Electronic Supplementary Information

Formation of Zn(II) and Pb(II) coordination polymers of tetrakis(4-pyridyl)cyclobutane controlled by benzene and toluene

Ming Dai,[a] Tian-Yi Gu,[a] Xin Zhao,[a] Hong-Xi Li,[a*] and Jian-Ping Lang[a,b*]

[a] College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, P. R. China

[b] State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 210032, P. R. China

Table of Contents

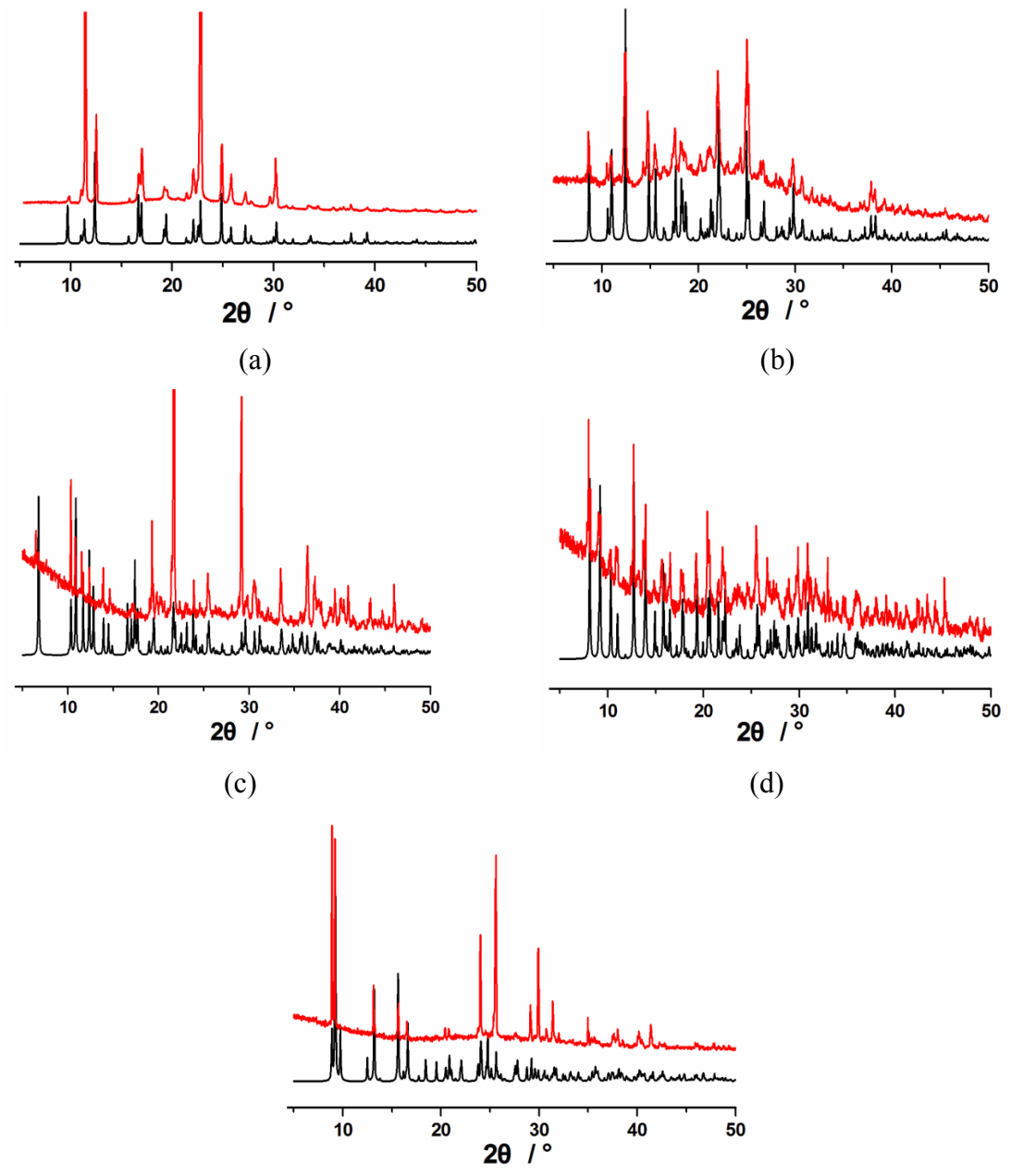


Fig. S1 PXRD patterns for compounds **1** (a), **2** (b), **3** (c), **4** (d) and **5** (e). Simulated (black) and single-phase polycrystalline sample (red).

