Electronic Supplementary Material for CrystEngComm

Designed self-assembly of a reactive metal-organic framework with quasi α-Po topology

Adonis Michaelides,* Stavroula Skoulika and Michael G. Siskos

Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece. Fax: 30-26510-98798; Tel: 30-26510-98447; E-mail: amihail@cc.uoi.gr

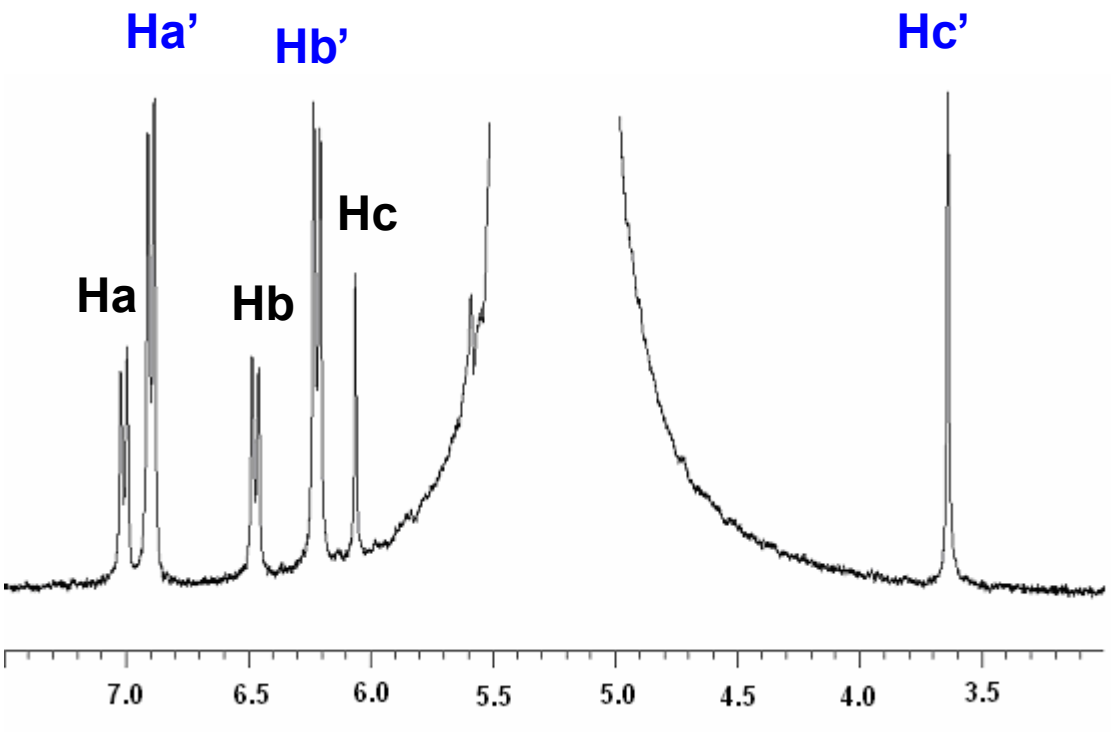

Fig. 1S: ^{1}H-NMR spectrum of a mixture of compounds **2** and **3** in HNO_3/D_2O = 3/2. The mixture was obtained by irradiation of **2** for 45 min.**T**he chemical shifts of the non-irradiated sample (compound **2**) are the following: 7.06 ppm (4H, d, *J*=6.25 Hz, Ha), 6.53 ppm (4H, d, *J*=6.25 Hz, Hb) and the olefinic protons at 6.12 ppm (2H, s, olefinic Hc). In this case the band of the hydrogens of fumaric acid is covered by the solvent. The chemical shifts of the product after isomerization (compound **3**) appear at 6.95 ppm (8H, d, *J*=6.25 Hz, Ha'), 6.27 ppm (8H, d, *J*=6.25 Hz, Hb') and at 3.70 ppm (8H, s) the cyclobutane ring hydrogens.

