

Supplementary Information

B_{31}^- and B_{32}^- : Chiral Quasi-Planar Boron Clusters†

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Table S1. Comparison of the experimental VDEs of B_{31}^- and the calculated VDEs for the low-lying isomers of B_{31}^- .

Table S2. Comparison of the experimental VDEs of B_{32}^- and the calculated VDEs for the low-lying isomers of B_{32}^- .

Figure S1. Low-lying isomers of B_{31}^- at CCSD(T)/6-311G(d)//PBE0/6-311+G(d) and PBE0/6-311+G(d) levels of theory.

Figure S2. Low-lying isomers of B_{32}^- at UCCSD(T)/6-31G(d)//PBE0/6-311+G(d) and PBE0/6-311+G(d) levels of theory.

Figure S3. Comparison of the experimental PES spectrum of B_{31}^- and the simulated spectra for some low-lying isomers of B_{31}^- .

Figure S4. The AdNDP bonding patterns for the closed-shell $C_2 B_{32}^{2-}$.

Figure S5 Calculated IRC reaction path of B_{31}^- at PBE0/6-311+G(d) level.

Figure S6 Calculated IRC reaction path of B_{32}^- at PBE0/6-311+G(d) level.

Table S3. Optimized cartesian coordinates of the key structures of B_{31}^- and B_{32}^- .

Table S1. Experimental vertical detachment energies (VDEs) of B_{31}^- , compared to the calculated values of the low-lying isomers of B_{31}^- at the TD-PBE0/6-311+G(d) level. All energies are in eV.

Feature	VDE (expt.)	Final state and electronic configuration	VDE (theo.) TD-PBE0
B_{31}^- Isomer I/II (C_1 1A)			
X	4.07	2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a ² 45a ² 46a ² 47a¹ }	3.89
A	4.24	2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a ² 45a ² 46a¹ 47a ² }	4.07
B	4.60	2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a ² 45a¹ 46a ² 47a ² }	4.49
C	5.11	2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a¹ 45a ² 46a ² 47a ² }	5.09
D	5.30	2A {... 39a ² 40a ² 41a ² 42a ² 43a¹ 44a ² 45a ² 46a ² 47a ² }	5.22
E	~5.7	2A {... 39a ² 40a ² 41a ² 42a¹ 43a ² 44a ² 45a ² 46a ² 47a ² }	5.54
F	6.00	2A {... 39a ² 40a ² 41a¹ 42a ² 43a ² 44a ² 45a ² 46a ² 47a ² }	5.92
G	~6.2	2A {... 39a ² 40a¹ 41a ² 42a ² 43a ² 44a ² 45a ² 46a ² 47a ² }	6.19
		2A {... 39a¹ 40a ² 41a ² 42a ² 43a ² 44a ² 45a ² 46a ² 47a ² }	6.40
B_{31}^- Isomer III (C_2 1A)			
		2B {... 19b ² 20a ² 21a ² 20b ² 22a ² 23a ² 21b ² 22b ² 24a ² 23b¹ }	4.07
		2B {... 19b ² 20a ² 21a ² 20b ² 22a ² 23a ² 21b ² 22b ² 24a¹ 23b ² }	4.37
		2A {... 19b ² 20a ² 21a ² 20b ² 22a ² 23a ² 21b ² 22b¹ 24a ² 23b ² }	4.53
		2A {... 19b ² 20a ² 21a ² 20b ² 22a ² 23a ² 21b¹ 22b ² 24a ² 23b ² }	4.93
		2B {... 19b ² 20a ² 21a ² 20b ² 22a ² 23a¹ 21b ² 22b ² 24a ² 23b ² }	4.94
		2B {... 19b ² 20a ² 21a ² 20b ² 22a¹ 23a ² 21b ² 22b ² 24a ² 23b ² }	5.06
		2A {... 19b ² 20a ² 21a ² 20b¹ 22a ² 23a ² 21b ² 22b ² 24a ² 23b ² }	5.18
		2B {... 19b ² 20a ² 21a¹ 20b ² 22a ² 23a ² 21b ² 22b ² 24a ² 23b ² }	5.49
		2B {... 19b ² 20a¹ 21a ² 20b ² 22a ² 23a ² 21b ² 22b ² 24a ² 23b ² }	5.96
		2A {... 19b¹ 20a ² 21a ² 20b ² 22a ² 23a ² 21b ² 22b ² 24a ² 23b ² }	6.37
B_{31}^- Isomer IV (C_s 1A)			
		$^2A'$ {... 17a ² 22a ² 23a ² 18a ² 19a ² 24a ² 20a ² 21a ² 25a ² 26a¹ }	3.88
		$^2A'$ {... 17a ² 22a ² 23a ² 18a ² 19a ² 24a ² 20a ² 21a ² 25a¹ 26a ² }	4.62
		$^2A''$ {... 17a ² 22a ² 23a ² 18a ² 19a ² 24a ² 20a ² 21a¹ 25a ² 26a ² }	4.88
		$^2A''$ {... 17a ² 22a ² 23a ² 18a ² 19a ² 24a ² 20a¹ 21a ² 25a ² 26a ² }	5.16
		$^2A'$ {... 17a ² 22a ² 23a ² 18a ² 19a ² 24a¹ 20a ² 21a ² 25a ² 26a ² }	5.32
		$^2A''$ {... 17a ² 22a ² 23a ² 18a ² 19a¹ 24a ² 20a ² 21a ² 25a ² 26a ² }	5.50
		$^2A''$ {... 17a ² 22a ² 23a ² 18a¹ 19a ² 24a ² 20a ² 21a ² 25a ² 26a ² }	5.56
		$^2A'$ {... 17a ² 22a ² 23a¹ 18a ² 19a ² 24a ² 20a ² 21a ² 25a ² 26a ² }	5.60
		$^2A''$ {... 17a¹ 22a ² 23a ² 18a ² 19a ² 24a ² 20a ² 21a ² 25a ² 26a ² }	6.37
B_{31}^- Isomer V (C_1 1A)			
		2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a ² 45a ² 46a ² 47a¹ }	3.88
		2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a ² 45a ² 46a¹ 47a ² }	4.47
		2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a ² 45a¹ 46a ² 47a ² }	4.65
		2A {... 39a ² 40a ² 41a ² 42a ² 43a ² 44a¹ 45a ² 46a ² 47a ² }	4.92
		2A {... 39a ² 40a ² 41a ² 42a ² 43a¹ 44a ² 45a ² 46a ² 47a ² }	5.04
		2A {... 39a ² 40a ² 41a ² 42a¹ 43a ² 44a ² 45a ² 46a ² 47a ² }	5.30
		2A {... 39a ² 40a ² 41a¹ 42a ² 43a ² 44a ² 45a ² 46a ² 47a ² }	5.70
		2A {... 39a ² 40a¹ 41a ² 42a ² 43a ² 44a ² 45a ² 46a ² 47a ² }	5.98
		2A {... 39a¹ 40a ² 41a ² 42a ² 43a ² 44a ² 45a ² 46a ² 47a ² }	6.29

