

Supporting Information

A new Co-nitroimidazolate-dicarboxylate pillared-layer network with various types of channel and ultralarge cages for gas uptake

Xiao-Qing Guo, Miao Wang, Yan-Feng Tang, Fei Meng, Guo-Qing Jiang and Jin-Li Zhu

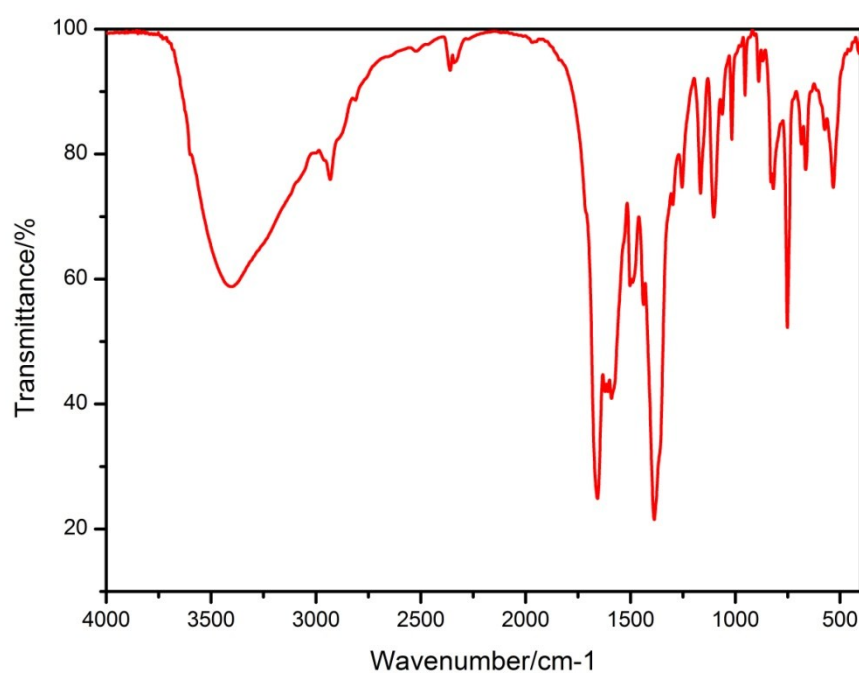


Figure S1. The IR spectrum of complex **1** in KBr pellets from 4000cm⁻¹ to 400cm⁻¹.

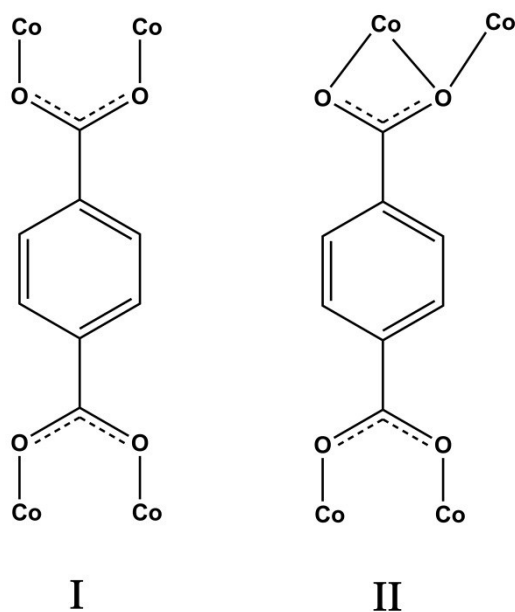


Figure S2. The coordination modes of H₂bdc in complex **1**.

