

Electronic Supplementary Information (ESI)

Hyperhalogen Properties of Early-Transition-Metal Borates

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Table S1. The VDE values (in eV) of $\text{Al}(\text{BO}_2)_n^-$ ^[a], $\text{Sc}(\text{BO}_2)_n^-$ ^[b], $\text{Sc}(\text{BH}_4)_n^-$ ^[c], ScF_n^- ^[d], $\text{Ti}(\text{BO}_2)_n^-$ ^[b], TiF_n^- ^[d], $\text{V}(\text{BO}_2)_n^-$ ^[b] and VF_n^- ^[d]

n	$\text{Al}(\text{BO}_2)_n^-$	$\text{Sc}(\text{BO}_2)_n^-$	$\text{Sc}(\text{BH}_4)_n^-$	ScF_n^-	$\text{Ti}(\text{BO}_2)_n^-$	TiF_n^-	$\text{V}(\text{BO}_2)_n^-$	VF_n^-
1	0.39	1.41	1.41	1.05	1.76	1.01	3.03	1.01
2	3.46	1.94	1.25	1.22	1.65	1.18	2.11	1.03
3	3.94	2.59	2.14	1.49	3.71	1.72	5.10	2.62
4	8.28	8.69	6.47	7.74	4.86	2.32	8.72	4.22
5					9.30	7.89	9.27	5.06
6							8.23	8.29

^[a] VDE values from reference [33].

^[b] VDE values of the lowest-energy configurations of $\text{TM}(\text{BO}_2)_n^-$ (TM = Sc, Ti, V)

^[c] VDE values from reference [52]

^[d] VDE values from reference [50]

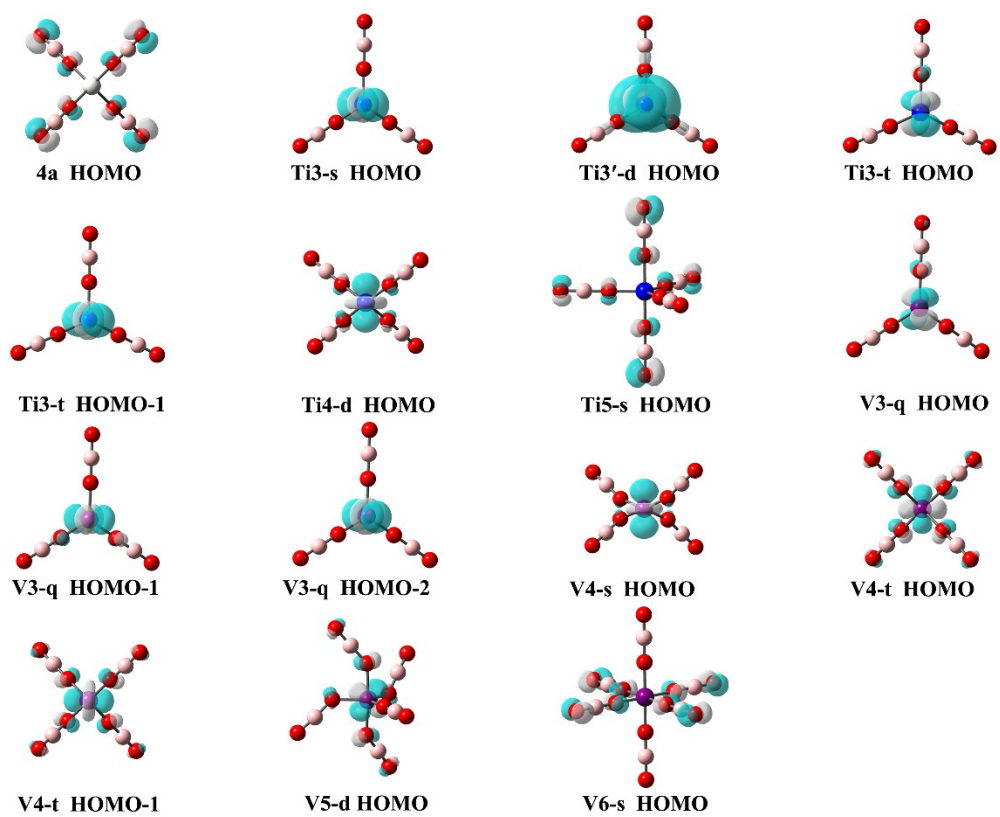


Figure S1. Critical MOs of 4a, Ti3-s, Ti3'-d, Ti3-t, Ti4-d, Ti5-s, V3-q, V4-s, V4-t, V5-d, and V6-s. (Color legend: Sc, grey; Ti, blue; V, purple; O, red; B, light pink.)