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Interplay of coordinative and supramolecular interactions in engineering unusual crystalline architectures of low-dimensional metal-pamoate complexes under co-ligand intervention

Miao Du,* Cheng-Peng Li, Xiao-Jun Zhao, and Qian Yu

Table S1 Hydrogen-bonding metrics for compounds **1**–**12**

Compound	D–H···A	D···A (Å)	H···A (Å)	D–H···A (°)
1	O(3)–H(3)···O(2)	2.569(3)	1.83	149
	O(4)–H(4)···O(5)	2.588(3)	1.86	147
	O(9)–H(9)···O(8)	2.560(3)	1.82	149
	O(12)–H(12)···O(11)	2.591(3)	1.86	148
	O(1)–H(1)···O(13)	2.548(3)	1.73	172
	O(6)–H(6)···O(14)[a]	2.624(3)	1.82	168
	O(7)–H(7)···O(16)[b]	2.515(3)	1.71	169
	O(10)–H(10)···O(15)[c]	2.570(3)	1.76	169
2	O(7)–H(7)···O(8)	2.503(2)	1.76	150
	O(10)–H(10)···O(11)	2.521(2)	1.78	149
	O(3)–H(3A)···O(9)[a]	2.741(3)	1.95	155
	O(3)–H(3B)···O(9)	2.710(3)	1.87	167
	O(4)–H(4A)···O(8)[b]	2.896(2)	2.06	167
	O(4)–H(4B)···O(8)	2.782(2)	1.98	156
	O(5)–H(5A)···O(12)[c]	2.763(3)	2.03	144
	O(5)–H(5B)···O(12)[d]	2.668(3)	1.82	177
	O(6)–H(6A)···O(11)[d]	2.690(2)	1.84	173
	O(6)–H(6B)···O(7)[b]	2.841(2)	2.01	166

3	O(1)–H(1)···O(2)	2.555(2)	1.82	148
	O(6)–H(6)···O(5)	2.550(2)	1.81	149
	O(9)–H(9A)···O(5)[a]	2.647(2)	1.81	169
	O(9)–H(9B)···O(2)[b]	2.646(2)	1.80	172
4	O(3)–H(3A)···O(2)	2.540(3)	1.80	149
	O(4)–H(4A)···O(5)	2.533(3)	1.79	149
5	O(3)–H(3)···O(2)	2.535(3)	1.79	150
	O(4)–H(4)···O(5)	2.541(3)	1.80	149
6	O(3)–H(3)···O(2)	2.525(2)	1.79	148
	O(4)–H(4)···O(5)	2.534(3)	1.79	149
7	O(3)–H(3)···O(2)	2.501(2)	1.75	151
	O(4)–H(4A)···O(1)	2.713(2)	1.92	155
	O(4)–H(4B)···O(1)[a]	2.656(2)	1.83	163
	O(5)–H(5')···O(2)	2.851(2)	2.10	144
8	O(3)–H(3)···O(1)	2.556(5)	1.82	149
	O(4)–H(4)···O(5)	2.543(5)	1.80	150
	O(7)–H(7A)···O(1)	2.683(5)	1.85	163
	O(7)–H(7B)···O(8)[a]	2.648(6)	1.82	161
9	O(3)–H(3)···O(2)	2.528(5)	1.78	150
	O(4)–H(4)···O(5)	2.561(5)	1.82	149
	O(7)–H(7A)···O(9)[a]	2.649(6)	1.81	167
	O(7)–H(7B)···O(5)[b]	2.678(5)	1.84	165
10	O(5)–H(5)···O(4)	2.565(3)	1.84	146
	O(6)–H(6)···O(1)	2.536(3)	1.79	150
11	O(3)–H(3)···O(2)	2.511(2)	1.77	149
12	O(3)–H(3)···O(2)	2.491(6)	1.84	135
	O(4)–H(4)···O(5)	2.552(6)	1.83	147

For **1**: [a] $-x+2, -y+1, -z+1$; [b] $-x+1, y-1/2, -z+3/2$; [c] $-x, -y+1, -z+1$. For **2**: [a] $-x+1, -y+2, -z+1$; [b] $-x, -y+2, -z+1$; [c] $-x, -y+1, -z+1$; [d] $x, y+1, z-1$. For **3**: [a] $-x+1/2, y-1/2, -z+3/2$; [b] $-x, -y+1, -z+1$. For **7**: [a] $-x+1, -y+1, -z+1$. For **8**: [a] $-x+1, -y, -z+2$. For **9**: [a] $-x+1, y+1/2, -z+1/2$; [b] $x, -y+5/2, z+1/2$.

