Electronic Supporting Informations

Tuned synthesis of two coordination polymers of Cd(II) using substituted bent 3-pyridyl linker and succinate: structures and their applications in anion exchange and sorption properties

Dilip Kumar Maity, Biswajit Bhattacharya, Arijit Halder and Debajyoti Ghoshal†*

Department of Chemistry, Jadavpur University, Jadavpur, Kolkata, 700 032, India

---

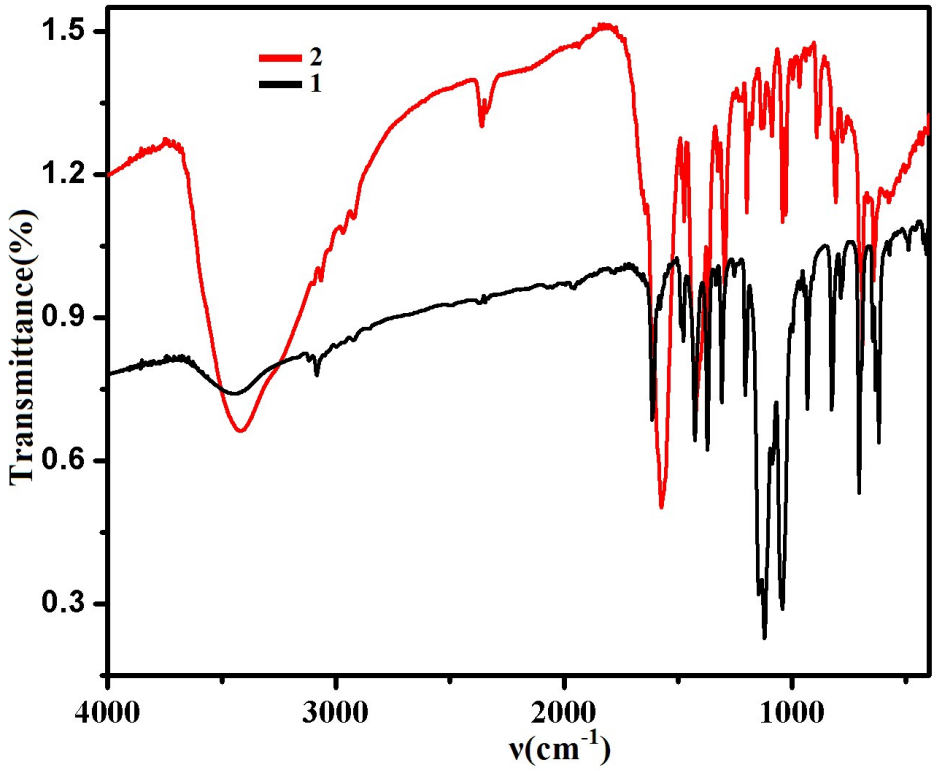

Fig. S1 FT-IR spectra of complexes **1-2**.

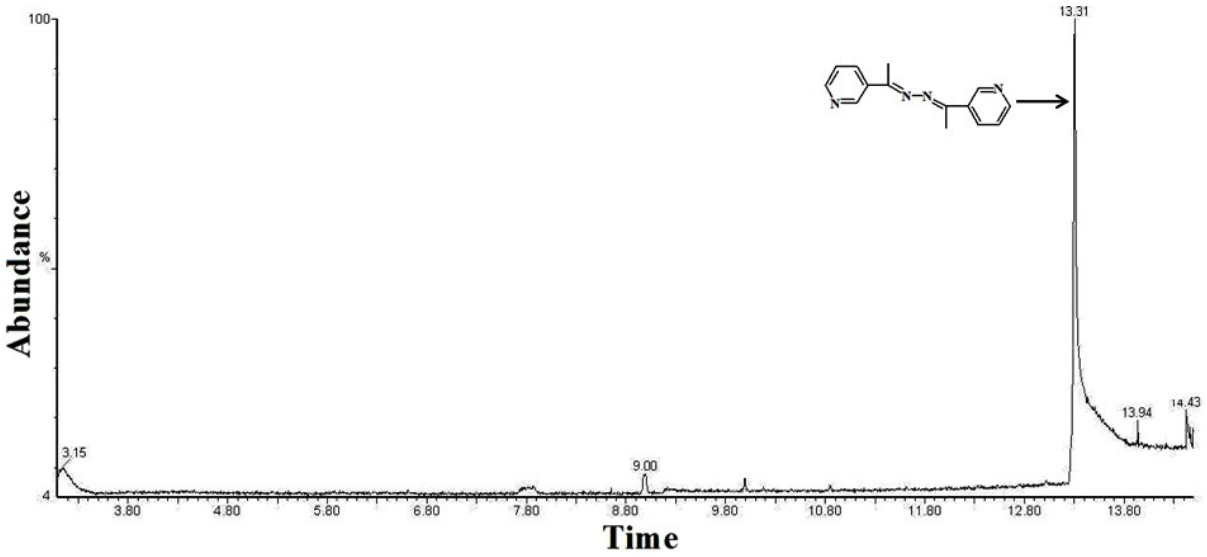

Fig. S2 GC trace of the 3-bpdh ligand in reaction medium at time interval 13.31 mins. The peak indicated above was identified by GC-MS spectra (see below).

