Electronic Supplementary Information (ESI) for:

Zn- and Cd-based coordination polymers with a novel anthracene dicarboxylate ligand for highly selective detection of hydrogen peroxide

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1. Crystal structure parameters and bond length and angles for 1, 2 and H_2L

Table S1 Crystal structure parameters for **1** and **2** and **H_2L**

Compound	**1**	**2**	**H_2L**
Empirical formula	$C_{38}H_{34}N_2O_6Zn$	$C_{38}H_{34}N_2O_6Cd$	$C_{40}H_{40}N_2O_6$
Molecular formula	$C_{32}H_{20}O_4Zn \cdot 2$ DMF	$C_{32}H_{20}CdO_4 \cdot 2$ DMF	$C_{32}H_{22}O_4 \cdot 2$ DMF
Formula weight	680.04	727.07	644.74
Temperature [K]	130(2)	130(2)	130(2)
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	*Pc*	$P2_1/n$	$P\bar{1}$
Unit cell dimensions			
a [pm]	1761.62(5)	805.84(2)	788.64(4)
b [pm]	910.37(2)	940.51(2)	920.43(4)
c [pm]	1039.73(3)	4192.84(8)	1191.98(6)
α [°]	90	90	76.155(4)
β [°]	105.338(3)	91.246(2)	81.642(4)
γ [°]	90	90	75.045(4)
Volume [nm^3]	1.60805(8)	3.1770(1)	0.80842(7)
Z	2	4	1
$\rho_{(calc.)}$ [Mg/m^3]	1.404	1.520	1.324
μ [mm^{-1}]	0.815	0.739	0.089
F(000)	708	1488	342
Crystal size [mm^3]	0.20 x 0.20 x 0.05	0.26 x 0.15 x 0.05	0.30 x 0.20 x 0.05
Θ_{min} - Θ_{max} [°]	2.237 - 32.555	1.943 - 26.406	1.767 - 30.623
Index ranges	$-24 \le h \le 26$ $-13 \le k \le 13$ $-15 \le l \le 15$	$-10 \le h \le 10$ $-11 \le k \le 11$ $-37 \le l \le 51$	$-10 \le h \le 10$, $-12 \le k \le 13$, $-17 \le l \le 16$
Reflections collected	21936	7479	11121
Independent reflections [$R_{(int)}$]	9615 [0.0422]	7479 [0.0474]	4475 [0.0228]
Completeness (Θ [°])	100.0 % (30.5)	100.0 % (25.4)	100.0 % (28.3)
T_{Min} / T_{Max}	1.00000 / 0.95114	1.00000 / 0.80567	1.00000 / 0.99331
Restraints / parameters	2 / 428	28 / 465	41 / 352
Goodness-of-fit on F^2	1.059	0.983	1.015
Absolute structure parameter	-0.004(6)	-	-
R1, wR2 [I>2σ(I)]	0.0458, 0.1044	0.0387, 0.0860	0.0500, 0.1171
R1, wR2 (all data)	0.0577, 0.1116	0.0489, 0.0943	R 0.0702, 0.1291
Residual electron density [$e \cdot Å^{-3}$]	1.373 / -0.463	1.386 / -0.970	0.474 / -0.291
Comments	-	Twinned crystal	

Table S2. Bond lengths [pm] and angles [°] for $\{[Zn(L)(DMF)_2]\}_n$ (**1**).

Zn(1)-O(1)	191.7(3)
Zn(1)-O(4)	197.7(3)
Zn(1)-O(5)	197.1(3)
Zn(1)-O(3)’	250.9(3)
Zn(1)-O(6)	204.7(3)
Zn(1)-C(32)’	257.3(4)
O(1)-C(1)	127.1(5)
O(2)-C(1)	123.3(5)
O(3)-C(32)	128.0(5)
O(4)-C(32)	123.1(4)
O(5)-C(35)	123.6(5)
O(6)-C(38)	125.0(5)
O(1)-Zn(1)-O(5)	124.2(1)
O(1)-Zn(1)-O(3)’	115.9(1)
O(5)-Zn(1)-O(3)’	116.0(1)
O(1)-Zn(1)-O(6)	102.9(1)
O(5)-Zn(1)-O(6)	93.3(1)
O(3)’-Zn(1)-O(6)	93.5(1)
O(2)-C(1)-O(1)	125.1(4)
O(4)-C(32)-O(3)	121.7(3)

Symmetry transformations used to generate equivalent atoms: ‘: x-1,-y,z+1/2

Table S3. Bond lengths [pm] and angles [°] for $\{[Cd(L)(DMF)]\cdot DMF\}_n$ (**2**).

