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

SUPPLEMENTARY INFORMATION

Magnetically induced current density in triple-layered beryllium-boron clusters

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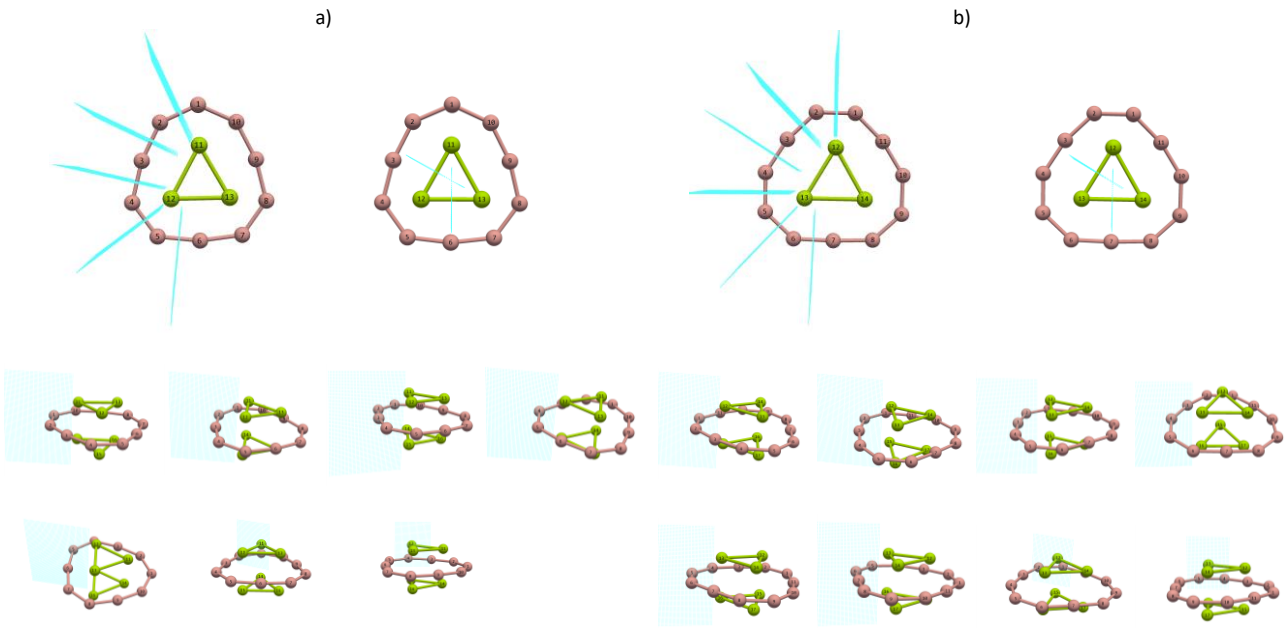

Fig. S1 Schematic representation of the bond-crossing planes used for the integration of the current density flow through the symmetry-unique bonds in: **1** (a) and **2** (b); top view (top) and side view (bottom).

