

Description of Additional Supplementary Files

Supplementary Data 1. Calculated average partial charges (e^-) for the various chemically distinct atoms for the fragments that were selected for **Zn-atz-oba**. The average and standard deviation between the fragments are also included. Labeling of atoms and fragments correspond to **Supplementary Figures 15** and **16**, respectively.

Supplementary Data 2. Parameters for the chemically distinct atoms in **Zn-atz-oba** that were used for the simulations. Atom labels correspond to the **Supplementary Figure 15**.

Supplementary Data 3. The crystallographic distances (in Å) between various atoms in **Zn-atz-oba**. Atom labels correspond to the **Supplementary Figure 15**.