507400
B	-0.25280700	-0.76874000	3.33652500
B	-0.71900900	-0.78398500	1.69638700
B	-0.71281000	0.65639400	0.81839500
B	-0.63674400	-2.21235700	0.82878300
B	0.41840400	-2.16111400	4.12165700
B	-0.31950800	3.53329700	0.84889200
B	-0.10758900	-2.15586700	2.44753000
B	0.08384300	3.51355300	2.54030900
B	0.51736700	-0.72952000	4.79498300
B	0.47430900	-3.58046100	3.27758400
B	-0.08861500	-3.61335600	1.64268300
B	0.44060600	-5.02366300	0.82299400
B	-0.71900900	-0.78398500	-1.69638700
B	-0.10758900	-2.15586700	-2.44753000
B	-0.08861500	-3.61335600	-1.64268300
B	0.44060600	-5.02366300	-0.82299400
B	0.69067000	-4.86403500	-2.37415700
B	0.47430900	-3.58046100	-3.27758400
B	0.41840400	-2.16111400	-4.12165700
B	-0.25280700	-0.76874000	-3.33652500
B	0.51736700	-0.72952000	-4.79498300
B	-0.02215300	2.09383600	-3.34567900
B	0.19646500	0.68144300	-4.18507400
B	-0.44975600	2.10339000	-1.72114700
B	0.08384300	3.51355300	-2.54030900
B	-0.31950800	3.53329700	-0.84889200
B	-0.46810600	0.67909900	-2.51998800
B	-0.46810600	0.67909900	2.51998800
B	-0.37225500	-3.65983200	0.00000000
B	-0.71281000	0.65639400	-0.81839500
B	0.69067000	-4.86403500	2.37415700
B	0.43931800	4.88327500	1.73423700
B	0.21207900	4.86684700	0.00000000
B	0.43931800	4.88327500	-1.73423700
B	0.93092500	6.09442200	-0.77877700
B	0.93092500	6.09442200	0.77877700
B	-0.63674400	-2.21235700	-0.82878300
B	-0.66944200	2.10176100	0.00000000

II C_s B_{41}^- ($^1A'$)

B	-0.34697400	1.95938300	1.65987000
B	0.02498000	1.92654300	3.31082700
B	0.18773900	0.55492900	4.18429300
B	-0.24379700	-0.92146300	3.30975400
B	-0.68923800	-0.91253600	1.63723600
B	-0.72618400	0.52189400	0.80710600
B	-0.66348400	-2.38890900	0.82182100
B	0.32879100	-2.29858700	4.11317900
B	-0.06138900	3.44986400	0.80826000
B	-0.30339700	-2.32941600	2.45358800
B	0.12507600	3.33623200	2.49816500
B	0.44195300	-0.87634200	4.80160500
B	0.40228900	-3.75019900	3.28205500
B	-0.12922500	-3.78054100	1.66576700
B	0.48946700	-5.17548600	0.81624200
B	-0.68923800	-0.91253600	-1.63723600
B	-0.30339700	-2.32941600	-2.45358800
B	-0.12922500	-3.78054100	-1.66576700
B	0.48946700	-5.17548600	-0.81624200
B	0.69686200	-5.00771700	-2.38754400
B	0.40228900	-3.75019900	-3.28205500
B	0.32879100	-2.29858700	-4.11317900
B	-0.24379700	-0.92146300	-3.30975400
B	0.44195300	-0.87634200	-4.80160500
B	0.02498000	1.92654300	-3.31082700
B	0.18773900	0.55492900	-4.18429300
B	-0.34697400	1.95938300	-1.65987000
B	0.12507600	3.33623200	-2.49816500
B	-0.06138900	3.44986400	-0.80826000
B	-0.39947400	0.56265700	-2.44987500
B	-0.39947400	0.56265700	2.44987500
B	-0.18250700	-3.79348600	0.00000000
B	-0.72618400	0.52189400	-0.80710600
B	0.69686200	-5.00771700	2.38754400
B	0.26269900	4.76899100	1.84440600
B	0.18165700	5.09377500	0.00000000
B	0.26269900	4.76899100	-1.84440600
B	0.40755900	6.24650800	-1.34957800
B	0.40755900	6.24650800	1.34957800
B	-0.66348400	-2.38890900	-0.82182100
B	0.39234400	6.92809800	0.00000000