Cd(1)-O(1)	219.3(3)
Cd(1)-O(5)	227.0(3)
Cd(1)-O(2)’	228.8(3)
Cd(1)-O(4)’’	232.6(2)
Cd(1)-O(3)’’	240.0(3)
Cd(1)-O(4)’’’	243.9(3)
O(1)-C(1)	128.2(5)
O(2)-C(1)	124.9(5)
O(3)-C(32)	125.0(5)
O(4)-C(32)	128.4(5)
O(5)-C(35)	124.9(5)
O(1)-Cd(1)-O(5)	115.8(1)
O(1)-Cd(1)-O(2)’	101.1(1)
O(5)-Cd(1)-O(2)’	86.8(1)
O(1)-Cd(1)-O(4)’’	141.9(1)
O(5)-Cd(1)-O(4)’’	95.4(1)
O(2)’-Cd(1)-O(4)’’	101.86(9)
O(1)-Cd(1)-O(3)’’	97.3(1)
O(5)-Cd(1)-O(3)’’	146.7(1)
O(2)’-Cd(1)-O(3)’’	83.8(1)
O(4)’’-Cd(1)-O(3)’’	55.9(1)
O(1)-Cd(1)-O(4)’’’	87.5(1)
O(5)-Cd(1)-O(4)’’’	83.4(1)
O(2)’-Cd(1)-O(4)’’’	169.1(1)
O(4)’’-Cd(1)-O(4)’’’	74.5(1)
O(3)’’-Cd(1)-O(4)’’’	101.9(1)
O(2)-C(1)-O(1)	123.5(4)
O(3)-C(32)-O(4)	121.8(3)

Symmetry transformations used to generate equivalent atoms:
‘: -x+1,-y+1,-z+1 ‘’: x-3/2,-y+1/2,z-1/2 ‘’’: -x+3/2,y+1/2,-z+3/2

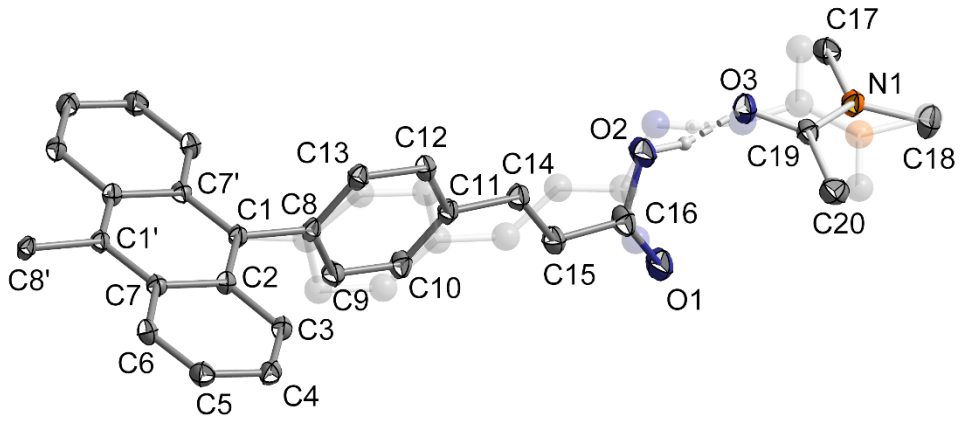

Figure S1 Labelling scheme and ellipsoidal plot of **H_2L**·2DMF (ellipsoids are drawn with 50% probability; most hydrogen atoms are omitted for clarity). Only half of the molecule is given, as it is located on a centre of inversion. The disordered part (7%) is presented in transparent mode.

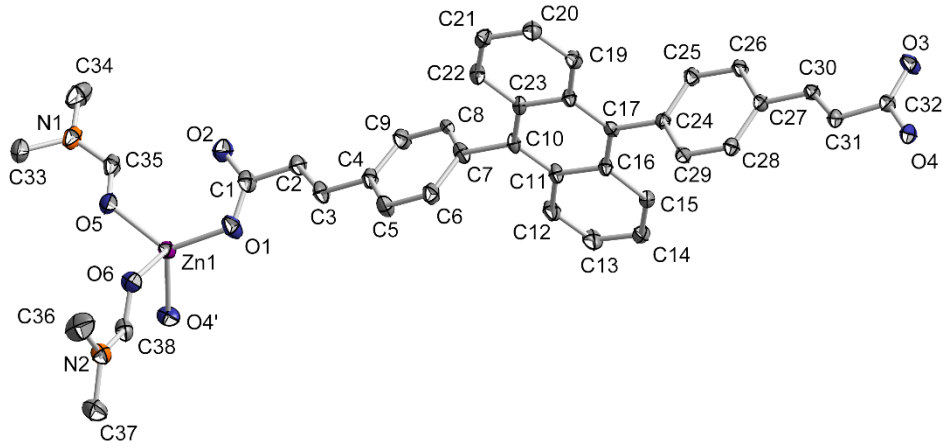

Figure S2 Labelling scheme and ellipsoidal plot of **1** (ellipsoids are drawn with 50% probability; hydrogen atoms are omitted for clarity).

