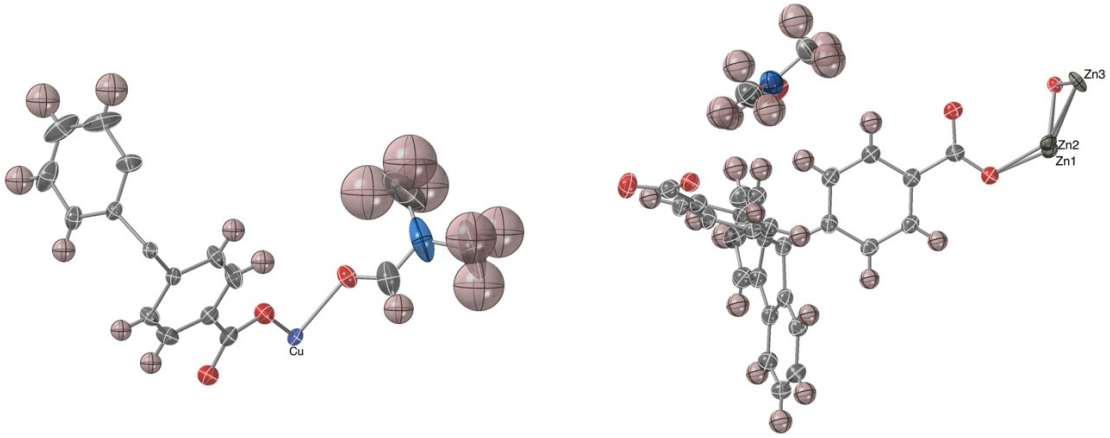
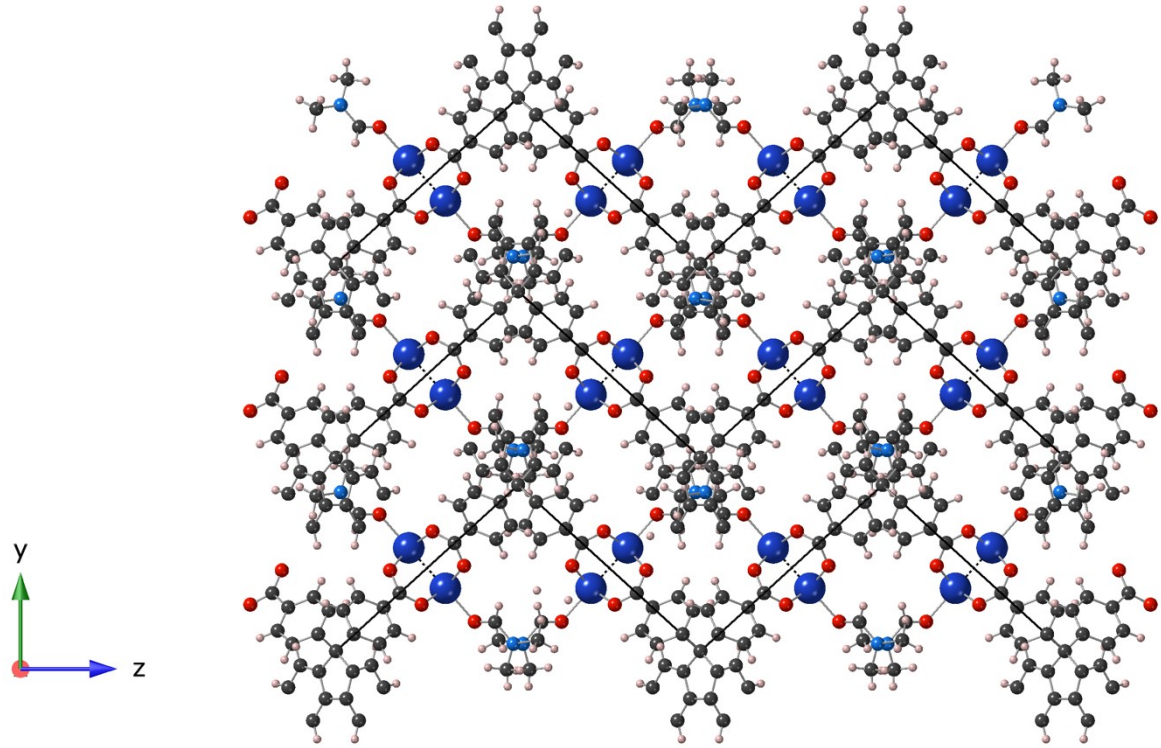
Exploring the formation of Coordination Polymers based on dicarboxylic ligand derived from fluorene and their adsorption abilities