III C_s B_{41}^- ($^1A'$)

B	-0.40837900	2.08506500	1.71774500
B	0.01078700	2.09462400	3.39381700
B	0.21845700	0.68366400	4.20103600
B	-0.22691500	-0.77380600	3.35004100
B	-0.66972000	-0.77521100	1.67376100
B	-0.64076200	0.65598600	0.83450100
B	-0.63408300	-2.20033300	0.85118700
B	0.33187400	-2.18162900	4.15306300
B	-0.25726700	3.47542700	0.85292000
B	-0.42805900	-2.21272600	2.53269400
B	0.13013400	3.49657200	2.55505900
B	0.49254800	-0.74879700	4.82534900
B	0.39107000	-3.59661200	3.33658000
B	-0.10341900	-3.59037700	1.66073700
B	0.49698200	-4.95919300	0.83449200
B	-0.66972000	-0.77521100	-1.67376100
B	-0.42805900	-2.21272600	-2.53269400
B	-0.10341900	-3.59037700	-1.66073700
B	0.49698200	-4.95919300	-0.83449200
B	0.64904500	-4.84788600	-2.41423000
B	0.39107000	-3.59661200	-3.33658000
B	0.33187400	-2.18162900	-4.15306300
B	-0.22691500	-0.77380600	-3.35004100
B	0.49254800	-0.74879700	-4.82534900
B	0.01078700	2.09462400	-3.39381700
B	0.21845700	0.68366400	-4.20103600
B	-0.40837900	2.08506500	-1.71774500
B	0.13013400	3.49657200	-2.55505900
B	-0.25726700	3.47542700	-0.85292000
B	-0.15358700	0.67353800	-2.46137900
B	-0.15358700	0.67353800	2.46137900
B	-0.08039400	-3.54737600	0.00000000
B	-0.64076200	0.65598600	-0.83450100
B	0.64904500	-4.84788600	2.41423000
B	0.37527400	4.89168100	1.74851100
B	0.25400100	4.81297100	0.00000000
B	0.37527400	4.89168100	-1.74851100
B	0.75601300	6.13639400	-0.78419500
B	0.75601300	6.13639400	0.78419500
B	-0.63408300	-2.20033300	-0.85118700
B	-0.83359300	2.12164000	0.00000000

VII C_2 B_{42}^- (^{2}A)

B	0.46562000	1.32134600	4.70474000
B	0.82846200	2.73239800	3.99001900
B	0.55906700	2.86119400	2.29462100
B	0.15355200	1.54394300	1.24014100
B	0.00000000	0.00000000	1.96655300
B	0.00000000	0.00000000	3.72009900
B	-0.00363400	0.87293200	-1.78168700
B	0.00000000	3.62897800	-0.82538100
B	0.07601200	1.91961800	-0.45377000
B	0.39185900	3.12333000	0.68397200
B	-0.47309300	2.52882500	-1.97309200
B	-0.24345100	1.61492700	-3.33976100
B	-0.07601200	-1.91961800	-0.45377000
B	0.47309300	-2.52882500	-1.97309200
B	0.24345100	-1.61492700	-3.33976100
B	0.60025600	-3.28225500	-3.60083100
B	0.45717200	-4.28729500	-2.34816500
B	0.00000000	-3.62897800	-0.82538100
B	0.14644900	-5.25518600	-1.15816200
B	-0.28801900	-4.89017800	0.28608300
B	-0.39185900	-3.12333000	0.68397200
B	0.53438500	1.32408800	2.89739600
B	0.00000000	0.00000000	-3.22036900
B	0.00363400	-0.87293200	-1.78168700
B	-0.53438500	-1.32408800	2.89739600
B	0.98077800	4.12291400	3.30095300
B	0.72461400	4.49782600	1.81498700
B	0.28801900	4.89017800	0.28608300
B	-0.21599500	0.79331900	-4.83417100
B	0.21599500	-0.79331900	-4.83417100
B	0.54619300	-2.30857200	-4.82452000
B	-0.55906700	-2.86119400	2.29462100
B	-0.72461400	-4.49782600	1.81498700
B	-0.98077800	-4.12291400	3.30095300
B	-0.14644900	5.25518600	-1.15816200
B	-0.45717200	4.28729500	-2.34816500
B	-0.60025600	3.28225500	-3.60083100
B	-0.54619300	2.30857200	-4.82452000
B	0.00000000	0.00000000	5.38697500
B	-0.46562000	-1.32134600	4.70474000
B	-0.82846200	-2.73239800	3.99001900
B	-0.15355200	-1.54394300	1.24014100