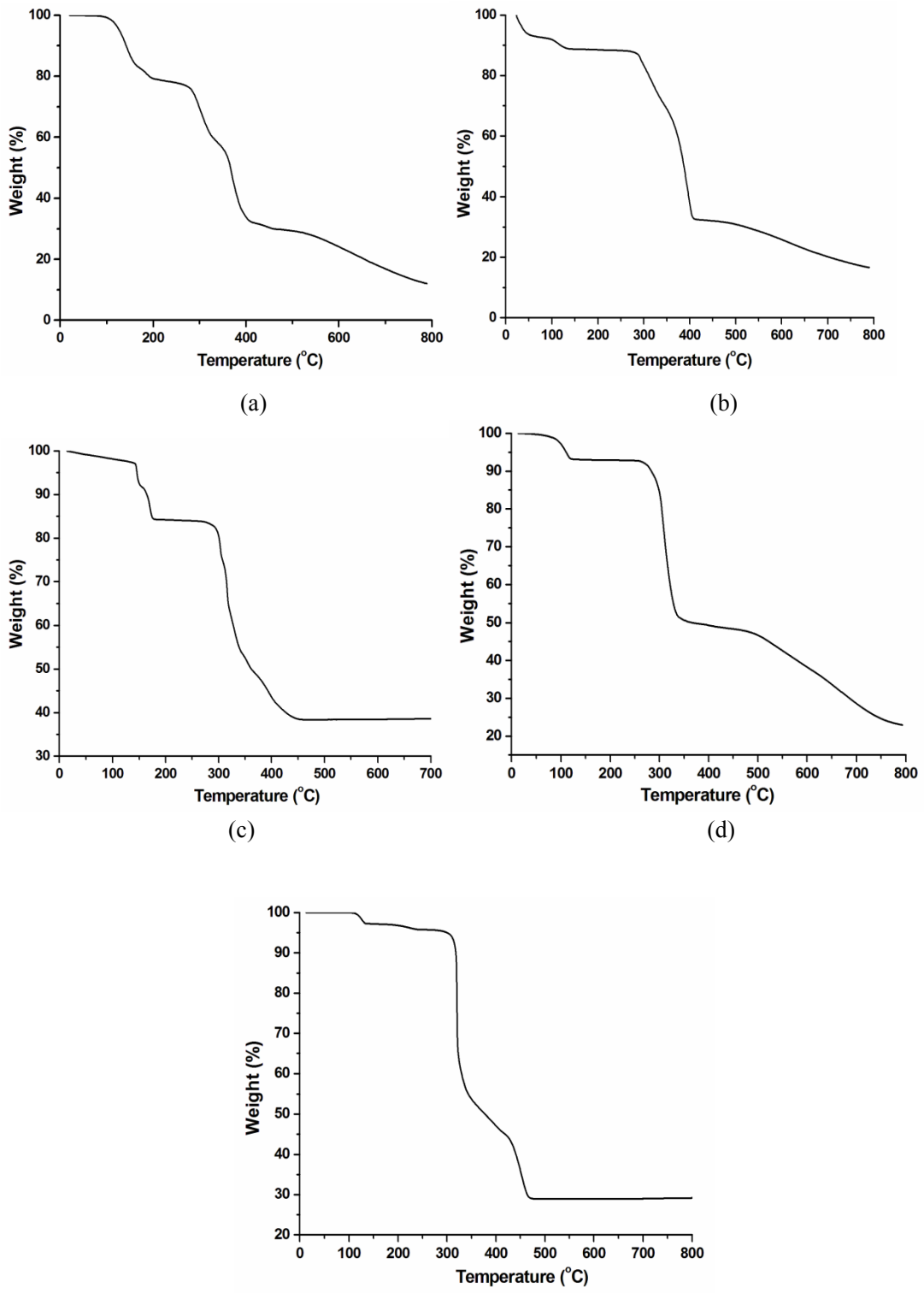


Fig. S2 TGA curves for compounds **1** (a), **2** (b), **3** (c), **4** (d) and **5** (e).