Nizami Israfilov,[a] Nathalie Kyritsakas,[b] Abdelaziz Jouaiti[a*] and Sylvie Ferlay[a*]



a



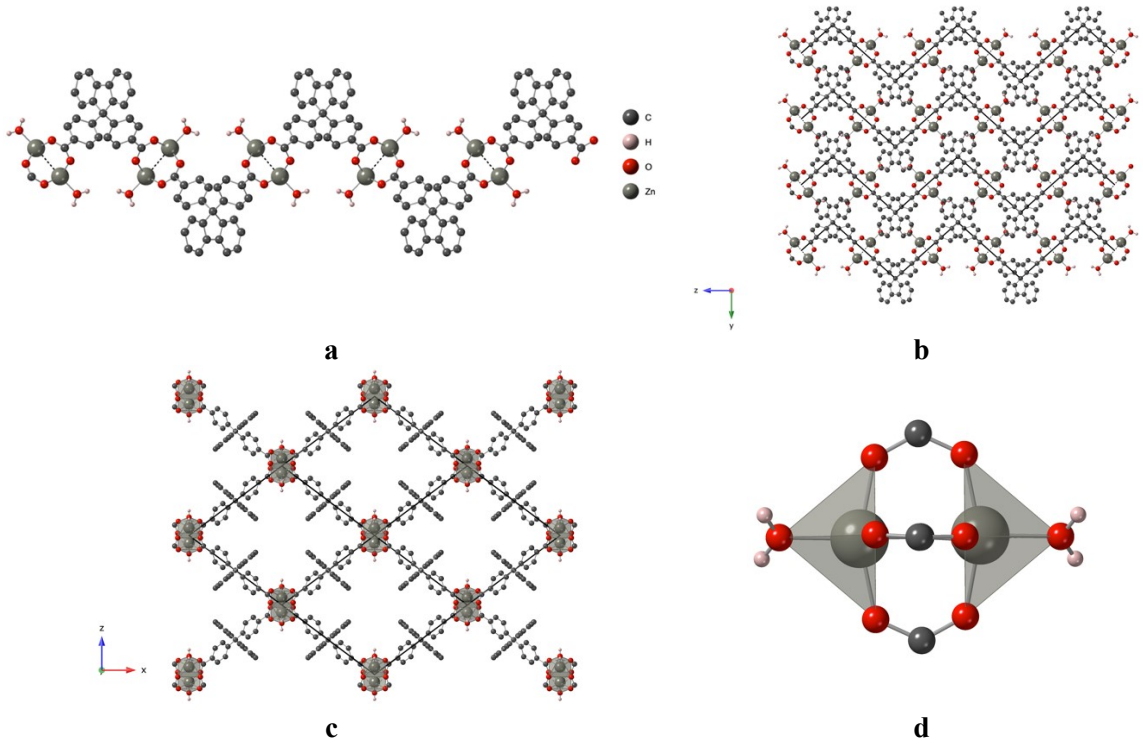
b

Figures S1: a) The asymmetric units for of **1** (left) and **2**(right). Thermal ellipsoids are at 50% probability b) the stacking of the planes in **1**

