

Novel complexes constructed by flexible 1,2,3,4,5,6-cyclohexanhexacarboxylate and transition metal ions - From 0D mononuclear to 3D porous coordination polymers[†]

Feifei Xing,^a Yueling Bai,^a Xiang He,^a Juan Jia,^a Dong Zhou,^a Min Shao^b and Shourong Zhu^{*a}

Supplementary materials

Fig. S1 The topologic net of complex **2, 3, 4**.

Fig. S2 Crystal packing diagram of complex **6**

Fig. S3 Crystal packing diagram of complex **7**

Fig. S4 Crystal packing diagram of complex **8**

Fig. S5 Crystal packing diagram of complex **9**

Fig. S6- S7 IR spectra of complexes.

Fig. S8- S14 TGA and DSC curves of complexes.

Fig. S15 Solid state fluorescence spectra of complex **1, 5, 6** and **7**.

Table S1 Bond lengths [Å] and angles [°] for complex **1-9**.

Table S2 Hydrogen bonds for complex **1-9** [Å and °].

^a Department of Chemistry, College of Science, Shanghai University Shanghai, 200444, China. E-mail: shourongzhu@shu.edu.cn; Fax: +86-21-66134594; Tel: +86-21-66132403

^b Instrumental Analysis and Research Centre, Shanghai University, Shanghai, 200444, China

[†] Electronic supplementary information (ESI) available: Crystal packing diagram of complex **5,6,7,8** and **9**; Solid state fluorescence spectra of **1, 5, 6** and **7**; IR spectra of complex **1-9**; TG and DSC curves of complexes **2-7** and **9**; Bond distances and angles for complexes **1-9**. CCDC reference numbers 848873–848881. For ESI and crystallographic data in CIF or other electronic format see DOI:

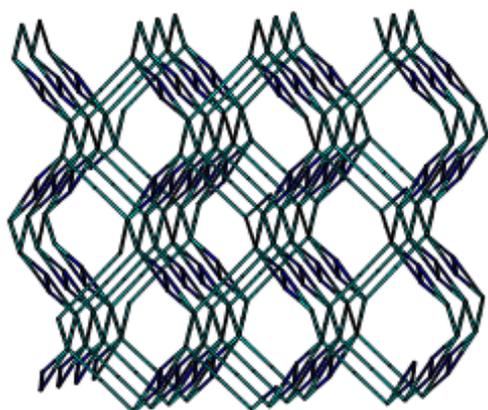


Fig. S1a The $\{3^2;4\}\{3;6^3;8^6\}$ topologic net of complex 2.

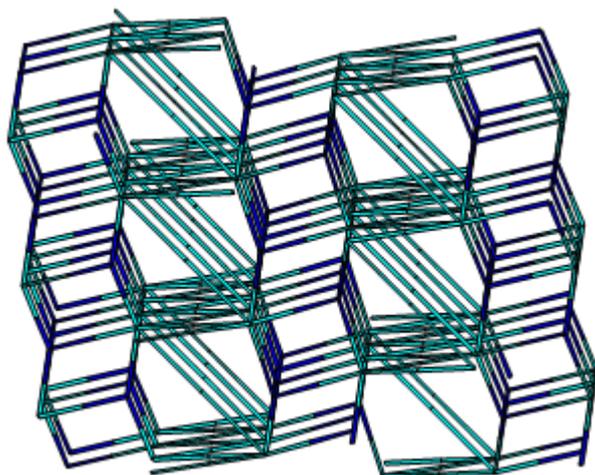


Fig. S1b The $\{4^3\}\{4^5;6^7;8^3\}$ topologic net of complex 3.