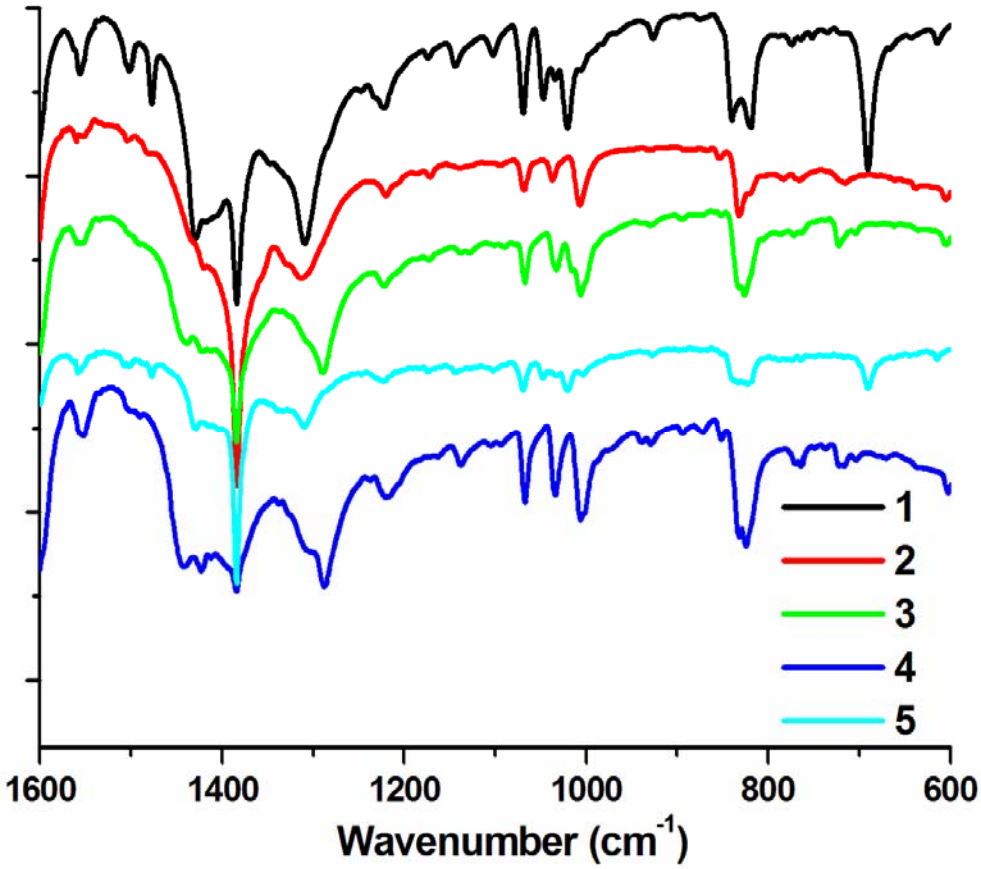
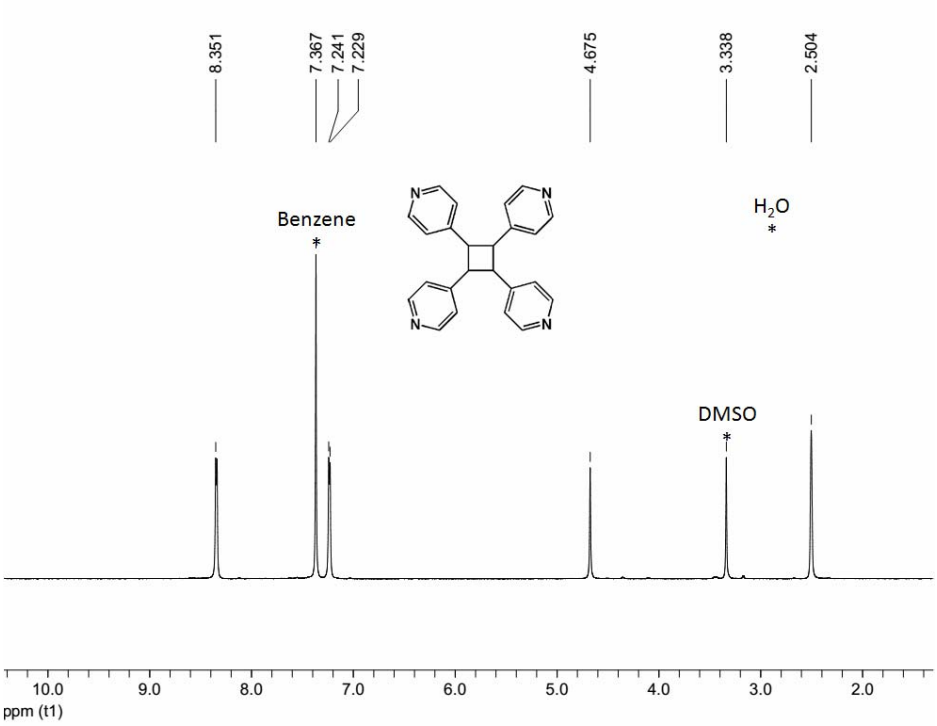
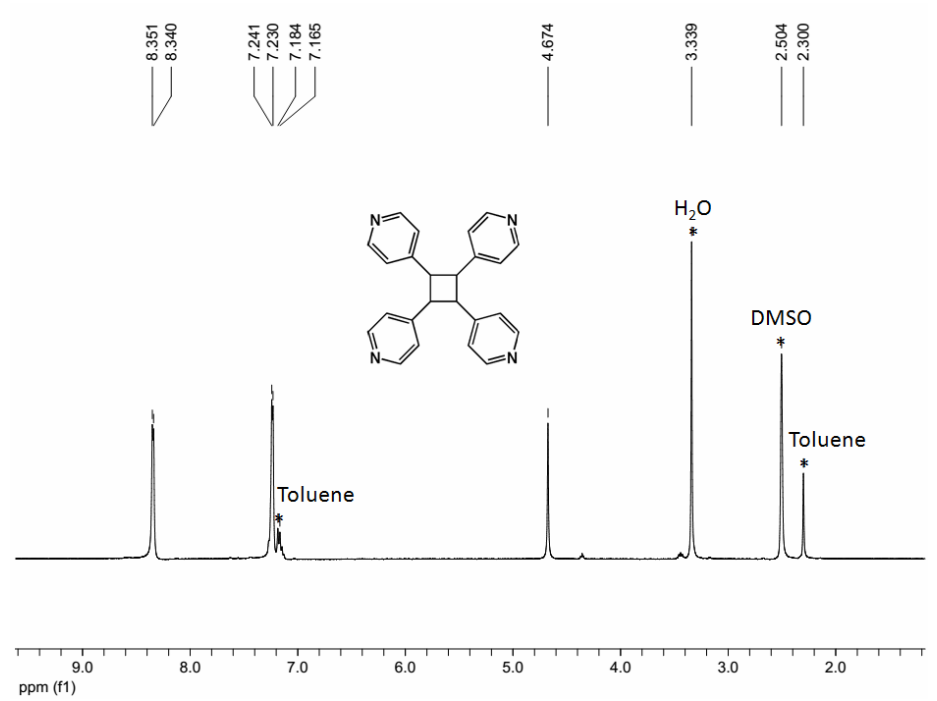


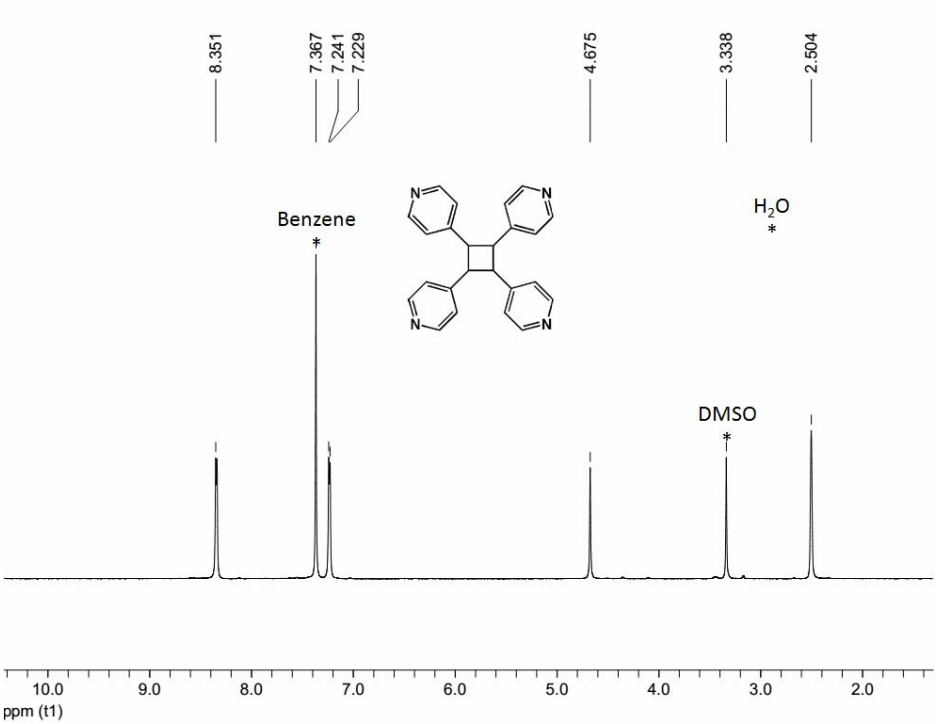
Fig. S3 IR spectra of **1-5**


8.351
7.367
7.241
7.229
4.675
3.338
2.504
Benzene
H2O
DMSO
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)