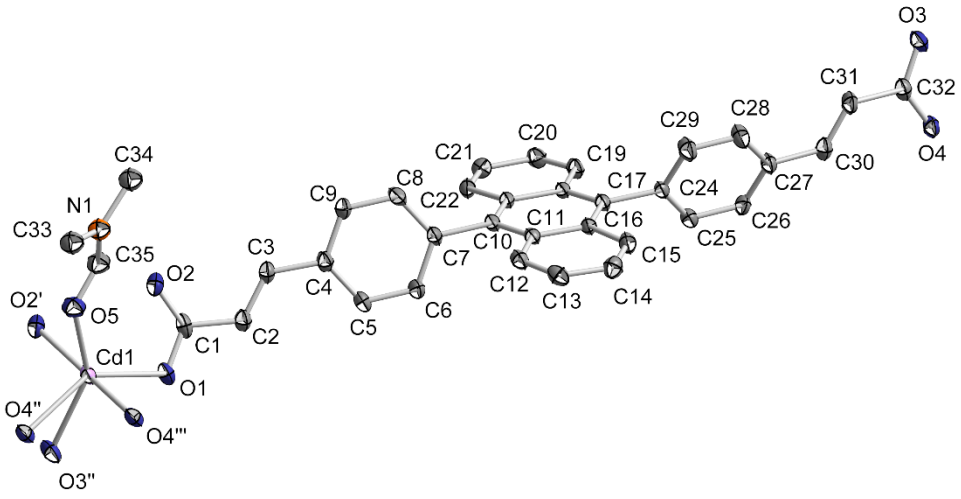

Figure S3 Labelling scheme and ellipsoidal plot of **2** (ellipsoids are drawn with 50% probability; all hydrogen atoms are omitted for clarity).