Table S2. Experimental vertical detachment energies (VDEs) of B_{32}^- , compared to the calculated values of the low-lying isomers of B_{32}^- at the TD-PBE0/6-311+G(d) level. All energies are in eV.

Feature	VDE (expt.)	Final state and electronic configuration	VDE (theo.) TD-PBE0
B_{32}^- Isomer VI/VII (C_2^2A)			
X'	3.57		
X	3.82	$^1A \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 23b^2 24b^2 24a^2 \mathbf{25a}^0 \}$	3.78
A	4.30	$^3A \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 23b^2 24b^2 \mathbf{24a}^1 25a^1 \}$	4.12
		$^1A \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 23b^2 24b^2 \mathbf{24a}^1 25a^1 \}$	4.38
B	5.04	$^3B \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 23b^2 \mathbf{24b}^1 24a^2 25a^1 \}$	4.71
		$^3B \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 \mathbf{23b}^1 24b^2 24a^2 25a^1 \}$	4.87
C	5.17	$^3A \{ \dots 21b^2 21a^2 22b^2 22a^2 \mathbf{23a}^1 23b^2 24b^2 24a^2 25a^1 \}$	5.00
		$^1B \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 23b^2 \mathbf{24b}^1 24a^2 25a^1 \}$	5.06
		$^1B \{ \dots 21b^2 21a^2 22b^2 22a^2 23a^2 \mathbf{23b}^1 24b^2 24a^2 25a^1 \}$	5.20
		$^1A \{ \dots 21b^2 21a^2 22b^2 22a^2 \mathbf{23a}^1 23b^2 24b^2 24a^2 25a^1 \}$	5.22
D	5.80	$^3A \{ \dots 21b^2 21a^2 22b^2 \mathbf{22a}^1 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	5.48
		$^3B \{ \dots 21b^2 21a^2 \mathbf{22b}^1 22a^2 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	5.58
		$^1A \{ \dots 21b^2 21a^2 22b^2 \mathbf{22a}^1 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	5.80
E	~6.10	$^3B \{ \dots \mathbf{21b}^1 21a^2 22b^2 22a^2 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	5.87
		$^3A \{ \dots 21b^2 \mathbf{21a}^1 22b^2 22a^2 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	5.89
		$^1B \{ \dots \mathbf{21b}^1 21a^2 22b^2 22a^2 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	6.02
		$^1A \{ \dots 21b^2 \mathbf{21a}^1 22b^2 22a^2 23a^2 23b^2 24b^2 24a^2 25a^1 \}$	6.05
B_{32}^- Isomer VIII ($C_i^2A_u$)			
X'	3.57		
X	3.82	$^1A_g \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_u^2 24a_g^2 \mathbf{25a_u}^0 \}$	3.77
A	4.30	$^3A_g \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_u^2 24a_g^2 \mathbf{24a_u}^1 25a_u^1 \}$	4.10
		$^1A_g \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_u^2 \mathbf{24a_g}^1 25a_u^1 \}$	4.32
B	5.04	$^3A_u \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 \mathbf{24a_g}^1 24a_u^2 25a_u^1 \}$	4.49
		$^1A_u \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 \mathbf{24a_g}^1 24a_u^2 25a_u^1 \}$	4.84
C	5.17	$^3A_g \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 \mathbf{23a_g}^1 24a_g^2 24a_u^2 25a_u^1 \}$	5.17
		$^3A_u \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 \mathbf{23a_g}^1 23a_u^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.32
		$^1A_g \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 23a_u^2 \mathbf{23a_g}^1 24a_g^2 24a_u^2 25a_u^1 \}$	5.35
		$^3A_u \{ \dots 21a_u^2 21a_g^2 22a_u^2 \mathbf{22a_g}^1 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.36
		$^3A_g \{ \dots 21a_u^2 21a_g^2 \mathbf{22a_u}^1 22a_g^2 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.42
		$^1A_u \{ \dots 21a_u^2 21a_g^2 22a_u^2 22a_g^2 \mathbf{23a_g}^1 23a_u^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.48
D	5.80	$^1A_g \{ \dots 21a_u^2 21a_g^2 \mathbf{22a_u}^1 22a_g^2 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.79
		$^3A_g \{ \dots \mathbf{21a_u}^1 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.84
		$^3A_u \{ \dots 21a_u^2 \mathbf{21a_g}^1 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	5.88
		$^1A_g \{ \dots \mathbf{21a_u}^1 21a_g^2 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	6.05
E	~6.10	$^1A_u \{ \dots 21a_u^2 \mathbf{21a_g}^1 22a_u^2 22a_g^2 23a_u^2 23a_g^2 24a_g^2 24a_u^2 25a_u^1 \}$	6.14