Table S2 Selected bond distances (Å) and angles (°) for compounds **1**–**12**[a]

Compound 1

C(1)–O(1)	1.309(3)	C(1)–O(2)	1.222(3)
C(16)–O(5)	1.224(3)	C(16)–O(6)	1.326(3)
C(24)–O(7)	1.297(3)	C(24)–O(8)	1.231(3)
C(45)–O(10)	1.312(3)	C(45)–O(11)	1.226(3)
C(46)–O(12)	1.353(3)	C(34)–O(9)	1.365(3)
C(11)–O(3)	1.365(3)	C(14)–O(4)	1.357(3)
C(10)–C(12)–C(13)	116.0(2)	C(33)–C(35)–C(36)	115.5(2)

Compound 2

Mn(1)–O(1)	2.135(2)	Mn(1)–O(2)	2.130(2)
Mn(1)–O(3)	2.175(2)	Mn(1)–O(4)	2.224(2)
Mn(1)–O(5)	2.133(2)	Mn(1)–O(6)	2.196(2)
O(7)–C(17)	1.363(2)	O(10)–C(20)	1.351(3)
O(8)–C(7)	1.271(3)	O(9)–C(7)	1.240(3)
O(11)–C(22)	1.261(3)	O(12)–C(22)	1.249(3)
O(1)–Mn(1)–O(2)	100.2(1)	O(1)–Mn(1)–O(3)	91.41(9)
O(1)–Mn(1)–O(4)	174.39(8)	O(1)–Mn(1)–O(5)	88.92(9)
O(1)–Mn(1)–O(6)	85.33(8)	O(2)–Mn(1)–O(3)	90.71(8)
O(2)–Mn(1)–O(4)	84.12(8)	O(2)–Mn(1)–O(5)	88.37(8)
O(2)–Mn(1)–O(6)	172.55(8)	O(3)–Mn(1)–O(4)	84.86(7)
O(3)–Mn(1)–O(5)	179.07(6)	O(3)–Mn(1)–O(6)	94.20(7)
O(4)–Mn(1)–O(5)	94.87(7)	O(4)–Mn(1)–O(6)	90.75(7)
O(5)–Mn(1)–O(6)	86.69(7)	C(16)–C(18)–C(19)	118.7(2)

Compound 3

Cu(1)–O(3)	1.956(1)	Cu(1)–O(4A)	1.959(1)
Cu(1)–O(7)	2.306(2)	Cu(1)–O(8)	1.952(2)
Cu(1)–O(9)	1.945(1)	O(1)–C(11)	1.358(3)
O(6)–C(23)	1.356(2)	O(2)–C(1)	1.256(3)
O(3)–C(1)	1.266(3)	O(4)–C(22)	1.258(3)
O(5)–C(22)	1.259(3)		

O(3)–Cu(1)–O(4A)	176.71(6)	O(3)–Cu(1)–O(7)	93.89(6)
O(3)–Cu(1)–O(8)	91.38(6)	O(3)–Cu(1)–O(9)	89.42(6)
O(4A)–Cu(1)–O(7)	88.94(6)	O(4A)–Cu(1)–O(8)	89.97(7)
O(4A)–Cu(1)–O(9)	88.88(6)	O(7)–Cu(1)–O(8)	96.30(6)
O(7)–Cu(1)–O(9)	90.55(6)	O(8)–Cu(1)–O(9)	173.02(7)
C(10)–C(12)–C(13)	116.1(2)		

Compound 4

Cd(1)–O(1)	2.557(2)	Cd(1)–O(2)	2.295(2)
Cd(1)–O(5B)	2.528(2)	Cd(1)–O(6B)	2.337(2)
C(1)–O(1)	1.238(3)	C(1)–O(2)	1.275(4)
C(16)–O(5)	1.264(3)	C(16)–O(6)	1.252(3)
C(3)–O(3)	1.346(3)	C(14)–O(4)	1.358(3)
O(1)–Cd(1)–O(1A)	128.1(1)	O(1)–Cd(1)–O(2)	53.35(7)
O(1)–Cd(1)–O(2A)	89.34(7)	O(1)–Cd(1)–O(5B)	135.63(6)
O(1)–Cd(1)–O(5C)	81.09(7)	O(1)–Cd(1)–O(6B)	83.70(6)
O(1)–Cd(1)–O(6C)	128.97(7)	O(2)–Cd(1)–O(2A)	91.9(1)
O(2)–Cd(1)–O(5B)	170.07(7)	O(2)–Cd(1)–O(5C)	84.57(8)
O(2)–Cd(1)–O(6B)	136.26(7)	O(2)–Cd(1)–O(6C)	95.93(7)
O(5B)–Cd(1)–O(5C)	100.4(1)	O(5B)–Cd(1)–O(6B)	53.52(6)
O(5B)–Cd(1)–O(6C)	80.49(7)	O(6B)–Cd(1)–O(6C)	107.2(1)
C(4)–C(12)–C(13)	113.5(2)		

