

Supporting Information

A novel trinuclear Cd(II) cluster-based Metal–Organic Framework: synthesis, structure and luminescence property

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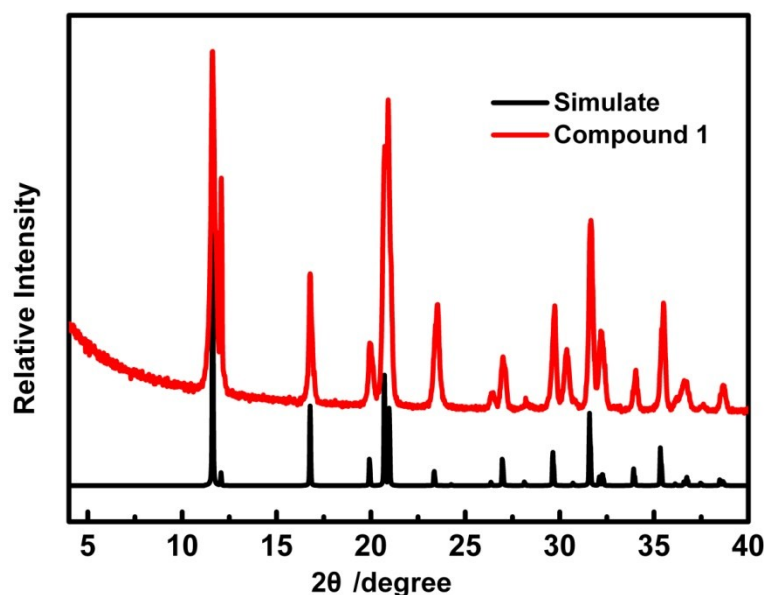


Fig. S1 Experimental and simulated PXRD patterns for compound **1**, indicating the phase purity of the as-synthesized samples.

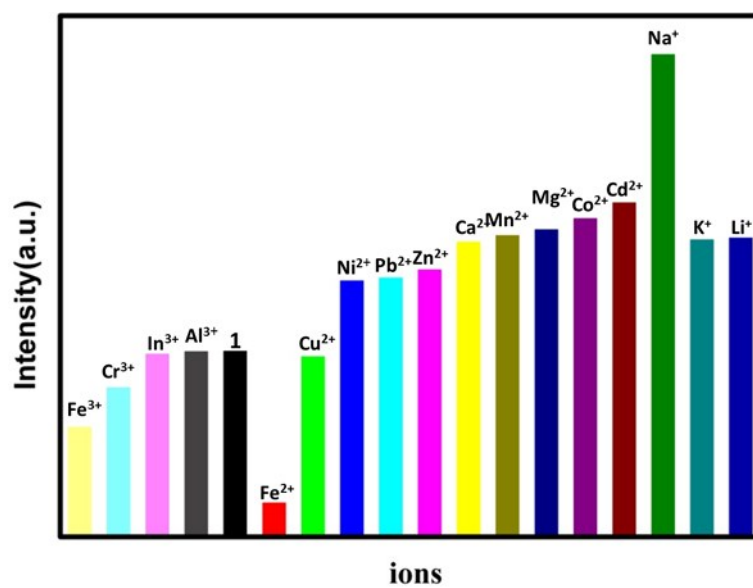


Fig. S2 Emission spectra of compound **1** in different metal ions.

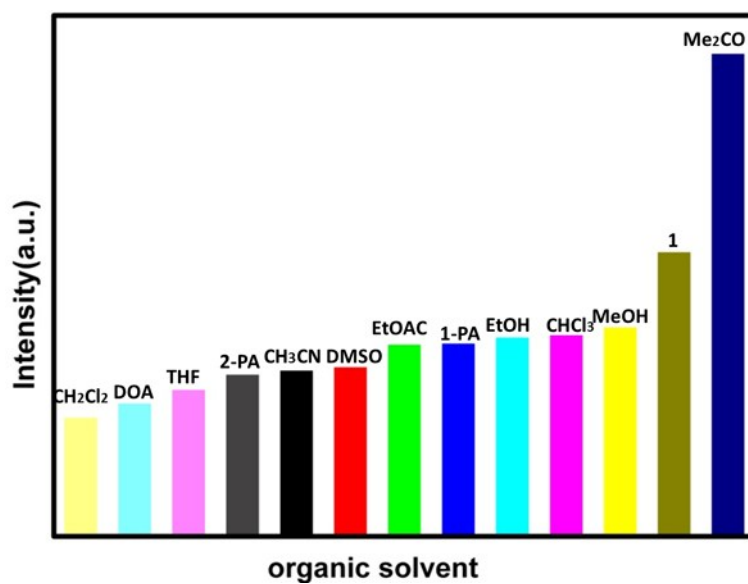


Fig. S3 Emission spectra of compound **1** in different volatile organic solvent.