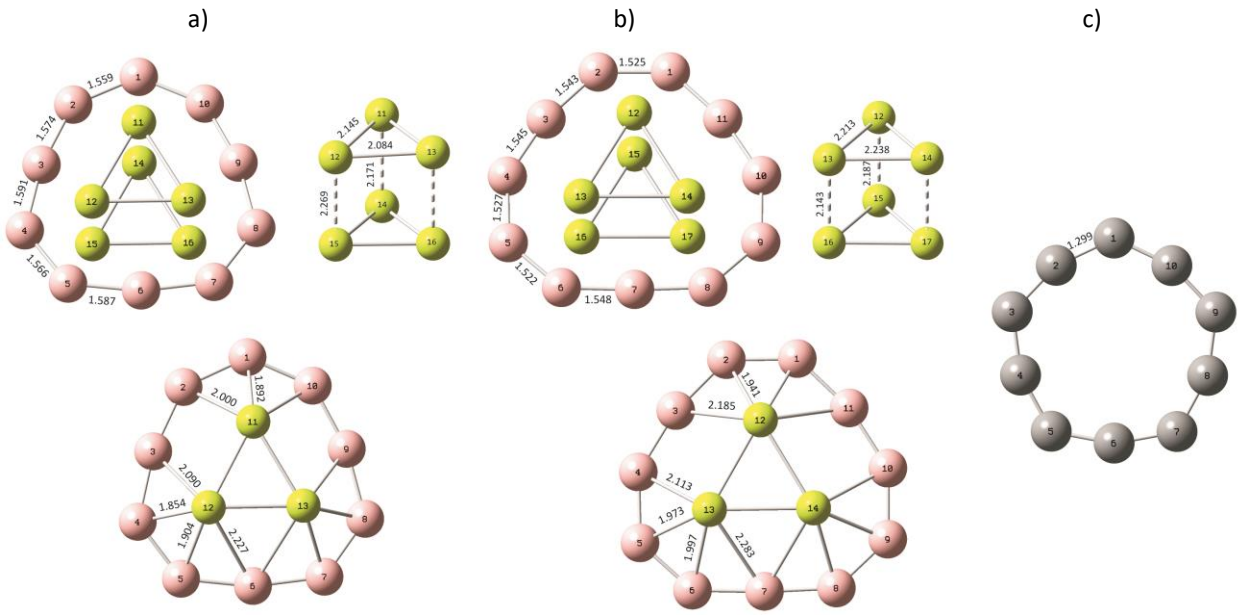

Fig. S2 Optimized geometries obtained at the BLYP/6-311+G(d) level of theory of: a) $Be_6B_{10}^{2-}$ (**1**); b) $Be_6B_{11}^{-}$ (**2**) and c) C_{10} (**3**). Bond lengths (in Å) are indicated.

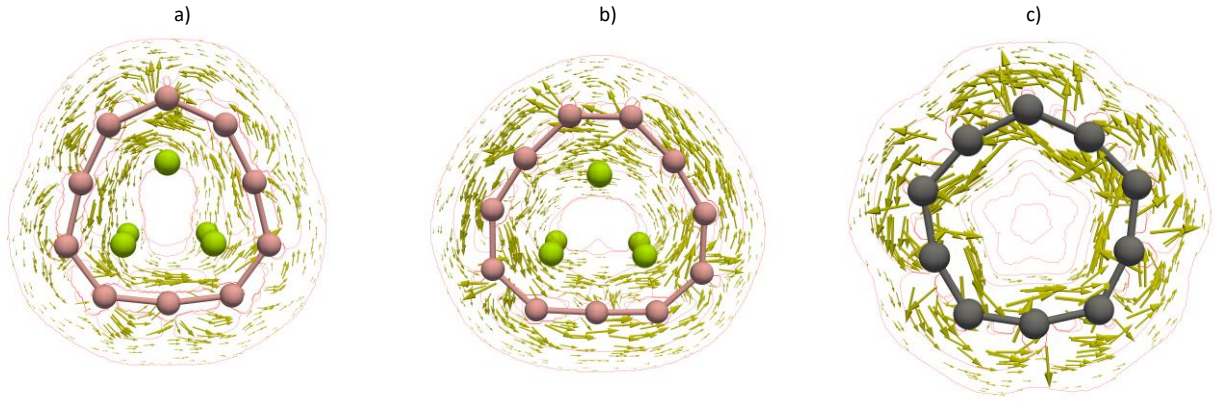

Fig. S3 Maps of the current density arising from the four σ electrons calculated in the $B_{10}/B_{11}/C_{10}$ ring plane: a) **1** (HOMO, HOMO-1); b) **2** (HOMO, HOMO-1) and c) **3** (HOMO).