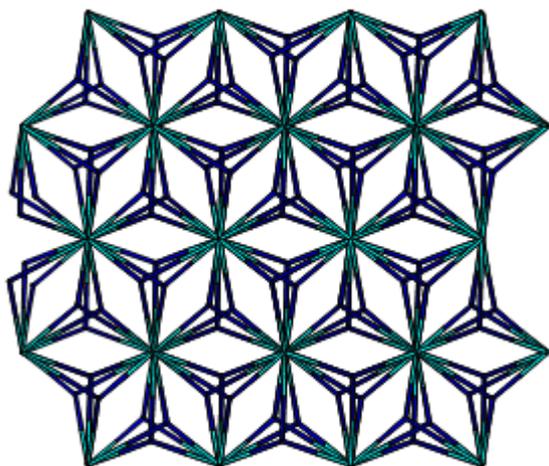


Fig. S1c The $\{4^2;6\}_3\{4^6;6^{21};8^9\}$ topologic net of complex 4.

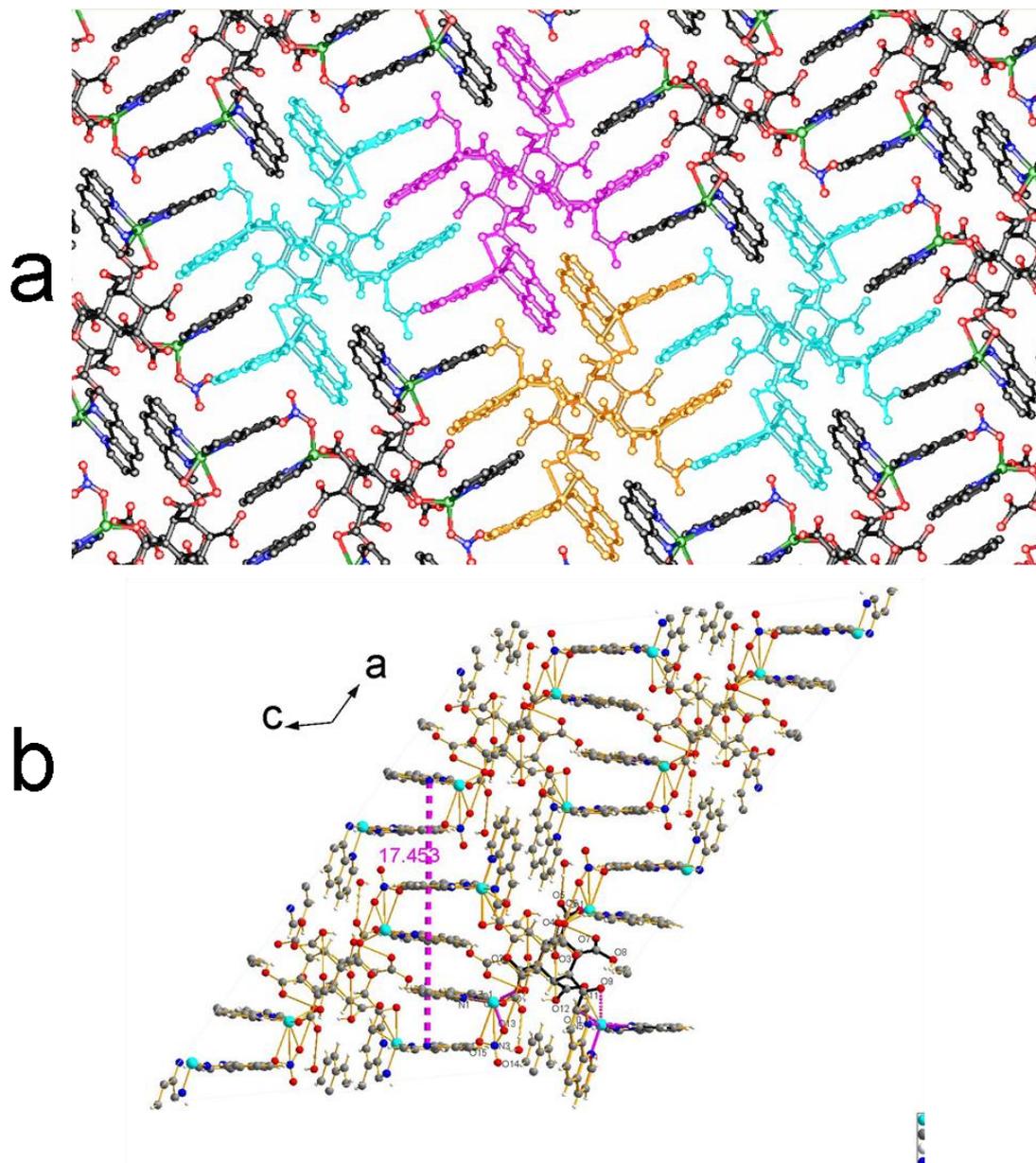