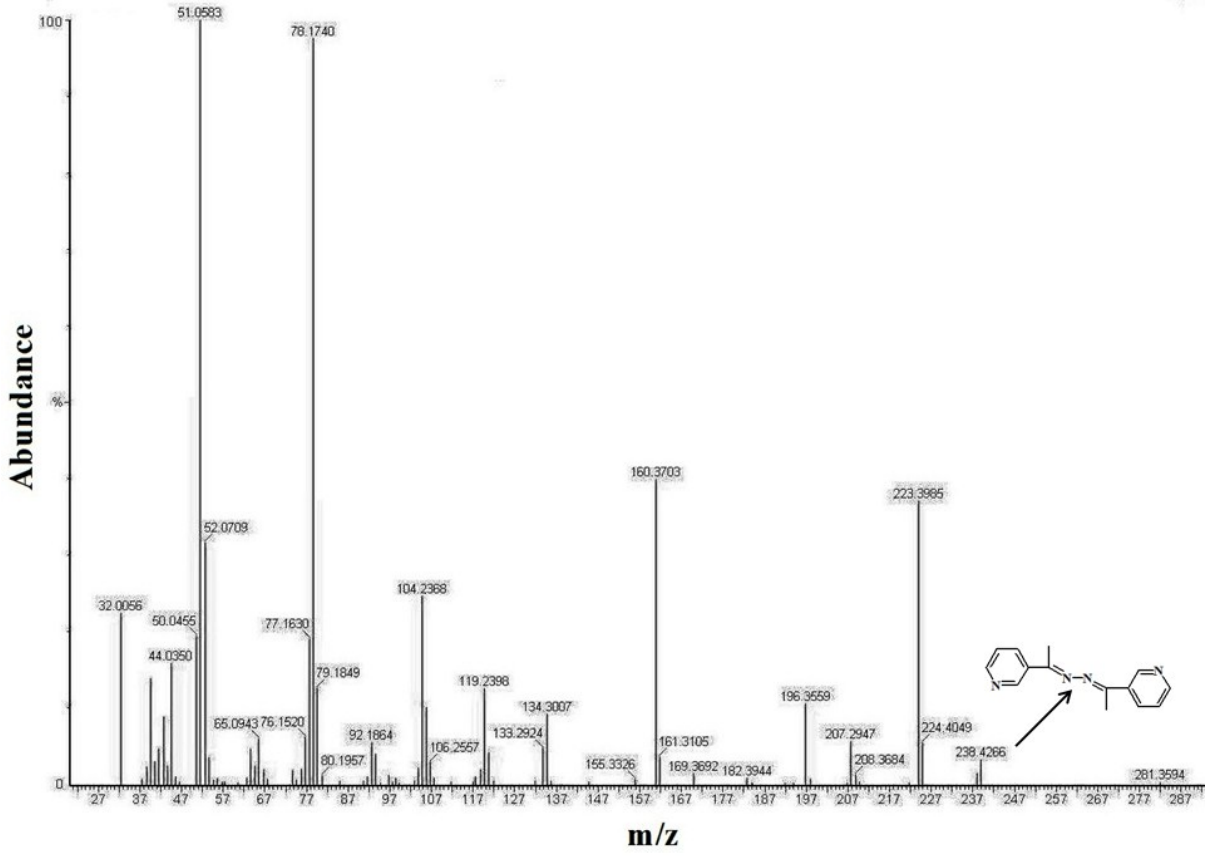

Fig. S3 Mass spectrum of the peak at 10.37 min showing the value at 238.4266 of 3-bpdh ligand in reaction mixture.

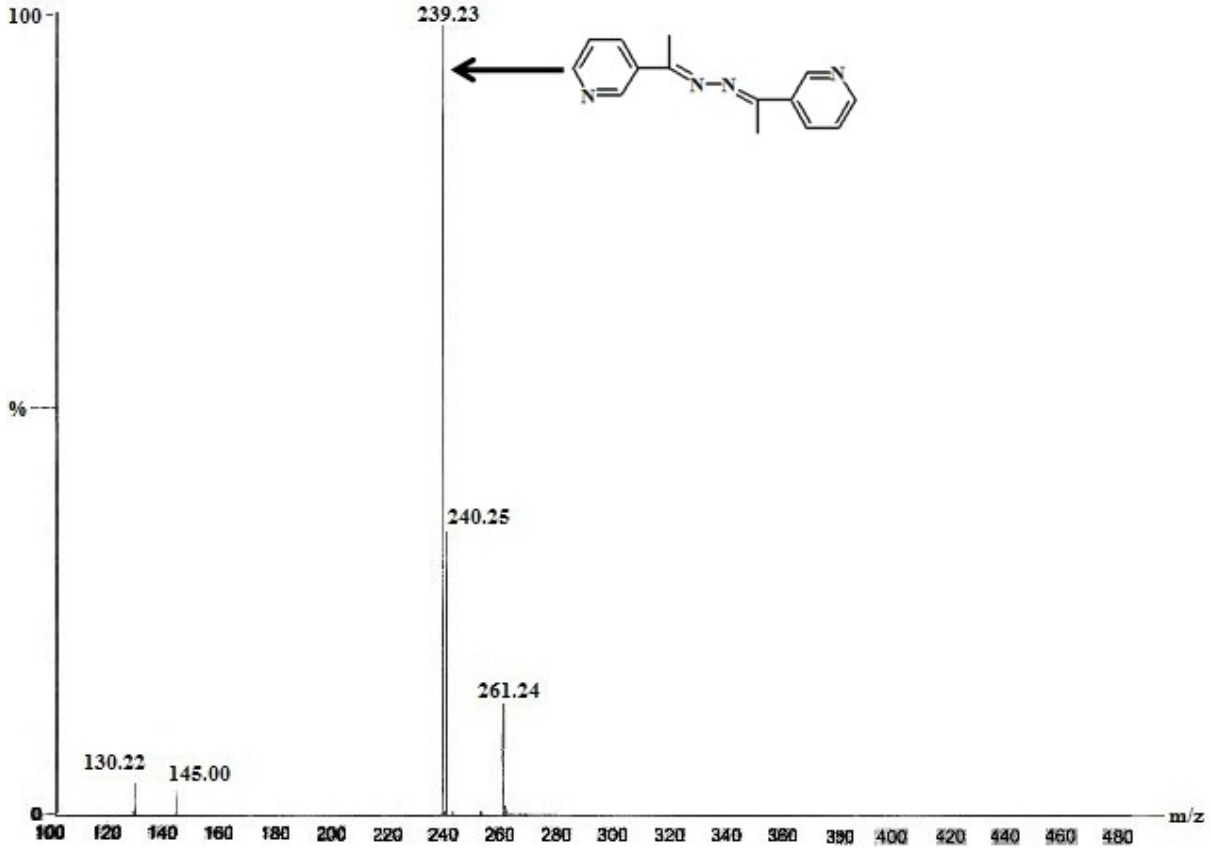

Fig. S4 ESI mass spectrum of yellow residue in reaction mixture.

