

Supplementary Information

Structural stability and evolution of medium-sized tantalum doped boron clusters: A half-sandwich-structured TaB_{12}^- cluster

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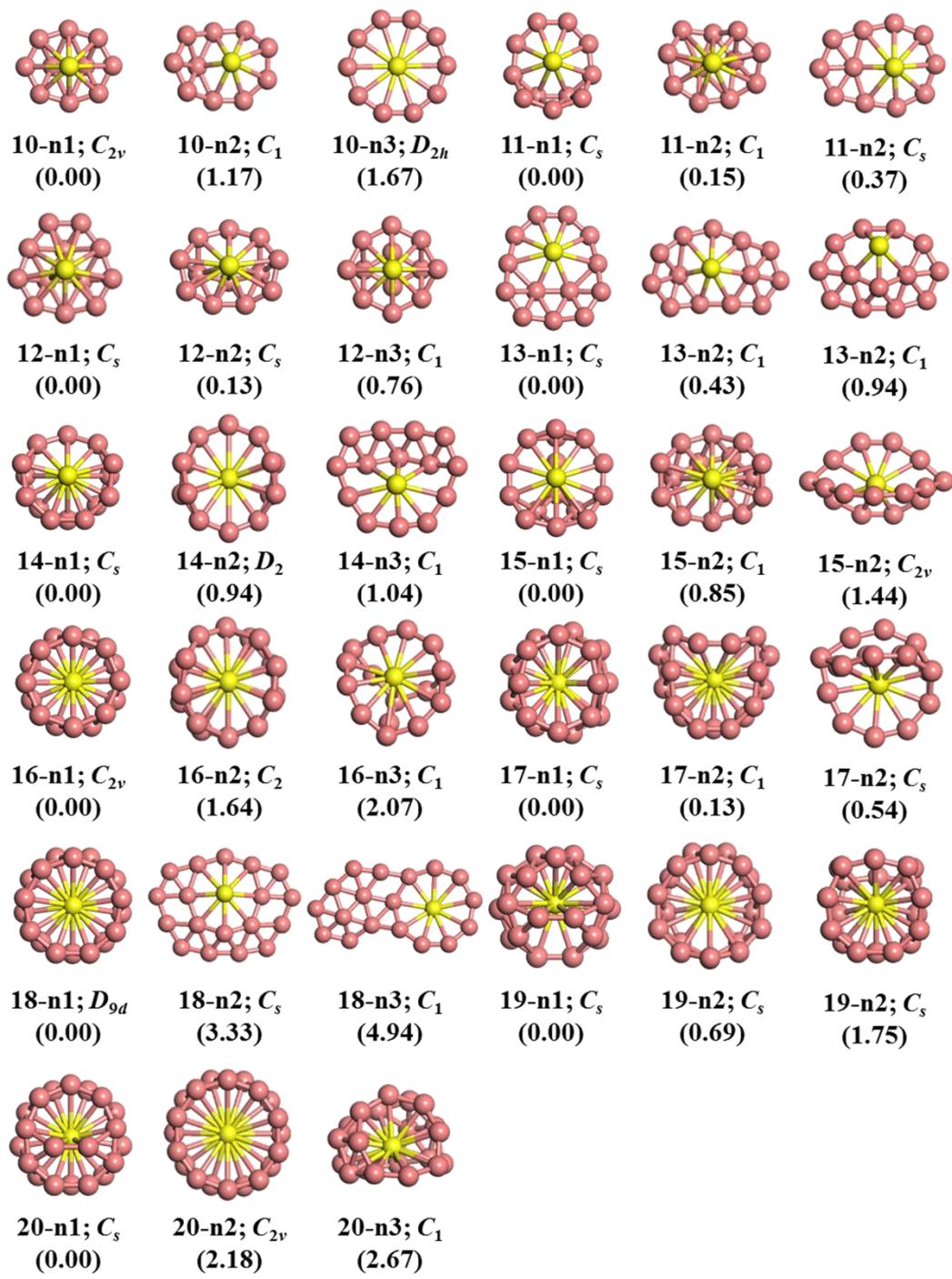


Figure S1. Low-lying isomers of TaB_n ($n = 10\text{--}20$) clusters, along with the point group symmetry and relative energy (eV).