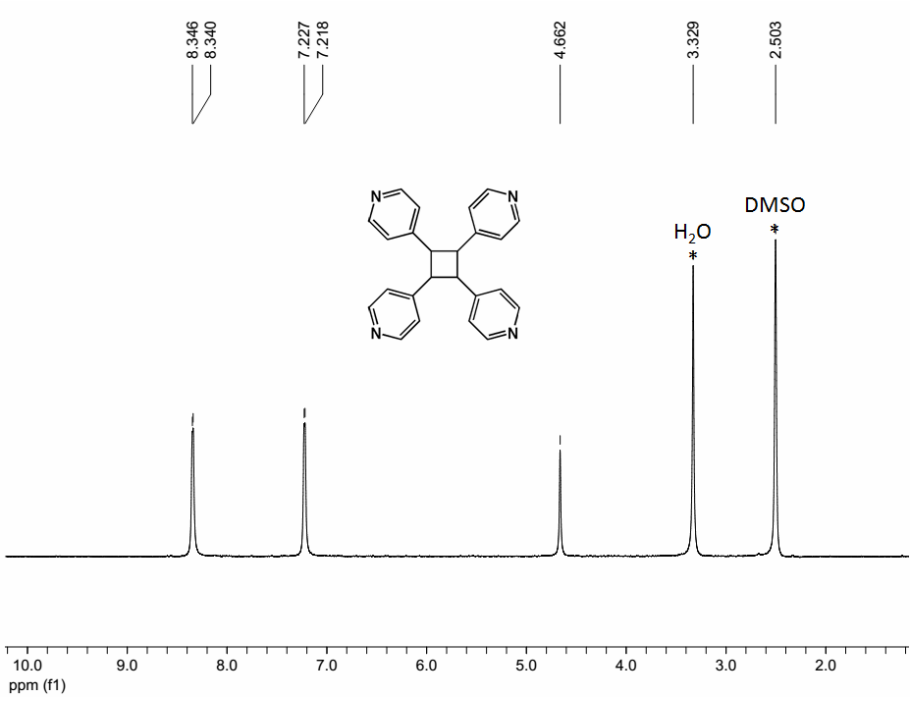
(a)


8.351
8.340
7.241
7.230
7.184
7.165
4.674
3.339
2.504
2.300
H2O
DMSO
Toluene
Toluene
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (f1)

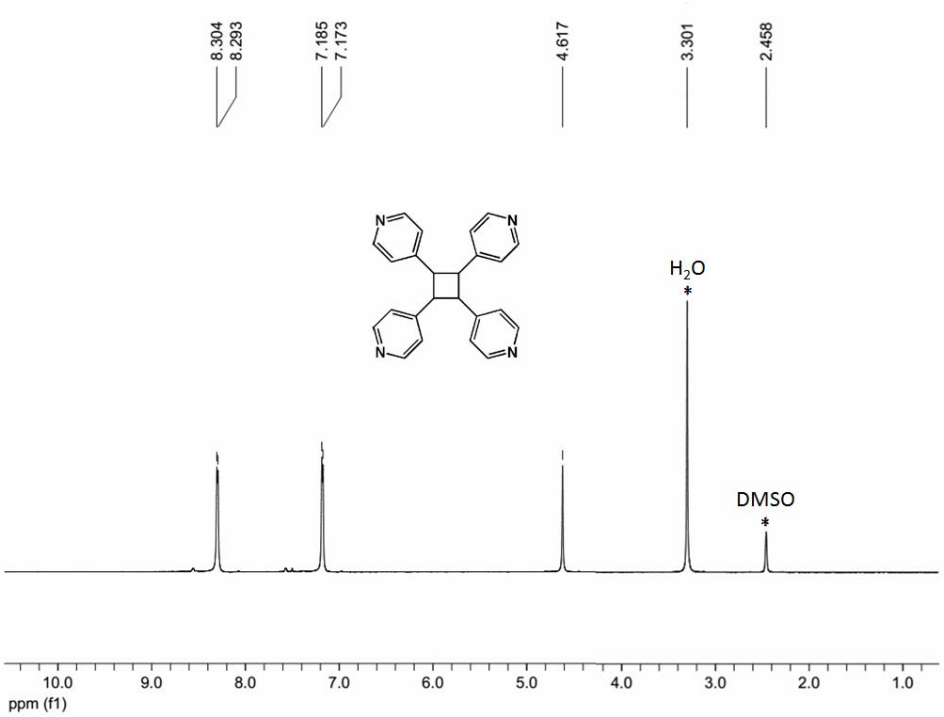
(b)


8.351
7.367
7.241
7.229
4.675
3.338
2.504
Benzene
*
H2O
*
DMSO
*
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (t1)

(c)