Figure S1. Low-lying isomers of B_{31}^- . The relative energies are given in eV at CCSD(T)/6-311G(d)//PBE0/6-311+G(d) and PBE0/6-311+G(d) (in square brackets) levels of theory.

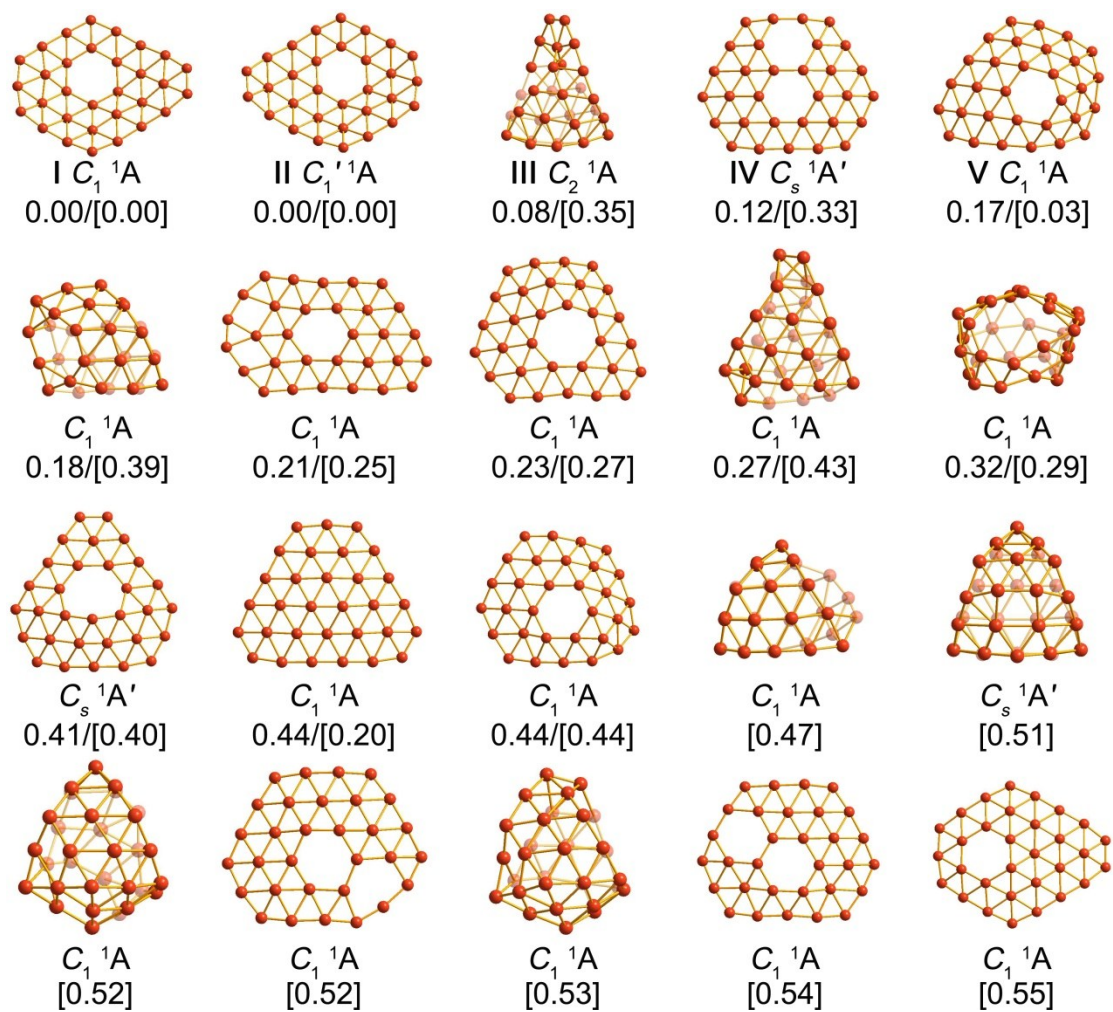


Figure S2. Low-lying isomers of B_{32}^- . The relative energies are given in