**Supplementary Material**

**C20 fullerene** **and its boron- and nitrogen-doped counterparts as an efficient catalyst for CO oxidation**

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**0.00**

**0.00**

**0.00**

**4.26**

**4.81**

**2.85**

**7.63**

**8.90**

**2.96**

**9.61**

**10.16**

**9.65**

**Fig. S1.** The top and side views of the optimized structures of the cage-like isomers of C20, BC19, and NC19 fullerene-like clusters with the bond distances in Å. The numbers under the structures are relative energy (in eV) with respect to the most stable fullerene-like C20 cluster. Color scheme: M, red; B, yellow; N, dark blue.

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