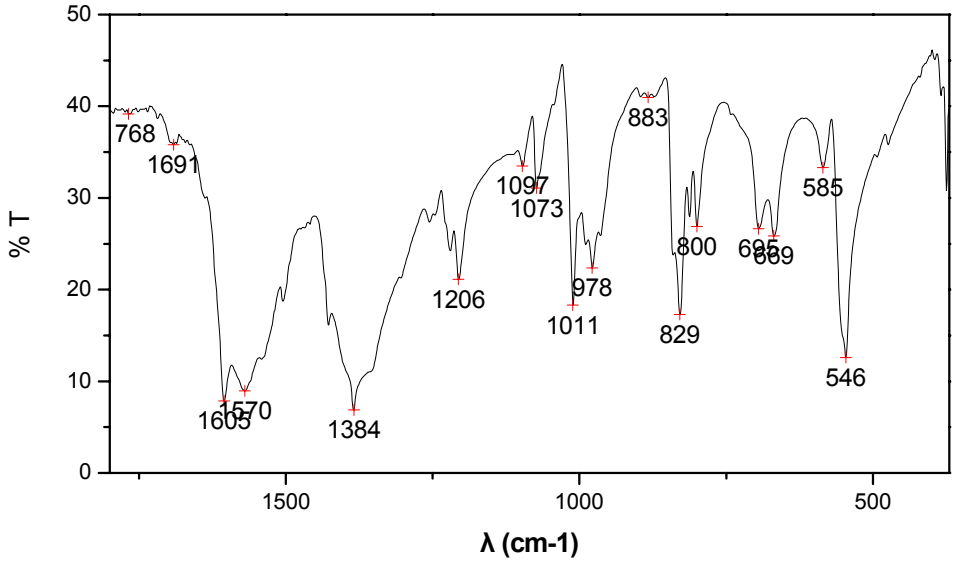

Fig. 2S. IR spectrum of compound **2** (KBr pellet)

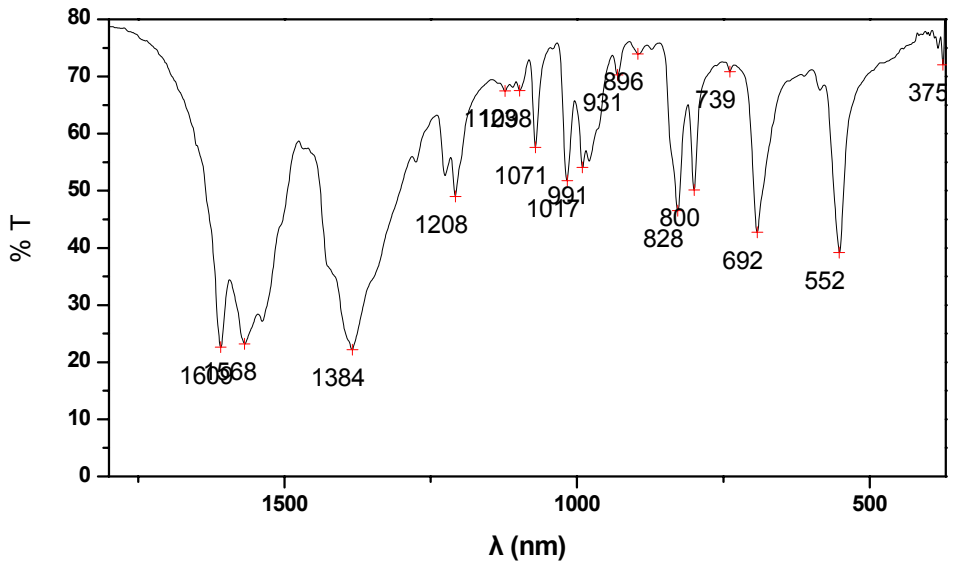

Fig. 3S. IR spectrum of compound **3** (irradiation of **2** for 5 ½ hours ,KBr pellet).