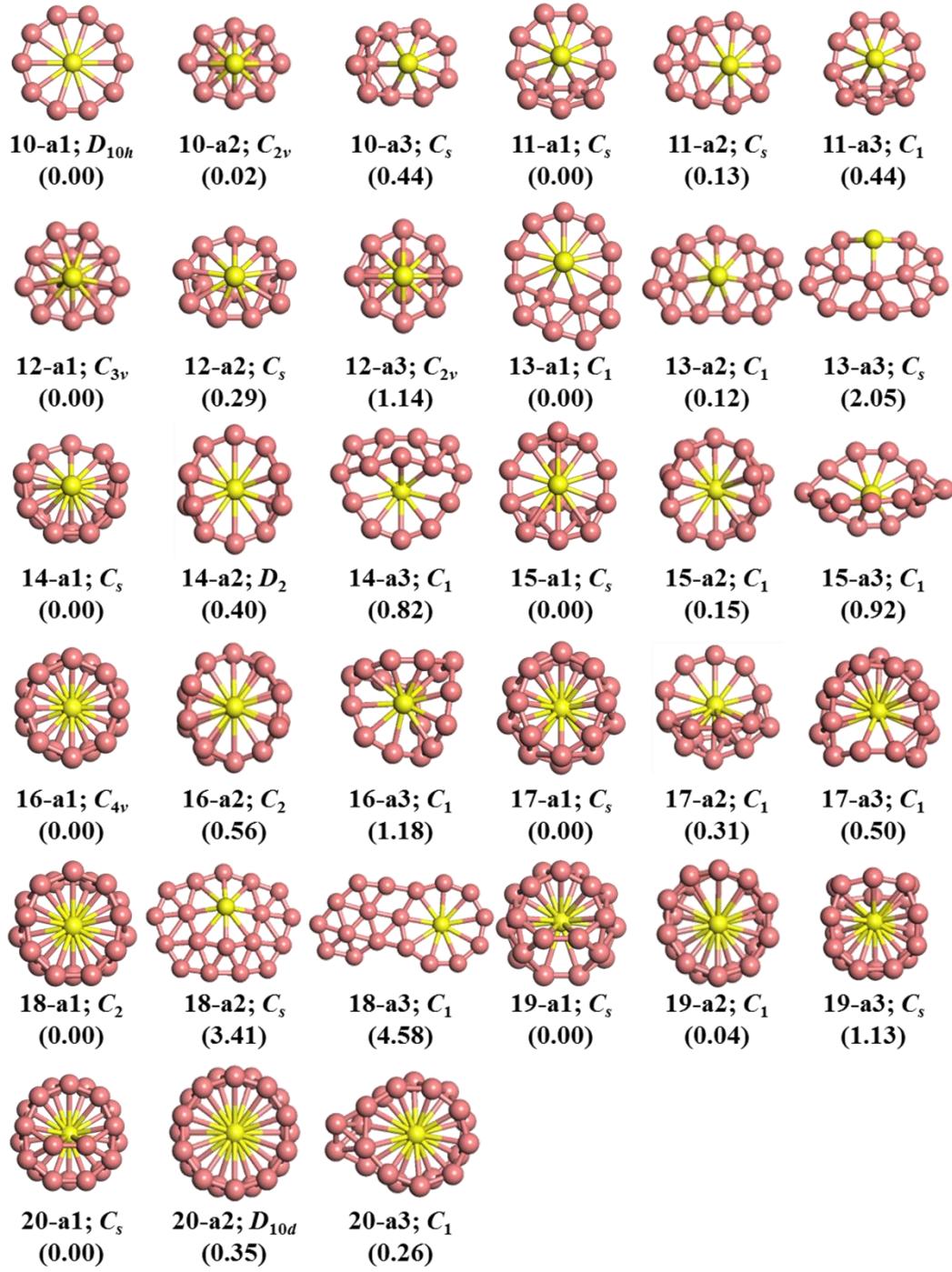


Figure S2. Low-lying isomers of TaB_n^- ($n = 10\text{--}20$) cluster, along with the point group symmetry and relative energy (eV).

