Heterometallic MOFs constructed from thiophene- and furandicarboxylate ligands for heavy metals luminescent sensing

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Comment about space group in **3**. Checking the ADDSYM in PLATON finds a higher symmetry and proposes to refine the structure in *Pnma*. We have resolved structure in this group However, it turned out that the collected X-ray data set correlates significantly worse with this solution compared to the solution in $Pna2_1$ (Final R indices [$I > 2\sigma(I)$] - 0.0918 for *Pnma* versus 0.0365 for $Pna2_1$). In this case, it is more appropriate to make the solution in $Pna2_1$.

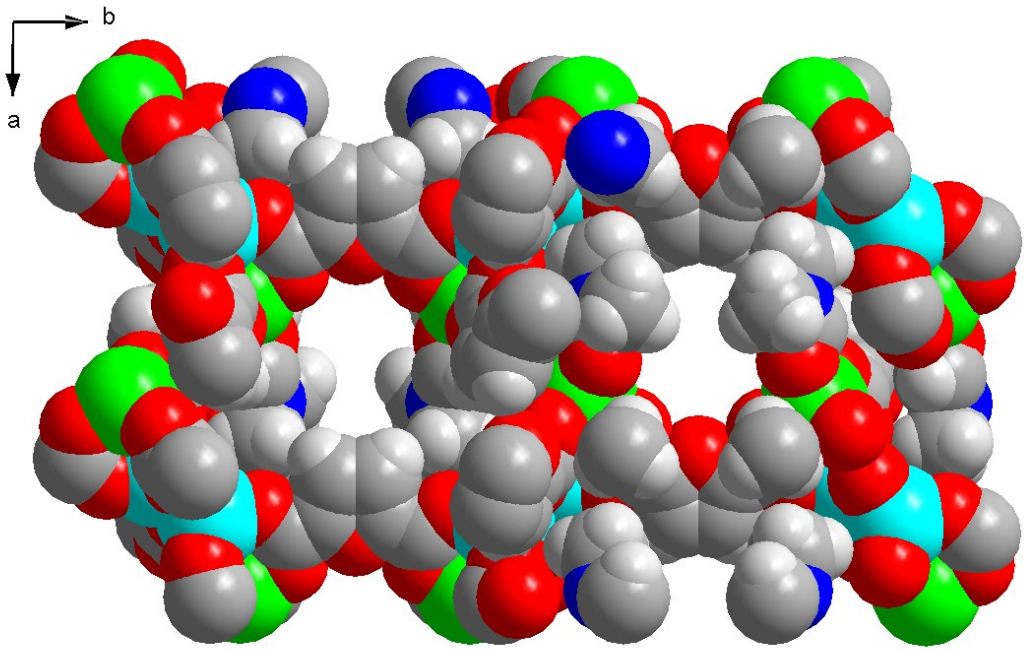

Figure S1. Structure projection of **3** with narrow channels which connect large channels with each other.

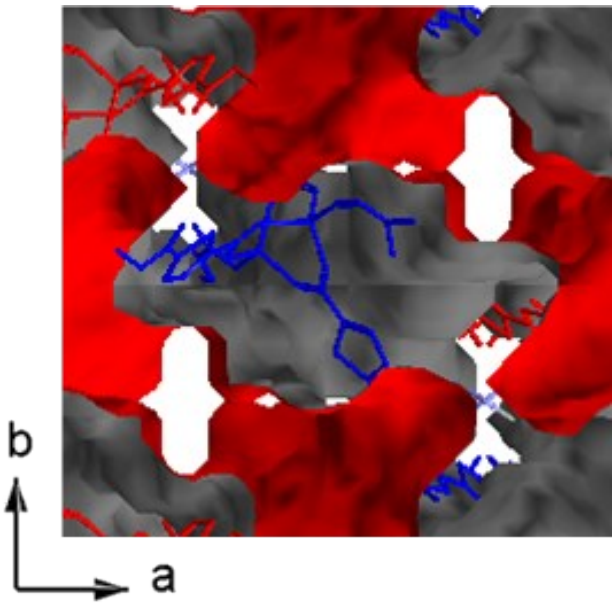

Figure S2. Calculated surface area in **1**.