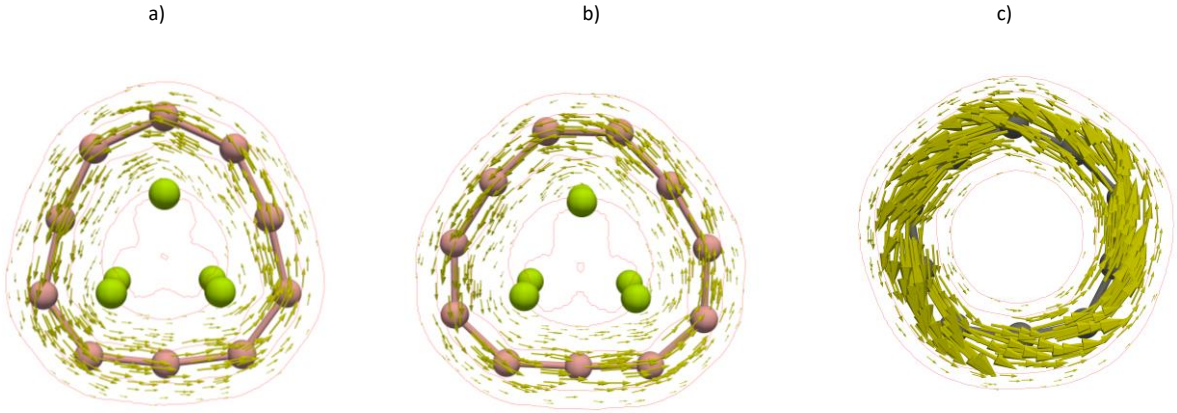

Fig. S4 Maps of the current density arising from the four π electrons calculated 1 bohr above the $B_{10}/B_{11}/C_{10}$ ring plane in: a) **1** (HOMO-2, HOMO-3); b) **2** (HOMO-2, HOMO-3) and c) **3** (HOMO-1)

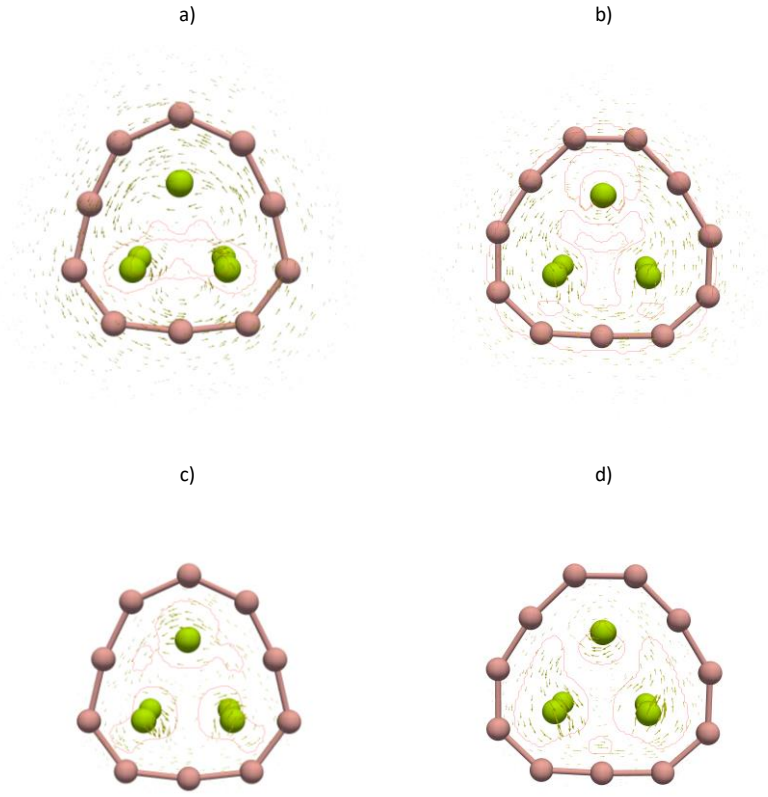

Fig. S5 Current density maps calculated 1 bohr above the Be_3 ring plane of **1** and **2**: total current density (a and b); the current density obtained by using only the atomic orbitals of Be atoms (c and d).