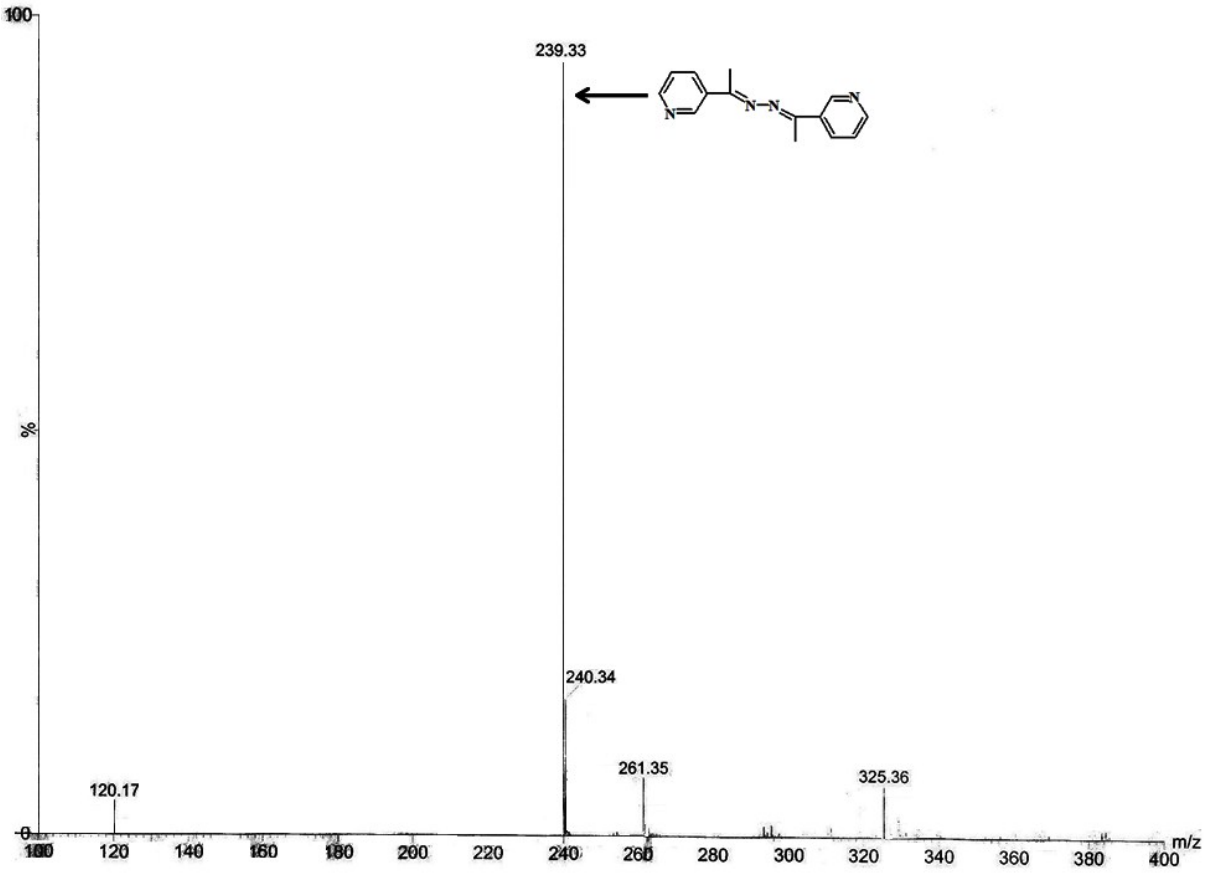

Fig. S5 ESI mass spectrum of pure 3-bpdh ligand.

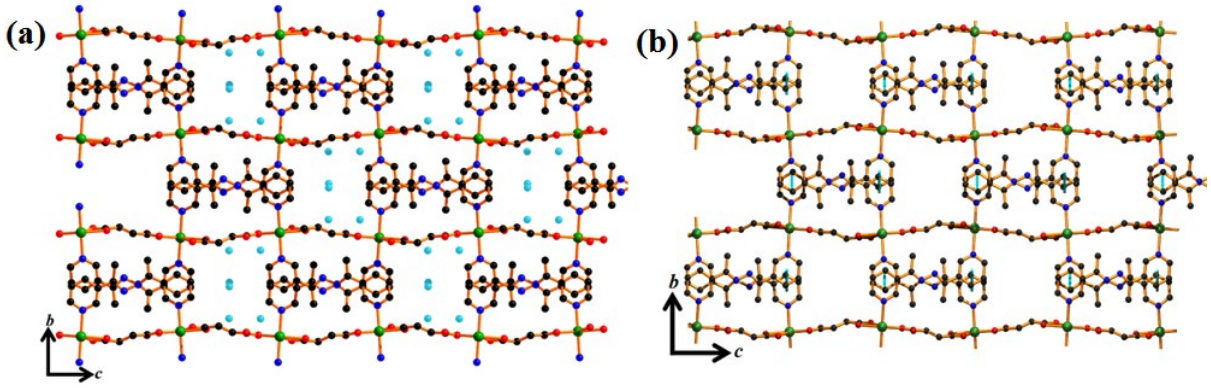

Fig. S6 (a) 3D porous framework showing 1D chanel of guest water molecules along *a*-axis. (b) Supramolecular 3D structure through intramolecular π-π interactions in **2** (π-π interactions: cyan dotted lines).