Table S1. Selected bond lengths and angles for 1

Bond	*d*, Å	Bond	*d*, Å
Zn1–O12	1.935(3)	Li1–O11	1.919(6)
Zn1–O13	1.948(3)	Li1–O14	1.909(7)
Zn1–O22	1.950(3)	Li1–O21	1.923(7)
Zn1–O24	1.964(2)	Li1–O1D	1.910(7)
Angle	ω, deg.	Angle	ω, deg.
O12–Zn1–O13	117.79(13)	O11–Li1–O21	107.0(3)
O12–Zn1–O22	108.86(12)	O14–Li1–O11	108.9(3)
O12–Zn1–O24	98.21(11)	O14–Li1–O21	106.5(3)
O13–Zn1–O22	119.38(12)	O14–Li1–O1D	112.2(3)
O13–Zn1–O24	100.25(11)	O1D–Li1–O11	110.8(3)
O22–Zn1–O24	109.36(12)	O1D–Li1–O21	111.2(3)

Table S2. Selected bond lengths and angles for 2

Bond	*d*, Å	Bond	*d*, Å
Zn1–O12	1.939(4)	Li1–O11	1.859(11)
Zn1–O21	1.934(5)	Li1–O22	1.832(11)
Zn1–O32	1.930(4)	Li1–O31	1.919(10)
Zn1–O1D	1.979(5)	Li1–O31	1.947(12)
Zn2–O14	1.925(4)	Li2–O13	1.909(5)
Zn2–O24	1.906(5)	Li2–O23	1.944(6)
Zn2–O33	1.927(4)	Li2–O34	1.862(6)
Zn2–O2D	1.992(4)	Li2–O3D	1.976(6)
Zn2'–O13	1.909(5)	Li2'–O14	1.925(4)
Zn2'–O23	1.944(6)	Li2'–O24	1.906(5)
Zn2'–O34	1.862(6)	Li2'–O33	1.927(4)
Zn2'–O3D	1.976(6)	Li2'–O2D	1.992(4)
Angle	ω, deg.	Angle	ω, deg.
O12–Zn1–O1D	97.4(2)	O11–Li1–O31	113.1(6)
O21–Zn1–O12	116.1(2)	O11–Li1–O31	115.2(6)
O21–Zn1–O1D	101.3(2)	O22–Li1–O11	110.7(6)
O32–Zn1–O12	114.5(2)	O22–Li1–O31	109.8(5)
O32–Zn1–O21	119.0(2)	O22–Li1–O31	112.8(6)
O32–Zn1–O1D	103.8(2)	O31–Li1–O31	94.4(5)
O14–Zn2–O33	111.9(2)	O13–Li2–O23	108.9(3)
O14–Zn2–O2D	99.02(19)	O13–Li2–O3D	107.1(3)
O24–Zn2–O14	114.9(2)	O23–Li2–O3D	108.8(3)
O24–Zn2–O33	120.3(2)	O34–Li2–O13	109.1(3)
O24–Zn2–O2D	99.92(19)	O34–Li2–O23	117.0(3)
O33–Zn2–O2D	107.34(18)	O34–Li2–O3D	105.6(3)
O13–Zn2'–O23	108.9(3)	O14–Li2'–O33	111.9(2)
O13–Zn2'–O3D	107.1(3)	O14–Li2'–O2D	99.02(19)
O23–Zn2'–O3D	108.8(3)	O24–Li2'–O14	114.9(2)
O34–Zn2'–O13	109.1(3)	O24–Li2'–O33	120.3(2)
O34–Zn2'–O23	117.0(3)	O24–Li2'–O2D	99.92(19)
O34–Zn2'–O3D	105.6(3)	O33–Li2'–O2D	107.34(18)