CCDC	2383979 (for comparison)	2379879	2379878
	1	**4**	**3**
Empirical formula	$C_{30}H_{23}CuNO_5$,solvent	$C_{27}H_{18}O_5Zn$, solvent	$C_{27}H_{18}CuO_5$
Formula weight	541.03	487.78	485.95
Temperature	120 (2) K		173(2) K
Wavelength	0.71073 A		
Crystal system, space group	Orthorhombic *C* mca		Monoclinic, *C* 2/c
Unit 2D Cocell dimensions	a = 23.4998(8) Å α = 90 deg. b = 18.6597(6)Å β = 90 deg. c = 17.5655(6) Å γ = 90 deg.	a = 23.673(4) Å α = 90 deg. b = 18.677(4) Å β = 90 deg. c = 17.763(4) Å γ = 90 deg.	a = 28.644(6) Å α = 90 deg. b = 7.1941(14) Å β = 113.655(4) deg. c = 23.764(5) Å γ = 90 deg.
Volume	7702.5(4) $Å^3$	7854(3) $Å^3$	4485.6(16)
Z, Calculated density	8, 0.933 Mg/m^3	8, 0.825 Mg/m^3	8, 1.439 Mg/m^3
Absorption coefficient	0.594 mm^{-1}	0.646 mm^{-1}	1.010 mm^{-1}
F(000)	2232	2000	1992
Crystal size	0.150 x 0.120 x 0.100 mm	0.16 x 0.12 x 0.10 mm	0.12 x 0.09 x 0.09 mm
Theta range for data collection	2.472 to 27.898 deg.	1.720 to 27.932 deg.	2.88 to 27.00 deg.
Limiting indices	-30<=h<=26 -24<=k<=23 -23<=l<=23	-31<=h<=28, -24<=k<=16, -23<=l<=22	-36<=h<=36, -9<=k<=7, -30<=l<=24
Reflections collected / unique	44079 / 4717 [R(int) = 0.0763]	28888 / 4819 [R(int) = 0.1231]	12288/ 4300 [R(int) = 0.0347]
Goodness-of-fit on F^2	1.046	1.021	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0464, wR2 = 0.1285	R1 = 0.0932, wR2 = 0.2610	R1 = 0.0641, wR2 = 0.0737
R indices (all data)	R1 = 0.0631, wR2 = 0.1400	R1 = 0.1622, wR2 = 0.3010	R1 = 0.1694, wR2 = 0. 0.1812
Largest diff. peak and hole	0.656 and -0.633 e. $Å^3$	0.614 and -1.373 e. $Å^3$	1.911 and -1.468 e. $Å^3$

Table S1. Crystallographic data for **1** (for comparison), **4** and **3**

Compound 4 (isomorphous to 1)