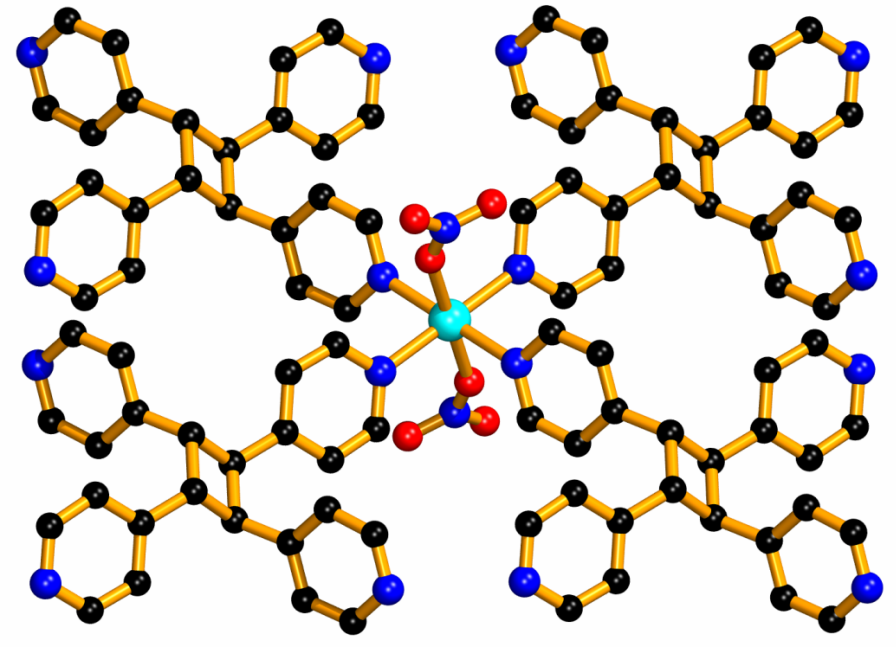

8.346
8.340
7.227
7.218
4.662
3.329
2.503
H2O
*
DMSO
*
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm (f1)

(d)

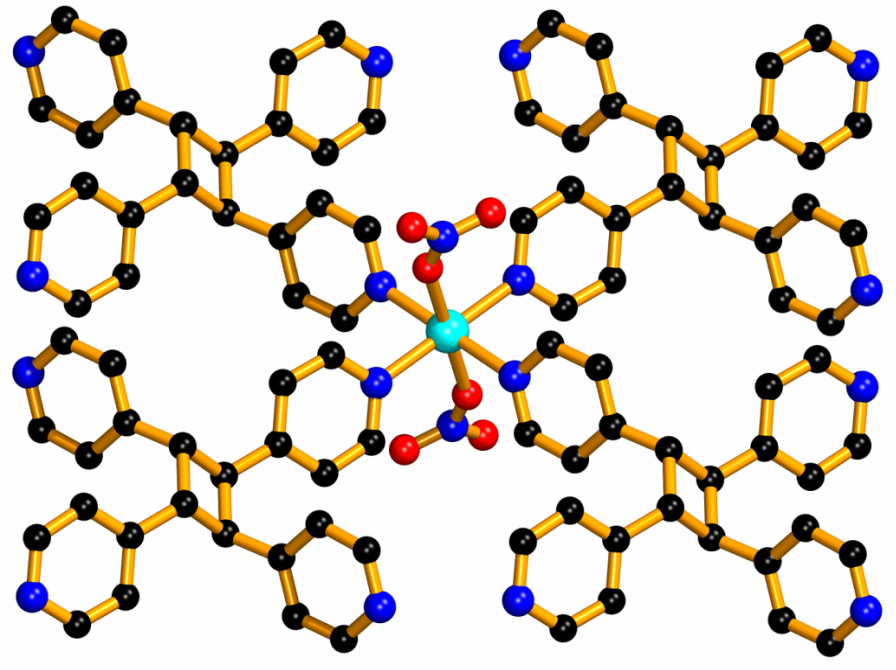


(e)

Fig. S4 ^{1}H NMR spectrum of compounds **1** (a), **2** (b), **3** (c), **4** (d) and **5** (e). The benzene and toluene signals are marked for clarity.



(a)



(b)

Fig. S5 View of the coordination environment of the Zn center in **1** (a) and **2** (b).

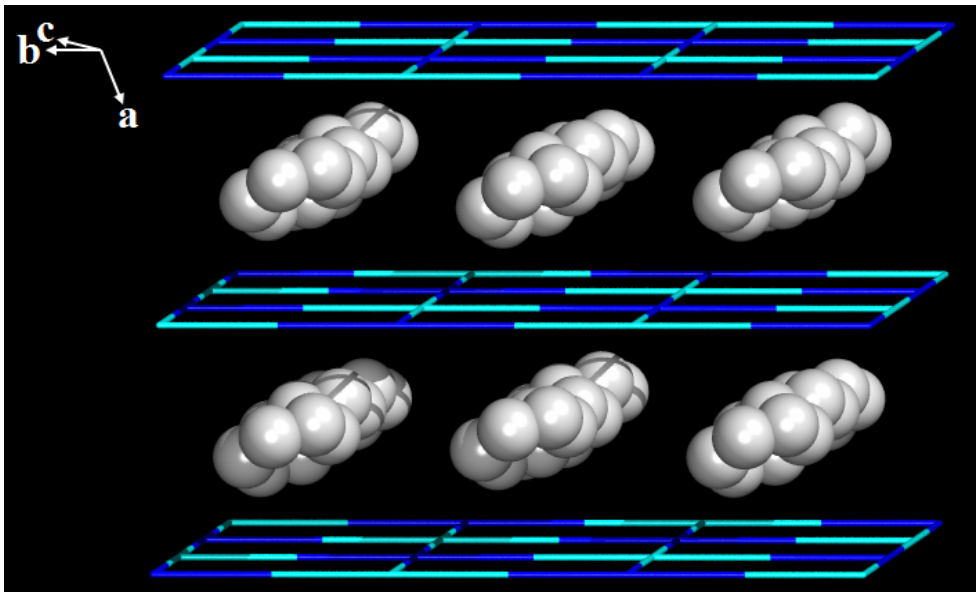


Fig. S6 View of the topological (4,4)-connected structure of **1**. The benzene molecules are shown as space-filling model, which are stuck between the 2D layers.

