SUPPORTING INFORMATION

Double-Ring Tubular (B₂O₂)ₙ Clusters (n=6-42) Rolled up from the Most Stable BO Double-Chain Ribbon in Boron Monoxides

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**Figure S1.** Optimized planar and tubular structures of \((\text{B}_2\text{O}_2)_n\) \((n=6-12, 21, 42)\) with their relative energy in eV at the PBE0/6-311+G* level. The B atom is in blue and O in red.

**Figure S2.** Optimized alternative low-lying structures of \(\text{B}_{12}\text{O}_{12}\), with their relative energy in eV at PBE0/6-311+G*. Also shown are the relative energies at the single-point CCSD(T)//PBE0/6-311+G* (in *italic*), TPSSh/6-311+G* (in curly brackets), and B3LYP/6-311+G* levels (in square brackets), respectively. The B atom is in blue and O in red.

**Figure S3.** AdNDP bonding patterns of \(\text{B}_{14}\text{O}_{14}\) \((3, D_{7h})\) (a) and \(\text{B}_{16}\text{O}_{16}\) \((4, D_{8h})\) (b) with their occupation numbers (ONs) indicated.

**Figure S4.** Simulated (a) IR, (b) Raman, and (c) UV-Vis spectra of \(D_{6h} \text{B}_{12}\text{O}_{12}\) (2) at the PBE0/6-311+G* level.

**Figure S5.** Simulated photoelectron spectra of \(\text{B}_{12}\text{O}_{12}^-\) on the basis of TD-PBE0 calculations. The simulations were done by fitting the distribution of the calculated VDEs with unit-area Gaussian functions of 0.04 eV half-width.

**Table S1.** Optimized coordinates \((x, y, z)\) in Å of tubular \((\text{B}_2\text{O}_2)_n\) \((n=6-9)\) at the PBE0/6-311+G* level.
Figure S1. Optimized planar and tubular structures of \((\text{B}_2\text{O}_2)_n\) \((n=6-12, 21, 42)\) with their relative energy in eV at the PBE0/6-311+G* level. The B atom is in blue and O in red.

(a) \(\text{B}_6\text{O}_8\)

(b) \(\text{B}_{10}\text{O}_{10}\)

(c) \(\text{B}_{12}\text{O}_{12}\)

(d) \(\text{B}_{18}\text{O}_{18}\)

(e) \(\text{B}_{22}\text{O}_{22}\)
(f) $B_{24}O_{24}$

(g) $B_{42}O_{42}$

(h) $B_{84}O_{84}$
Figure S2 Optimized alternative low-lying structures of $\text{B}_{12}\text{O}_{12}$, with their relative energy in eV at PBE0/6-311+G*. Also shown are the relative energies at the single-point CCSD(T)//PBE0/6-311+G* (in italic), TPSSh/6-311+G* (in curly brackets), and B3LYP/6-311+G* levels (in square brackets), respectively. The B atom is in blue and O in red.
Figure S3. AdNDP bonding patterns of $\text{B}_{14}\text{O}_{14}$ (3, $D_{7h}$) (a) and $\text{B}_{16}\text{O}_{16}$ (4, $D_{8h}$) (b) with their occupation numbers (ONs) indicated.
Figure S4. Simulated (a) IR, (b) Raman, and (c) UV-Vis spectra of $D_{6h}$ $\text{B}_{12}\text{O}_{12}$ (2) at the PBE0/6-311+G* level.
Figure S5. Simulated photoelectron spectra of $\text{B}_{12}\text{O}_{12}^-$ on the basis of TD-PBE0 calculations. The simulations were done by fitting the distribution of the calculated VDEs with unit-area Gaussian functions of 0.04 eV half-width.
Table S1. Optimized coordinates ((x, y, z) in Å) of tubular (B$_2$O$_2$)$_n$ (n=6-9) at PBE0/6-311+G*.

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