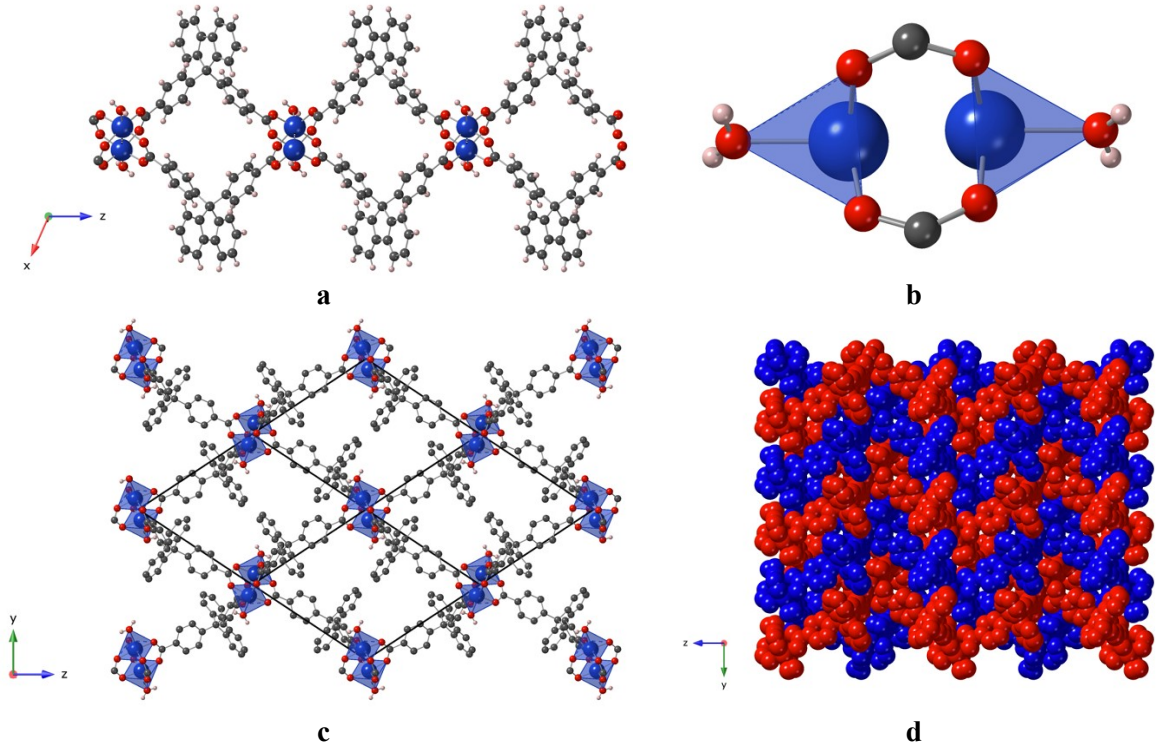


Figures S2: Portion of the X-ray structure for **4** showing a) the formation of the 2D neutral coordination network resulting from the bridging of consecutive ligand $\mathbf{L^{2-}}$ by Zn^{2+} b) view of the corrugated plane along the *b* axis, c) view of the grid in the xOz plane c) details of the environment of the Zn^{2+} cations. H atoms are not all presented for clarity.