VIII C_1 B_{42}^- ($_2$A)

B	-0.93827600	2.86018000	0.37455200
B	-0.16483300	4.28288400	-0.18602100
B	1.46409400	4.36341300	-0.42343000
B	2.34949800	2.93069700	0.06979600
B	1.58948600	1.49064500	0.66659400
B	-0.05361700	1.44374600	0.77202600
B	2.48266700	0.07686300	0.64115100
B	3.94821700	2.95022400	-0.53770200
B	-2.58106500	2.82721800	0.20215800
B	3.19416300	1.52556600	0.22071400
B	-1.80204100	4.31455400	-0.23297600
B	2.99857500	4.21910900	-0.73018900
B	4.84980800	1.56492200	-0.51946600
B	4.08035600	0.12477400	0.08211400
B	4.93987700	-1.28053400	-0.42423600
B	0.02800500	-1.42055200	0.92794000
B	0.87501900	-2.79236600	0.31062500
B	2.53894300	-2.77429900	0.22060200
B	4.15773100	-2.72565100	-0.38074200
B	3.28718400	-4.02134200	-0.57849000
B	1.73691800	-4.21625900	-0.33195400
B	0.10034400	-4.21133300	-0.20708100
B	-0.75647300	-2.90039800	0.43444300
B	-1.51491300	-4.28763200	-0.37474300
B	-3.31729600	-1.47457800	0.30518600
B	-2.35503000	-2.79420700	-0.11784600
B	-2.60809200	-0.05046800	0.85567100
B	-3.95731700	-0.03054200	-0.16478900
B	-3.37126700	1.39493300	0.48561300
B	-1.62140200	-1.42579800	0.67915000
B	0.64910700	2.87603800	0.30548500
B	3.33954000	-1.32719800	0.38063900
B	-0.83972700	0.02350600	0.87348000
B	5.53230500	0.16547400	-0.71108600
B	-3.37428800	4.16020000	-0.40235300
B	-4.19589900	2.80801700	-0.25457700
B	-4.92136600	1.34809500	-0.44387800
B	1.69423500	-1.39644500	0.80076400
B	-3.08748200	-4.17696600	-0.65772600
B	-4.00875600	-2.89153900	-0.55251500
B	-4.83736000	-1.47976500	-0.62754100
B	-5.52957400	-0.07318500	-0.74936400

IX $C_1B_{42}^-$ (2A)