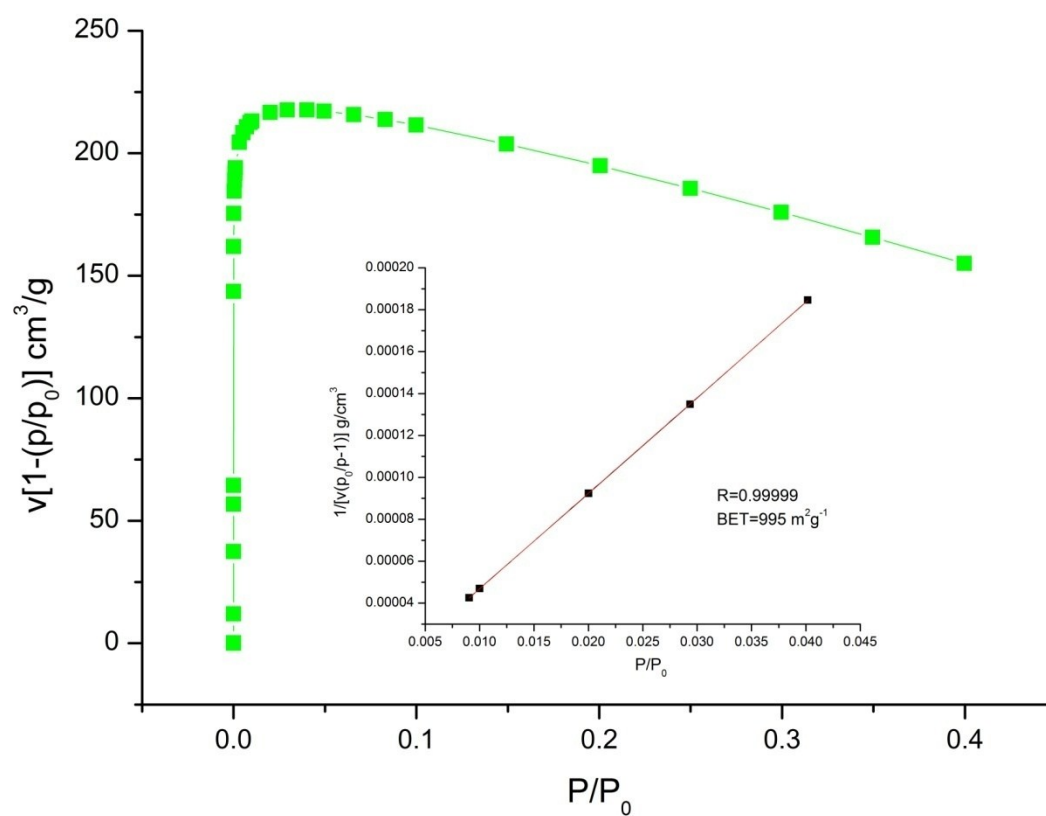


Figure S3. $V[1-(P/P_0)]$ vs. P/P_0 for **1**, only the range below $P/P_0=0.028$ satisfies the first consistency criterion for applying the BET theory. Insert: Plot of the linear region for the BET equation.

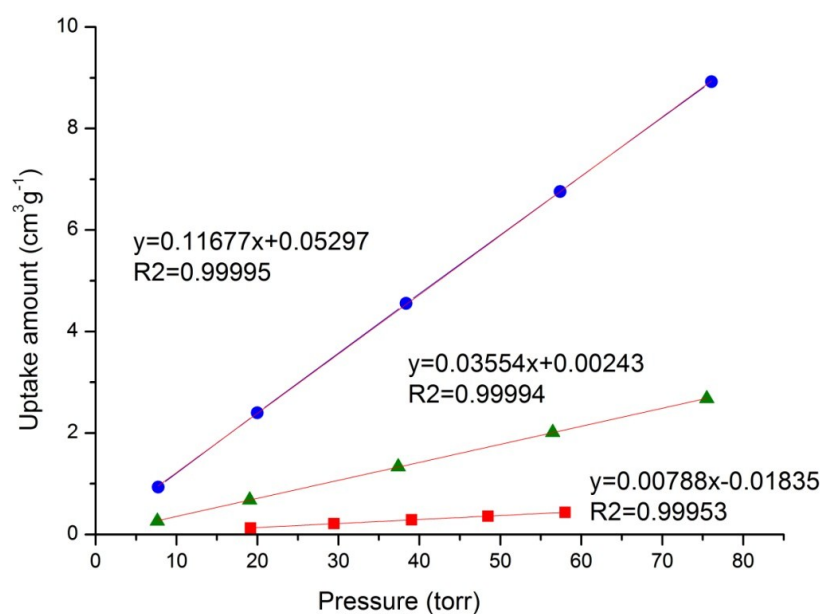


Figure S4. The fitting initial slope for CO₂, CH₄ and N₂ isotherms for complex 1 collected at 273 K. CO₂ (blue circle), CH₄ (green triangle), N₂ (red square).