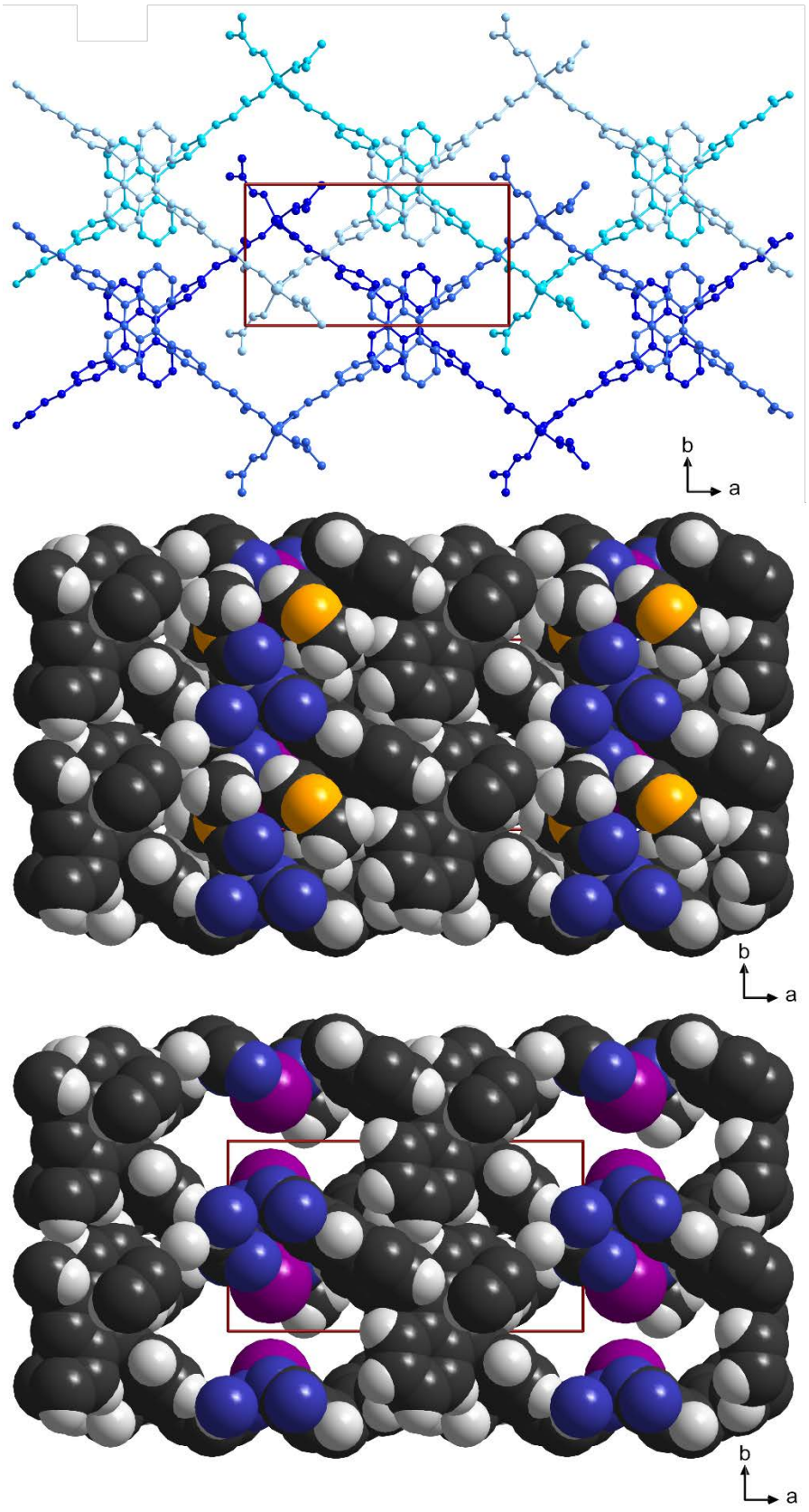

Figure S4 Molecular packing of the one-dimensional "chain-structured" coordination polymer **1** (ball and stick model with chains in different colours (top)). In space-filling mode with (middle) and without (bottom) solvent molecules; channels parallel to the *c* axis of the unit cell are observed. The unit cell is visualised in red.

