SUPPORTING INFORMATION

Competition between Drum and Quasi-planar Structures in RhB_{18}^-: Motifs for Metallo-Boronanotubes and Metallo-Borophenes

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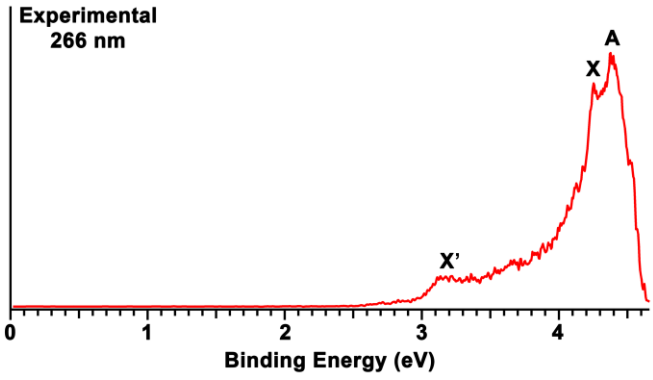

Figure S1. The photoelectron spectrum of RhB_{18}^- at 266 nm (4.661 eV).

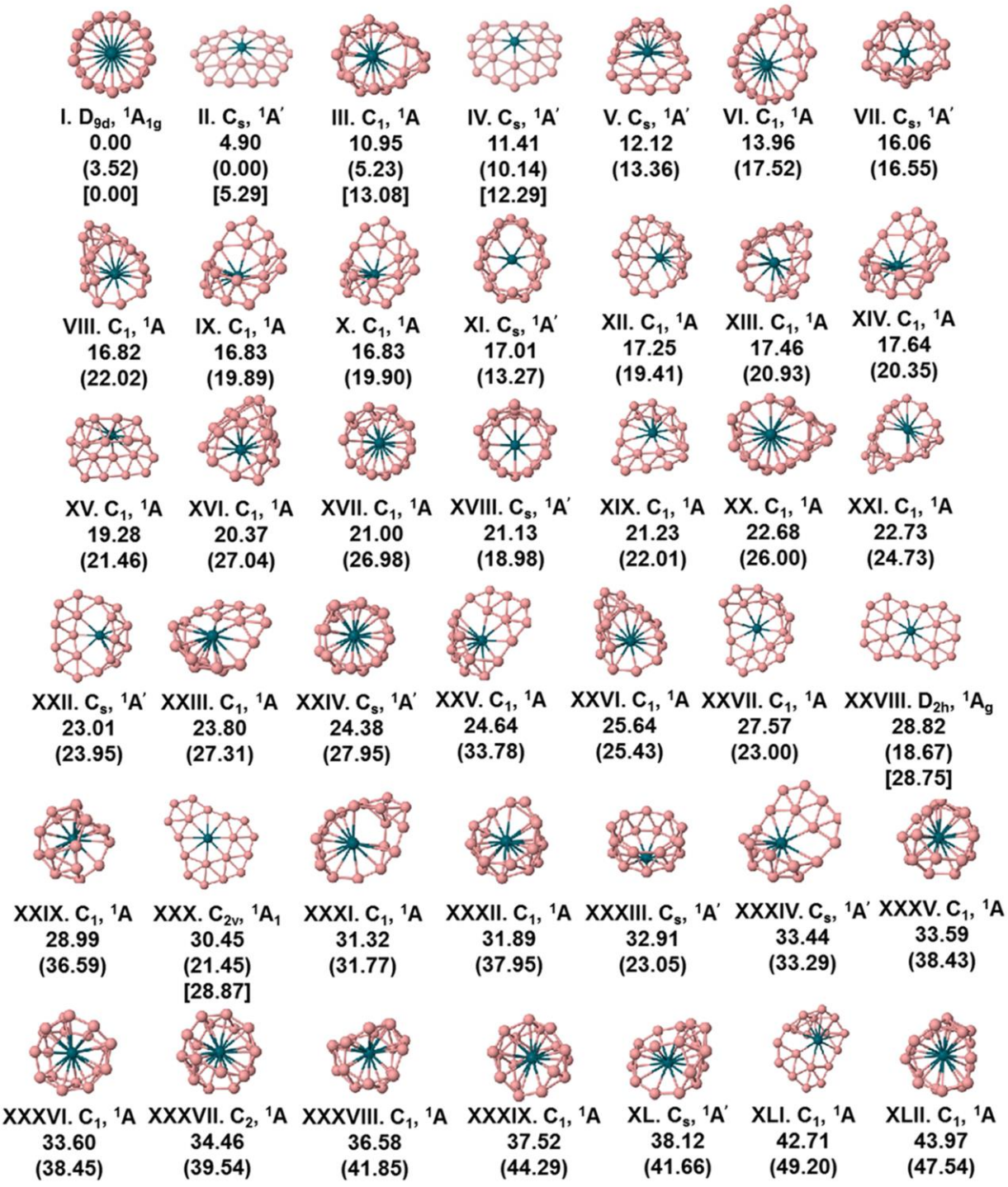

Figure S2. Relative energies in kcal/mol of the low-lying isomers of RhB_{18}^- within 45.0 kcal/mol at PBE0/TZP, PBE/TZP in brackets and CCSD(T) levels in square brackets.