Fig. S2 (a) Linkage scheme of the 1D coordination polymer, (b) Crystal packing diagram from the b-axis of complex **6**

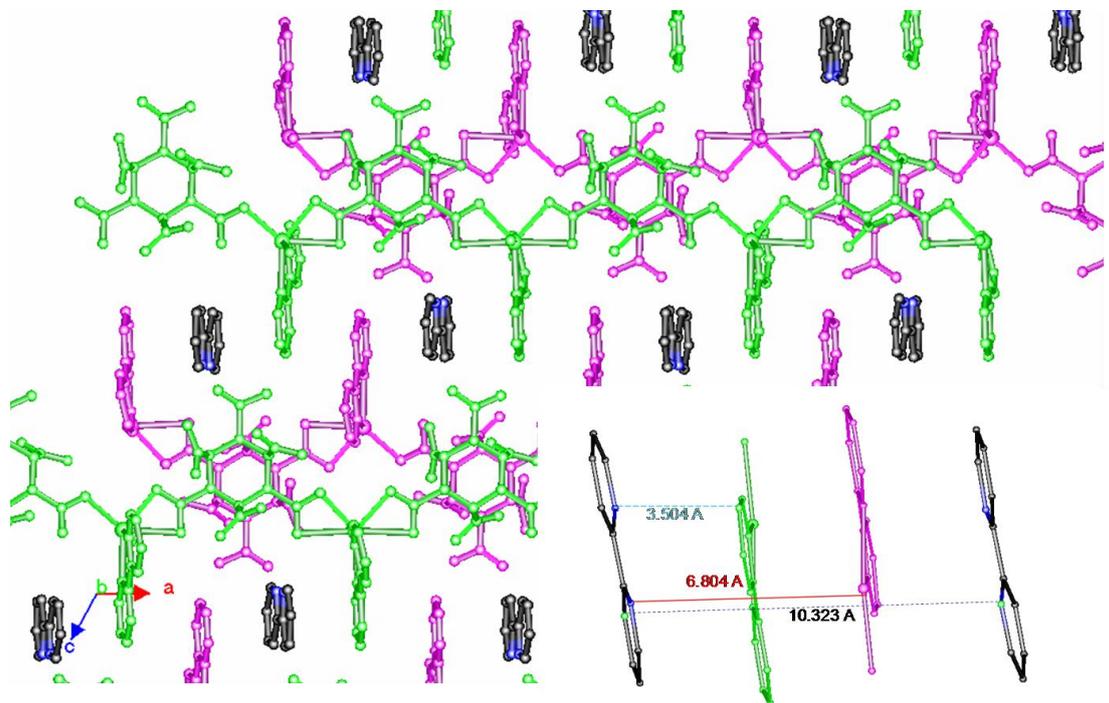
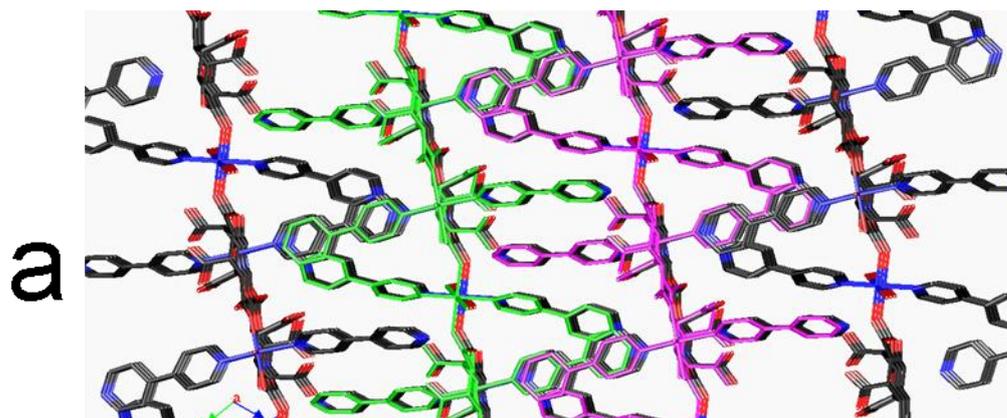