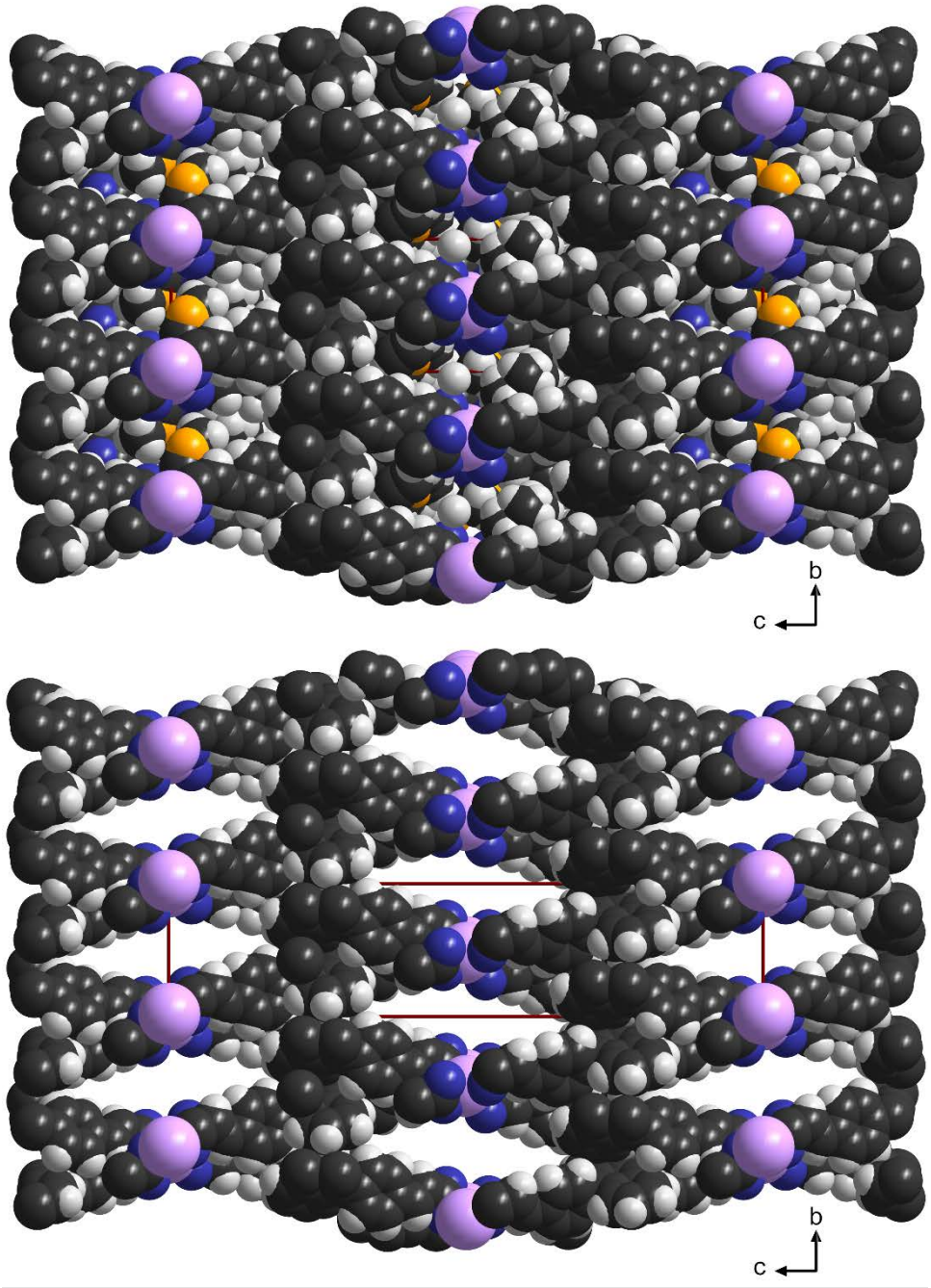

Figure S5 Molecular packing diagram of the three-dimensional coordination polymer **2** in space-filling mode with (top) and without (bottom) solvent molecules (DMF). The DMF molecules are located in elliptical channels of dimensions 1200 pm x 400 pm, parallel to the *a* axis of the unit cell. The unit cell is visualised in red.