eV at UCCSD(T)/6-31G(d)/PBE0/6-311+G(d) and PBE0/6-311+G(d) (in square brackets) levels of theory.

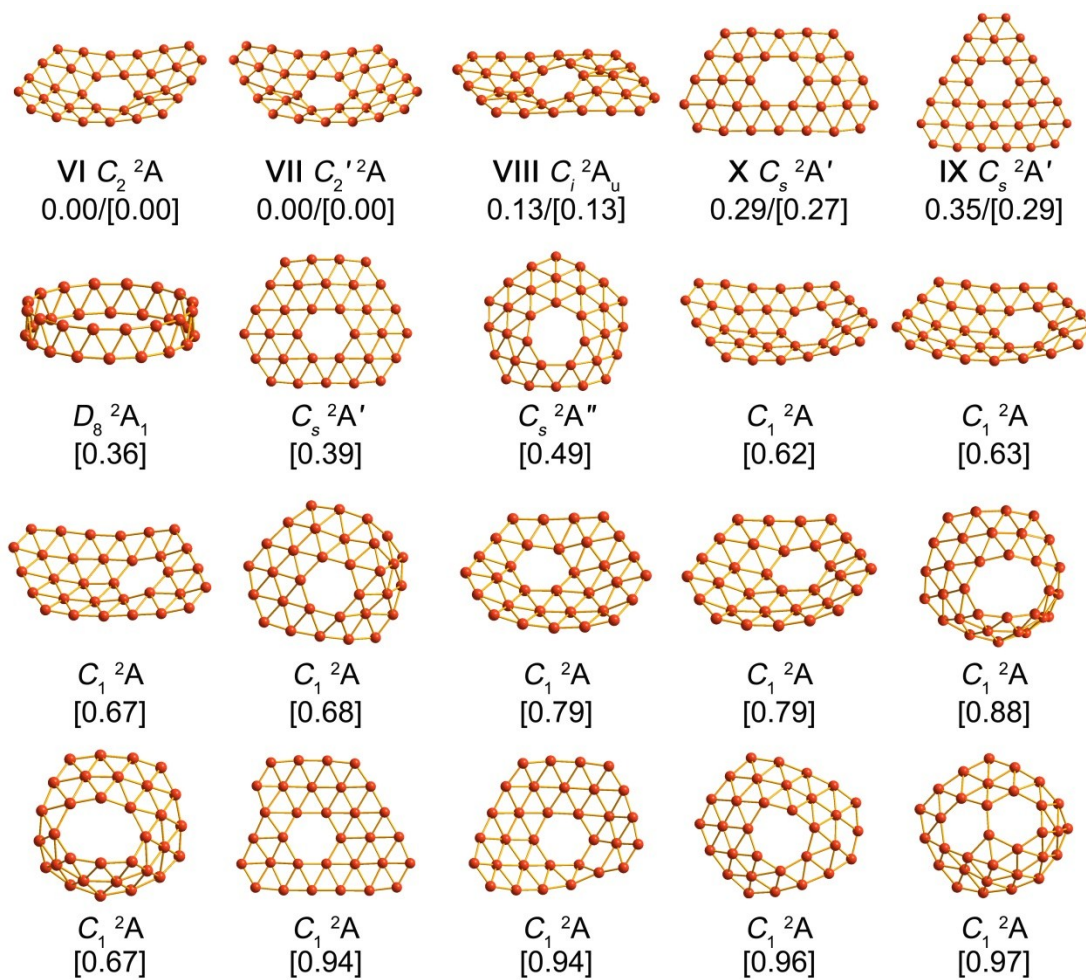


Figure S3. The experimental PES spectrum of (a) B_{31}^- at 193 nm (6.424 eV), compared to (b-d) the simulated spectra of some low-lying isomers of B_{31}^- .