Fig. S3 Crystal packing diagram of complex 7 from the b-axis. The nearest atom distances among the adjacent aromatic rings are ~ 3.50 Å.



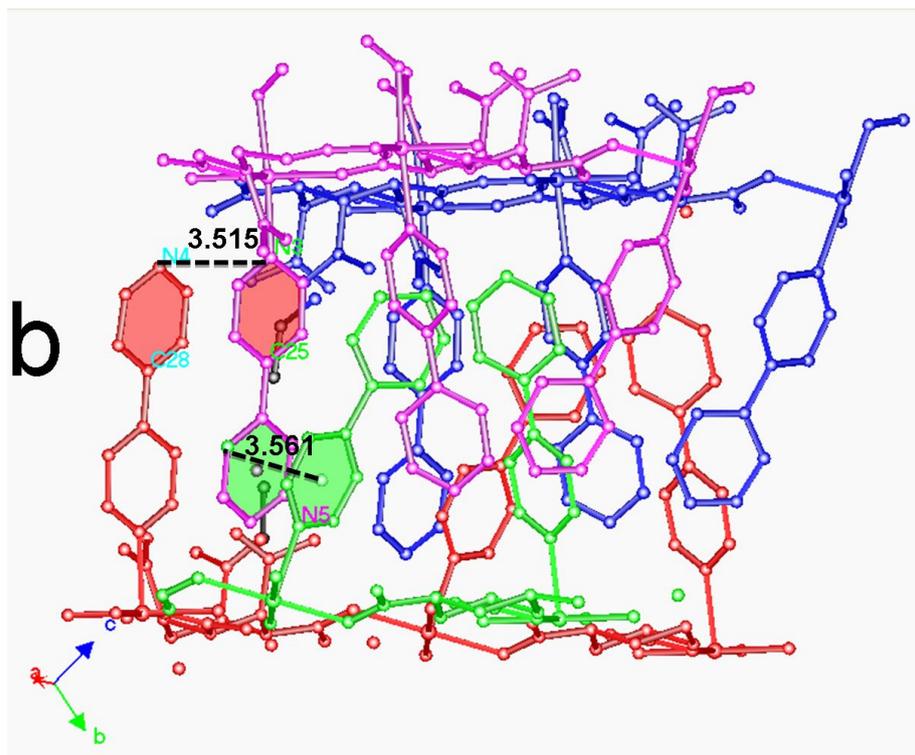


Fig. S4 (a) Crystal packing diagram of complex **8** from the a-axis. (b) The nearest atom-atom or atom-centroid distances among the adjacent aromatic rings are 3.5 Å ~3.6 Å.