2. Powder X-ray diffractograms

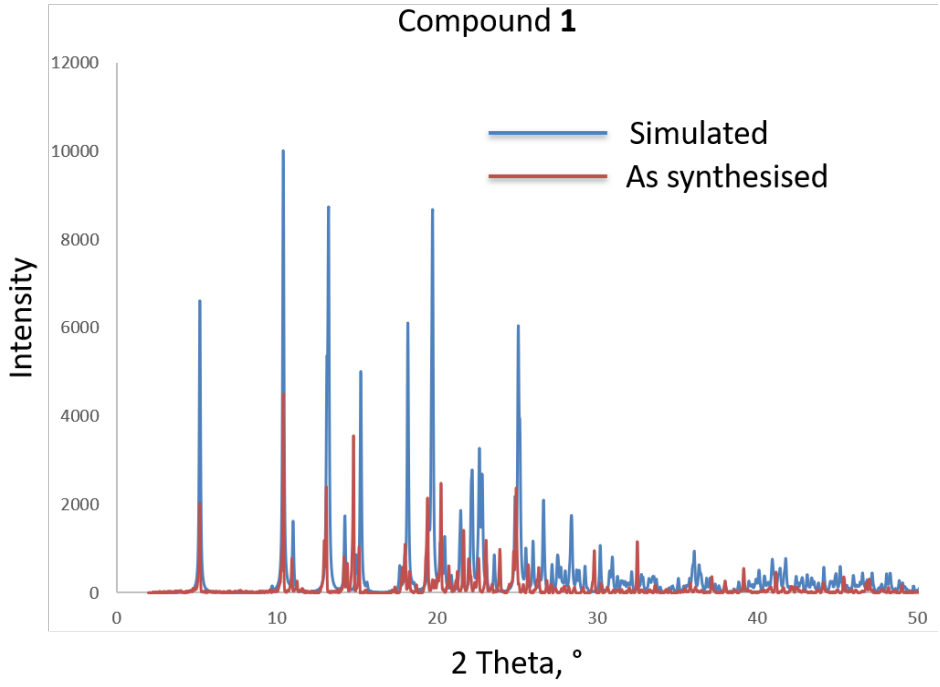

Figure S6. Powder X-ray diffractogram of compound **1**

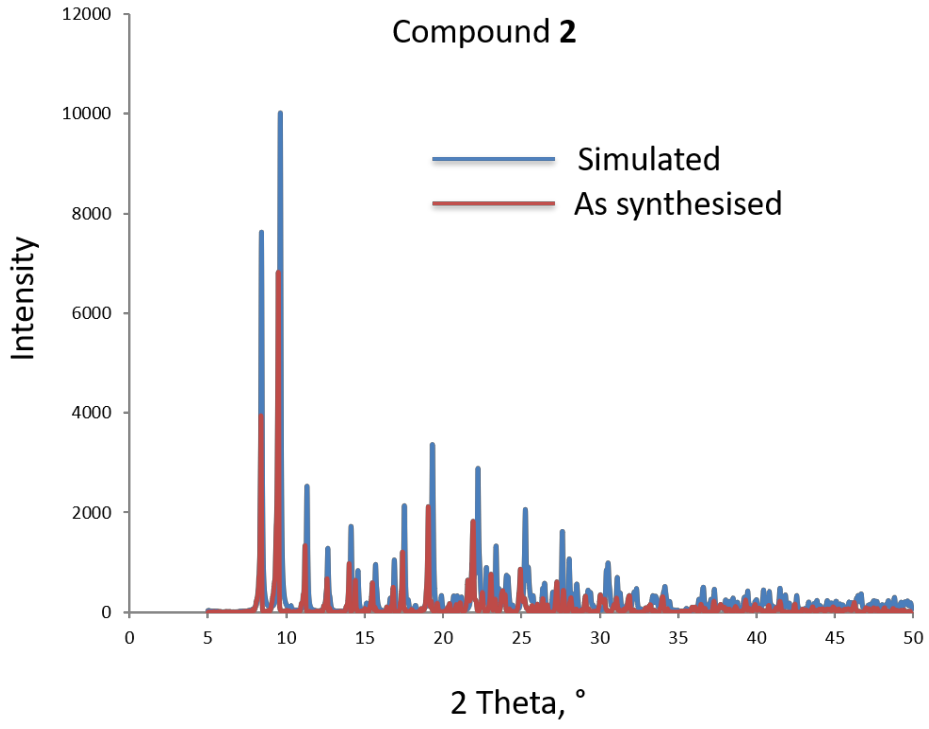

Figure S7. Powder X-ray diffractogram of compound **2**

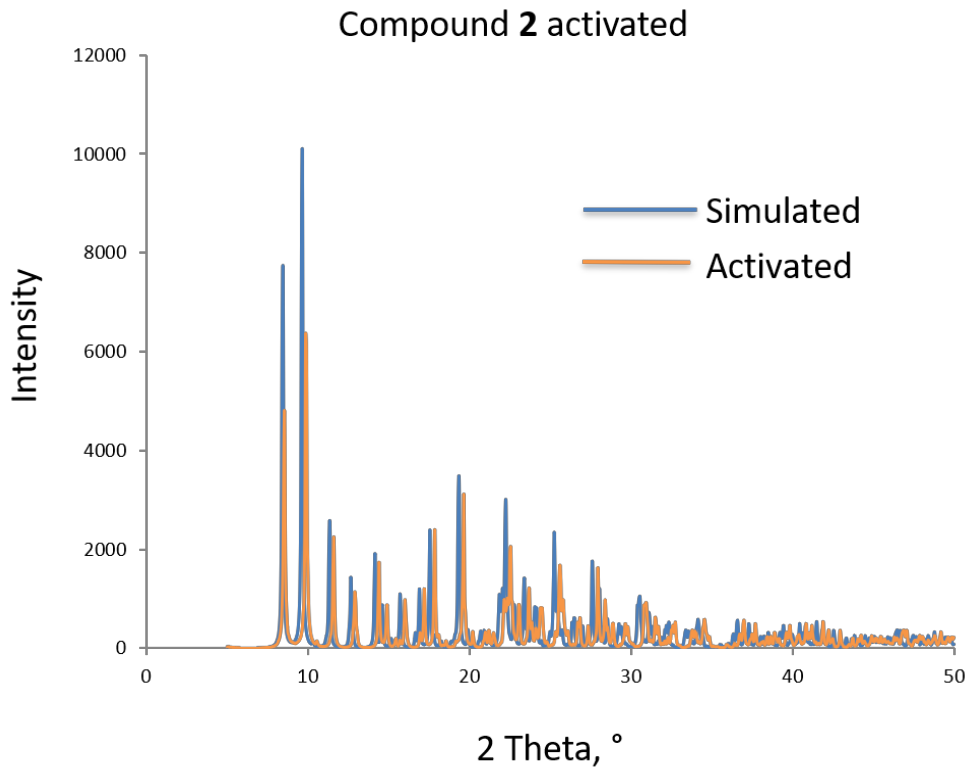

Figure S8. Powder X-ray diffractogram of compound **2** activated - after washing with methanol and heating to 200 °C for 120 min (compound **2** activated)

