Electronic Supplementary Material (ESI) for CrystEngComm.

A new 3D four-fold interpenetrated dia-like polymer: gas sorption and computational analyses

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Supporting Information

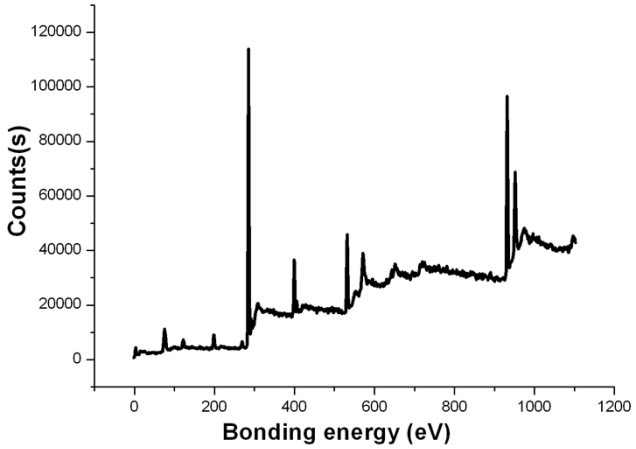

Fig. S1 view of XPS in **1**.

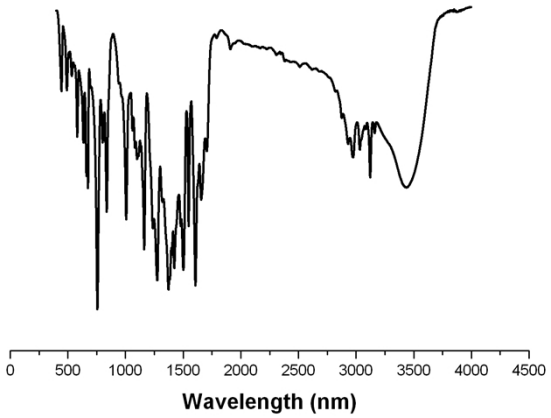

Fig. S2 View of the IR in **1**.

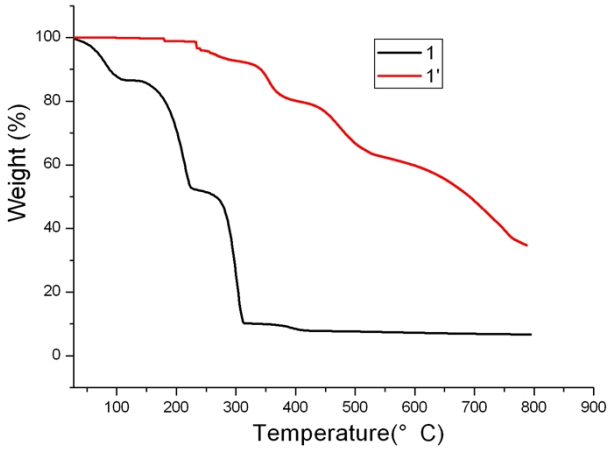

Fig. S3 View of the TGA in **1** and **1'.**

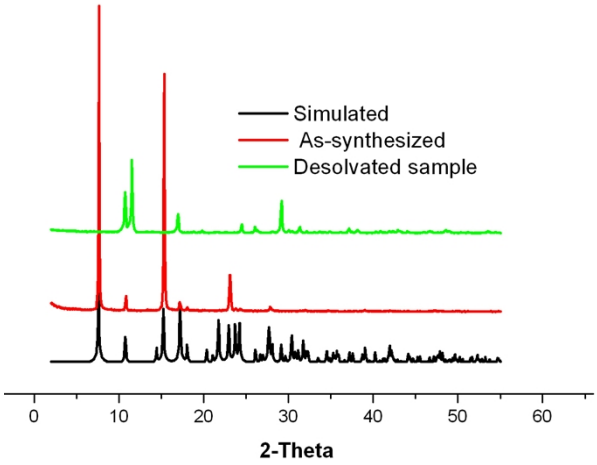

Fig. S4 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination, the as-synthesized product of **1** and desolved in compound **1'**.