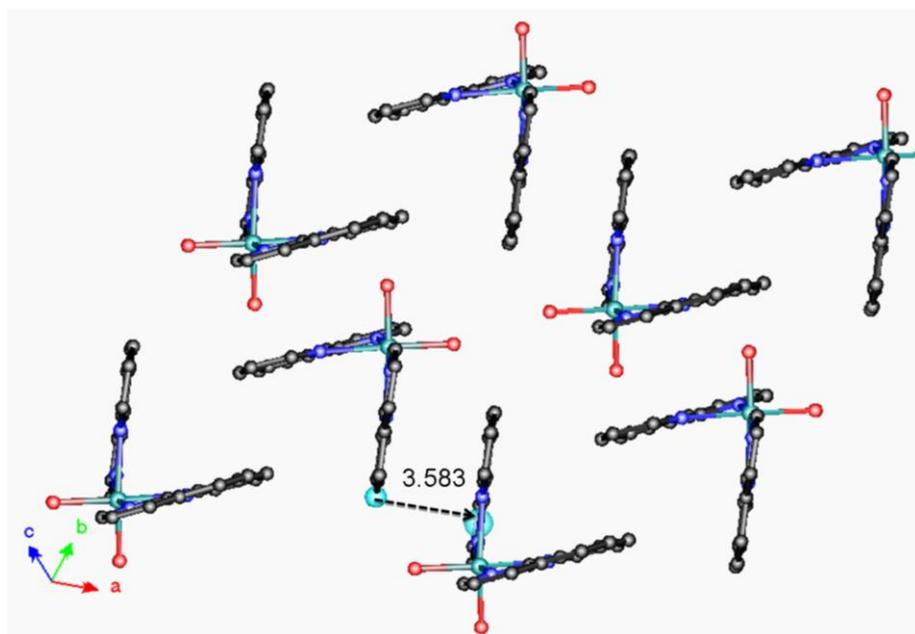


Fig. S5 Crystal packing diagram of complex **9**, the nearest atom-centroid distances among the adjacent aromatic rings are ~3.6 Å.

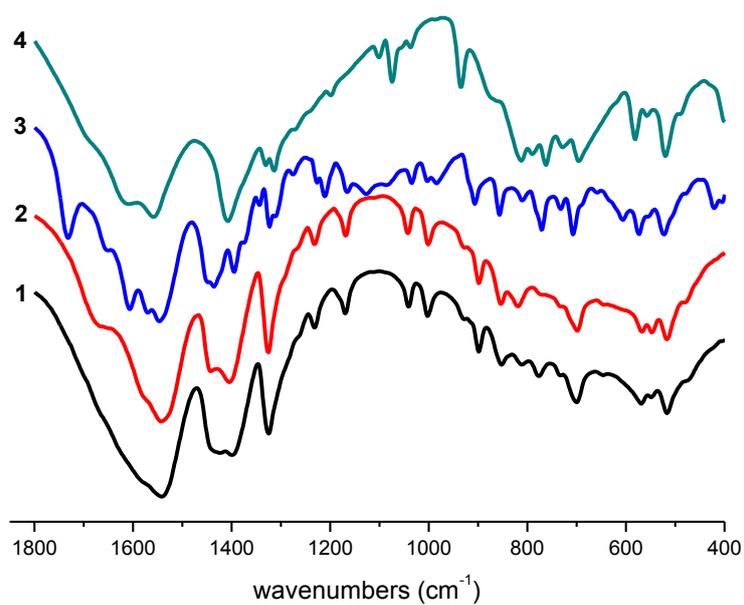


Fig. S6 IR spectra of complex 1-4.

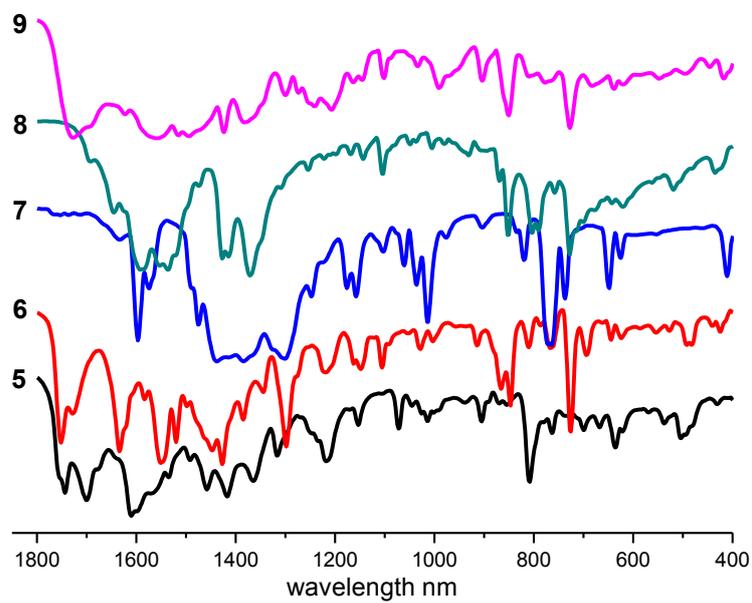


Fig. S7 IR spectra of complex 5-9.