Compound 5

Zn(1)–O(1)	2.000(2)	Zn(1)–O(7)	2.135(3)
Zn(1)–O(6A)	1.974(2)	Zn(1)–N(1)	2.127(3)
Zn(1)–N(2)	2.147(3)	O(1)–C(11)	1.275(3)
O(2)–C(11)	1.242(4)	O(5)–C(26)	1.248(4)
O(6)–C(26)	1.274(4)	O(3)–C(12)	1.364(3)
O(4)–C(24)	1.370(3)		
O(1)–Zn(1)–O(6A)	101.79(9)	O(1)–Zn(1)–O(7)	94.7(1)
O(1)–Zn(1)–N(1)	94.8(1)	O(1)–Zn(1)–N(2)	157.8(1)
O(6A)–Zn(1)–O(7)	93.9(1)	O(6A)–Zn(1)–N(1)	117.67(9)
O(6A)–Zn(1)–N(2)	100.4(1)	O(7)–Zn(1)–N(1)	144.2(1)
O(7)–Zn(1)–N(2)	83.1(1)	N(1)–Zn(1)–N(2)	75.4(1)
C(13)–C(22)–C(23)	115.1(2)		

Compound 6

Cd(1)–O(1)	2.436(2)	Cd(1)–O(2)	2.405(2)
Cd(1)–O(6A)	2.247(2)	Cd(1)–O(7)	2.305(2)
Cd(1)–N(1)	2.332(2)	Cd(1)–N(2)	2.343(2)
O(1)–C(1)	1.249(3)	O(2)–C(1)	1.264(3)
O(5)–C(16)	1.263(3)	O(6)–C(16)	1.253(3)
O(3)–C(3)	1.356(3)	O(4)–C(14)	1.355(3)
O(1)–Cd(1)–O(2)	53.65(6)	O(1)–Cd(1)–O(6A)	98.50(7)
O(1)–Cd(1)–O(7)	80.94(7)	O(1)–Cd(1)–N(1)	135.89(7)
O(1)–Cd(1)–N(2)	92.28(7)	O(2)–Cd(1)–O(6A)	98.46(7)
O(2)–Cd(1)–O(7)	133.29(7)	O(2)–Cd(1)–N(1)	83.95(7)
O(2)–Cd(1)–N(2)	85.66(7)	O(6A)–Cd(1)–O(7)	98.50(8)
O(6A)–Cd(1)–N(1)	99.34(7)	O(6A)–Cd(1)–N(2)	168.86(7)
O(7)–Cd(1)–N(1)	134.96(8)	O(7)–Cd(1)–N(2)	85.89(8)
N(1)–Cd(1)–N(2)	70.69(7)	C(4)–C(12)–C(13)	115.4(2)

Compound 7

Mn(1)–O(4)	2.139(1)	Mn(1)–N(1)	2.264(2)
Mn(1)–N(2)	2.317(2)	O(3)–C(15)	1.362(2)
C(13)–O(1)	1.253(2)	C(13)–O(2)	1.261(2)
O(4)–Mn(1)–O(4A)	80.35(7)	O(4)–Mn(1)–N(1)	91.98(5)
O(4)–Mn(1)–N(1A)	157.55(5)	O(4)–Mn(1)–N(2)	106.48(5)
O(4)–Mn(1)–N(2A)	89.46(6)	N(1)–Mn(1)–N(1A)	102.29(8)
N(1)–Mn(1)–N(2)	72.41(6)	N(1)–Mn(1)–N(2A)	94.42(6)
N(2)–Mn(1)–N(2A)	159.32(9)	C(16)–C(17)–C(16B)	115.9(2)