Table S1. Comparing calculated vertical detachment energy with available experimental data.

Cluster	VDE(eV)	
	Theo.	Exp.
TaB ₁₀ ⁻	4.0024	4.04 ^a
TaB ₁₁ ⁻	3.4725	
TaB ₁₂ ⁻	3.2427	
TaB ₁₃ ⁻	4.0454	
TaB ₁₄ ⁻	3.8138	
TaB ₁₅ ⁻	3.3052	
TaB ₁₆ ⁻	3.8316	
TaB ₁₇ ⁻	3.6989	
TaB ₁₈ ⁻	3.6745	
TaB ₁₉ ⁻	3.9457	
TaB ₂₀ ⁻	3.0026	3.30 ^b

^a Ref.1. ^b Ref.2.

Table S2. Natural electron configuration (NEC) of Ta and B atoms for the lowest-energy structures of TaB_n ($n = 10\text{-}20$) clusters.

n	NEC(Ta)	NEC(B)
10	$6S^{0.25}5d^{3.8}6p^{0.33}6d^{0.02}$	$2S^{0.76-0.82}2p^{2.15-2.30}3p^{0.01-0.02}3d^{0.01}$
11	$6S^{0.24}5d^{3.90}6p^{0.47}7S^{0.01}6d^{0.02}$	$2S^{0.76-0.88}2p^{1.93-2.24}3p^{0.01}3d^{0.01}4p^{0.01}$
12	$6S^{0.19}5d^{3.76}6p^{0.34}6d^{0.04}$	$2S^{0.57-0.83}2p^{2.18-2.40}3p^{0.01-0.02}3d^{0.01}$
13	$6S^{0.21}5d^{4.01}6p^{0.37}6d^{0.02}$	$2S^{0.62-0.88}2p^{2.01-2.45}3S^{0.0-0.01}3p^{0-0.01}3d^{0-0.01}4p^{0-0.01}$
14	$6S^{0.23}5d^{4.01}6p^{0.56}7S^{0.01}6d^{0.06}$	$2S^{0.69-0.84}2p^{1.82-2.49}3p^{0.01-0.02}3d^{0.01}$
15	$6S^{0.20}5d^{3.94}6p^{0.59}7S^{0.01}6d^{0.05}$	$2S^{0.69-0.88}2p^{1.57-2.48}3p^{0-0.01}3d^{0-0.01}4p^{0-0.02}$
16	$6S^{0.20}5d^{4.49}6p^{0.69}7S^{0.02}6d^{0.13}$	$2S^{0.69-0.72}2p^{2.21-2.29}3p^{0.02}3d^{0.01}$
17	$6S^{0.20}5d^{4.36}6p^{0.68}7S^{0.02}6d^{0.10}$	$2S^{0.66-0.87}2p^{1.79-2.48}3p^{0-0.02}3d^{0-0.01}4p^{0-0.02}$
18	$6S^{0.19}5d^{4.29}6p^{0.61}7S^{0.02}6d^{0.11}$	$2S^{0.71}2p^{2.25}3p^{0.02}3d^{0.01}$
19	$6S^{0.18}5d^{4.29}6p^{0.70}7S^{0.01}6d^{0.10}$	$2S^{0.65-0.86}2p^{2-2.40}3S^{0-0.01}3p^{0-0.02}3d^{0.01}4p^{0-0.02}$
20	$6S^{0.19}5d^{4.60}6p^{0.80}7S^{0.02}6d^{0.13}$	$2S^{0.63-0.72}2p^{2.08-2.42}3S^{0-0.01}3p^{0.02}3d^{0.01}$

Table S3. Natural electron configuration (NEC) of Ta and B atoms for the lowest-energy structures of TaB_n^- ($n = 10\text{-}20$) clusters.