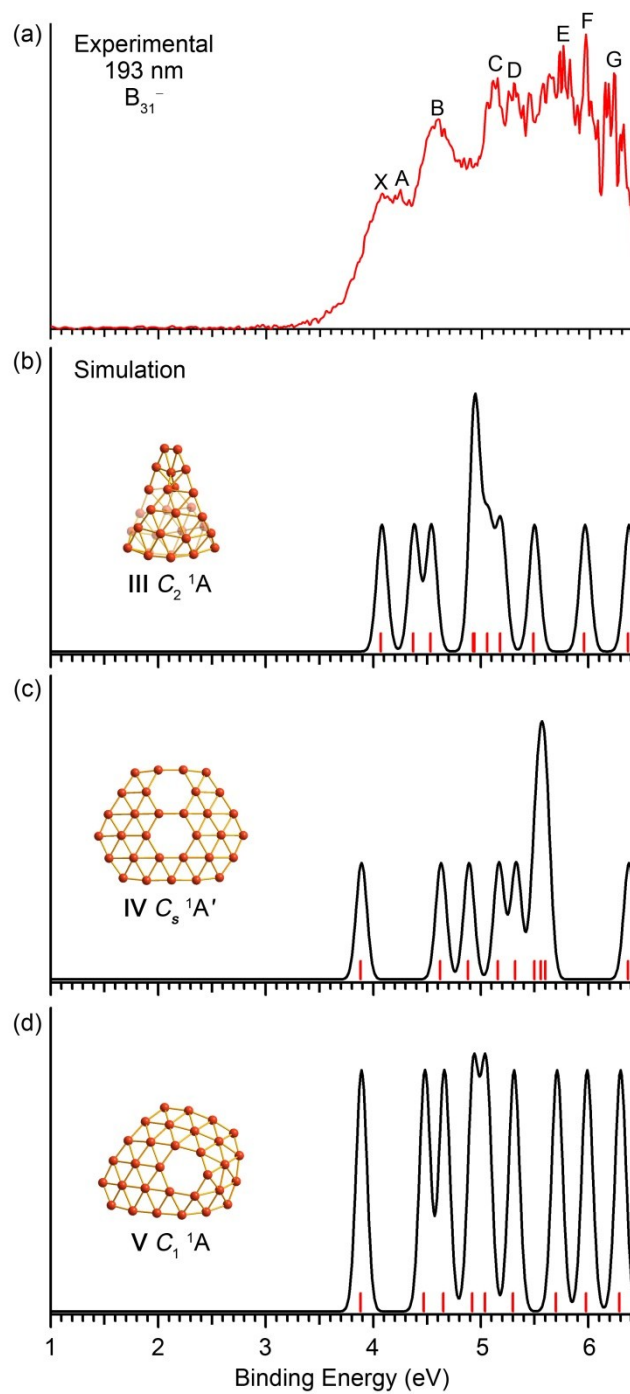


Figure S4. The AdNDP bonding patterns for the closed-shell $C_2 B_{32}^{2-}$.

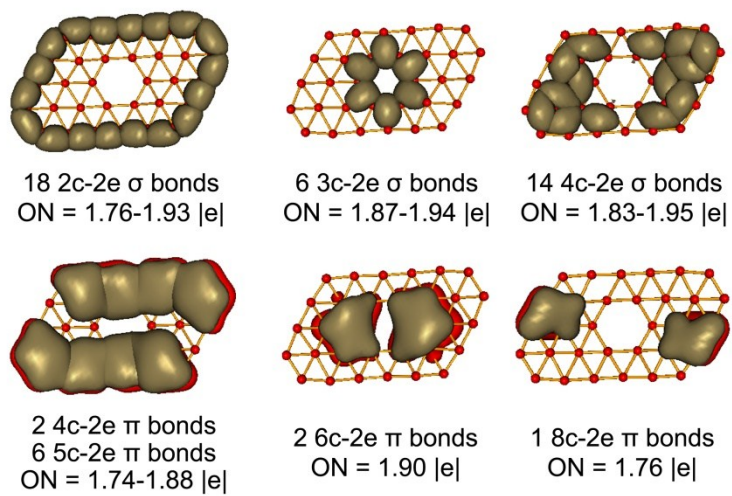


Figure S5. Calculated IRC reaction path of B_{31}^- from the global minimum $C_1 B_{31}^-$ (I) to its enantiomer $C_1' B_{31}^-$ (II) via the transition state $C_1 B_{31}^-$ (TS1) at PBE0/6-311+G(d) level.