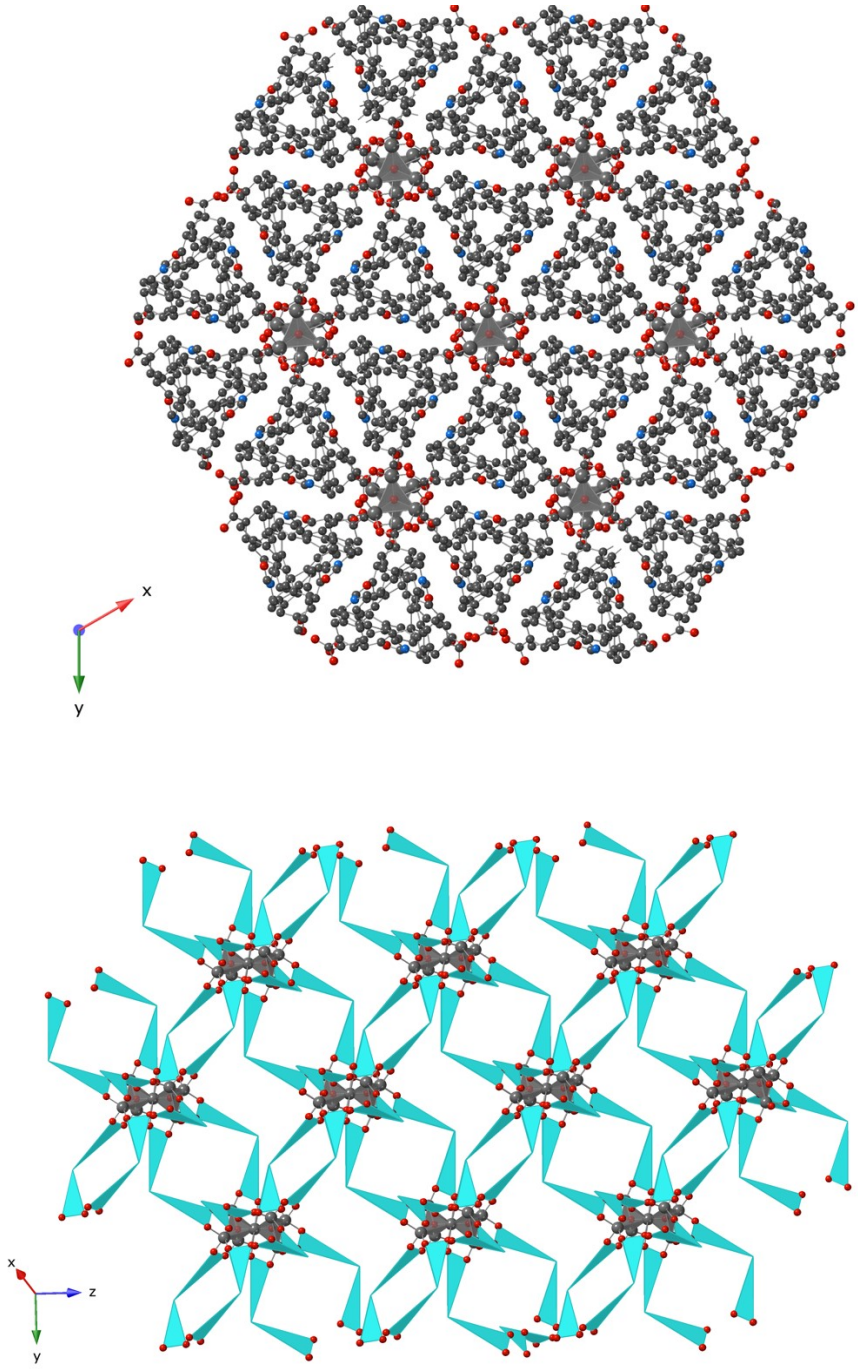
	1	**4**	**3**
M–O (Å)	1.9619(15) 1.9684(16)	2.032(5) 2.035(5)	1.951(3) 1.953(3) 1.972(3) 1.980(3)
$M–O_{(solvent)}$ (Å)	2.142(3)	1.990(7)	2.205(3)
M-M (Å)	2.6302(7)	2.994(2)	2.5938(11)
α angle (figure 1) (°)	102.19	103.88	101.82

Table S2. Selected bonds lengths (Å) around the M(II) ions for **1**, **4** and **3**

Compound 3



Figures S3: Portion of the X-ray structure for **3** showing a) the formation of the 2D neutral coordination network resulting from the bridging of consecutive ligand $\mathbf{L}^{2-}$ by Cu^{2+} b) details of the environment of the Cu^{2+} cations c) view of the grid in the yOz plane, and d) space filling representation of interpenetration of two 2D grids. H atoms are not all presented for clarity.



Figures S4: Portion of the X-ray structure for 3D **2** showing the resulting 3D coordination polymer, with uncoordinated DMF molecules located in the free space. H atoms and the disordered Zn cations are not represented, for the sake of clarity.