Table S3. Selected bond lengths and angles for 3

Bond	*d*, Å	Bond	*d*, Å
Li1–O12	1.871(11)	Zn1–O11	1.944(4)
Li1–O15	1.936(11)	Zn1–O22	1.939(5)
Li1–O21	1.957(13)	Zn1–O34	1.941(4)
Li1–O35	1.89(2)	Zn1–O1D	1.985(4)
Li1–O35'	1.88(2)	Zn2–O14	1.921(4)
Li2–O15	1.928(12)	Zn2–O25	1.960(5)
Li2–O21	1.931(11)	Zn2–O32	1.946(4)
Li2–O24	1.875(11)	Zn2–O2D	1.989(4)
Li2–O31	1.844(18)		
Li2–O31'	2.01(2)		
Angle	ω, deg.	Angle	ω, deg.
O12–Li1–O15	116.2(6)	O11–Zn1–O1D	97.13(19)
O12–Li1–O211	12.3(6)	O22–Zn1–O11	126.7(2)
O12–Li1–O35	105.4(7)	O22–Zn1–O34	111.28(19)
O12–Li1–O35'	113.2(7)	O22–Zn1–O1D	101.86(19)
O15–Li1–O21	91.8(5)	O34–Zn1–O11	112.79(19)
O35–Li1–O15	121.0(8)	O34–Zn1–O1D	101.8(2)
O35–Li1–O21	109.6(7)	O14–Zn2–O25	127.0(2)
O35'–Li1–O21	96.4(7)	O14–Zn2–O32	111.69(18)
O15–Li2–O21	92.8(5)	O14–Zn2–O2D	102.78(19)
O15–Li2–O31'	97.4(7)	O25–Zn2–O2D	97.91(19)
O21–Li2–O31'	119.0(6)	O32–Zn2–O25	110.9(2)
O24–Li2–O15	112.9(5)	O32–Zn2–O2D	101.73(19)
O24–Li2–O21	114.4(7)		
O24–Li2–O31'	115.9(6)		
O31–Li2–O15	111.0(8)		
O31–Li2–O21	119.2(7)		
O31–Li2–O24	106.2(6)		

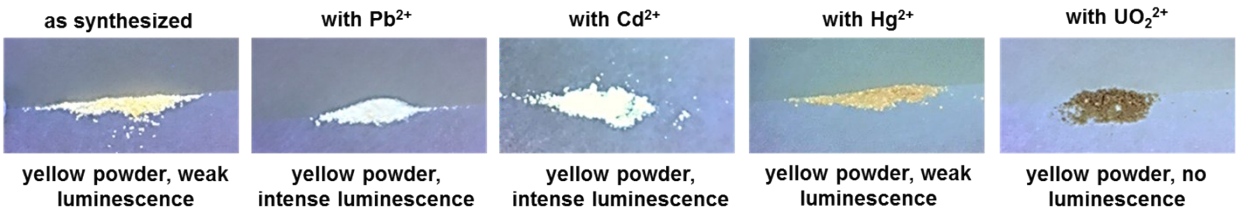

Figure S3. Differences in emission of **2** and its inclusion compounds. 365 nm excitation lamp.