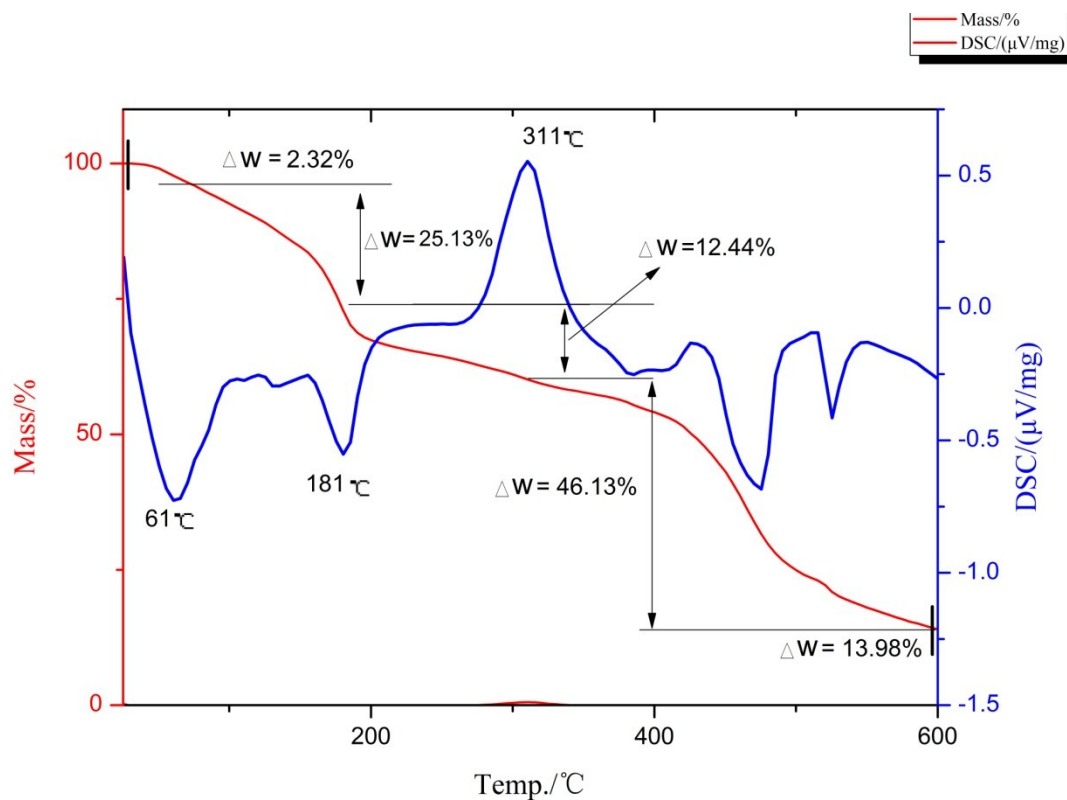


Figure S5. TGA/DSC curves for complex 1.