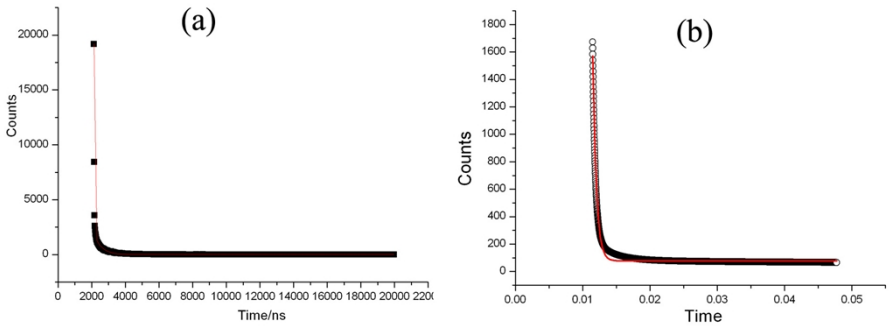

Fig.S5 View of lifetime for **1** and **1'** at room temperature.

Calculated section

Compound has been formally partially de-solvated (water crystallization molecules have been withdrawn). Uncoordinated NO_3^- ion was also removed.

The computational method, based on Connolly's algorithm[1] has already been described and successfully used elsewhere[2-4]. Thanks to this method, porosity profile can be calculated on the basis of the crystal structure.

The compound exhibits quite sizeable potential porosity. The square cross-section channels that spread along the c axis can host guest molecules that present a kinetic radius as large as 3.8 Å (Figure S6). Accessible solvent surface area versus kinetic radius is drawn on Figure S6. The potential porosity has been calculated for several probe sphere radii that correspond to different guest molecules kinetic radii[5].

Table S1 different calculated potential gas adsorption feature in **1**

Probe sphere radius (Å)	Guest molecule	potential porosity ($m^2.g^{-1}$)
1.3	He	2921(6)
1.45	H_2	2847(6)
1.65	CO_2	2763(6)
1.7	Ar	2741(6)
1.8	N_2	2670(6)
1.9	CO	2641(6)
2.9	C_6H_6	23085(8)

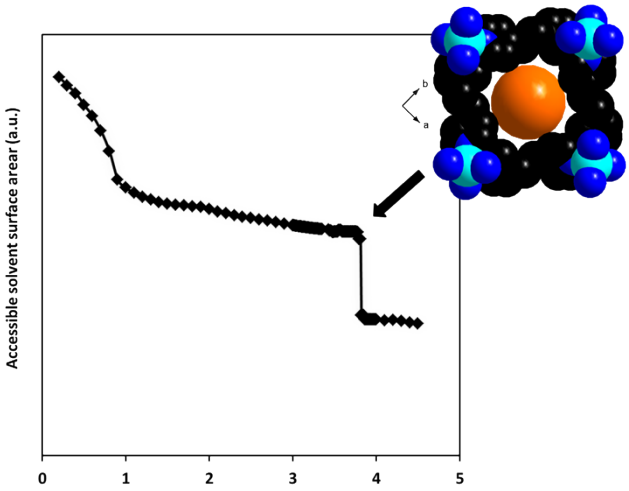

Figure S6. Porosity profile for the compound $\{[Cu(bib)_2].NO_3.4H_2O]_n$.

References

(1) M. L. Connolly, *Science,* 1983, **221**,709.

(2) C. Daiguebonne, N. Kerbellec, K. Bernot, Y. Gérault, A. Deluzet and O. Guillou, *Inorg. Chem.,* 2006, **45**, 5399.

(3) Y. Qiu, H. Deng, S. Yang, J.Mou, C. Daiguebonne, N. Kerbellec, O. Guillou and

S. R. Batten, *Inorg. Chem.,* 2009, **48**, 3976.
(4) N. Kerbellec, C. Daiguebonne, K. Bernot, O. Guillou and X. Le Guillou, *J. All Comp.* 2008, **451**, 377.
(5) N. Rosi, J. Kim, M. Eddaoudi, B. Chen, M. O'Keeffe and O. M. Yaghi, *J. Am Chem. Soc.,* 2005, **127**, 1504.