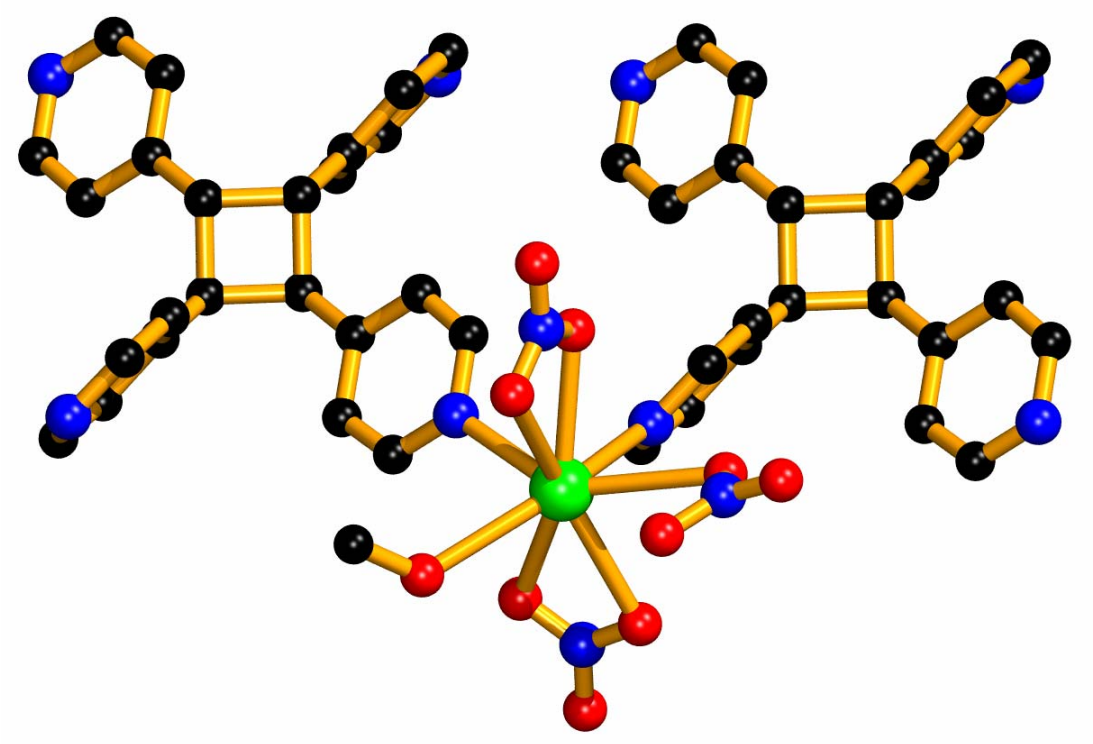


Fig. S7 View of the coordination environment of the Pb center in **3**.

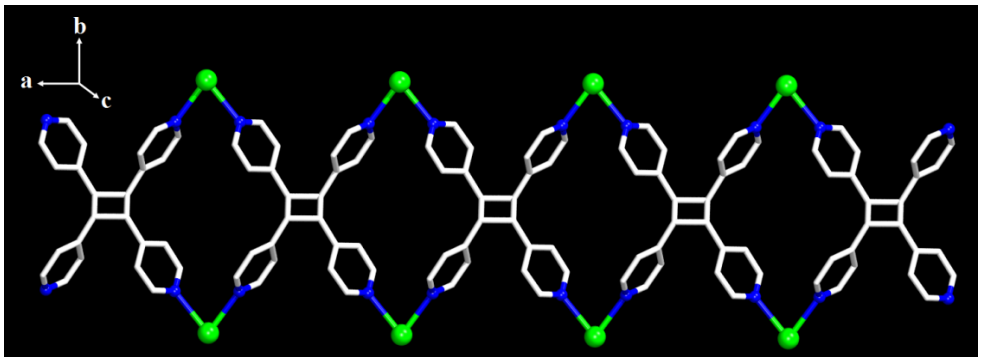


Fig. S8 View of a section of the 1D $[Pb_2(tpcb)]_n$ chain extending along the *c* axis.

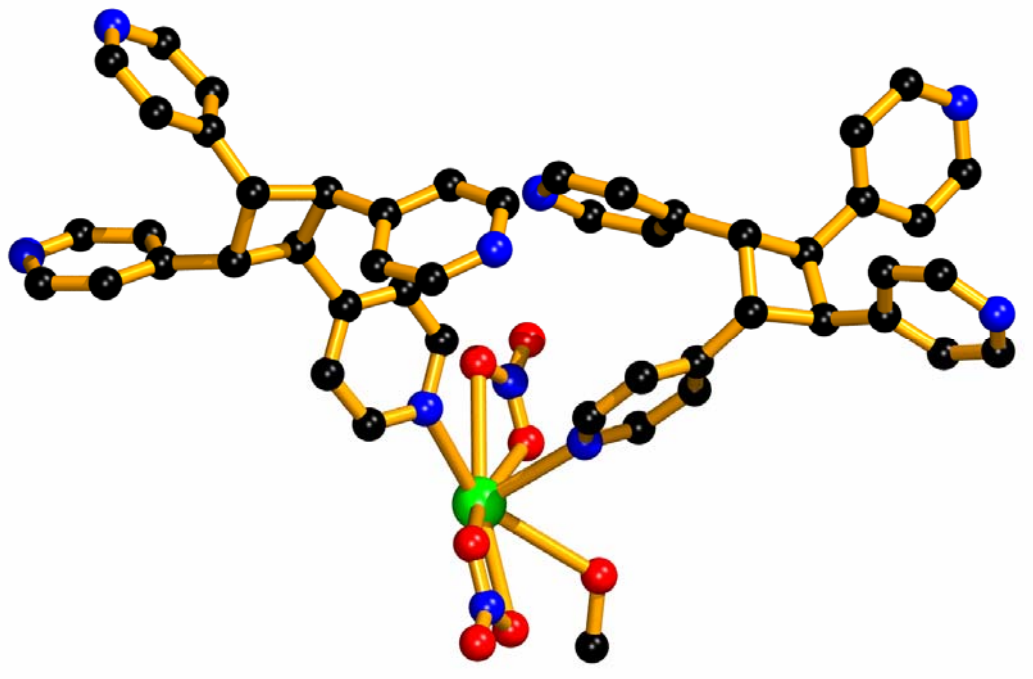


Fig. S9 View of the coordination environment of the Pb center in **4**.

