Supplementary materials

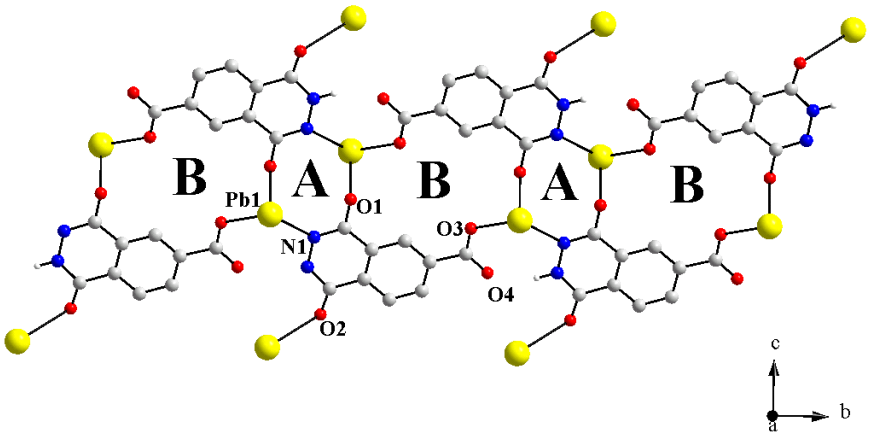

Fig. S1 The 1-D chain structure in [Pb(CPTH)(phen)] **1**.

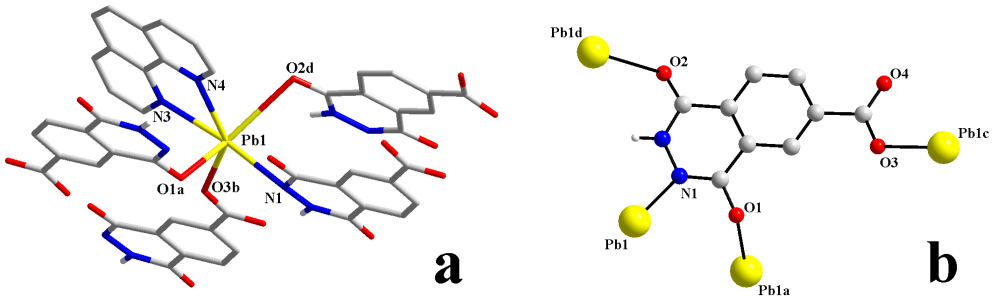

Fig. S2 The coordination environment of Pb center (a) and the bridging mode of CPTH ligand (b) in [Pb(CPTH)(phen)] **1** (a: -*x*+1, -*y*, -*z*; b: *x*, *y*+1, *z*; c: *x*, *y*-1, *z*; d: -*x*+1, *y*, -*z*+0.5).