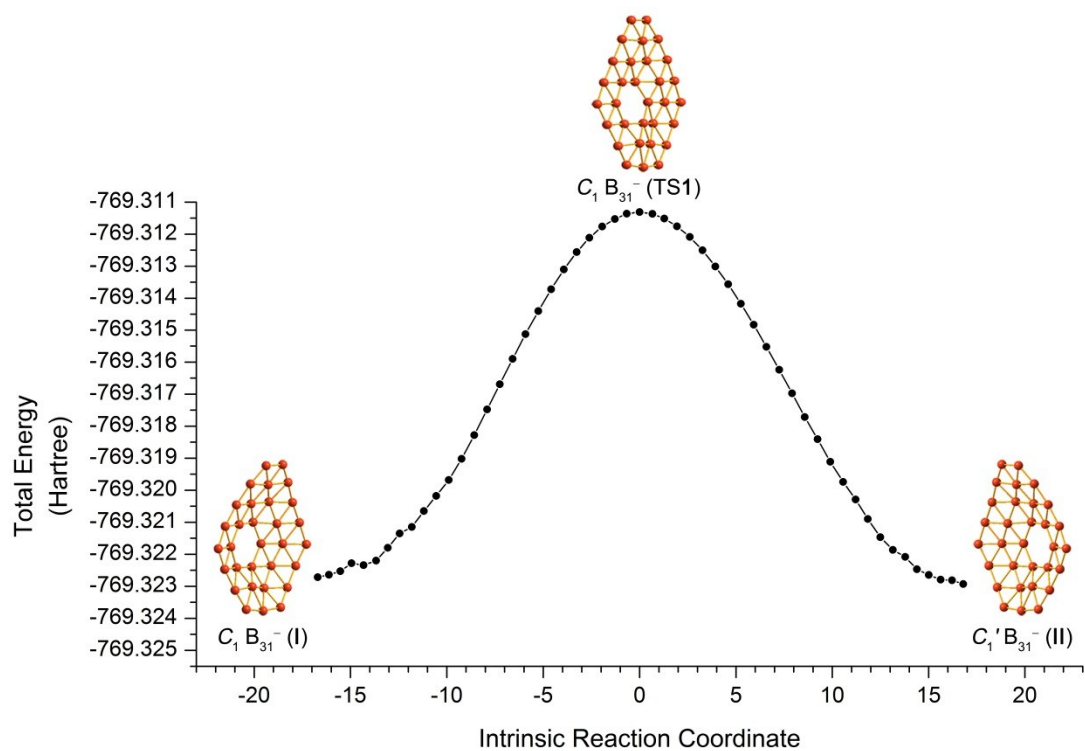


Figure S6. Calculated IRC reaction path of B_{32}^- from global minimum $C_2 B_{32}^-$ (VI) to intermediate $C_i B_{32}^-$ (VIII) via the transition state $C_1 B_{32}^-$ (TS2) at PBE0/6-311+G(d) level.