B	-2.488530	0.321521	1.352198
B	-3.120802	1.597290	0.343915
B	-2.070587	2.818426	-0.149069
B	-0.489643	2.946116	0.468492
B	0.217849	1.467034	1.144406
B	-0.768981	0.131746	1.342756
B	1.848167	1.255701	0.894038
B	0.453020	4.058048	-0.365323
B	-3.453716	-0.992020	1.434090
B	1.123064	2.689421	0.373456
B	-4.016091	0.219190	0.495347
B	-1.140176	4.171836	-0.679270
B	2.092842	3.972659	-0.455517
B	2.789387	2.517680	0.205064
B	4.360514	2.283169	-0.436000
B	1.405521	-1.619437	0.805398
B	2.982335	-1.825598	0.242841
B	4.000200	-0.523639	0.057330
B	5.003453	0.764674	-0.441035
B	5.413245	-0.721610	-0.777863
B	4.558769	-2.029692	-0.591679
B	3.476174	-3.264312	-0.666991
B	1.919304	-3.082703	0.024401
B	2.340910	-4.340637	-0.955846
B	-0.790055	-3.941255	-0.349420
B	0.810087	-4.252698	-0.629203
B	-1.305309	-2.628928	0.594629
B	-2.354372	-3.544268	-0.367308
B	-2.958773	-2.339169	0.693470
B	0.282007	-2.824106	0.413149
B	-1.480671	1.587445	0.932840
B	3.464963	1.005888	0.433489
B	-0.209154	-1.390003	1.102182
B	3.610808	3.647257	-0.677702
B	-4.754508	-0.180409	-1.206445
B	-4.192332	-1.366144	-0.039717
B	-3.676080	-2.754875	-0.908554
B	2.444158	-0.307309	0.706707
B	-2.650372	4.010442	-1.139849
B	-3.637532	2.782968	-0.900821
B	-4.408076	1.359331	-0.724418
B	-4.631015	-1.679027	-1.598163

X C_1 B_{42}- ($_2$A)

B	-0.77582500	3.57538400	-0.09335300
B	0.32582300	4.88675600	-0.08144400
B	1.92932800	4.57429800	-0.03810400
B	2.45664200	2.93049900	-0.02244100
B	1.39474000	1.54869500	0.02916100
B	-0.28899000	1.91710000	0.03679100
B	2.10233000	-0.01602900	0.00807900
B	4.16595500	2.85566300	0.01727100
B	-1.49563400	0.82042100	0.13246000
B	3.05278200	1.40920600	0.07198800
B	-1.24005800	5.16662100	-0.10992700
B	3.46880100	4.24844500	-0.01269900
B	4.85033900	1.37247100	0.04904200
B	3.85514600	-0.03129400	0.01310100
B	4.82559500	-1.45160400	0.03237000
B	-0.32575600	-1.91430200	0.14075100
B	0.76442100	-3.18842300	-0.02903300
B	2.40367700	-2.96595900	-0.04559000
B	4.11441600	-2.92118000	-0.02460500
B	3.39395800	-4.30003000	-0.09385500
B	1.84962900	-4.59944800	-0.11389900
B	0.24154900	-4.88302300	-0.16219000
B	-0.83928500	-3.56535100	0.00929600
B	-1.32759800	-5.13744900	-0.18696900
B	-3.61603200	-2.89624700	0.00718300
B	-2.49472200	-4.10431300	-0.08904400
B	-3.18392200	-1.28328300	0.23284600
B	-4.80904200	-1.83361200	0.01958800
B	-3.14990500	1.31803900	-0.03228900
B	-1.98682400	-2.34492900	0.09883700
B	0.82104900	3.18163100	0.01488500
B	3.02693900	-1.45740200	0.06970600
B	-1.51680400	-0.80151200	0.27630400
B	5.51406000	-0.04562900	0.05150100
B	-2.42279200	4.14746900	-0.10457100
B	-1.94314800	2.37156900	-0.02362900
B	-5.91389200	-0.71116600	0.01443700
B	-4.77633300	1.90973200	-0.04115400
B	-3.56230500	2.94954600	-0.09811900
B	1.36434100	-1.56809400	0.03748100
B	-4.35454000	0.03104700	0.05307900
B	-5.89811300	0.80568500	-0.01324100

XI C_s B_{42-} ($^2A'$)