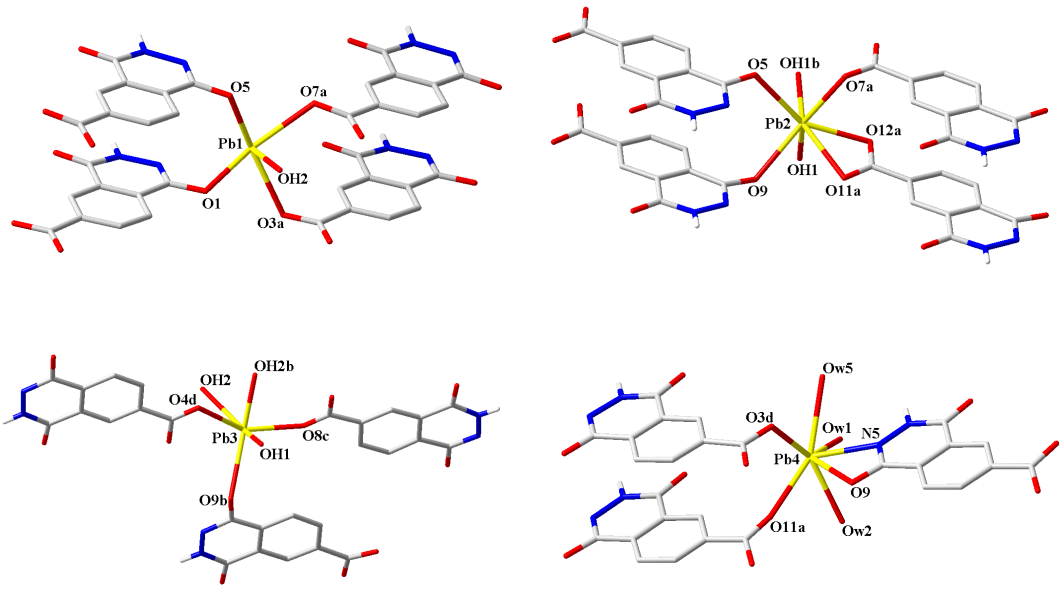

Fig. S3 The coordination environments of four Pb(II) centers in $[Pb_4(OH)_2(H_2O)_3(CPTH)_3] \cdot 2H_2O$ **2** (a: *x*-1, *y*, *z*; b: -*x*-2, -*y*+2, -*z*+1; c: -*x*-1, -*y*+2, -*z*+1; d: *x*-1, *y*+1, *z*).

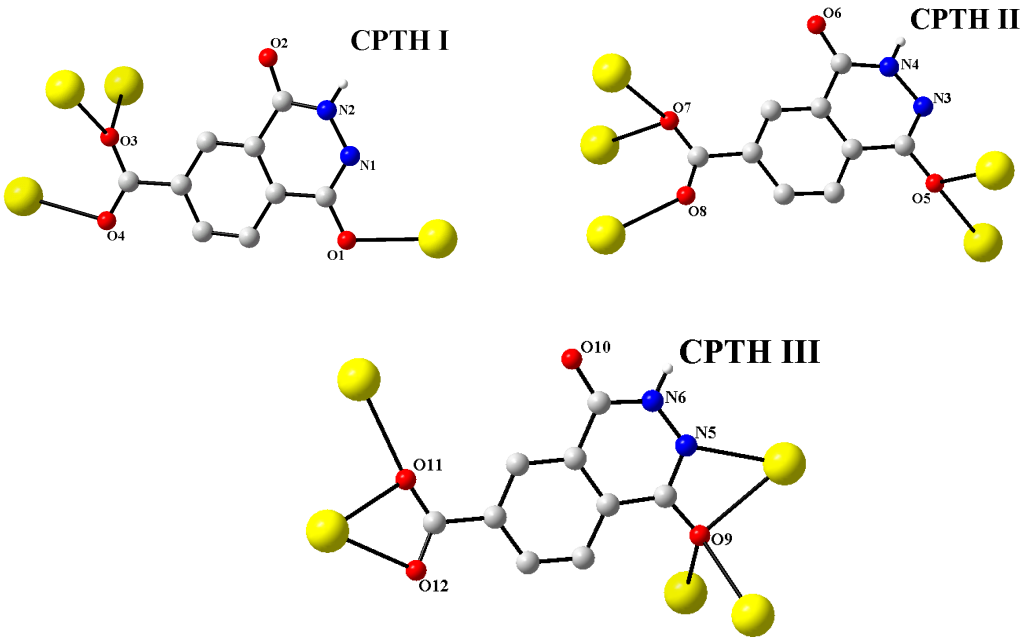

Fig. S4 The bridging modes of CPTH ligands in $[Pb_4(OH)_2(H_2O)_3(CPTH)_3] \cdot 2H_2O$ **2**.