3. IR Spectra

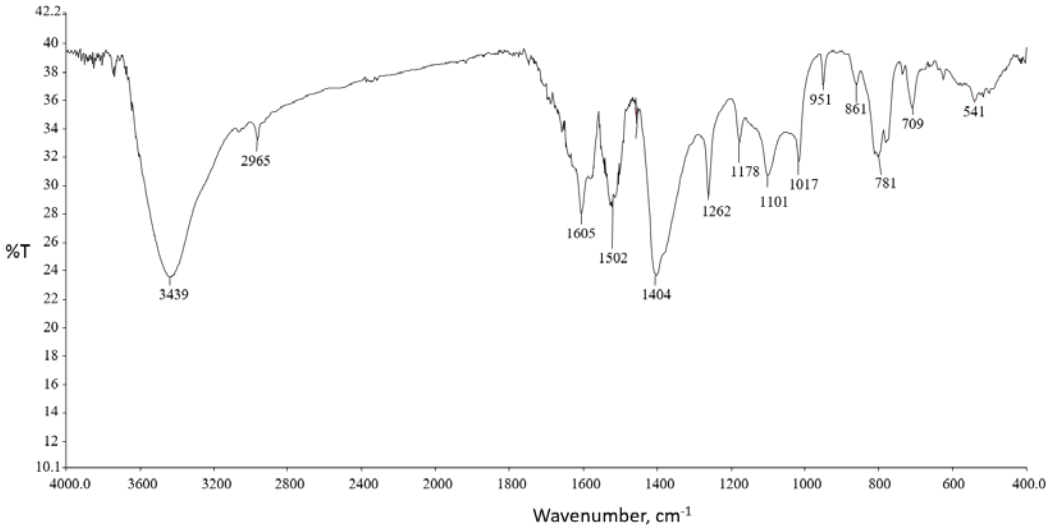

Figure S9. IR spectrum of compound **1**

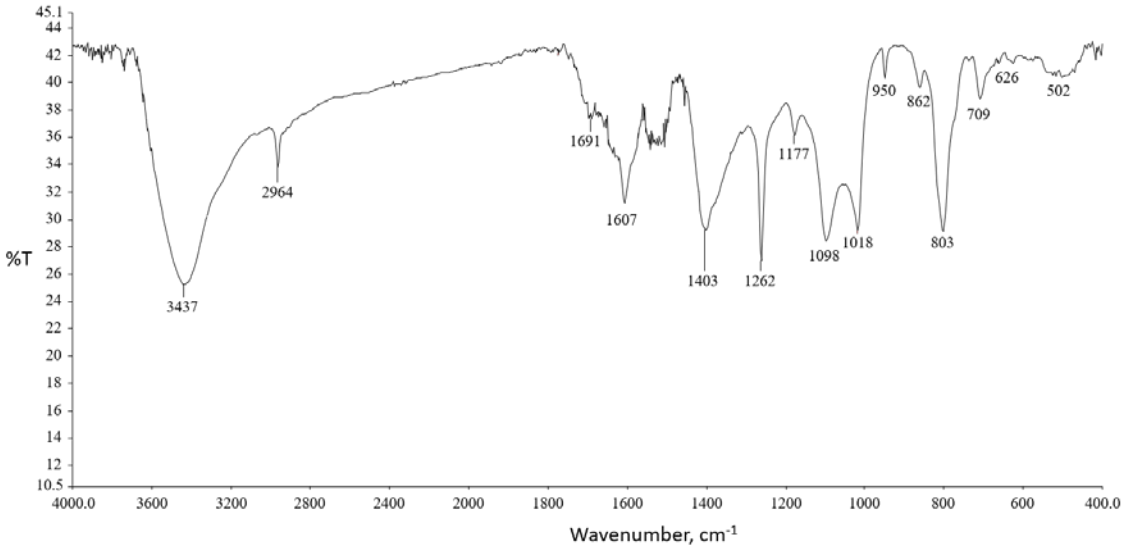

Figure S10. IR spectrum of compound **2**

4. UV-vis spectrum of H_2L

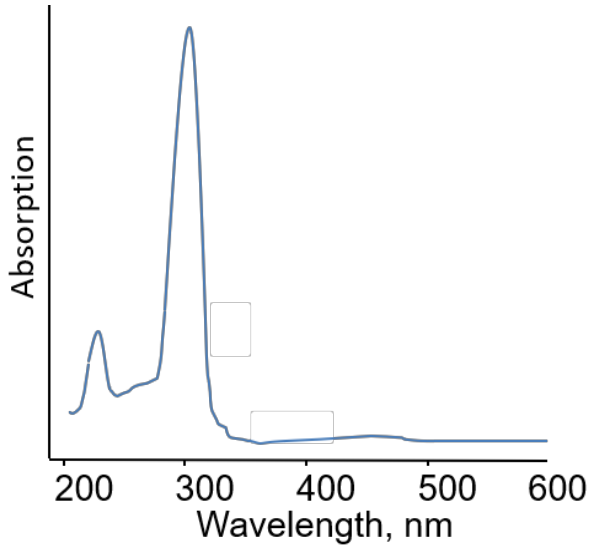

Figure S11. UV-Vis spectrum of H_2L in DCM

The UV-Vis spectrum of H_2L (concentration 10^{-7} mol·L^{-1}) was obtained with a Perkin-Elmer Lambda 900 spectrometer, in DCM at room temperature.

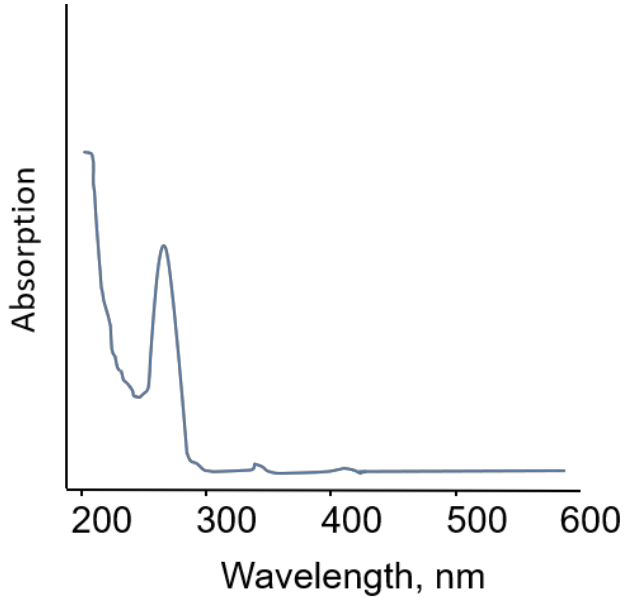

Figure S12. UV-Vis spectrum of H_2L in H_2O

The UV-Vis spectrum of H_2L (concentration 10^{-7} mol·L^{-1}) was obtained with a Perkin-Elmer Lambda 900 spectrometer, in H_2O at room temperature.