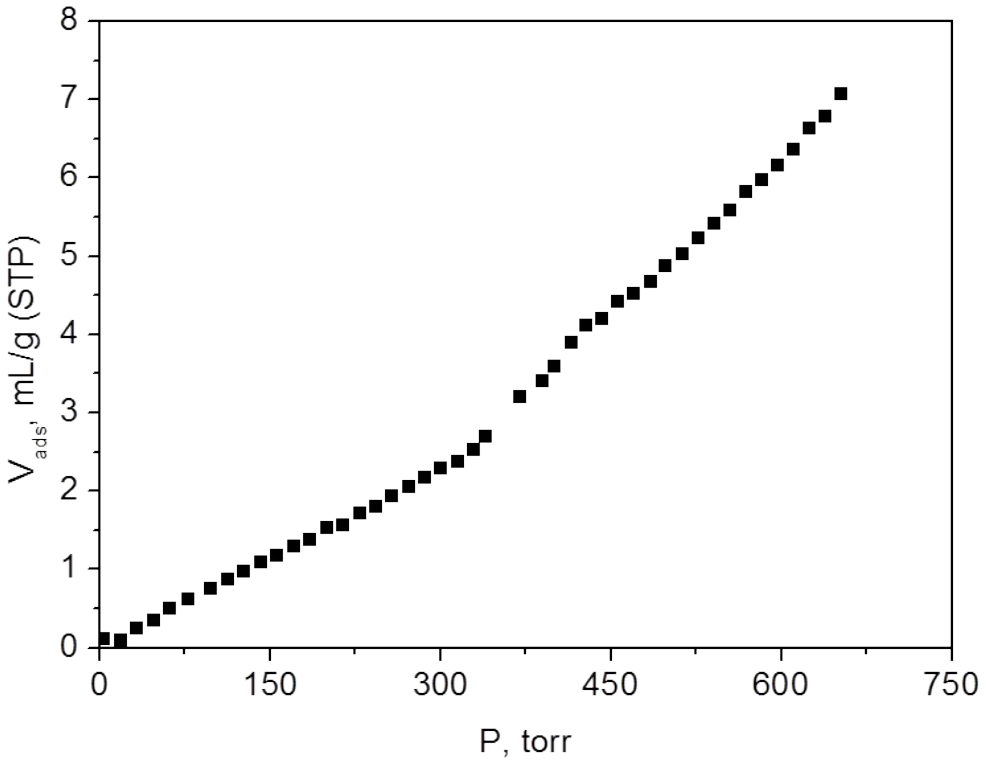

Figure S4. Nitrogen adsorption curve for activated **2** at 77K.

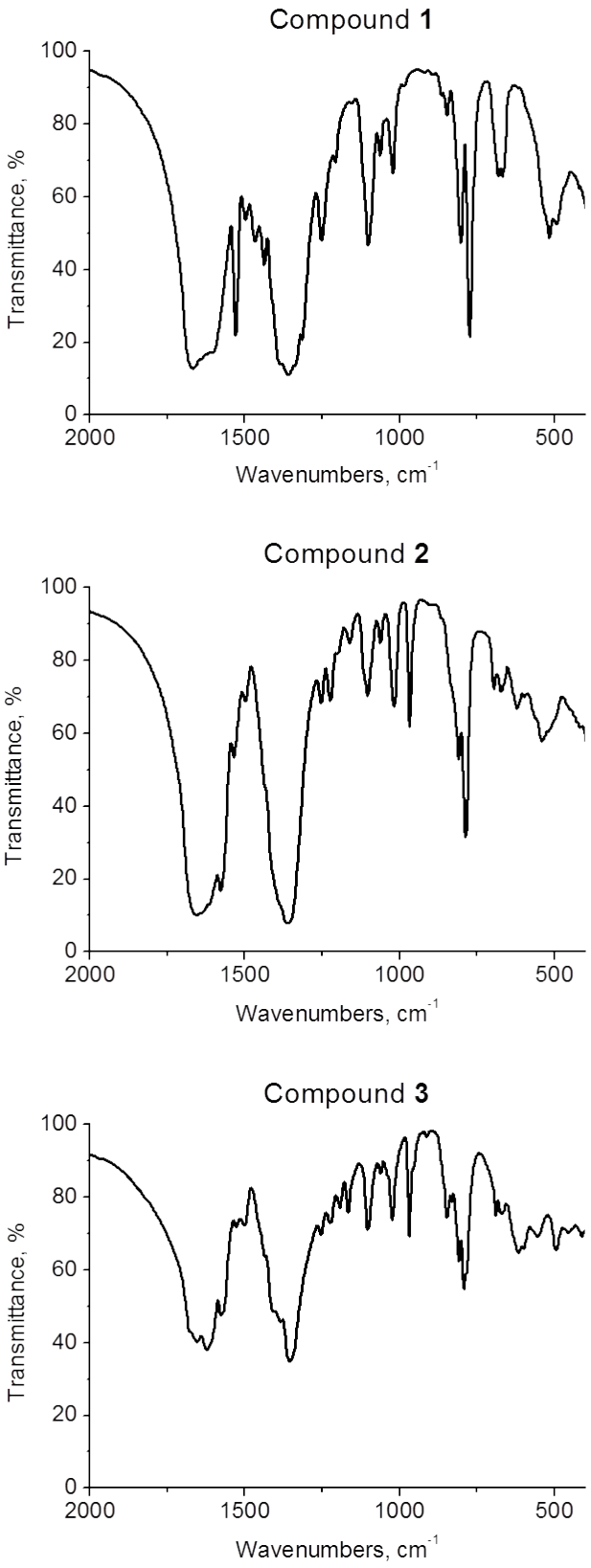

Figure S4. FT-IR spectra of **1**-**3**.