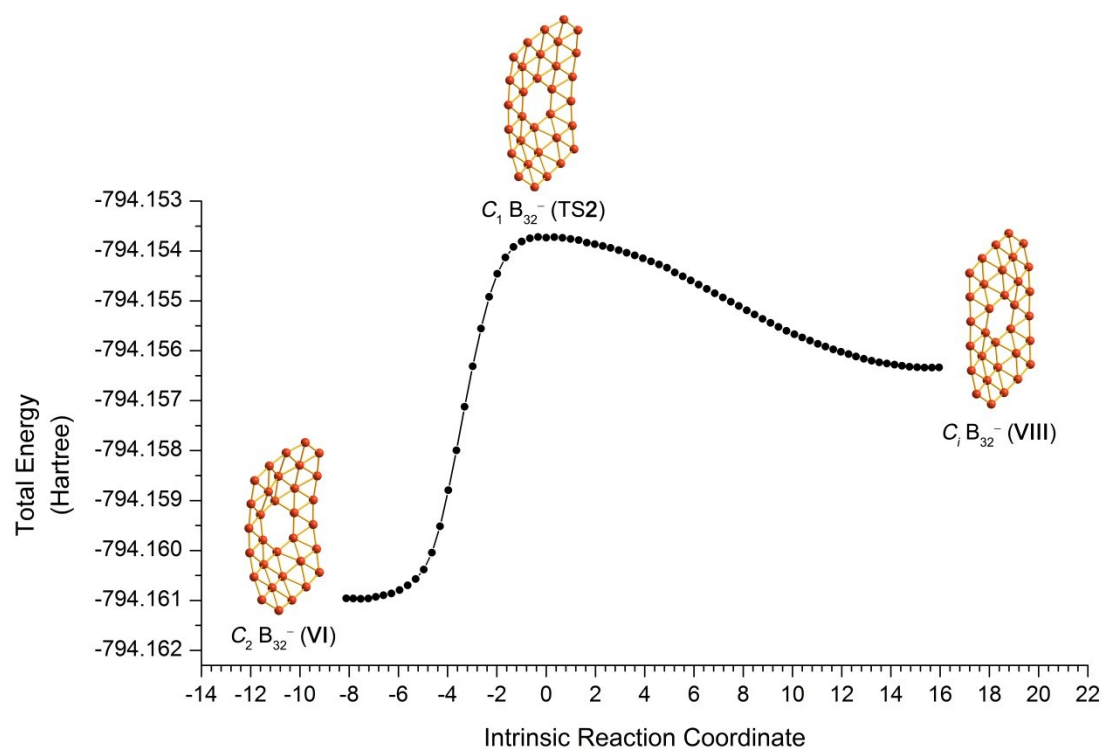


Table S3. Optimized coordinates of the key structures of B_{31}^- and B_{32}^- at the PBE0/6-311+G(d) level of theory.

$C_1 B_{31}^- (\mathbf{I})$				$C_1 B_{31}^- (\mathbf{TS1})$			
B	-1.79900600	1.66898700	0.36543300	B	1.04538800	-1.61434800	0.22262800
B	-0.43947200	4.01059600	-0.43895000	B	2.46561200	-0.86212400	-0.11899200
B	-0.40998700	2.54933000	0.33201800	B	2.43671600	0.87935500	-0.01812500
B	1.04433700	0.02998900	0.55457200	B	1.06957200	1.70204600	-0.09439500
B	2.44635900	0.92366300	0.38196500	B	-0.33670700	-0.75470600	-0.03885300
B	-0.35527600	-0.81701100	0.81877700	B	-1.76717000	1.70024600	-0.00070900
B	5.09880900	0.84671000	-0.70047000	B	1.07988400	3.45564300	-0.14147900
B	-4.46330100	1.52245500	-0.48306300	B	1.06710600	-3.41830300	-0.00794100
B	3.88501300	0.08662200	0.10216400	B	-0.35522700	2.53684600	0.03764500
B	-3.25403900	2.45674100	-0.11672400	B	2.50355600	-2.58155900	0.12415000
B	-1.84014700	-0.01180500	0.72080500	B	2.50581500	2.57023400	-0.07200800
B	1.04822500	1.72779500	0.40943200	B	-0.37368000	4.15888400	-0.16528700
B	2.41416500	2.55682600	-0.11511700	B	-1.78774500	3.41685200	-0.02319800
B	3.87673600	1.79592300	-0.32440800	B	-3.10977900	0.86220200	0.45642300
B	5.08328100	-0.70856000	-0.70077700	B	-3.18127400	-0.76683500	0.03925500
B	1.08791200	-1.65128400	0.67006000	B	-4.74334100	0.01670400	0.04985700
B	2.48059800	-0.81172000	0.38607600	B	-4.54292200	1.61807500	-0.00045200
B	2.53612700	-2.50905900	0.11419000	B	-4.60702900	-1.58028000	-0.00454500
B	1.15032400	-3.33220100	-0.10563200	B	-1.84607200	-3.33990000	-0.09549200
B	-0.32569600	-2.45417300	0.33824000	B	-0.40336200	-4.06822200	-0.07751900
B	-0.27196500	-3.92887100	-0.43743200	B	-3.28415000	-2.50579100	-0.06365200
B	-4.66323800	-0.04943800	-0.47779800	B	1.06391700	0.00443900	-0.37457700
B	-4.44062700	-1.60167000	-0.62479900	B	-3.25041500	2.55332100	0.11051200
B	-3.18211400	-0.81603900	0.13473800	B	-1.78605600	-1.58874900	-0.32472600
B	-1.70983200	-3.26874200	-0.33194500	B	3.92973100	-1.77686100	0.09390500
B	-3.21884500	0.82819500	0.46431400	B	3.84281900	0.02045500	0.27243800
B	-3.14988900	-2.48699700	-0.39524800	B	3.98447000	1.76272800	0.04873400
B	-1.82788500	3.30947500	-0.16130400	B	-0.37219800	-2.43101400	-0.05062300
B	3.89019400	-1.69250600	-0.19401400	B	5.26306800	0.78153800	0.04528600
B	-1.70027600	-1.56107600	0.03575700	B	5.23963900	-0.79210100	0.01220100
B	1.00951500	3.38784600	-0.22086000	B	-1.75016700	0.04122400	0.15953900

Table S3. Continued.