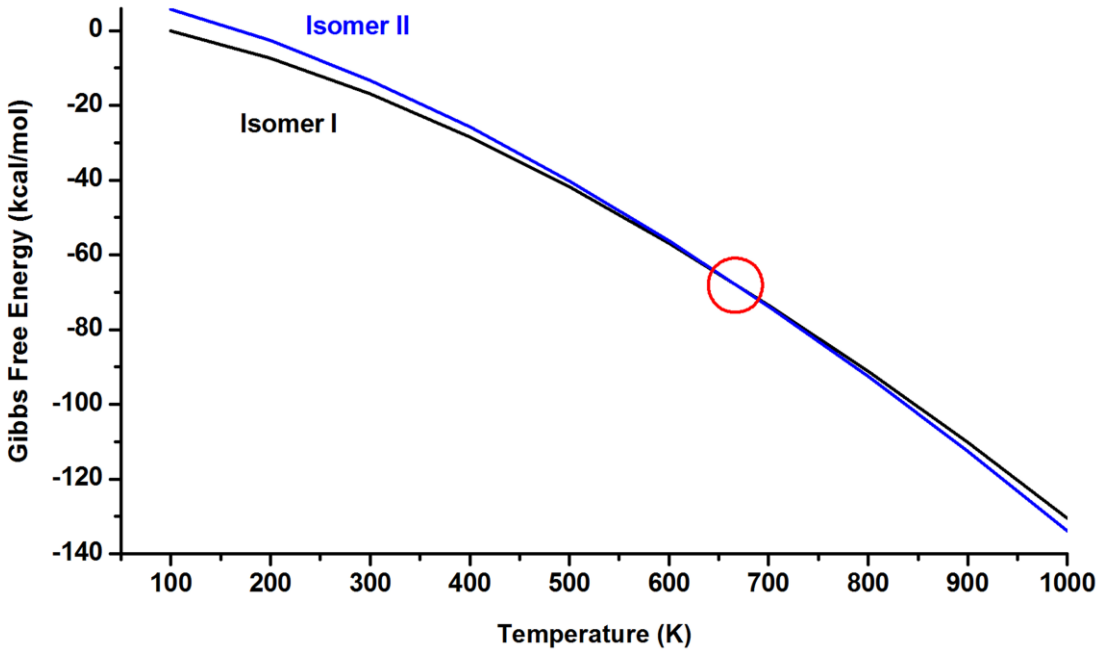

Figure S3. Relative Gibbs free energies (kcal/mol) of the *drum* isomer I and *quasi-planar* isomer II of RhB_{18}^- in the temperature range from 100 to 1000 K at the PBE0/B/cc-pVTZ/Rh/ECP10MDF_VTZ level of theory. Note that the two isomers are nearly degenerate within a wide range of temperature; while PBE0 and CCSD(T) calculations predict that the isomer I is slightly more stable than isomer I, PBE ones predict the opposite.