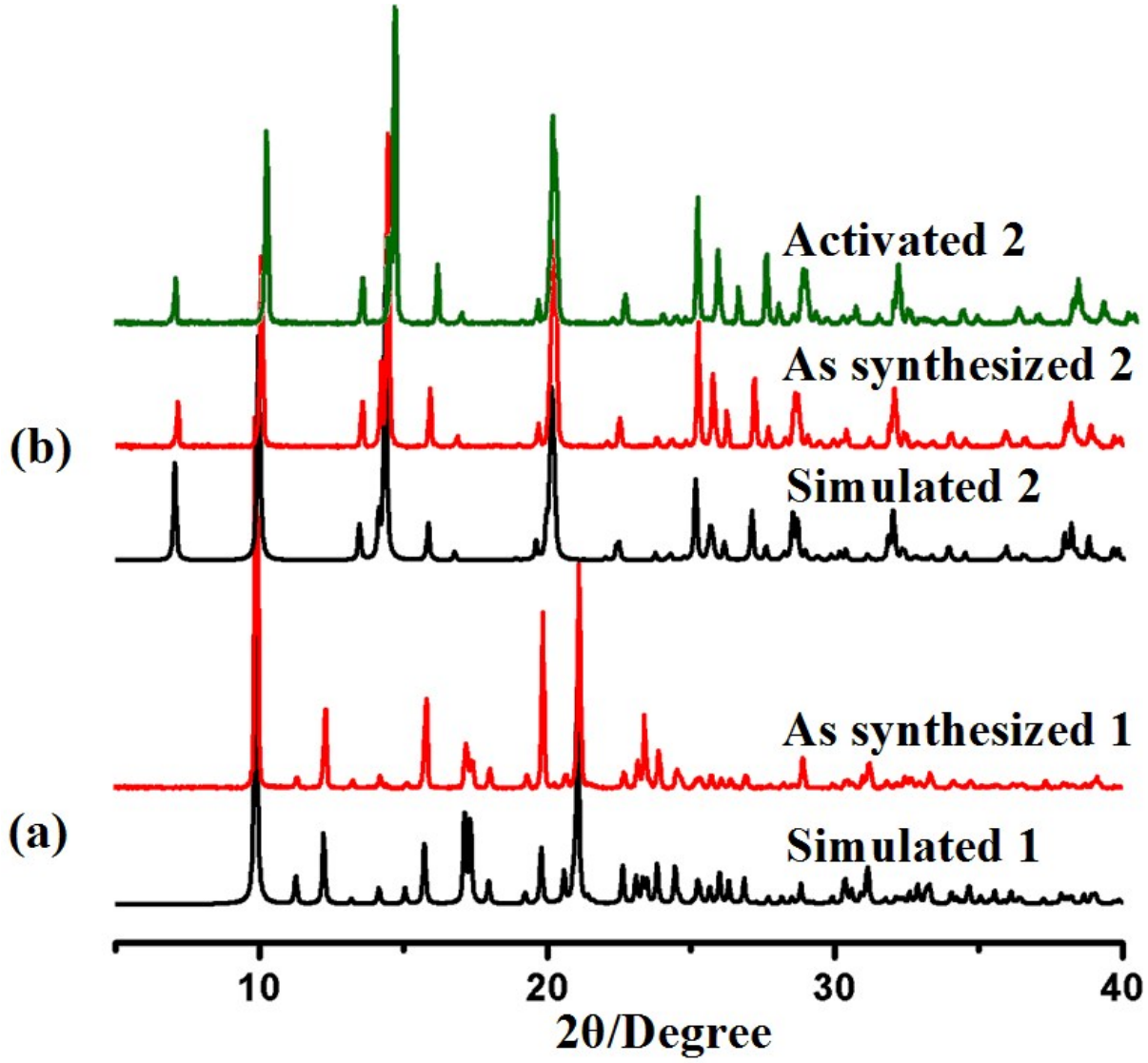

Fig. S7 PXRD spectra of **(a) s**imulated and as synthesized of **1**; **(b)** Simulated, as synthesized, activated at 130 ^{o}C.

