

Supplemental Materials to Accompany the Communication
Entitled:

First hexanuclear zirconium macrocycle in a chair-like confirmation sustained by glycolic acids

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Figure S1: structure of $ZrOCl_2$ indicating how A^4 and B^2 units can form a square. Color Code: Light Blue, Zr; Red, O.

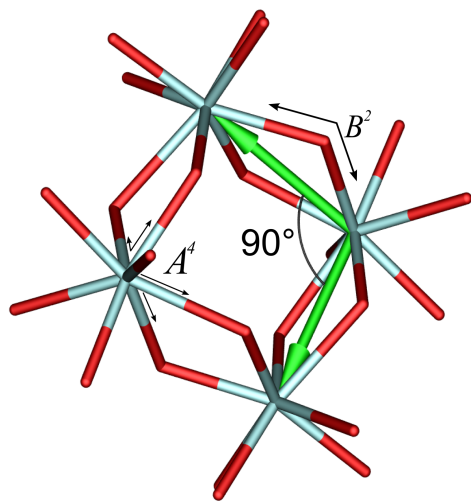


Figure S2: structure of CP-3 indicating how A^4 and B^2 units can form a hexagon. Color Code: Light Blue, Zr; Red, O.

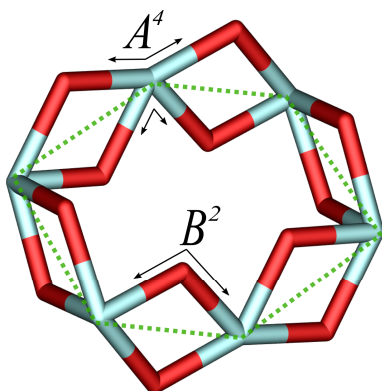


Figure S3. MOOP's of the Zr-Zr and Zr-O (bridging) bonds calculated for the Zr crown structure.

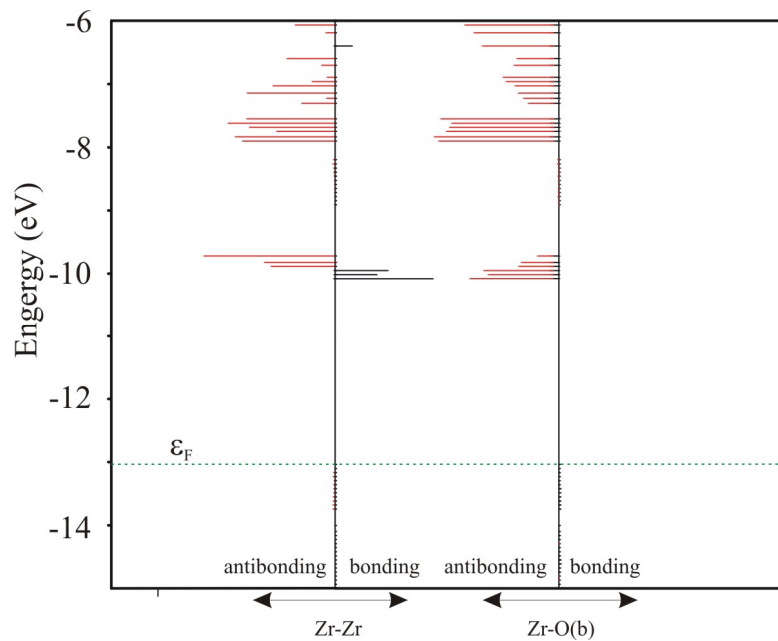


Figure S4: IR spectrum of CP-3

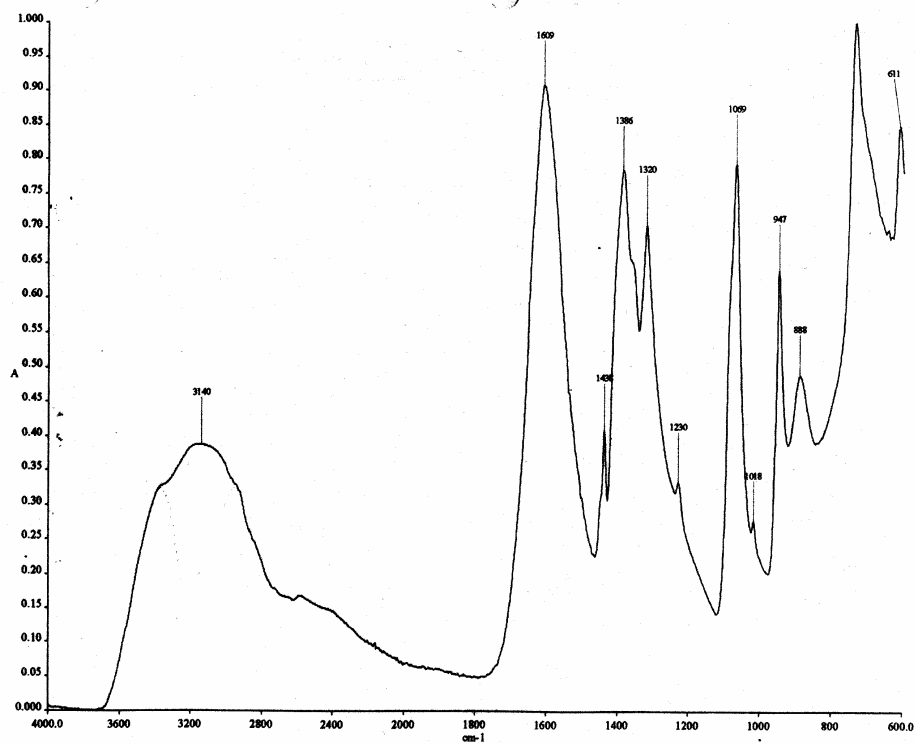


Figure S5: The PXRD patterns of two batches of CP-3 (Blue, Green) compared with a simulated XRD pattern (red).