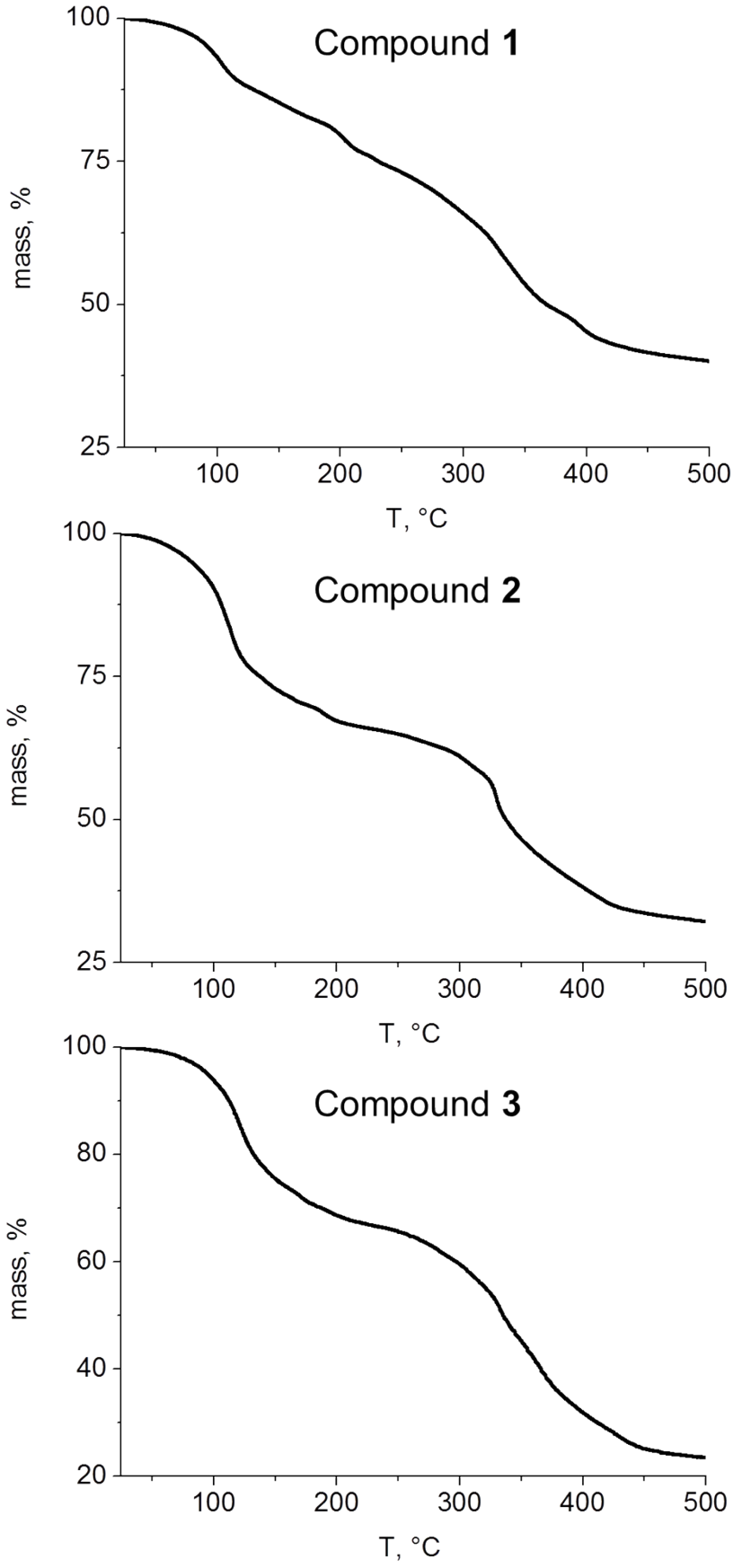

Figure S5. TGA plots for **1**–**3**.