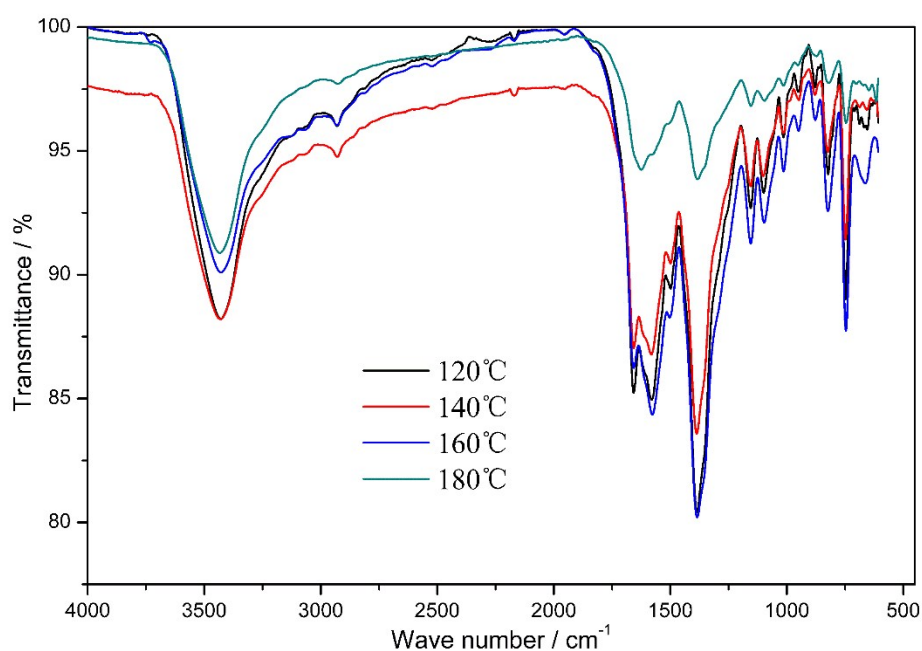


Figure. S6 IR spectra of compound **1** at different temperature

In order to confirm the solvent loss, the FTIR spectra of as-synthesized **1** which was heated by TGA analyzer to different temperatures (120 - 180°C) were collected (see Fig. 2). The typical absorption bands for benzene skeleton vibration (C=C) are observed at 1600-1450 cm^{-1} . The adsorption peak at 1385 cm^{-1} may be associated with the symmetric stretching vibration of $-\text{NO}_2$ group in 2-nitroimidazole ligand, respectively. With the temperature increasing, the disappearance of characteristic adsorption peaks of $-\text{CHO}$ group at 2931 cm^{-1} (C-H) and 1655 cm^{-1} (C=O) at 180°C indicates the loss of DMF molecules. However, the adsorption peak of $-\text{OH}$ group at 3430 cm^{-1} remains the same (we tried the experiment again and again, even if the temperature was raised to 320°C). Generally, the guest and coordinated water molecules can be removed completely under the aforementioned condition. Therefore, we speculated that the activated material is easily adsorbed water molecules in the air due to the special porosity.

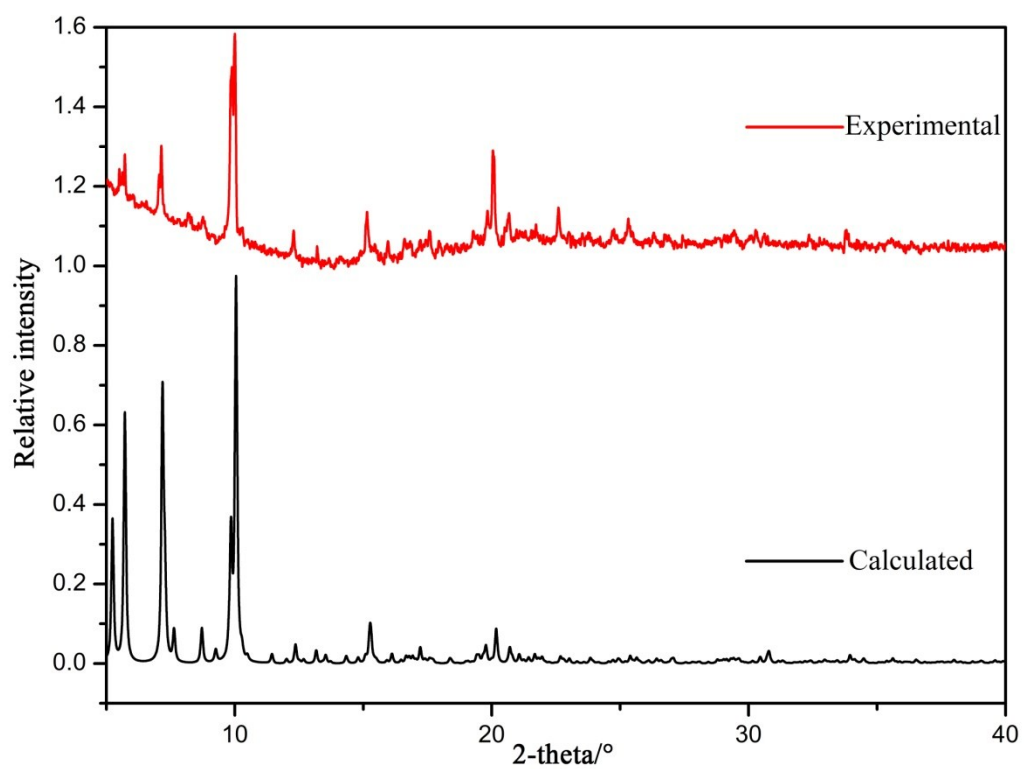


Figure S7. The calculated X-ray powder diffraction patterns (lower) and the experimental one (upper) of complex **1**.