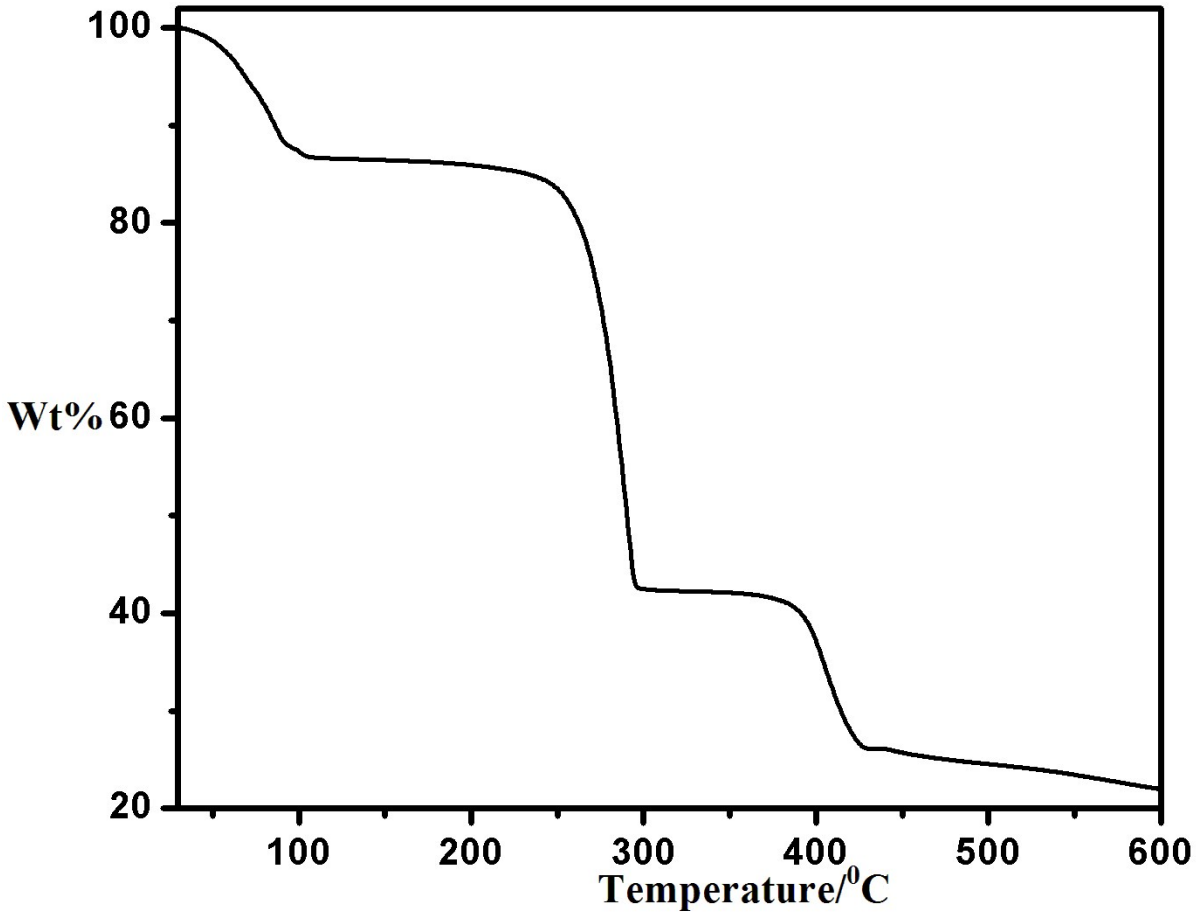

Fig. S8 Thermogravimetric analysis of **2** in the temperature range 30-600 ^{o}C.

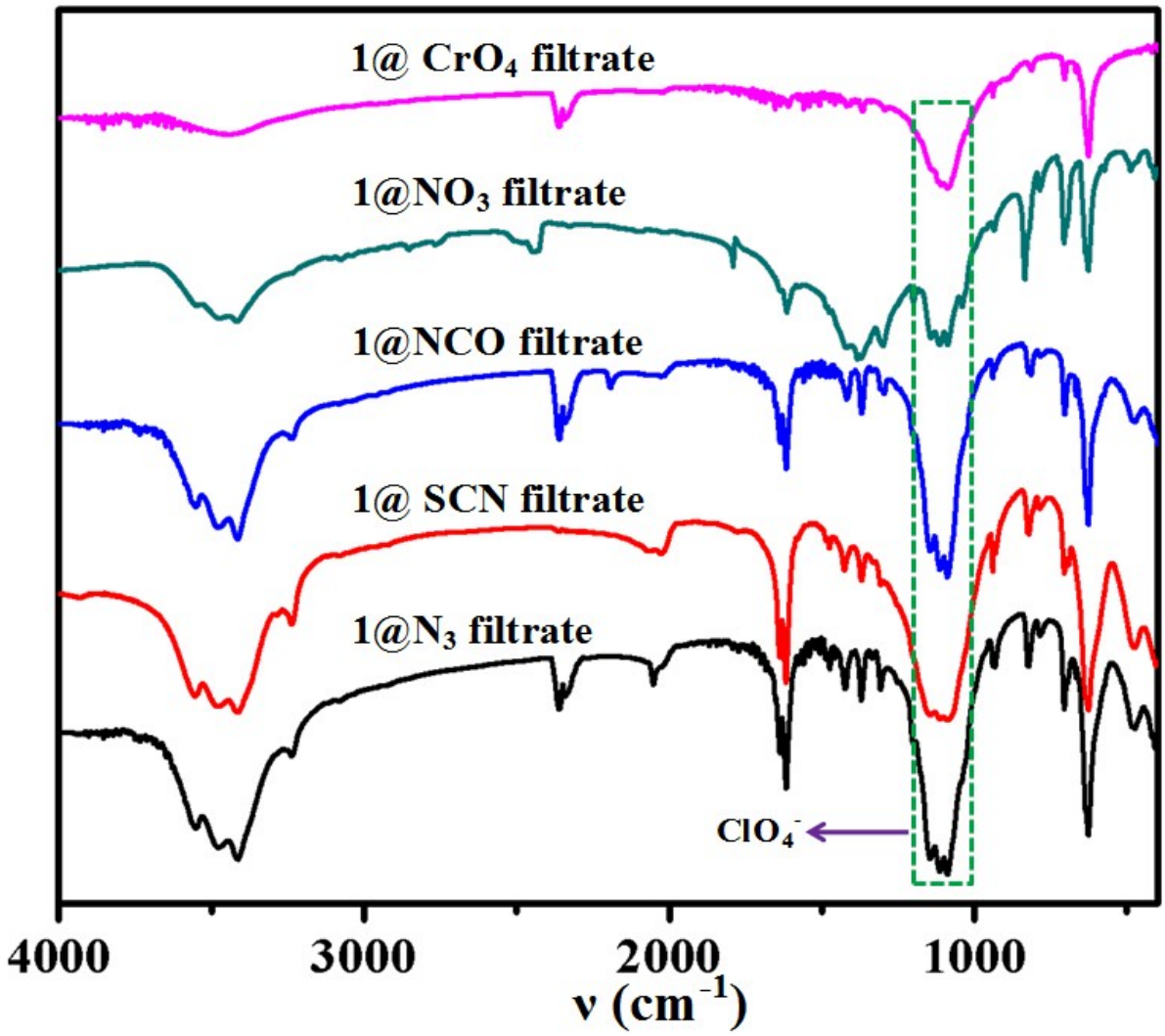

Fig. S9 Combined IR spectra of the filtrate after anion-exchange with the corresponding anions which show the presence of perchlorate ions in all the cases.