n	NEC(Ta)	NEC(B)
10	$6S^{0.15}5d^{3.96}6p^{0.49}6d^{0.01}$	$2S^{0.87}2p^{2.25}3p^{0.01}3d^{0.01}$
11	$6S^{0.22}5d^{4.10}6p^{0.48}7S^{0.01}6d^{0.03}$	$2S^{0.69-0.86}2p^{2.13-2.55}3p^{0.01-0.02}3d^{0.01}$
12	$6S^{0.19}5d^{3.88}6p^{0.35}6d^{0.04}$	$2S^{0.57-0.82}2p^{2.34-2.39}3p^{0-0.02}3d^{0.01}4p^{0-0.02}$
13	$6S^{0.21}5d^{4.11}6p^{0.42}6d^{0.02}$	$2S^{0.62-0.86}2p^{2.09-2.51}3S^{0-0.01}3p^{0.01-0.02}3d^{0-0.01}$
14	$6S^{0.22}5d^{4.08}6p^{0.57}7S^{0.01}6d^{0.07}$	$2S^{0.70-0.84}2p^{1.92-2.53}3p^{0-0.01}3d^{0.01}4p^{0.01-0.02}$
15	$6S^{0.18}5d^{4.25}6p^{0.65}7S^{0.01}6d^{0.06}$	$2S^{0.72-0.83}2p^{1.60-2.54}3p^{0.01-0.02}3d^{0.01}$
16	$6S^{0.19}5d^{4.57}6p^{0.65}7S^{0.02}6d^{0.13}$	$2S^{0.68-0.71}2p^{2.17-2.45}3p^{0.01-0.02}3d^{0.01}4p^{0-0.01}$
17	$6S^{0.19}5d^{4.38}6p^{0.73}7S^{0.02}6d^{0.11}$	$2S^{0.65-0.80}2p^{2.17-2.44}3S^{0-0.01}3p^{0.01-0.02}3d^{0.01}$
18	$6S^{0.02}5d^{4.31}6p^{0.61}7S^{0.18}6d^{0.11}$	$2S^{0.68-0.75}2p^{2.17-2.38}3p^{0-0.01}3d^{0.01}4p^{0-0.02}$
19	$6S^{0.18}5d^{4.35}6p^{0.69}7S^{0.01}6d^{0.11}$	$2S^{0.62-0.85}2p^{2.14-2.50}3S^{0-0.01}3p^{0.02}3d^{0.01}$
20	$6S^{0.01}5d^{4.67}6p^{0.82}7S^{0.19}6d^{0.13}$	$2S^{0.64-0.72}2p^{2.14-2.44}3S^{0-0.01}3p^{0-0.02}3d^{0.01}4p^{0-0.02}$

Table S4. Cartesian coordinates of optimized lowest-energy structure of half-sandwich TaB_{12}^- (C_{3v} , $^1\text{A}_1$) cluster.

B	0.85303900	-0.49250200	-1.41605200
B	1.78448300	1.03027200	-0.64228100
B	-0.76616800	2.18820400	-0.41978700
B	0.00000000	0.98500400	-1.41605200
B	0.76616800	2.18820400	-0.41978700
B	-1.78448300	1.03027200	-0.64228100
B	-0.85303900	-0.49250200	-1.41605200
B	-2.27812400	-0.43058100	-0.41978700
B	2.27812400	-0.43058100	-0.41978700
B	1.51195600	-1.75762300	-0.41978700
B	-1.51195600	-1.75762300	-0.41978700
B	0.00000000	-2.06054400	-0.64228100
Ta	0.00000000	0.00000000	0.59546000

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- 2 Li, W. L.; Jian, T.; Chen, X.; Li, H. R.; Chen, T. T.; Luo, X. M.; Li, S. D.; Li, J.; Wang, L. S. Observation of a metal-centered $\text{B}_2\text{-TaB}_{18}^-$ tubular molecular rotor and a perfect TaB_{20}^- boron drum with the record coordination number of twenty. *Chem. Commun.* **2017**, *53*, 1587–1590.