Compound 8

Cu(1)–O(5A)	1.971(3)	Cu(1)–O(7)	1.980(4)
Cu(1)–N(1)	2.015(4)	Cu(1)–N(2)	2.021(4)
Cu(1)–O(2)	2.252(3)	O(1)–C(13)	1.259(6)
O(2)–C(13)	1.253(6)	O(5)–C(28)	1.313(6)
O(6)–C(28)	1.224(6)	O(3)–C(15)	1.366(6)
O(4)–C(26)	1.353(5)		
O(2)–Cu(1)–O(5A)	93.7(1)	O(2)–Cu(1)–O(7)	86.6(1)
O(2)–Cu(1)–N(1)	95.4(1)	O(2)–Cu(1)–N(2)	99.1(1)
O(5A)–Cu(1)–O(7)	94.1(2)	O(5A)–Cu(1)–N(1)	92.9(2)
O(5A)–Cu(1)–N(2)	166.3(2)	O(7)–Cu(1)–N(1)	172.6(1)

O(7)–Cu(1)–N(2)	91.6(2)	N(1)–Cu(1)–N(2)	81.1(2)
C(16)–C(24)–C(25)	116.4(4)		

Compound 9

Zn(1)–O(1)	2.416(4)	Zn(1)–O(2)	2.107(3)
Zn(1)–O(6A)	2.064(3)	Zn(1)–O(7)	2.075(3)
Zn(1)–N(1)	2.127(4)	Zn(1)–N(2)	2.156(4)
O(1)–C(13)	1.240(6)	O(2)–C(13)	1.287(7)
O(5)–C(28)	1.264(6)	O(6)–C(28)	1.263(5)
O(3)–C(15)	1.359(6)	O(4)–C(26)	1.374(5)
O(1)–Zn(1)–O(2)	57.7(1)	O(1)–Zn(1)–O(6A)	150.5(1)
O(1)–Zn(1)–O(7)	87.3(1)	O(1)–Zn(1)–N(1)	111.4(1)
O(1)–Zn(1)–N(2)	90.2(1)	O(2)–Zn(1)–O(6A)	93.4(2)
O(2)–Zn(1)–O(7)	96.7(2)	O(2)–Zn(1)–N(1)	165.1(2)
O(2)–Zn(1)–N(2)	92.1(2)	O(6A)–Zn(1)–O(7)	91.0(1)
O(6A)–Zn(1)–N(1)	98.0(1)	O(6A)–Zn(1)–N(2)	97.1(1)
O(7)–Zn(1)–N(1)	92.6(2)	O(7)–Zn(1)–N(2)	167.7(2)
N(1)–Zn(1)–N(2)	77.1(1)	C(16)–C(24)–C(25)	117.0(4)

Compound 10

Cd(1)–O(1)	2.441(2)	Cd(1)–O(2)	2.311(2)
Cd(1)–O(3)	2.275(2)	Cd(1)–N(2)	2.312(3)
Cd(1)–O(4)	2.251(2)	Cd(1)–N(1)	2.338(3)
O(1)–C(1)	1.263(4)	O(2)–C(1)	1.253(4)
O(3A)–C(12)	1.244(4)	O(4)–C(12)	1.260(4)
O(5)–C(22)	1.355(3)	O(6)–C(11)	1.356(4)
O(1)–Cd(1)–O(2)	54.91(7)	O(1)–Cd(1)–O(3)	148.46(8)
O(1)–Cd(1)–O(4)	90.44(9)	O(1)–Cd(1)–N(1)	91.08(9)
O(1)–Cd(1)–N(2)	87.98(9)	O(2)–Cd(1)–O(3)	94.23(8)
O(2)–Cd(1)–O(4)	97.76(9)	O(2)–Cd(1)–N(1)	89.48(9)
O(2)–Cd(1)–N(2)	138.44(9)	O(3)–Cd(1)–O(4)	101.2(1)
O(3)–Cd(1)–N(1)	81.4(1)	O(3)–Cd(1)–N(2)	117.80(9)
O(4)–Cd(1)–N(1)	172.1(1)	O(4)–Cd(1)–N(2)	100.8(1)
N(1)–Cd(1)–N(2)	71.5(1)	C(10)–C(23)–C(10A)	118.2(3)
C(21)–C(24)–C(21B)	117.6(3)		

Compound 11

Cu(1)–O(1)	1.974(1)	Cu(1)–N(1)	2.026(2)

Cu(1)–N(2B)	1.996(2)	Cu(1)–O(4)	2.561(2)
O(1)–C(12)	1.270(2)	O(2)–C(12)	1.250(3)
O(3)–C(2)	1.355(2)		
O(1)–Cu(1)–O(1A)	176.24(7)	O(1)–Cu(1)–N(1)	88.12(4)
O(1)–Cu(1)–N(2B)	91.88(4)	O(1)–Cu(1)–O(4)	97.11(6)
O(1)–Cu(1)–O(4A)	82.56(6)	N(1)–Cu(1)–O(4)	84.89(4)
N(2B)–Cu(1)–O(4)	95.11(4)	N(2B)–Cu(1)–N(1)	180
O(4A)–Cu(1)–O(4)	169.78(6)	C(3)–C(11)–C(3C)	118.0(3)

