Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

NbB_{12}^-: A new member of half-sandwich type doped boron clusters with high stability

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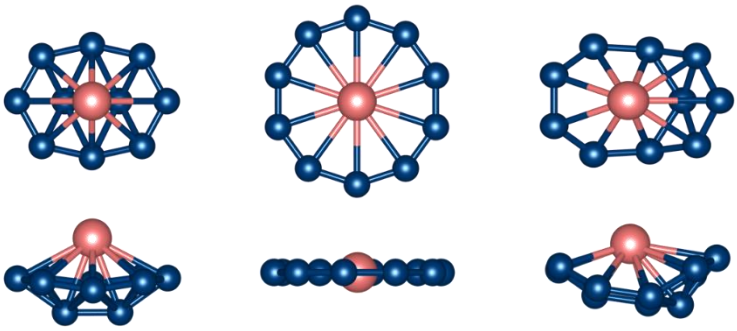

Isomers	10B', C_{2v},	10A', D_{10h},	10C', C_S,
PBE0	0.00 eV	0.57 eV	0.84 eV
RCCSD(T)	0.56 eV	0.00 eV	0.98 eV
	(13.03 kcal·mol^{-1})	(0.00 kcal·mol^{-1})	(22.71 kcal·mol^{-1})

Figure S1. The low-energy isomers of NbB_{10}^- clusters, their point-group symmetries and relative energies. The isomers are optimized by PBE0/Nb/LANL2DZ/B/6-311+g(d). Single point total energies are calculated at the CCSD(T)/Nb/Stuttgart/B/aug-cc-pVTZ level.

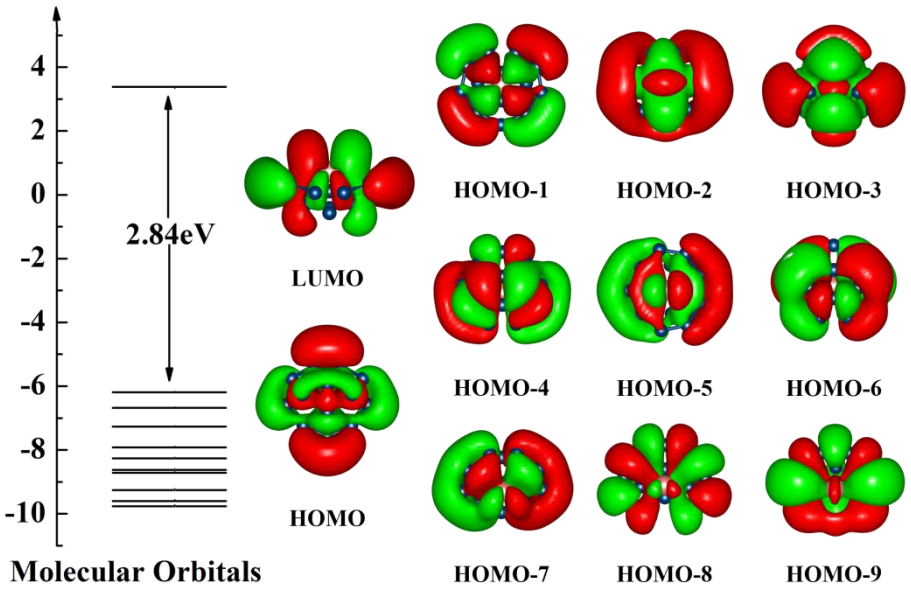

Figure S2. The molecular orbitals of the NbB_{13} cluster.

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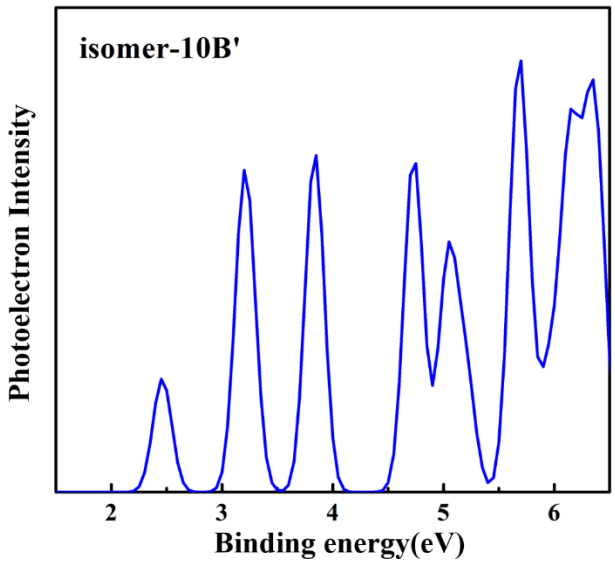

Figure S3. The photoelectron spectrum of the second isomer 10B' (C_{2v} symmetry) of NbB_{10}^- cluster.

Table S1. The electronic states of all metastable structures of neutral and anionic NbB_n clusters.

Neutral ions				Anions			
Isomer	State	Isomer	State	Isomer	State	Isomer	State
10B	^{4}A’	10C	^{2}A	10B’	^{1}A$_1$	10C’	^{1}A’
11B	^{1}A	11C	^{1}A’	11B’	^{2}A’’	11C’	^{2}A’
12B	^{2}A’’	12C	^{2}A’	12B’	^{1}A’	12C’	^{1}A’
13B	^{3}B	13C	^{1}A	13B’	^{2}A	13C’	^{2}A
14B	^{2}A’	14C	^{2}A’	14B’	^{3}A’’	14C’	^{1}A’
15B	^{1}A	15C	^{1}A’	15B’	^{2}A	15C’	^{2}A
16B	^{2}B	16C	^{2}A	16B’	^{1}A	16C’	^{1}A
17B	^{1}A	17C	^{1}A	17B’	^{2}A	17C’	^{2}A
18B	^{4}A	18C	^{2}A	18B’	^{1}A	18C’	^{1}A
19B	^{1}A	19C	^{1}A	19B’	^{2}A	19C’	^{2}A
20B	^{2}A	20C	^{2}A	20B’	^{1}A	20C’	^{1}A