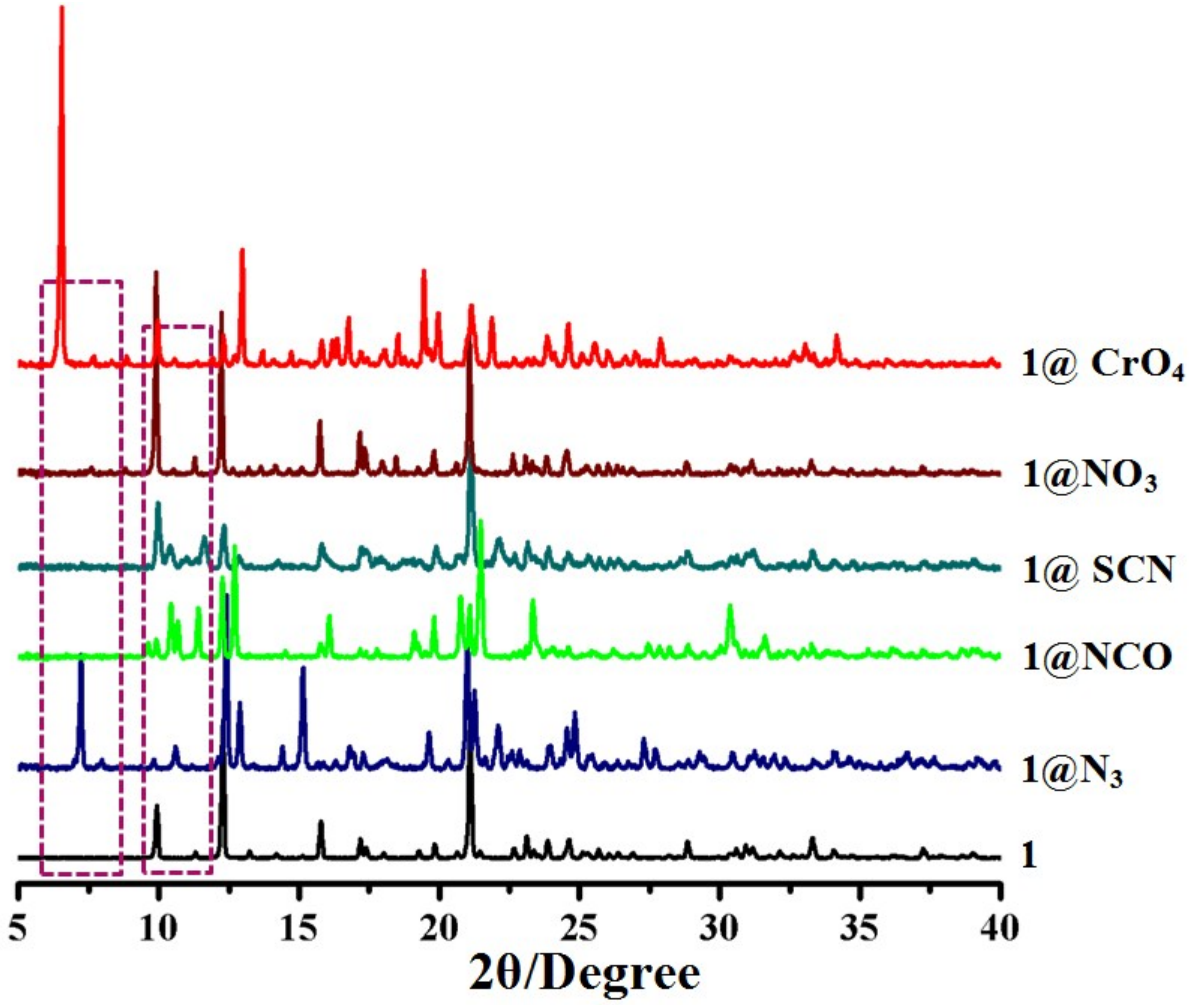

Fig. S10 Combined PXRD spectra of complex **1** and its anion-exchanged solids showing slight changes with highlighted bands.