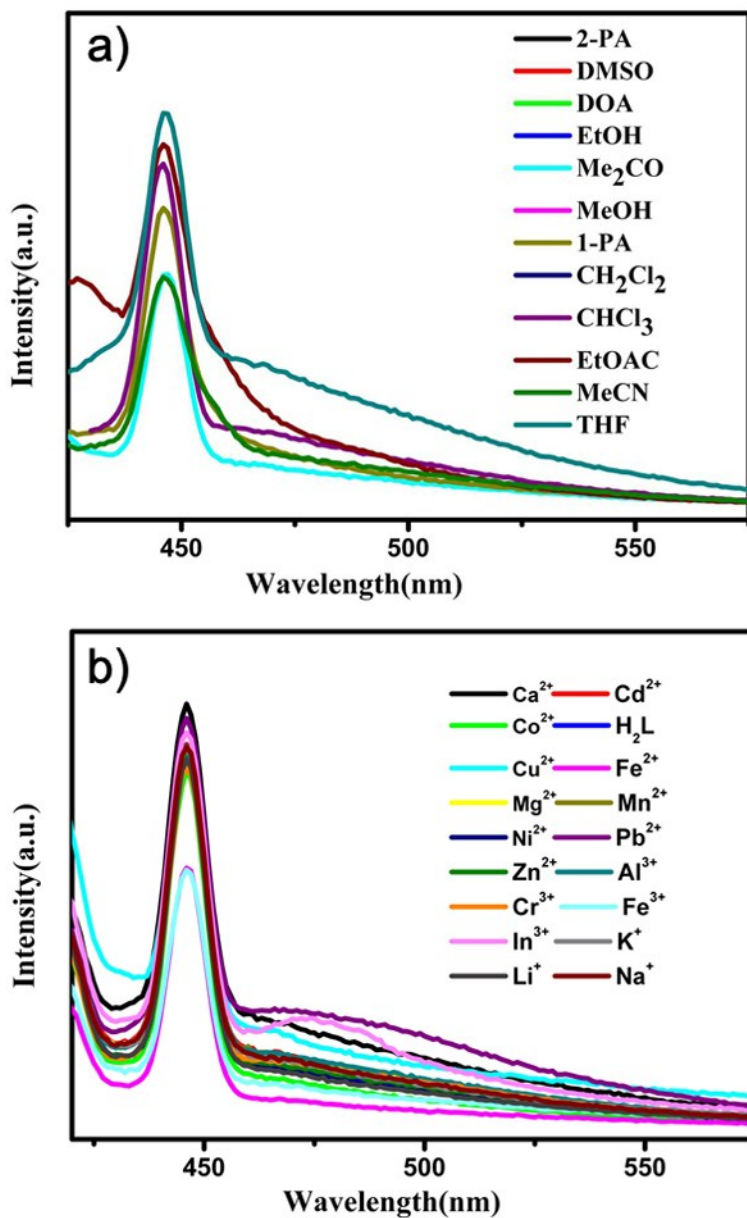


Fig. S4 Emission spectra of free H₂PZC ligand in different volatile organic solvents (a), and different metal ions (b).

Table S1 Selected bond lengths [Å] and angles [°] for compound **1**.

	compound 1
Cd(1)-N(1)#1	2.254(5)
Cd(1)-O(1)#2	2.254(5)
Cd(1)-O(2)	2.297(7)
Cd(1)-O(1)	2.366(4)
Cd(1)-O(1)#3	2.366(4)
Cd(1)-Cl(1)	2.6631(19)
Cl(1)-Cd(1)#4	2.6631(19)
Cl(1)-Cd(1)#5	2.6631(19)
N(1)-Cd(1)#6	2.254(5)

N(1)#1-Cd(1)-N(1)#2	107.3(3)
N(1)#1-Cd(1)-O(2)	90.7(2)
N(1)#2-Cd(1)-O(2)	90.7(2)
N(1)#1-Cd(1)-O(1)	153.62(18)
N(1)#2-Cd(1)-O(1)	98.6(2)
O(2)-Cd(1)-O(1)	84.3(3)
N(1)#1-Cd(1)-O(1)#3	98.6(2)
N(1)#2-Cd(1)-O(1)#3	153.62(18)
O(2)-Cd(1)-O(1)#3	84.3(3)
O(1)-Cd(1)-O(1)#3	55.1(2)
N(1)#1-Cd(1)-Cl(1)	94.73(15)
N(1)#2-Cd(1)-Cl(1)	94.73(15)
O(2)-Cd(1)-Cl(1)	170.8(3)
O(1)-Cd(1)-Cl(1)	87.55(15)
O(1)#3-Cd(1)-Cl(1)	87.55(15)
N(1)#1-Cd(1)-C(3)	125.96(16)
N(1)#2-Cd(1)-C(3)	125.96(16)
O(2)-Cd(1)-C(3)	81.1(3)
O(1)-Cd(1)-C(3)	27.67(11)
O(1)#3-Cd(1)-C(3)	27.67(11)
Cl(1)-Cd(1)-C(3)	89.7(2)
Cd(1)#4-Cl(1)-Cd(1)#5	98.29(9)
Cd(1)#4-Cl(1)-Cd(1)	98.29(9)
Cd(1)#5-Cl(1)-Cd(1)	98.29(9)
C(3)-O(1)-Cd(1)	92.5(4)
Cd(1)-O(2)-H(2A)	127(2)
C(2)-N(1)-Cd(1)#6	125.9(5)
N(1)#3-N(1)-Cd(1)#6	126.01(15)
O(1)#3-C(3)-Cd(1)	59.9(4)
O(1)-C(3)-Cd(1)	59.9(4)
C(1)-C(3)-Cd(1)	169.7(6)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/3, x-y+2/3, z+2/3$ #2 $-x+y+1/3, -x+2/3, z+2/3$
#3 $-y+1, -x+1, z$ #4 $-x+y+1, -x+1, z$ #5 $-y+1, x-y, z$
#6 $-y+2/3, x-y+1/3, z-2/3$