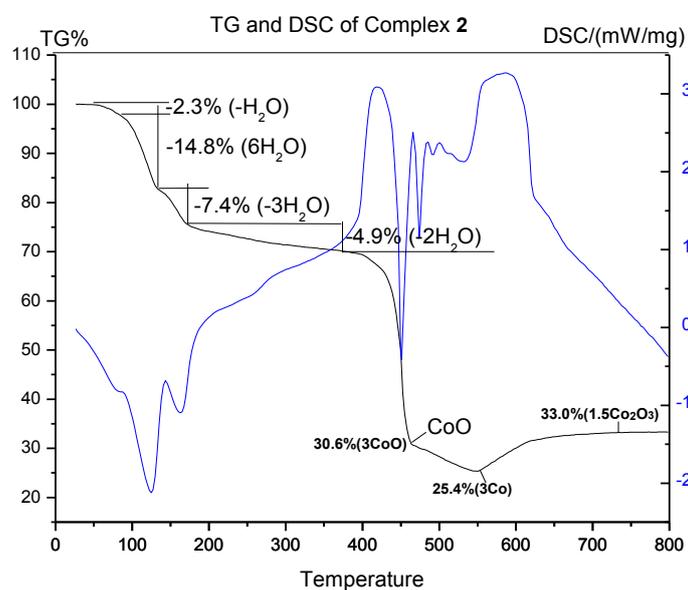


Fig. S8 TGA and DSC curve of $\{[\text{Co}_3(\eta_9\text{-L}^1)(\eta_2\text{-H}_2\text{O})_1(\eta_1\text{-H}_2\text{O})_7] \cdot (\text{H}_2\text{O})_5\}_n$ (**2**)

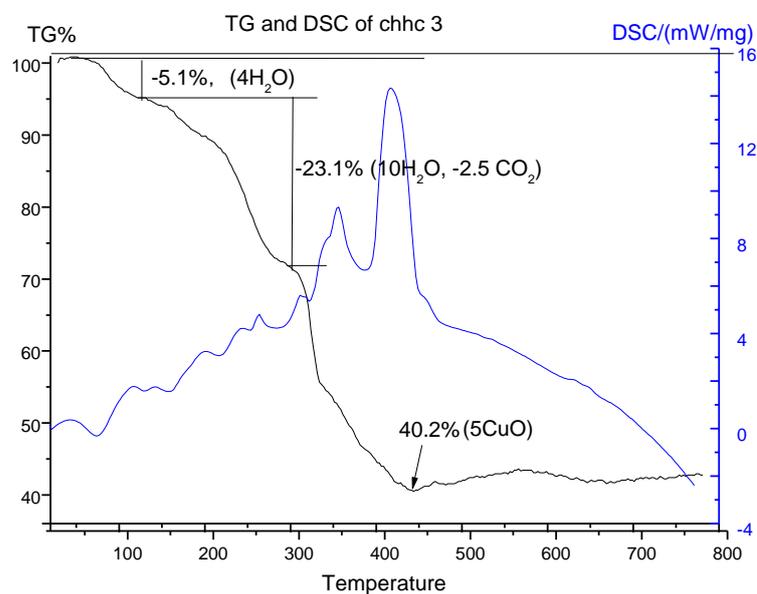


Fig. S9 TGA and DSC curve of $\{[\text{Cu}_5(\eta_8\text{-HL}^1)_2 \cdot 10\text{H}_2\text{O}] \cdot (\text{H}_2\text{O})_4\}_n$ (**3**)