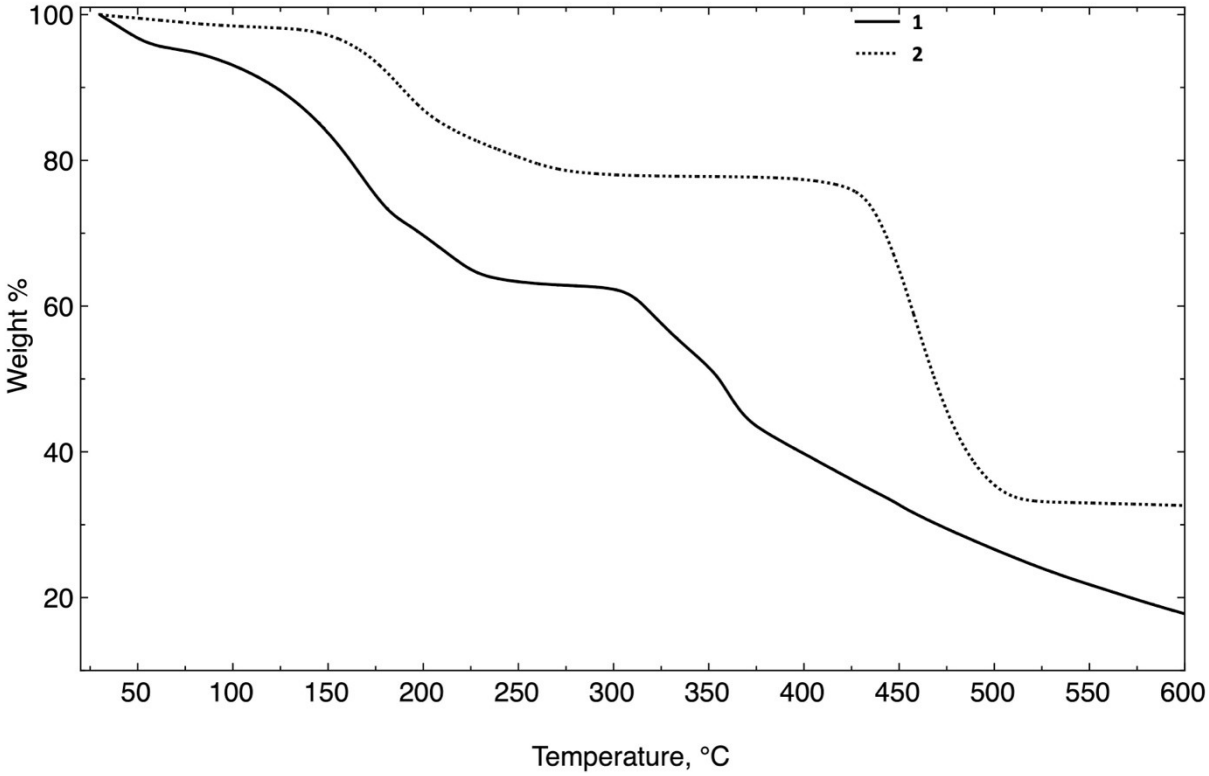
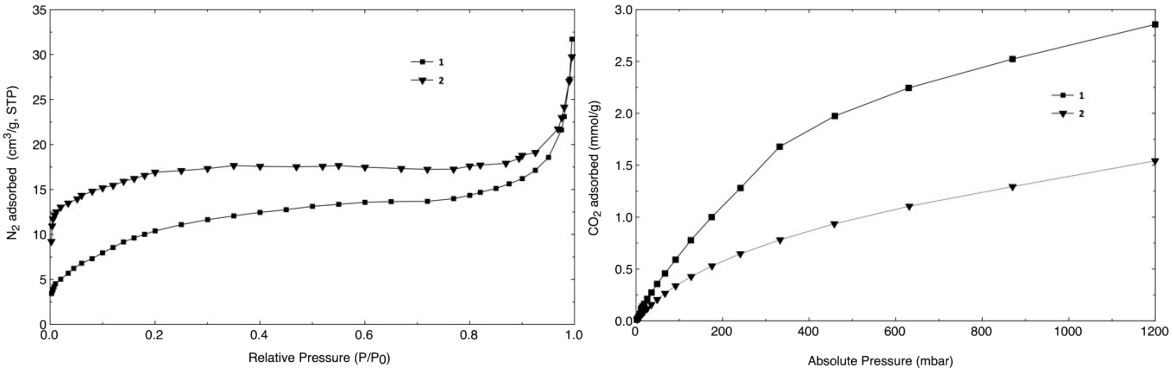


Figure S5. For **1** and **2**, TGA traces between T = 30°C and 500°C.