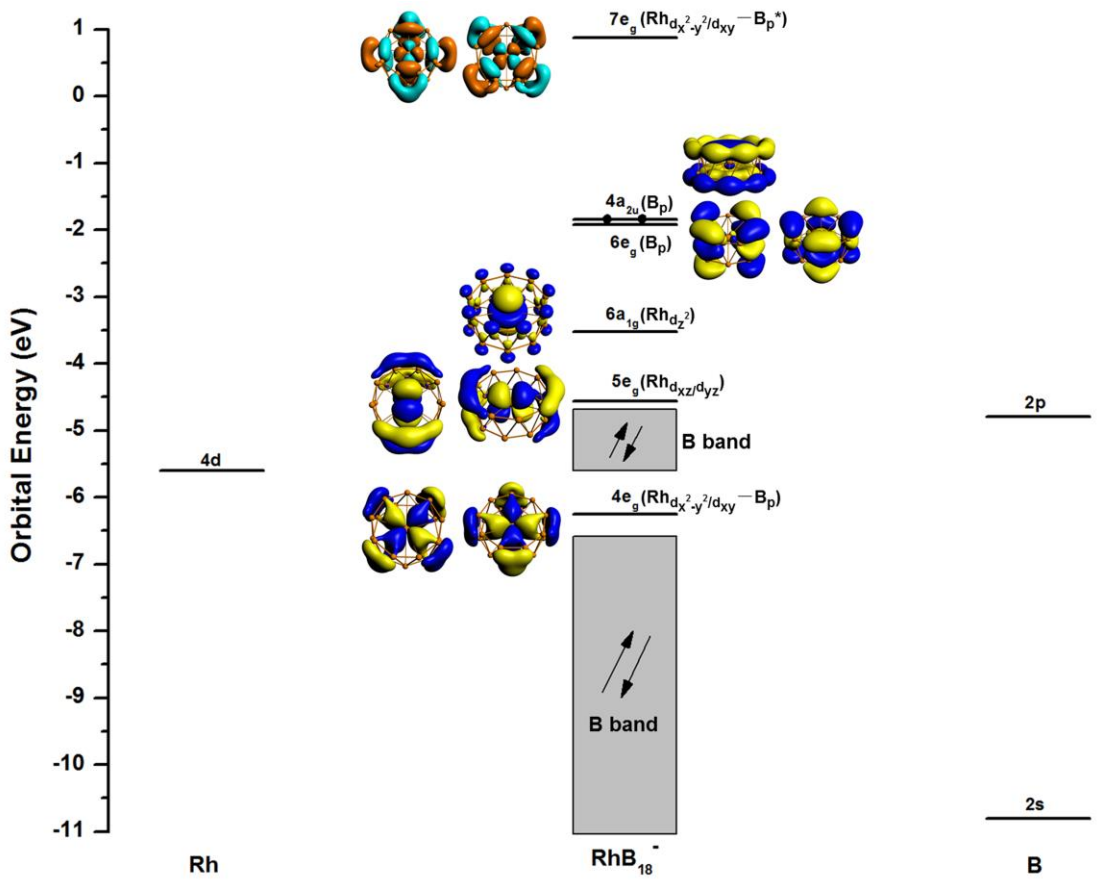

Figure S4. Kohn-Sham molecular orbital energy levels for the drum isomer of RhB_{18}^- with selected molecular orbital contours.

