Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Metalloborospherenes with a Stabilized Classical Fullerene-Like Borospherene $B_{36}$ as Electric Field Manipulated Second-Order Nonlinear Optical Switches

Weihong Chen,[a] Jiayuan Liu,[b] Weiming Sun,[c] Huimin He,[d] Shansheng Yu,*[a], Ying Li*[e], and Zhiru Li*[e]

[a] *Key Laboratory of Automobile Materials of MOE and Department of Materials Science, Jilin University, Changchun, 130012, China*

[b] *Institute of Applied Chemistry, Hebei North University, Zhangjiakou, 075000, China*

[c] *Department of Basic Chemistry, The School of Pharmacy, Fujian Medical University, Fuzhou, 350108, People's Republic of China*

[d] *Institute of Computational and Applied Physics, Department of Physics, Taiyuan Normal University, Jinzhong, 030600, China*

[e] *Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun, 130023, China*

**Corresponding Authors**

E-mail: yuss@jlu.edu.cn (Shansheng Yu)

E-mail: liyingedu@jlu.edu.cn (Ying Li)

E-mail: lzr@jlu.edu.cn (Zhiru Li)

Table S1. The symmetry, B-B bond lengths shared between two five-membered rings ($d_{5\text{-}5}$, in Å), B-B bond lengths shared between a five and a six membered ring ($d_{5\text{-}6}$, $d_{6\text{-}5}$, in Å), B-B bond lengths between two six-membered rings ($d_{6\text{-}6}$, in Å), B-Mg bond lengths ($d_1$, in Å), top and lumbar B-Li bond lengths ($d_2$, $d_3$, in Å), horizontal and vertical diameters ($D_1$, $D_2$ in Å) for $Mg_{12}Li_8\&B_{36}$.

| Level | Symmetry | $d_{5\text{-}5}$ | $d_{6\text{-}6}$ | $d_{6\text{-}5}$ | $d_{5\text{-}6}$ | $d_1$ | $d_2$ | $d_3$ | $D_1$ | $D_2$ |
|---|---|---|---|---|---|---|---|---|---|---|
| PBE0/6-311G(d) | $D_{6h}$ | 1.799 | 1.705 | 1.716 | 1.744 | 2.304 | 2.193 | 2.204 | 6.1 | 6.5 |
| PBE0/6-311+G(d) | $D_{6h}$ | 1.799 | 1.705 | 1.716 | 1.744 | 2.304 | 2.193 | 2.204 | 6.1 | 6.5 |
| TPSSH/6-311G(d) | $D_{6h}$ | 1.805 | 1.708 | 1.722 | 1.749 | 2.311 | 2.204 | 2.216 | 6.1 | 6.5 |
| B3LYP/6-311G(d) | $D_{6h}$ | 1.798 | 1.710 | 1.719 | 1.747 | 2.318 | 2.193 | 2.206 | 6.1 | 6.4 |

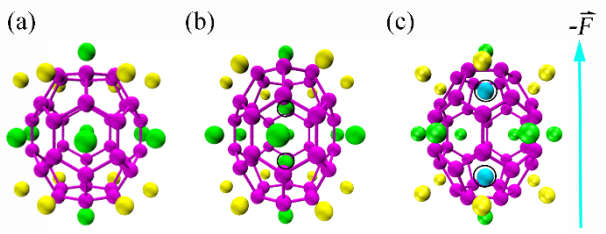


Figure. S1 Optimized structures of $Mg_{12}Li_8\&B_{36}$ (a), $Mg_{12}Li_8\&(Li_2@B_{36})$ (b), $Mg_{12}Li_8\&(Be_2@B_{36})$ (c) and the direction of external electric field (light blue arrow).

Table S2. $\beta_0$ ($10^4$ au) values of $Mg_{12}Li_8\&B_{36}$ calculated by different density functionals in conjunction with the 6-311+G(d) for Mg, and 6-31+G(d) for B as well as 6-31G(d) basis set for Li atoms.

| *F* | 0 | 5 | 10 | 15 | 20 | 30 | 40 | 45 | 50 | 55 | 60 | 70 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| M06-2X | 0.0 | 0.4 | 0.8 | 1.6 | 2.3 | 3.9 | 6.2 | 8.3 | 11.9 | 86.1 | 3.6 | 9.7 |
| LC-PBEPBE | 0.0 | 0.1 | 0.5 | 1.0 | 1.3 | 2.4 | 24.5 | 34.7 | 49.6 | 61.0 | 48.9 | 28.6 |