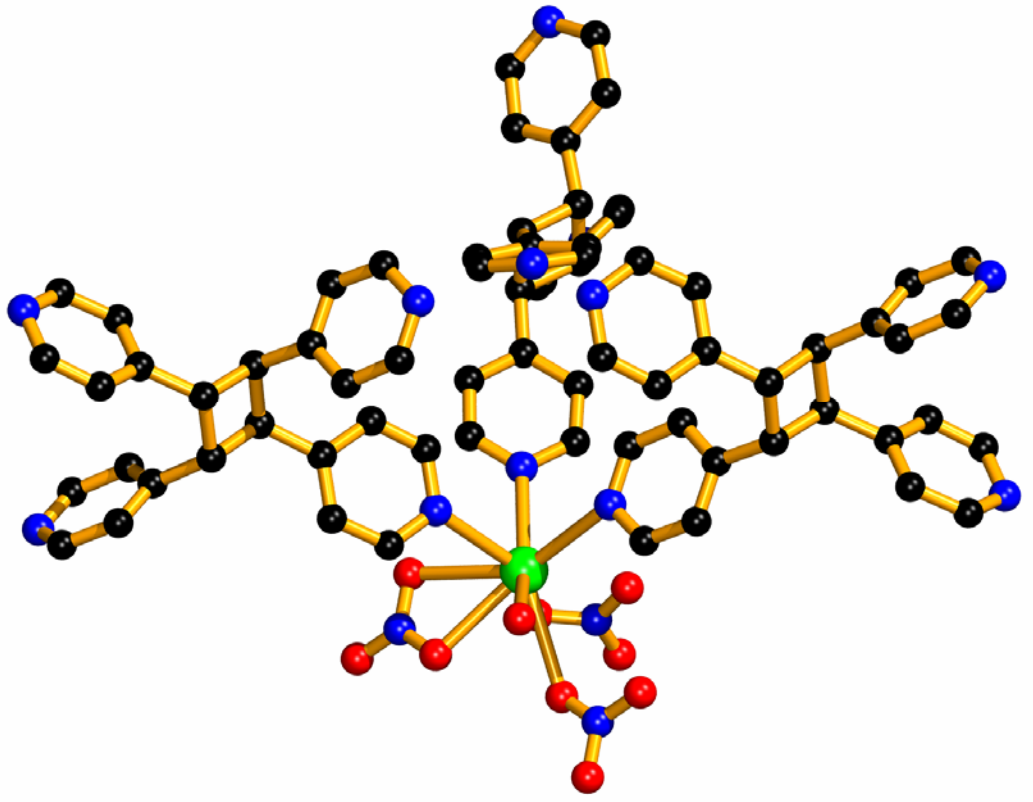


Fig. S10 View of the coordination environment of the Pb center in **5**.

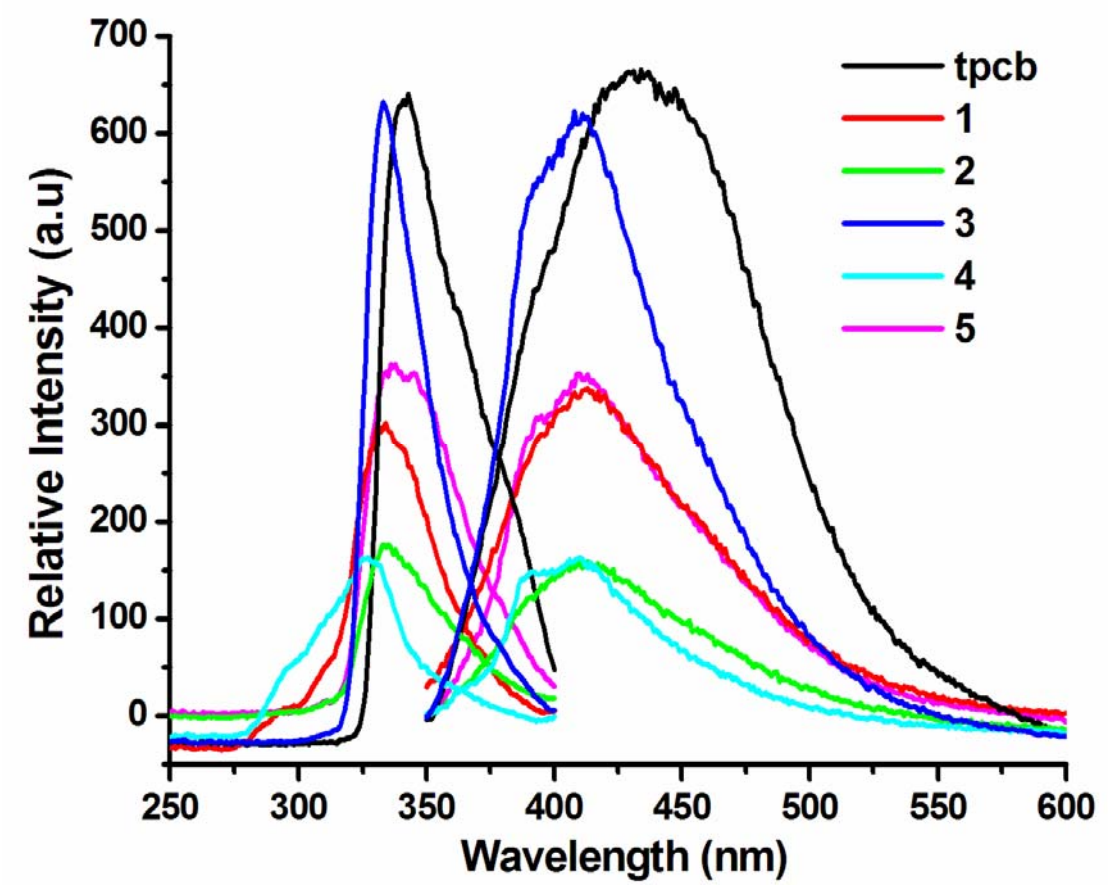


Fig. S11 Photoluminescence excitation and emission spectra of **1**-**5** in DMF.