Compound 12

Cd(1)–O(1)	2.572(4)	Cd(1)–O(2)	2.310(4)
Cd(1)–O(5A)	2.528(4)	Cd(1)–O(6A)	2.339(5)
Cd(1)–N(1B)	2.421(5)	Cd(1)–N(2)	2.369(5)
Cd(1)–N(3)	2.319(5)	O(1)–C(11)	1.250(7)
O(2)–C(11)	1.273(7)	O(5)–C(23)	1.267(7)
O(6)–C(23)	1.231(8)	O(3)–C(3)	1.358(6)
O(4)–C(14)	1.360(7)		
O(1)–Cd(1)–O(2)	53.0(1)	O(1)–Cd(1)–O(5A)	90.6(1)
O(1)–Cd(1)–O(6A)	142.1(1)	O(1)–Cd(1)–N(1B)	136.8(1)
O(1)–Cd(1)–N(2)	82.4(2)	O(1)–Cd(1)–N(3)	89.3(2)
O(2)–Cd(1)–O(5A)	143.5(2)	O(2)–Cd(1)–O(6A)	162.3(2)
O(2)–Cd(1)–N(1B)	83.9(1)	O(2)–Cd(1)–N(2)	85.3(2)
O(2)–Cd(1)–N(3)	95.9(2)	O(5A)–Cd(1)–O(6A)	53.2(2)
O(5A)–Cd(1)–N(1B)	132.4(2)	O(5A)–Cd(1)–N(2)	92.8(2)
O(5A)–Cd(1)–N(3)	79.4(2)	O(6A)–Cd(1)–N(1B)	80.7(2)
O(6A)–Cd(1)–N(2)	88.2(2)	O(6A)–Cd(1)–N(3)	93.7(2)
N(1B)–Cd(1)–N(2)	97.4(2)	N(1B)–Cd(1)–N(3)	94.1(2)
N(2)–Cd(1)–N(3)	168.6(2)	C(4)–C(12)–C(13)	114.1(5)

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[a] Symmetry transformations used to generate equivalent atoms. For **3**: A $x - 1/2, -y + 3/2, z - 1/2$. For **4**: A $-x + 2, y, -z + 1/2$; B $-x + 2, y + 1, -z + 1/2$; C $x, y + 1, z$. For **5**: A $x, -y + 2, z + 1/2$. For **6**: A $x - 1/2, -y + 1, z + 1/2$. For **7**: A $-x + 1, y, -z + 3/2$; B $-x, y, -z + 1/2$. For **8**: A $x, -y + 1/2, z + 1/2$. For **9**: A $x, -y + 5/2, z + 1/2$. For **10**: A $-x + 1, y, -z + 3/2$; B $-x + 1, y, -z + 1/2$. For **11**: A $-x + 1, y, -z + 3/2$; B $x, y - 1, z$; C $-x, y, -z + 1/2$. For **12**: A $x + 1, -y + 1/2, z + 1/2$; B $-x, y - 1/2, -z + 1/2$.

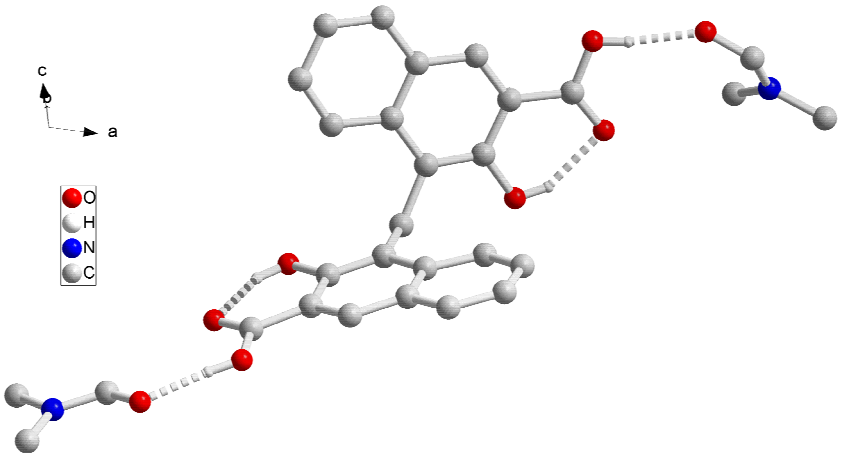

Fig. S1 A portion view of **1** showing the hydrogen bonding