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

SUPPORTING INFORMATION

Structural Transition Upon Hydrogenation of B_{20} at Different Charge States: From Tubular, Disk-, to Cage-Like

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Figure S1. The AdNDP bonding patterns of the second low-lying isomer $B_{20}H_4$ (**7.1**) (**a**) and the third low-lying isomer $B_{20}H_4$ (**7.2**) (**b**).

Figure S2. Optimized geometries of cage-like $B_{20}H_6$ and quasi-planar $B_{20}H_6$ at the B3LYP, with their symmetries, electronic states, and relative energies indicated in kcal mol^{-1} at CCSD(T) and B3LYP (in parentheses), respectively.

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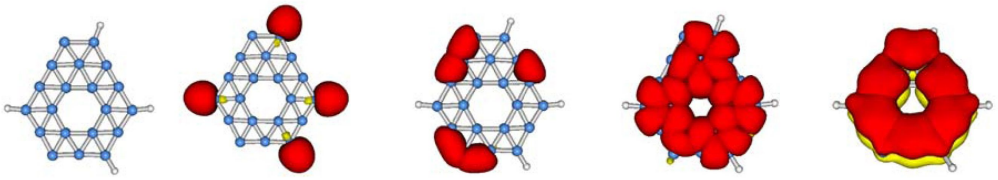
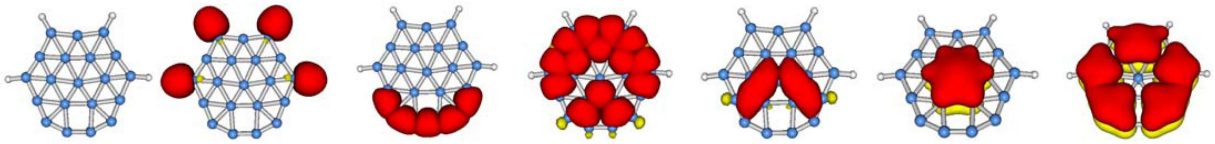
a.



C_s $B_{20}H_4$ | 4× 2c-2e B-H σ-bonds | 5× 2c-2e B-B σ-bonds | 14× 3c-2e σ-bonds, 2× 4c-2e σ-bonds, 1× 5c-2e σ-bond | 6× 5c-2e π-bonds

ON = 1.93|e| | ON = 1.77–1.87|e| | ON = 1.79–1.97|e| | ON = 1.87–1.97|e|

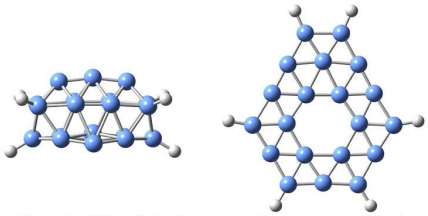
b.



C_{2v} $B_{20}H_4$ | 4× 4c-2e σ-bonds | 5× 2c-2e σ-bonds | 14× 3c-2e σ-bonds | 4× 4c-2e σ-bonds | 1× 7c-2e π-bond | 4× 4c-2e π-bonds, 1× 5c-2e π-bond

ON = 1.90–1.96|e| | ON = 1.89–1.97|e| | ON = 1.69–1.97|e| | ON = 1.67–1.72|e| | ON = 1.98|e| | ON = 1.77–1.81|e|

Figure S2. Optimized geometries of cage-like $B_{20}H_6$ and quasi-planar $B_{20}H_6$ at the B3LYP, with their symmetries, electronic states, and relative energies indicated in kcal mol^{-1} at CCSD(T) and B3LYP (in parentheses), respectively.



10. C_{2v} $B_{20}H_6$ ($^1A_1$) 0.00 (+22.65)

11. C_s $B_{20}H_6$ ($^1A'$) +40.51 (0.00)