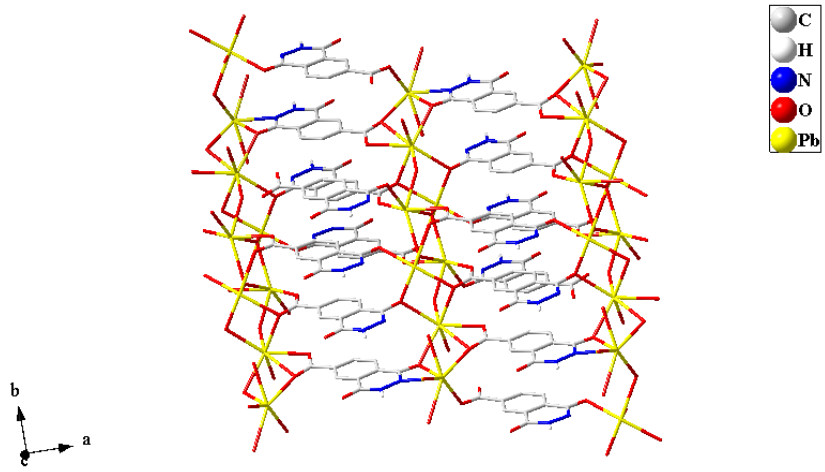

Fig. S5 The projection plot of $[Pb_4(OH)_2(H_2O)_3(CPTH)_3] \cdot 2H_2O$ **2** in *ab* plane.

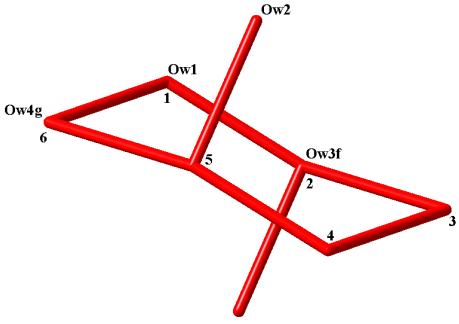

Fig. S6 The water octamer with a chairlike hexamer at the core in compound **2**

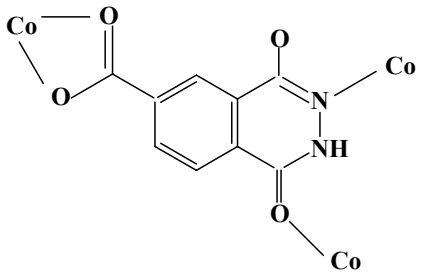

Fig. S7 The μ_3-bridging mode for 4-CPTH in reported compound [Co(CPTH)(bpy)].

Table S1 Selected bond lengths [Å] and angles [º] for the title compounds

Compound **1**			
Pb(1)-O(1)#1	2.310(5)	Pb(1)-O(3)#2	2.423(4)
Pb(1)-N(3)	2.673(5)	Pb(1)-N(4)	2.691(5)
Pb(1)-N(1)	2.677(5)	O(1)-C(7)	1.312(7)
O(2)-C(8)	1.242(7)		
O(1)#1-Pb(1)-O(3)#2	79.78(18)	O(3)#2-Pb(1)-N(1)	97.62(19)
O(1)#1-Pb(1)-N(3)	85.50(16)	N(3)-Pb(1)-N(1)	171.89(16)
O(3)#2-Pb(1)-N(3)	81.83(18)	O(1)#1-Pb(1)-N(4)	81.63(16)
O(1)#1-Pb(1)-N(1)	86.43(15)	O(3)#2-Pb(1)-N(4)	139.87(18)
N(3)-Pb(1)-N(4)	61.46(15)	N(1)-Pb(1)-N(4)	116.37(16)
Compound **2**			
Pb(1)-OH2	2.226(5)	Pb(1)-O(5)	2.400(6)
Pb(1)-O(1)	2.426(6)	Pb(1)-O(7)#1	2.637(6)
Pb(1)-O(3)#1	2.673(6)	Pb(2)-OH1	2.470(5)
Pb(2)-OH1#2	2.498(5)	Pb(2)-O(12)#1	2.612(6)
Pb(2)-O(11)#1	2.626(6)	Pb(2)-O(9)	2.660(5)
Pb(2)-O(7)#1	2.707(6)	Pb(2)-O(5)	2.738(6)
Pb(3)-OH2#2	2.346(5)	Pb(3)-OH1	2.374(5)
Pb(3)-O(8)#3	2.507(7)	Pb(3)-O(4)#4	2.569(6)
Pb(4)-N(5)	2.484(7)	Pb(4)-OW2	2.584(7)
Pb(4)-O(3)#4	2.635(6)	Pb(4)-O(11)#1	2.680(5)
Pb(4)-O(9)	2.693(7)	Pb(4)-OW1	2.728(9)
O(1)-C(7)	1.294(9)	O(2)-C(8)	1.239(9)
O(5)-C(16)	1.318(9)	O(6)-C(17)	1.251(9)
O(9)-C(25)	1.293(9)	O(10)-C(26)	1.259(9)
OH2-Pb(1)-O(5)	83.4(2)	O(5)-Pb(1)-O(7)#1	81.04(19)
OH2-Pb(1)-O(1)	71.7(2)	O(1)-Pb(1)-O(7)#1	153.56(19)
O(5)-Pb(1)-O(1)	88.7(2)	OH2-Pb(1)-O(3)#1	78.84(19)
OH2-Pb(1)-O(7)#1	82.9(2)	O(5)-Pb(1)-O(3)#1	162.15(19)
O(1)-Pb(1)-O(3)#1	84.0(2)	O(7)#1-Pb(1)-O(3)#1	98.51(18)
OH1-Pb(2)-OH1#2	74.98(19)	O(12)#1-Pb(2)-O(11)#1	49.94(17)
OH1-Pb(2)-O(12)#1	72.3(2)	OH1-Pb(2)-O(9)	72.87(16)