Table S1. Selected bond distances (Å) and angles (°) for **1**−**5**

Compound **1**							
Zn(1)-O(1)	2.204(3)	Zn(1)-O(1A)	2.204(3)	Zn(1)-N(1B)	2.182(4)	Zn(1)-N(1A)	2.182(4)
Zn(1)-N(1)	2.182(4)						
N(1A)-Zn(1)-N(1)	180.0	N(1A)-Zn(1)-N(1B)	93.9(2)	N(1)-Zn(1)-N(1B)	86.1(2)	N(1A)-Zn(1)-O(1A)	91.0(1)
N(1)-Zn(1)-O(1A)	89.03(1)	O(1)-Zn(1)-O(1A)	180.0				
Compound **2**							
Zn(1)-O(1)	2.184(3)	Zn(1)-O(1A)	2.184(3)	Zn(1)-N(2B)	2.168(2)	Zn(1)-N(2C)	2.168(2)
Zn(1)-N(1)	2.183(3)	Zn(1)-N(1A)	2.183(3)				
N(2B)-Zn(1)-N(2C)	180.0	N(2B)-Zn(1)-N(1)	94.2(1)	N(2C)-Zn(1)-N(1)	85.8(1)	N(1)-Zn(1)-N(1A)	180.0
N(2B)-Zn(1)-O(1)	85.2(1)	N(2C)-Zn(1)-O(1)	94.8(1)	N(1)-Zn(1)-O(1)	94.5(1)	O(1)-Zn(1)-O(1A)	180.0
N(1)-Zn(1)-O(1A)	85.5(1)						
Compound **3**							
Pb(1)-N(1)	2.549(7)	Pb(1)-N(2A)	2.597(7)	Pb(1)-O(4)	2.733(2)	Pb(1)-O(2)	2.853(7)
Pb(1)-O(1)	2.640(7)	Pb(1)-O(5)	2.691(6)	Pb(1)-O(7)	2.762(7)		
N(2A)-Pb(1)-N(1)	75.2(2)	N(2A)-Pb(1)-O(1)	76.5(2)	O(1)-Pb(1)-O(4)	146.8(2)	N(2A)-Pb(1)-O(7)	83.1(2)
N(1)-Pb(1)-O(5)	83.9(2)	N(2A)-Pb(1)-O(5)	72.7(2)	O(1)-Pb(1)-O(7)	117.2(2)	O(5)-Pb(1)-O(7)	93.1(2)
O(1)-Pb(1)-O(5)	146.2(2)	N(2A)-Pb(1)-O(4)	114.6(2)	N(1)-Pb(1)-O(7)	151.5(2)	N(1)-Pb(1)-O(1)	75.7(2)
Compound **4**							
Pb(1)-N(1)	2.490(7)	Pb(1)-N(4A)	2.608(7)	Pb(1)-O(6)	2.960(9)	Pb(1)-O(4)	2.772(10)
Pb(1)-O(1)	2.608(8)	Pb(1)-O(3)	2.859(8)	Pb(1)-O(7)	2.807(9)		
N(4A)-Pb(1)-N(1)	78.1(2)	N(4A)-Pb(1)-O(1)	67.8(3)	N(1)-Pb(1)-O(1)	82.3(2)	O(6)-Pb(1)-O(1)	131.6(3)
N(4A)-Pb(1)-O(3)	112.3(2)	N(4A)-Pb(1)-O(6)	66.7(2)	N(1)-Pb(1)-O(3)	92.5(2)	N(1)-Pb(1)-O(7)	70.6(2)
N(4A)-Pb(1)-O(4)	109.5(3)	N(4A)-Pb(1)-O(7)	148.0(3)	O(6)-Pb(1)-O(7)	109.2(2)	O(1)-Pb(1)-O(7)	100.8(3)
N(1)-Pb(1)-O(6)	73.1(2)	N(1)-Pb(1)-O(4)	79.8(3)				
Compound **5**							
Pb(1)-O(4)	2.630(3)	Pb(1)-N(4A)	2.659(4)	Pb(1)-N(1)	2.743(4)	Pb(1)-O(1)	2.749(4)
Pb(1)-O(7)	2.660(4)	Pb(1)-N(3B)	2.671(4)	Pb(1)-O(5)	2.827(3)	Pb(1)-O(2)	2.905(5)
Pb(1)-O(4C)	2.831(3)						
O(7)-Pb(1)-O(4)	77.9(1)	N(4A)-Pb(1)-O(7)	72.5(1)	N(4A)-Pb(1)-O(1)	135.2(1)	O(1)-Pb(1)-O(7)	136.6(1)
N(3B)-Pb(1)-O(4)	120.4(1)	N(4A)-Pb(1)-N(3B)	82.1(1)	N(3B)-Pb(1)-O(1)	76.8(1)	O(1)-Pb(1)-N(1)	127.1(1)
N(3B)-Pb(1)-O(7)	146.5(1)	N(1)-Pb(1)-O(4)	153.1(1)	O(4C)-Pb(1)-N(1)	109.7(1)	O(4C)-Pb(1)-N(4A)	134.8(1)
N(4A)-Pb(1)-N(1)	88.0(1)	N(1)-Pb(1)-O(7)	75.2(1)	O(4C)-Pb(1)-N(3B)	139.6(1)	N(4A)-Pb(1)-O(4)	82.3(1)
N(1)-Pb(1)-N(3B)	82.7(1)	O(1)-Pb(1)-O(4)	75.3(1)				

[a]Symmetry codes for **1** A, -*x*, *y*, -*z* + 1; B, *x*, -*y* + 1, *z*; for **2** A, -*x* +3, -*y* + 1, -*z* + 1; B, *x* +1, *y*, *z*; C, -*x* +2, -*y* + 1, -*z* + 1; for **3** A, 1+*x*, *y*, *z*; for **4** A, *x*, -*y* – 1/2, *z* – 1/2; for **5** A, -*x* + 2, -*y*, -*z* + 1; B, -*x* + 5/2, *y* – 1/2, -*z* + 1/2; C, -*x* + 3, -*y*, -*z* + 2.