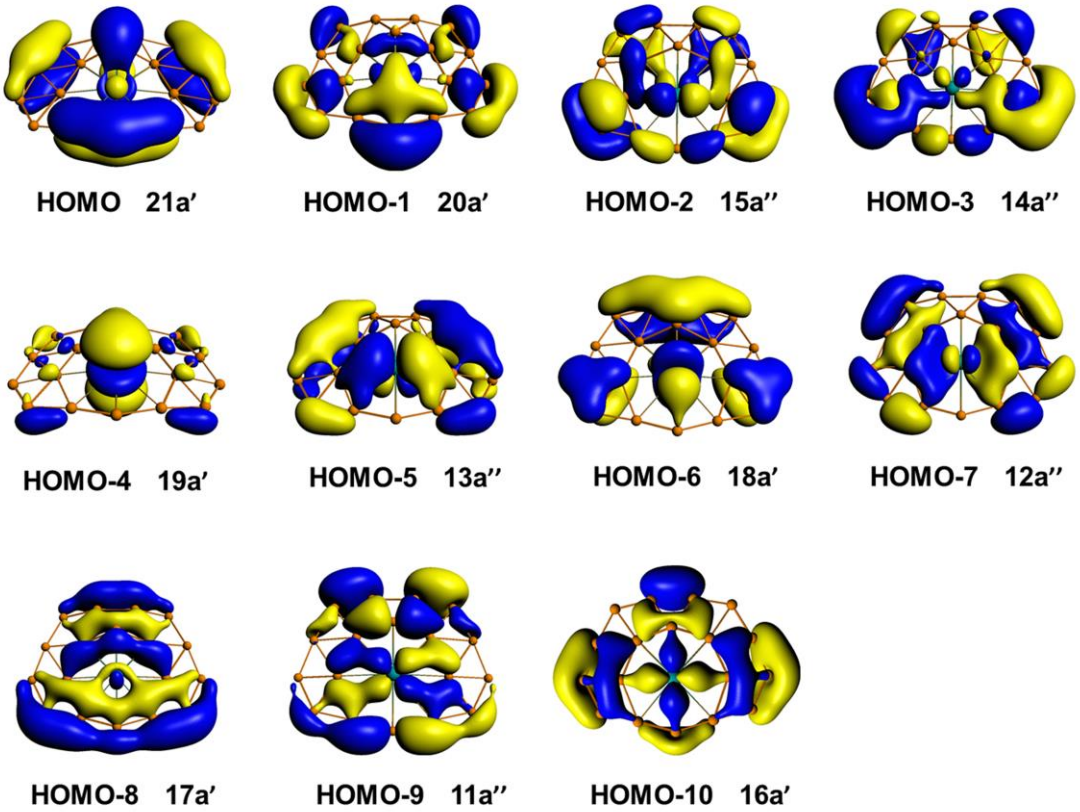

Figure S5. Valence Kohn-Sham molecular orbital contours for the quasi-planar isomer of RhB_{18}^-.

Table S1. Cartesian coordinates of the D_{9d} drum and C_s quasi-planar isomers of RhB_{18}^- at the PBE0/TZP level of theory.

D_{9d} drum isomer:

1.Rh	0.000000	0.000000	0.000000
2.B	0.000000	2.322405	0.827886
3.B	1.492892	1.779109	0.827806
4.B	-1.492892	-1.779109	-0.827806
5.B	0.000000	-2.322405	-0.827886
6.B	2.287200	0.403328	0.827806
7.B	1.492892	-1.779109	-0.827806
8.B	-2.287200	-0.403328	-0.827806
9.B	2.287200	-0.403328	-0.827806
10.B	-1.492892	1.779109	0.827806
11.B	2.011262	-1.161203	0.827886
12.B	-0.794308	-2.182437	0.827806
13.B	0.794308	-2.182437	0.827806
14.B	-2.011262	1.161203	-0.827886
15.B	0.794308	2.182437	-0.827806
16.B	-0.794308	2.182437	-0.827806
17.B	2.011262	1.161203	-0.827886
18.B	-2.287200	0.403328	0.827806
19.B	-2.011262	-1.161203	0.827886

C_s quasi-planar isomer:

1.Rh	-0.272015	0.450139	0.000000
2.B	0.012811	0.464003	-2.164864
3.B	0.117565	2.172161	-1.523826
4.B	0.054250	2.600605	0.000000
5.B	0.012811	0.464003	2.164864
6.B	-0.045689	-1.100916	1.461179
7.B	0.035083	-2.740446	0.861958
8.B	-0.726098	-1.508452	0.000000
9.B	-0.045689	-1.100916	-1.461179
10.B	0.480422	0.410499	-3.767007
11.B	0.382113	1.784396	3.076109
12.B	0.337400	-1.090381	3.189937
13.B	0.295152	-2.469353	-2.404338
14.B	0.337400	-1.090381	-3.189937
15.B	0.480422	0.410499	3.767007
16.B	0.382113	1.784396	-3.076109
17.B	0.117565	2.172161	1.523826
18.B	0.295152	-2.469353	2.404338
19.B	0.035083	-2.740446	-0.861958