OH1#2-Pb(2)-O(12)#1	93.46(18)	OH1#2-Pb(2)-O(9)	125.96(19)
OH1-Pb(2)-O(11)#1	86.1(2)	O(12)#1-Pb(2)-O(9)	115.91(19)
OH1#2-Pb(2)-O(11)#1	142.87(18)	O(11)#1-Pb(2)-O(9)	75.74(19)
OH1-Pb(2)-O(7)#1	143.15(18)	O(11)#1-Pb(2)-O(7)#1	87.4(2)
OH1#2-Pb(2)-O(7)#1	89.10(18)	O(9)-Pb(2)-O(7)#1	139.65(18)
O(12)#1-Pb(2)-O(7)#1	75.8(2)	OH1-Pb(2)-O(5)	133.38(19)
OH1#2-Pb(2)-O(5)	81.06(18)	O(9)-Pb(2)-O(5)	90.84(18)
O(12)#1-Pb(2)-O(5)	149.41(19)	O(7)#1-Pb(2)-O(5)	74.01(18)
O(11)#1-Pb(2)-O(5)	132.74(19)	OH2#2-Pb(3)-OH1	84.01(19)
OH1-Pb(3)-O(8)#3	88.8(2)	OH2#2-Pb(3)-O(8)#3	80.6(2)
OH2#2-Pb(3)-O(4)#4	68.5(2)	O(8)#3-Pb(3)-O(4)#4	146.1(2)
OH1-Pb(3)-O(4)#4	74.7(2)	N(5)-Pb(4)-OW2	78.1(3)
N(5)-Pb(4)-O(3)#4	104.4(2)	OW2-Pb(4)-O(11)#1	69.9(2)
OW2-Pb(4)-O(3)#4	140.2(2)	O(3)#4-Pb(4)-O(11)#1	76.1(2)
N(5)-Pb(4)-O(11)#1	122.4(2)	N(5)-Pb(4)-O(9)	50.41(19)
O(3)#4-Pb(4)-O(9)	79.31(19)	OW2-Pb(4)-O(9)	72.1(2)
O(11)#1-Pb(4)-O(9)	74.31(17)	N(5)-Pb(4)-OW1	78.6(3)
O(11)#1-Pb(4)-OW1	134.6(3)	OW2-Pb(4)-OW1	77.5(3)
O(9)-Pb(4)-OW1	124.3(3)	O(3)#4-Pb(4)-OW1	142.4(3)

Symmetry transformations used to generate equivalent atoms: #1 -*x*+1, -*y*, -*z* #2 *x*, *y*+1, *z* for **1**; #1 *x*-1, *y*, *z* #2 -*x*-2, -*y*+2, -*z*+1 #3 -*x*-1, -*y*+2, -*z*+1 #4 *x*-1, *y*+1, *z* for **2**

Table S2 Hydrogen-bonded parameters in compound **2**

D-H···A	*d*(D-H) (Å)	*d*(H···A) (Å)	*d*(D···A) (Å)	∠D-H···A (º)	Symmetry operation
N2-H2A···O10#1	0.86	1.951	2.798	167.72	#1: -*x*-1, -*y*+2, -*z*
N4-H4A···O6#1	0.86	2.046	2.905	178.27	
N6-H6A···O2#1	0.86	1.948	2.802	171.68	