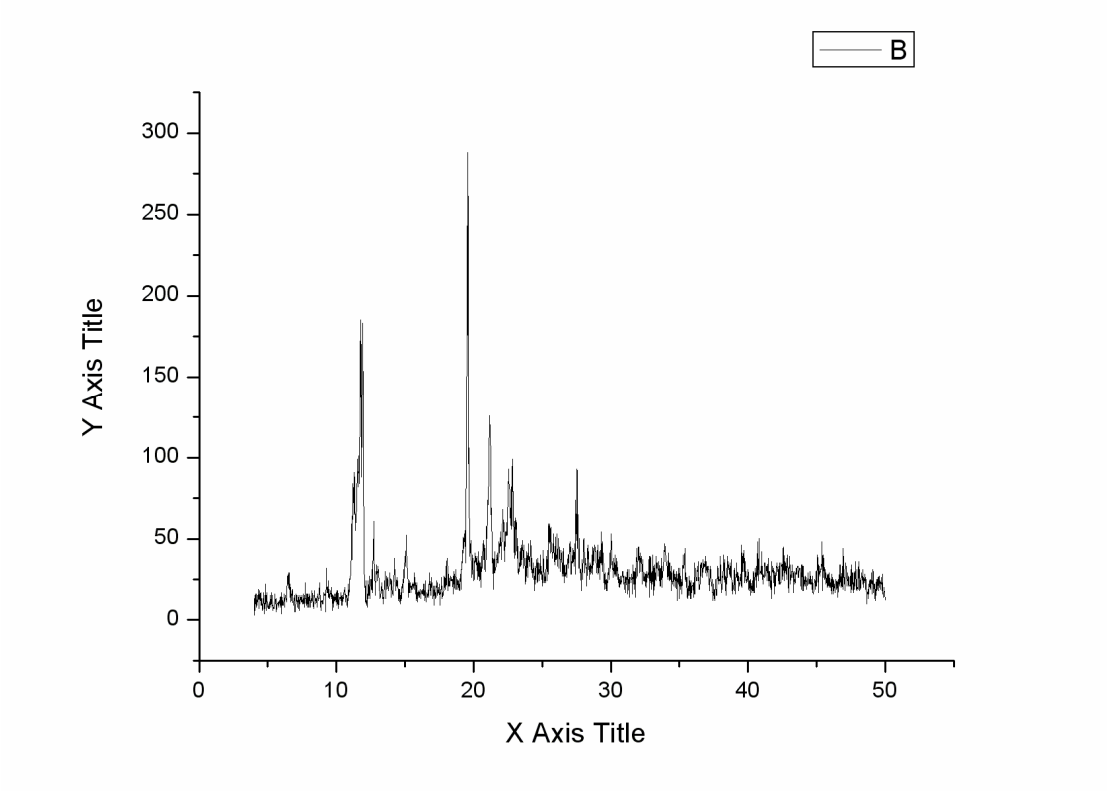

Fig 4S. XRPD pattern of compound **2**.

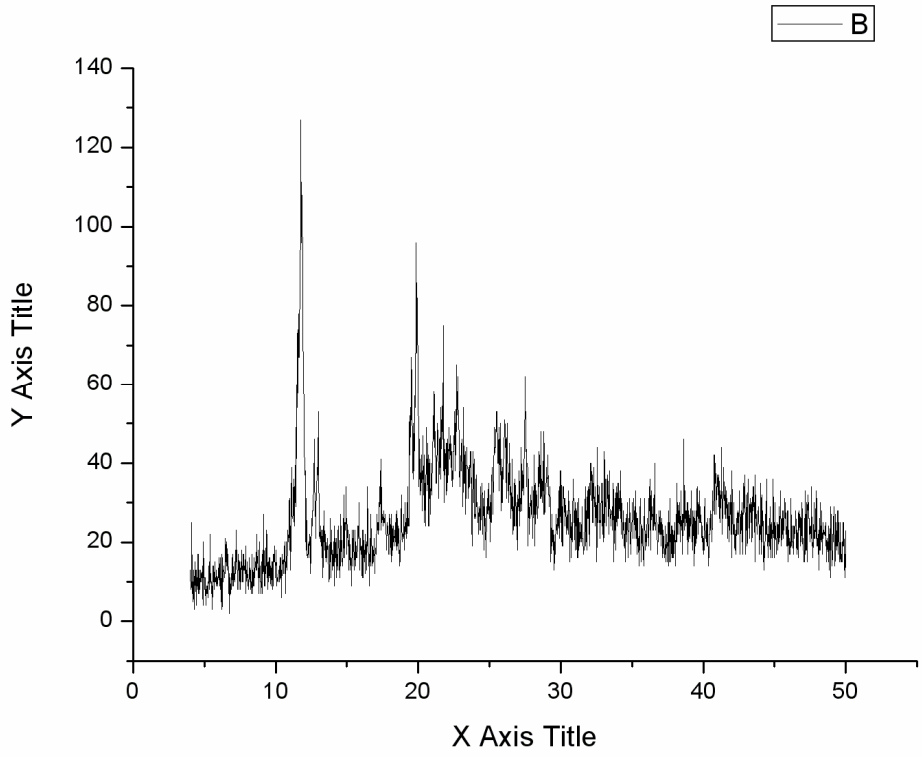

Fig 5S. XRPD pattern of compound **3**.