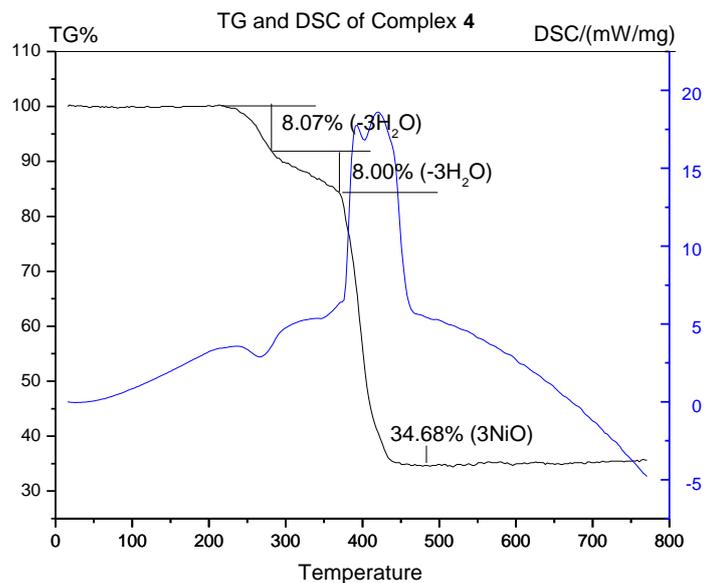


Fig. S10 TGA and DSC curve of $\{[\text{Ni}_3(\eta_{12}\text{-L}^{\text{II}})(\eta_1\text{-H}_2\text{O})_6] \cdot 1.5\text{H}_2\text{O}\}_n$ (**4**)

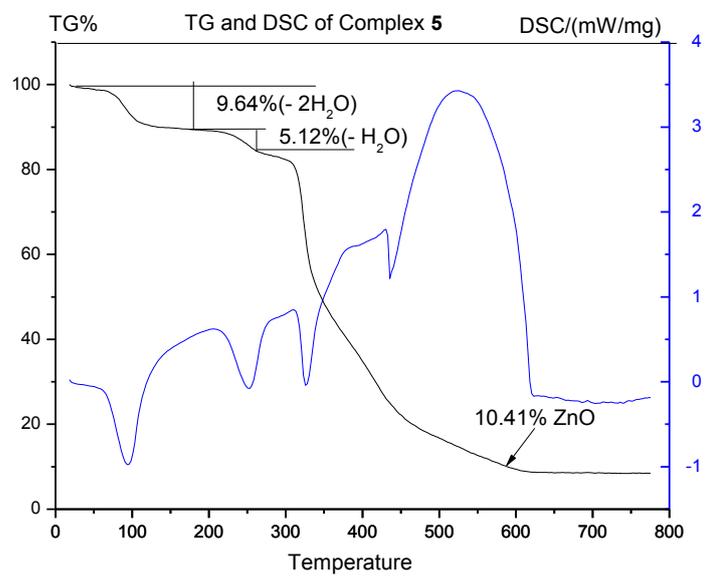


Fig. S11 TGA and DSC curves of $\{[\text{Zn}(\eta_3\text{-H}_4\text{L}^{\text{I}})(4,4'\text{-bipy})(\eta_1\text{-H}_2\text{O})] \cdot (\text{H}_2\text{O})_2\}_n$ (**5**)