$C_2 B_{32}^-$ (VI)				$C_i B_{32}^-$ (VIII)			
B	-1.43409000	0.84049000	-0.50880100	B	1.45172400	-0.83019300	0.03414900
B	-1.41110900	2.50846000	-0.26531400	B	2.91321100	0.01866900	0.00527700
B	-0.00183300	3.30204600	0.00455300	B	2.90673400	1.67091300	0.00703500
B	1.39041400	2.34138100	0.08283900	B	1.38117400	2.41368800	0.09883800
B	1.45662700	0.85522000	-0.77022900	B	0.00343000	1.59038800	-0.48456400
B	2.81516400	3.30046500	0.39453400	B	1.49482400	4.15583900	0.07033300
B	-0.02295900	-1.67072400	-0.67198900	B	-1.44355800	-0.78855300	0.37332600
B	2.86702700	-0.08329500	-0.44903200	B	-1.49612000	2.40400400	-0.39086200
B	-2.86702700	0.08329500	-0.44903200	B	1.49612000	-2.40400400	0.39086200
B	1.39041400	3.97693000	0.32274500	B	2.79729000	3.25354700	0.06762400
B	2.86397800	1.67848200	-0.31625900	B	0.03884700	3.27329200	-0.38613900
B	-1.45662700	-0.85522000	-0.77022900	B	-0.00343000	-1.59038800	0.48456400
B	-2.84406200	1.74334500	-0.21615600	B	2.95354900	-1.61793700	0.08571700
B	1.43409000	-0.84049000	-0.50880100	B	-1.45172400	0.83019300	-0.03414900
B	-4.25155100	0.99920100	0.18421700	B	2.99583400	-3.26656400	0.01621800
B	4.21891500	2.45577500	0.52180000	B	0.05107600	4.95851800	0.10809200
B	4.16006100	0.75255500	0.20814100	B	-1.41107300	4.03859700	-0.05905800
B	5.47559400	1.48408100	0.81486000	B	-1.42350400	5.62466500	0.25730000
B	5.48017800	-0.07860700	0.66409000	B	-2.79121100	4.85249400	0.19745900
B	2.84406200	-1.74334500	-0.21615600	B	-2.95354900	1.61793700	-0.08571700
B	1.41110900	-2.50846000	-0.26531400	B	-2.91321100	-0.01866900	-0.00527700
B	-1.39041400	-2.34138100	0.08283900	B	-1.38117400	-2.41368800	-0.09883800
B	-1.39041400	-3.97693000	0.32274500	B	-2.79729000	-3.25354700	-0.06762400
B	-2.86397800	-1.67848200	-0.31625900	B	-0.03884700	-3.27329200	0.38613900
B	-2.81516400	-3.30046500	0.39453400	B	-1.49482400	-4.15583900	-0.07033300
B	-4.21891500	-2.45577500	0.52180000	B	-0.05107600	-4.95851800	-0.10809200
B	-5.48017800	0.07860700	0.66409000	B	2.79121100	-4.85249400	-0.19745900
B	-5.47559400	-1.48408100	0.81486000	B	1.42350400	-5.62466500	-0.25730000
B	4.25155100	-0.99920100	0.18421700	B	-2.99583400	3.26656400	-0.01621800
B	0.00183300	-3.30204600	0.00455300	B	-2.90673400	-1.67091300	-0.00703500
B	-4.16006100	-0.75255500	0.20814100	B	1.41107300	-4.03859700	0.05905800
B	0.02295900	1.67072400	-0.67198900	B	1.44355800	0.78855300	-0.37332600

Table S3. Continued.

$C_1 B_{32}^-$ (TS2)			
B	-1.10775400	1.24871600	-0.39121800
B	-0.55433200	2.83442400	-0.19290300
B	1.06782200	3.17856500	-0.03936000
B	2.15470300	1.91417500	-0.35991400
B	1.60058400	0.31837000	-0.42975600
B	3.76877100	2.29260800	0.22890500
B	-0.54641700	-1.59843800	-0.68569300
B	2.63705400	-0.96846400	-0.12535000
B	-2.71208200	0.99002900	-0.45133800
B	2.61718000	3.38032600	0.21919200
B	3.19733300	0.66278200	-0.09570700
B	-1.64080100	-0.33940100	-0.72933900
B	-2.16408100	2.55117200	-0.12624300
B	1.10688600	-1.28964500	-0.56434000
B	-3.74628900	2.27774100	0.20286400
B	4.83889500	1.02393700	0.35238100
B	4.24678400	-0.59603400	0.10404800
B	5.73296100	-0.29652700	0.66995100
B	5.22568500	-1.78835300	0.60869900
B	2.14756000	-2.56579900	-0.08866000
B	0.53927100	-2.83062000	-0.18079300
B	-2.08009700	-1.81280100	0.00953300
B	-2.60795100	-3.36375600	0.21057900
B	-3.25491800	-0.68611300	-0.35123700
B	-3.74318800	-2.26408100	0.28214900
B	-4.79724700	-1.01792000	0.45771100
B	-5.20720900	1.77810700	0.66105600
B	-5.68754700	0.29190300	0.77985600
B	3.74489900	-2.30109700	0.22793600
B	-1.06491900	-3.16148100	-0.06285800
B	-4.22199600	0.58899300	0.14928000
B	0.51043900	1.54868200	-0.28942900