5. TG-DTA of 1 and 2

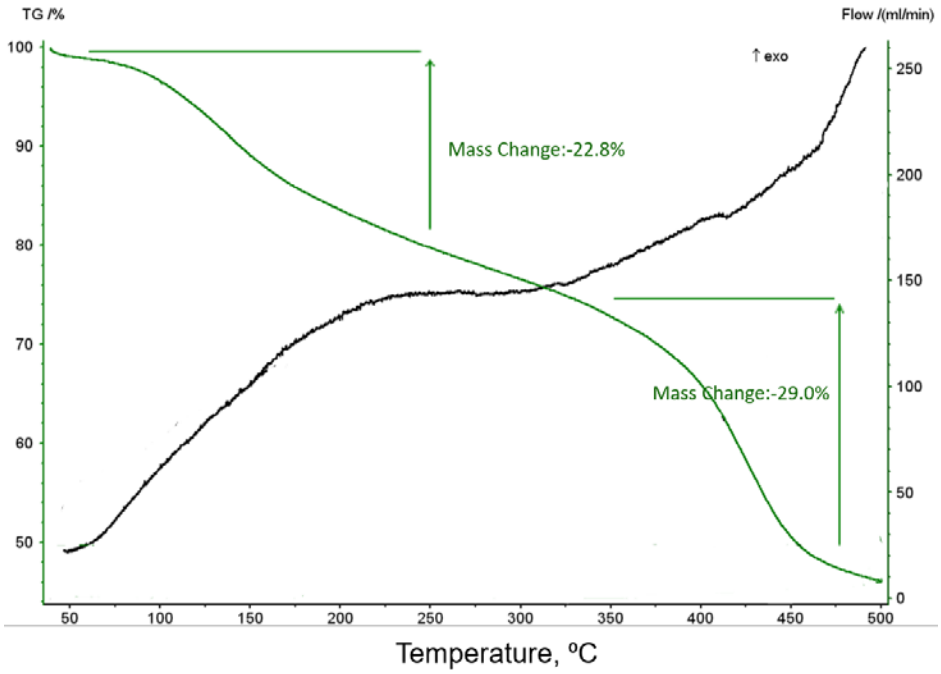

Figure S13. TG-DTA of compound **1**

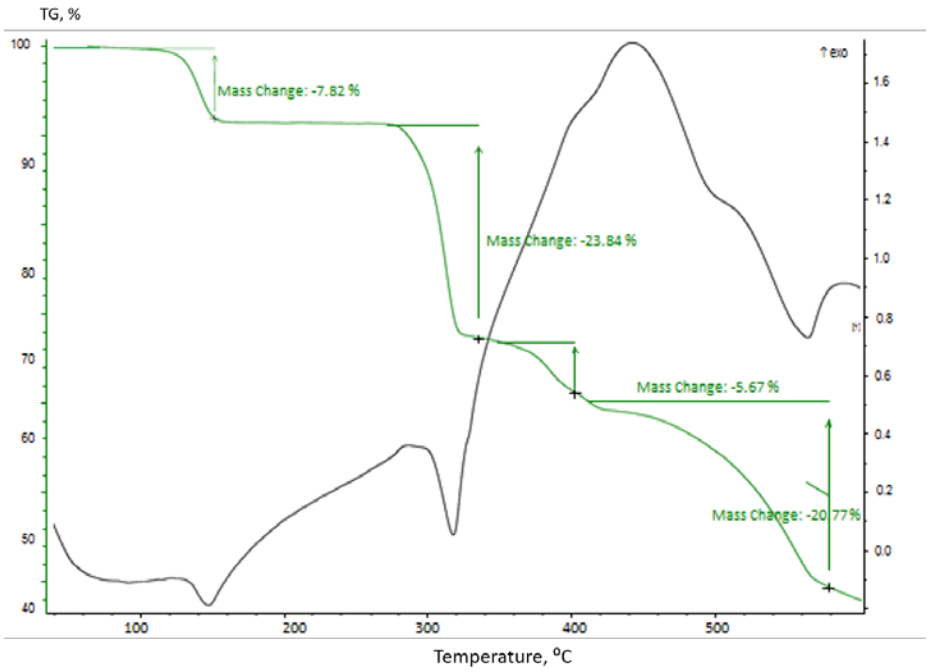

Figure S14. TG-DTA of compound **2**