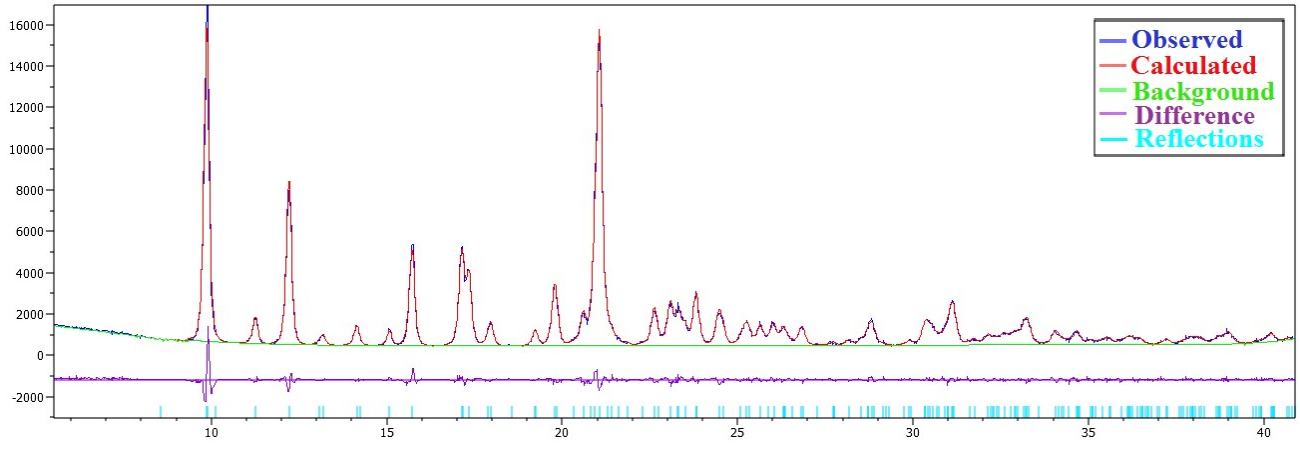

Fig. S11 LeBail fitting of X-ray powder pattern of **1@NO_3.**

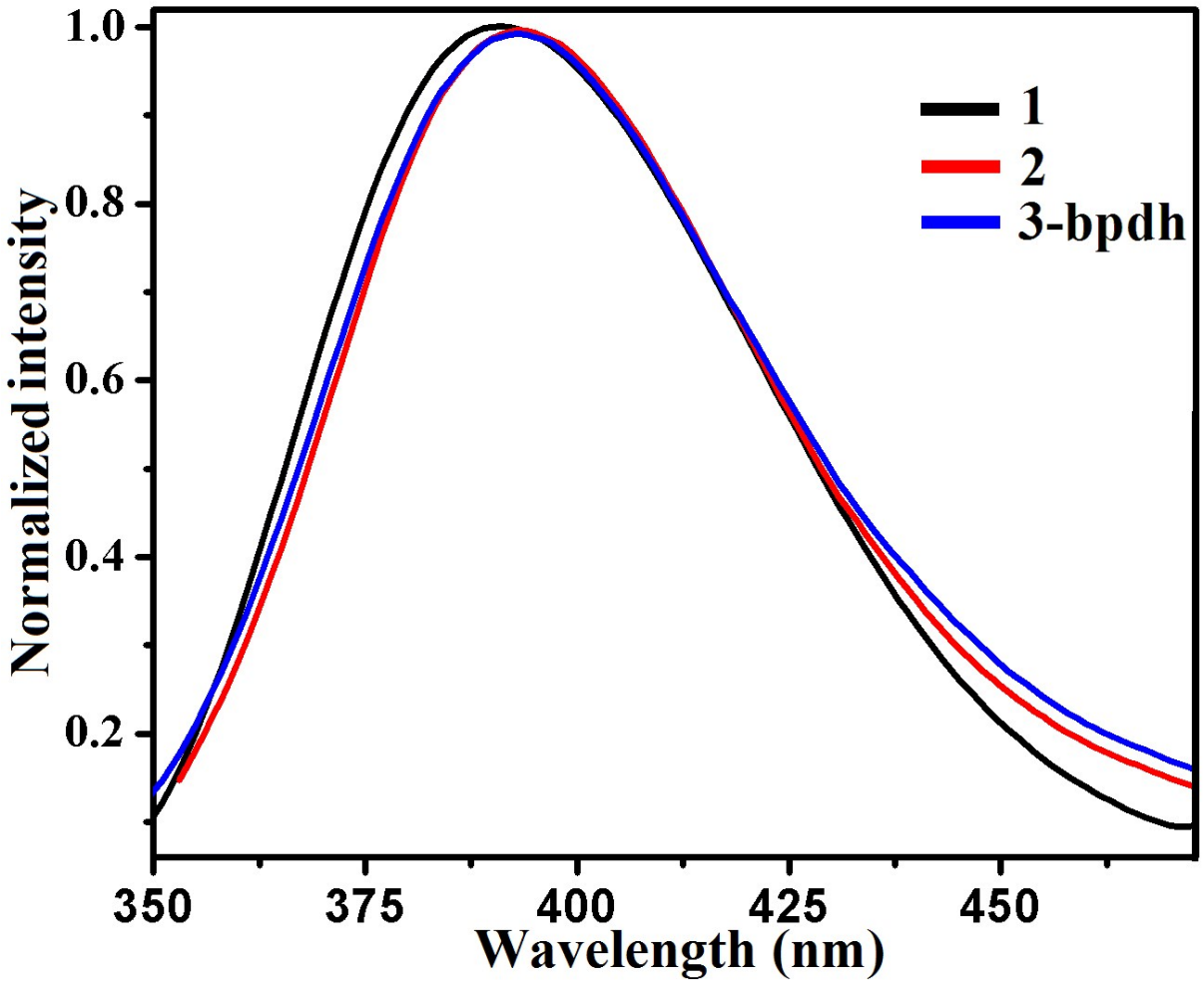

Fig. S12 Photoluminescence spectra of complexes **1-2** with free 3-bpdh ligand.

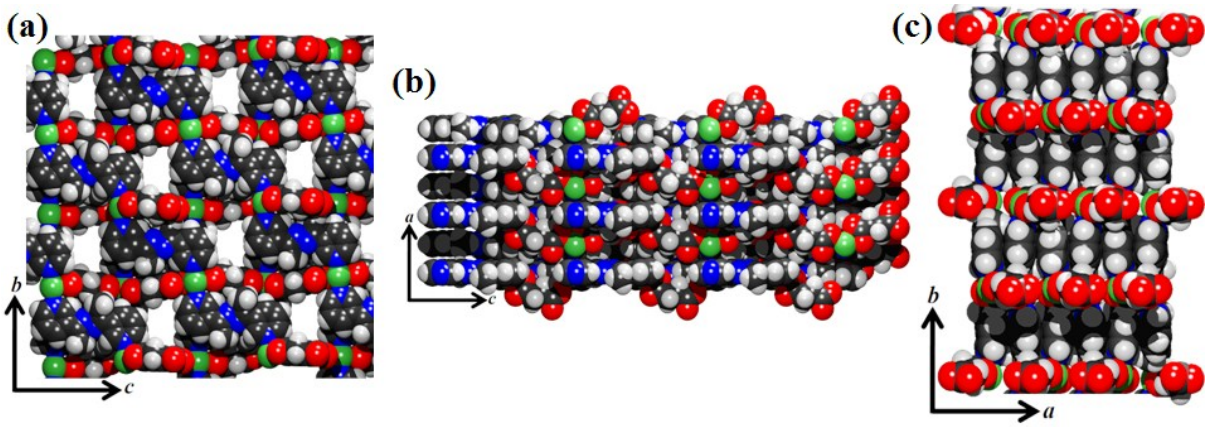

Fig. S13 (a, b, c) Space filling model of **2** viewed along crystallographic *a*, *b* and *c*-axis respectively (guest water molecules are removed for clarity).

