Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Geometrical Requirements for Transition-Metal-Centered Aromatic Boron Wheels: The Case of VB_{10}^-

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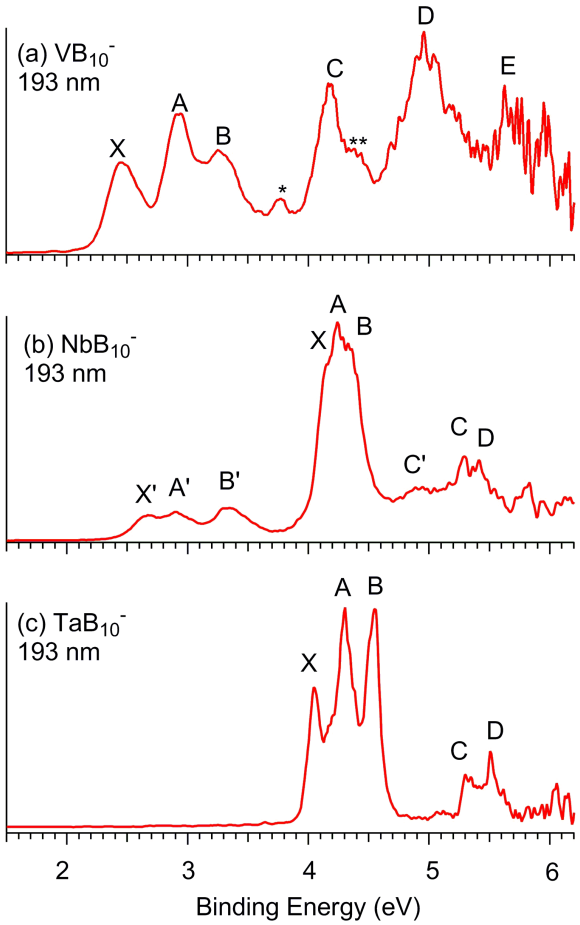

Fig. S1. Comparison of the photoelectron spectrum of VB_{10}^- with those of NbB_{10}^- and TaB_{10}^- at 193 nm.

Cartesian Coordinates of the VB_{10}^- Global Minimum and Low-Lying Isomers:
All coordinates reported at optimized BP86/6-311+G(d)/V/Stuttgart '97 geometries using the Gaussian 09 software package at the default geometric optimization settings

Isomer I:

V	0.00000000	0.00000000	0.92163800
B	-1.15462900	1.07520400	-0.60633200
B	1.15462900	-1.07520400	-0.60633200
B	1.92153400	0.20157400	0.01589800
B	1.44732300	1.69224500	-0.02600100
B	-0.62291400	-0.57423700	-1.10260100
B	0.62291400	0.57423700	-1.10260100
B	-1.92153400	-0.20157400	0.01589800
B	0.00000000	-2.12818800	-0.40073100
B	0.00000000	2.12818800	-0.40073100
B	-1.44732300	-1.69224500	-0.02600100

Isomer II:

V	0.00000000	0.00000000	0.92332400
B	-1.58642600	0.00000000	-0.62455700
B	1.58642600	0.00000000	-0.62455700
B	1.37902300	1.51685400	-0.18658400
B	0.00000000	2.22296300	-0.03622900
B	0.00000000	-0.85073400	-1.08969100
B	0.00000000	0.85073400	-1.08969100
B	-1.37902300	-1.51685400	-0.18658400
B	1.37902300	-1.51685400	-0.18658400
B	-1.37902300	1.51685400	-0.18658400
B	0.00000000	-2.22296300	-0.03622900

Isomer III:

B	-2.20433900	0.79728100	-0.51196000
B	-1.01433000	1.79207800	-0.43993600
B	0.57599500	1.73914700	-0.27900200
B	2.10389800	1.41709800	-0.09262800
B	2.81892200	0.00000000	-0.02953600
B	2.10389900	-1.41709800	-0.09262800
B	0.57599600	-1.73914600	-0.27900200
B	1.19352300	0.00000000	-0.35521700
B	-1.01432900	-1.79207900	-0.43993500
V	-0.63802100	0.00000000	0.65908800
B	-2.20433900	-0.79728200	-0.51195900

Isomer IV:

B	2.25437200	0.77263700	0.38696000

B	1.02244700	1.77831000	0.42913600
B	-0.54669300	1.78976400	0.37096000
B	-2.05462200	1.41868800	0.08282300
B	-2.75809900	-0.00047100	-0.06306000
B	-2.05345800	-1.41927800	0.08237000
B	-0.54589000	-1.78971800	0.37134700
B	-1.16995900	-0.00015600	0.38453700
B	1.02334700	-1.77786600	0.42958700
V	0.55958900	0.00000200	-0.62196400
B	2.25444500	-0.77192100	0.38637500

Isomer V:

B	0.29486800	1.62588600	0.87861300
B	1.38593900	0.71996500	0.00000000
B	0.29486800	1.62588600	-0.87861300
B	0.70573000	0.06773600	-1.48961200
B	0.29486800	-1.47449800	-1.39456800
B	0.07716500	-2.20405800	0.00000000
B	1.17508700	-0.89884600	0.00000000
B	0.29486800	-1.47449800	1.39456800
B	0.70573000	0.06773600	1.48961200
V	-0.90413700	-0.01474000	0.00000000
B	-1.07009200	2.01249700	0.00000000

Isomer VI:

V	0.00000000	0.00000000	1.02335900
B	-1.23439400	1.08935900	-0.55145300
B	1.23439400	-1.08935900	-0.55145300
B	2.02096700	0.21214500	-0.09760000
B	1.48392900	1.70879700	-0.16850000
B	-0.60451600	-0.59562600	-1.08195700
B	0.60451600	0.59562600	-1.08195700
B	-2.02096700	-0.21214500	-0.09760000
B	0.00000000	-2.10793300	-0.45421600
B	0.00000000	2.10793300	-0.45421600
B	-1.48392900	-1.70879700	-0.16850000

Isomer VII:

B	-2.33896000	0.75995800	-0.00038700
B	2.33896000	0.75995900	0.00032200
B	0.00000000	2.45941900	0.00003900
B	0.00000000	-2.45941900	0.00003900
B	1.44549600	-1.98955500	-0.00056200
B	-1.44549600	1.98955500	-0.00056200
B	1.44549600	1.98955500	0.00058700
B	-1.44549600	-1.98955500	0.00058700

B	2.33896000	-0.75995800	-0.00038700
V	0.00000000	0.00000000	0.00000000
B	-2.33896000	-0.75995900	0.00032200

Isomer VIII:

B	0.05070200	1.89137300	0.79307900
B	1.10851600	0.82766900	0.00000000
B	1.23488900	-0.66026400	0.82195000
B	0.18389800	-1.80958800	0.00000000
B	-0.19134300	-1.18164100	-1.55682900
B	0.31875900	0.49113900	-1.63629500
V	-0.89531000	-0.02158600	0.00000000
B	1.23488900	-0.66026400	-0.82195000
B	0.05070200	1.89137300	-0.79307900
B	0.31875900	0.49113900	1.63629500
B	-0.19134300	-1.18164100	1.55682900