B	-0.00487200	-0.92946300	3.49629000
B	-0.40307600	0.13448700	4.77299500
B	-0.17037600	1.74269800	4.53042800
B	-0.06614500	2.28762800	2.91325800
B	0.15806200	1.26902900	1.54396200
B	0.48468000	-0.41702300	1.90868500
B	0.11906200	1.99714500	0.00000000
B	-0.09892500	4.02504200	2.87494000
B	0.96736900	-1.57150500	0.87263800
B	0.13268000	2.93869500	1.42784800
B	-0.65887200	-1.40206500	4.94055900
B	-0.18762200	3.29138200	4.24613400
B	-0.07336100	4.73340900	1.41297900
B	-0.03824900	3.75149400	0.00000000
B	-0.07336100	4.73340900	-1.41297900
B	0.48468000	-0.41702300	-1.90868500
B	0.18445400	0.68723700	-3.15877300
B	-0.06614500	2.28762800	-2.91325800
B	-0.09892500	4.02504200	-2.87494000
B	-0.18762200	3.29138200	-4.24613400
B	-0.17037600	1.74269800	-4.53042800
B	-0.40307600	0.13448700	-4.77299500
B	-0.00487200	-0.92946300	-3.49629000
B	-0.65887200	-1.40206500	-4.94055900
B	-0.31221700	-3.65954400	-2.69284800
B	-0.51523700	-2.56451700	-3.88937600
B	0.65065900	-3.25571000	-1.40254400
B	-0.54838900	-4.64820300	-1.41653200
B	0.65065900	-3.25571000	1.40254400
B	-0.06037500	-2.02192900	-2.23926000
B	0.18445400	0.68723700	3.15877300
B	0.13268000	2.93869500	-1.42784800
B	0.96736900	-1.57150500	-0.87263800
B	-0.09926800	5.40926300	0.00000000
B	-0.51523700	-2.56451700	3.88937600
B	-0.06037500	-2.02192900	2.23926000
B	-0.80457800	-5.30245600	0.00000000
B	-0.54838900	-4.64820300	1.41653200
B	-0.31221700	-3.65954400	2.69284800
B	0.15806200	1.26902900	-1.54396200
B	1.44052500	-2.89263200	0.00000000
B	0.42563500	-4.24211000	0.00000000

XII C_{2h} B_{42}^{-} ($_2$Au)

B	-3.73333500	-0.10822000	0.00000000
B	2.25212900	2.99008100	0.00000000
B	3.34321600	1.73728300	0.00000000
B	2.42064500	-2.85275400	0.00000000
B	-0.72062600	-3.68544900	0.00000000
B	-3.34321600	-1.73728300	0.00000000
B	-3.44012500	1.53919100	0.00000000
B	3.73333500	0.10822000	0.00000000
B	-2.25212900	-2.99008100	0.00000000
B	3.44012500	-1.53919100	0.00000000
B	-2.42064500	2.85275400	0.00000000
B	0.72062600	3.68544900	0.00000000
B	-0.93465200	3.63948500	0.00000000
B	0.93465200	-3.63948500	0.00000000
B	1.64762600	-3.17502800	1.52913200
B	1.45920900	3.26570200	1.53005800
B	-0.10403000	3.59002000	1.50281600
B	-3.51375600	0.68823900	1.51739100
B	-2.73452000	-2.32209300	1.50619300
B	0.10403000	-3.59002000	1.50281600
B	2.86406200	-2.15886400	1.50769700
B	-1.64762600	3.17502800	1.52913200
B	-1.45920900	-3.26570200	1.53005800
B	-2.86406200	2.15886400	1.50769700
B	3.51375600	-0.68823900	1.51739100
B	2.73452000	2.32209300	1.50619300
B	3.46646800	0.89171000	1.51930700
B	-3.46646800	-0.89171000	1.51930700
B	-0.10403000	3.59002000	-1.50281600
B	2.86406200	-2.15886400	-1.50769700
B	1.64762600	-3.17502800	-1.52913200
B	-2.73452000	-2.32209300	-1.50619300
B	-3.51375600	0.68823900	-1.51739100
B	-1.64762600	3.17502800	-1.52913200
B	1.45920900	3.26570200	-1.53005800
B	0.10403000	-3.59002000	-1.50281600
B	-2.86406200	2.15886400	-1.50769700
B	-1.45920900	-3.26570200	-1.53005800
B	2.73452000	2.32209300	-1.50619300
B	3.51375600	-0.68823900	-1.51739100
B	3.46646800	0.89171000	-1.51930700
B	-3.46646800	-0.89171000	-1.51930700