Figures S6. For **1** and **2**, adsorption isotherms a) N_2 at T = 77 and b) CO_2 at T = 273 K.

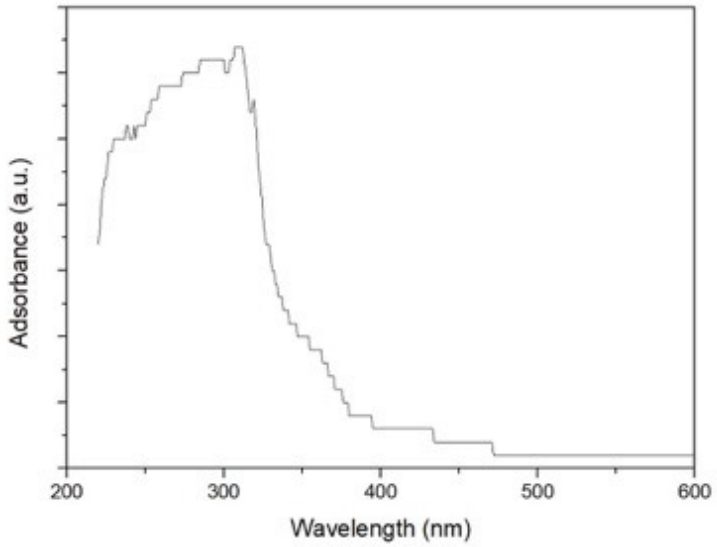


Figure S7. For **2**, solid-state reflectance spectra at RT.