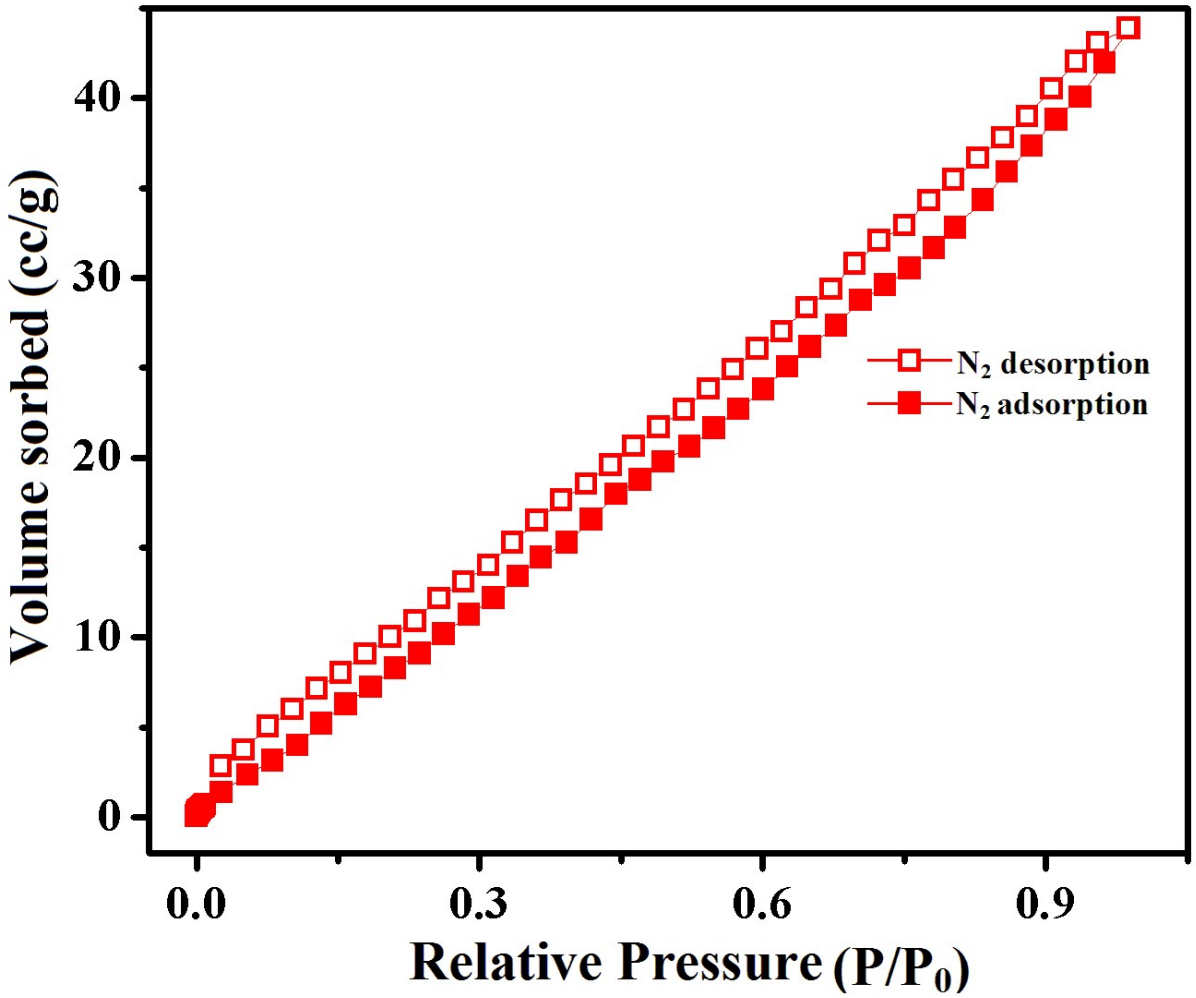

Fig. S14 N_2 adsorption isotherms for **2** at 77K: adsorption (filled squares), desorption (open squares).

Table S1 π-π interactions in **2**

2	ring(i) → ring(j)	distance of centroid(i) from ring(j),(Å)	dihedral angle (i,j) (deg)	Distance between the (i,j) ring centroids,(Å)
	R(1)→R(1)^{i}	3.685(3)	8	3.4358(11)
	R(1)→R(1)^{ii}	3.685(3)	8	-3.5759(11)
	R(2)→R(2)^{i}	4.000(3)	1	3.5263(12)
	R(2)→R(2)^{ii}	4.000(3)	1	3.5591(12)

Symmetry code: i = -1/2+X, -1/2-Y, Z; ii = 1/2+X, -1/2-Y, Z.

R(i)/R(j) denotes the ith/jth rings in the corresponding structures: R(1)=N(1)/C(1)/C(2)/C(3)/C(4)/C(5); R(2)=N(4)/C(10)/C(11)/C(12)/C(13)/C(14).

Table S2 Comparison of cell parameter of **1** with the indexed cell parameter (using TREOR 90 programme) **1@NO_3** from the powder data

	1	**1@NO_3**
Crystal system	Monoclinic	Monoclinic
Space group	*P21/n*	*P21/m*
a/ Å	8.840	8.8339
b/ Å	17.934	17.8997
c/ Å	10.458	10.4245
α/°	90.000	90
β/°	98.701	98.89
γ/°	90.000	90
V/ $Å^3$	1638.9	1628.58