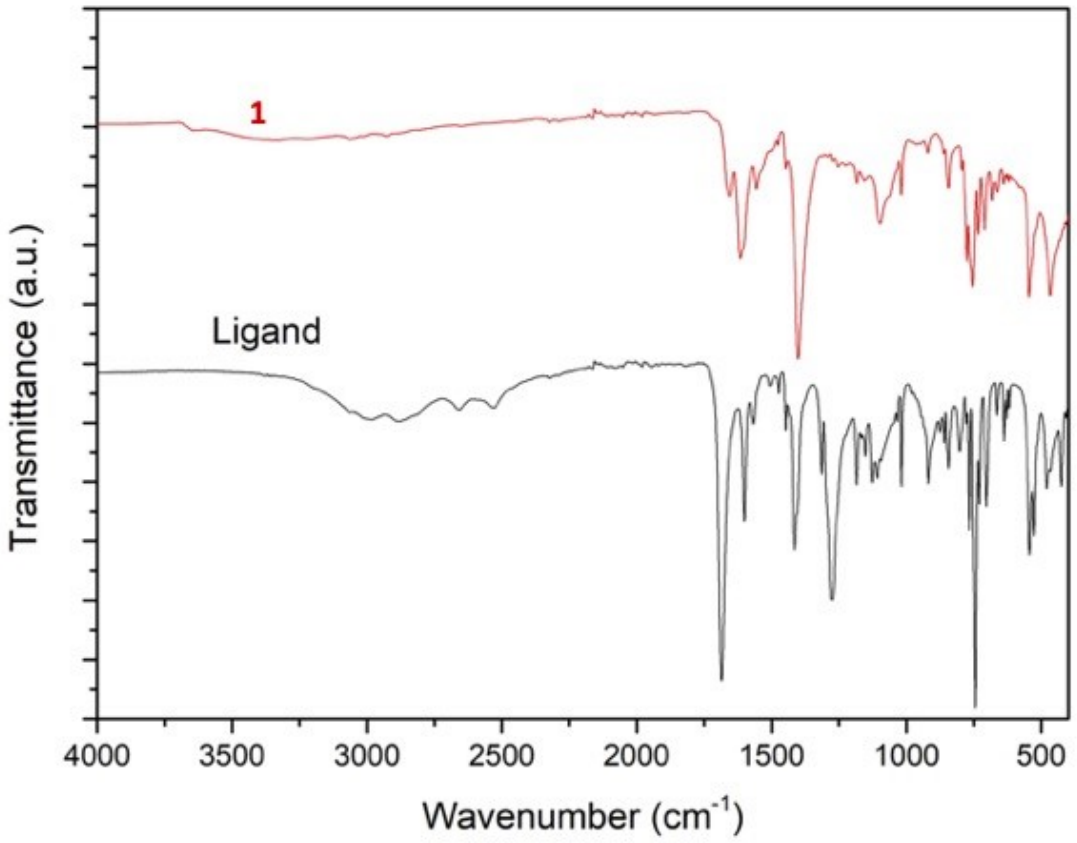


Figure S8. For **1**, IR spectrum in the solid-state (ATR), compared to the one of the ligand H_2**L**.

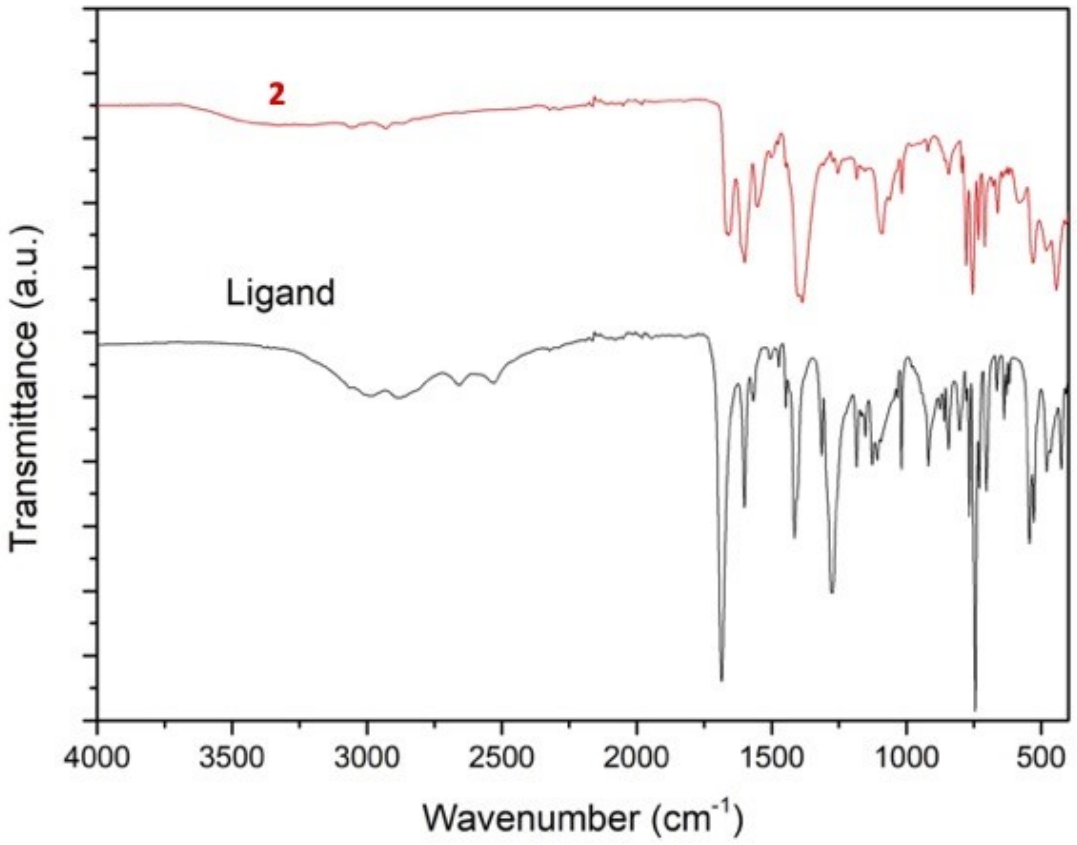


Figure S9. For **2**, IR spectrum in the solid-state (ATR), compared to the one of the ligand H_2**L**.