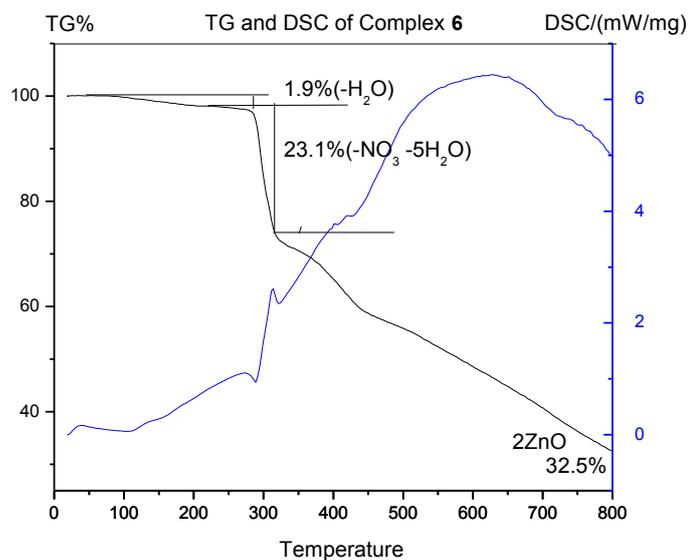


Fig. S12 TGA and DSC curves of $\{[\text{Zn}_2(\eta_4\text{-H}_3\text{L}^{\text{I}})(1,10\text{-phen})_3(\eta_1\text{-NO}_3)]\cdot\text{H}_2\text{O}\}_n$ (**6**)

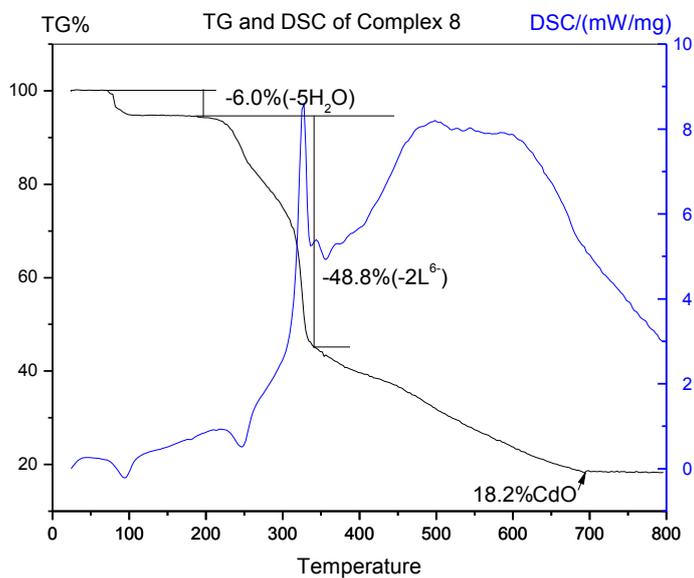


Fig. S13 TGA and DSC curves of $\{[\text{Cd}_2(\eta_4\text{-H}_4\text{L}^{\text{I}})_2(2,2'\text{-bipy})_2(\eta_1\text{-H}_2\text{O})_2]\cdot(2,2'\text{-bipy})\cdot(\text{H}_2\text{O})_3\}_n$ (**7**)

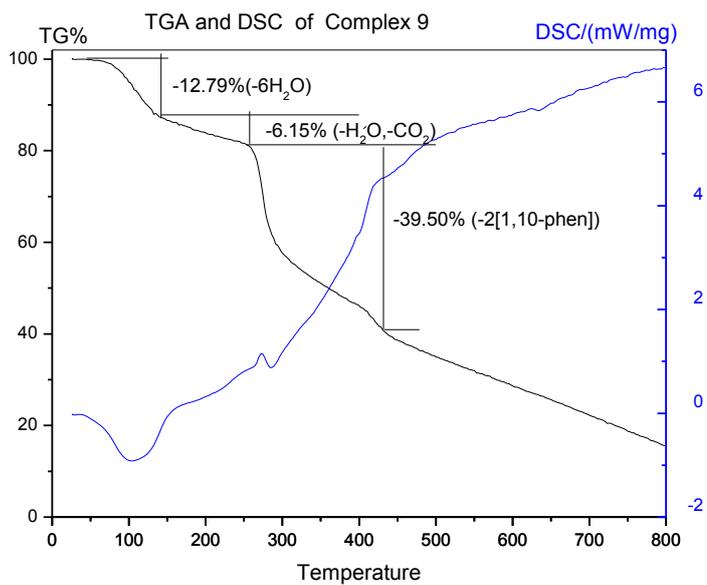


Fig. S14 TGA and DSC curves of $[\text{Mn}(1,10\text{-phen})_2(\text{H}_2\text{O})_2] \cdot (\text{H}_4\text{L}^1) \cdot (\text{H}_2\text{O})_5$ (**9**)

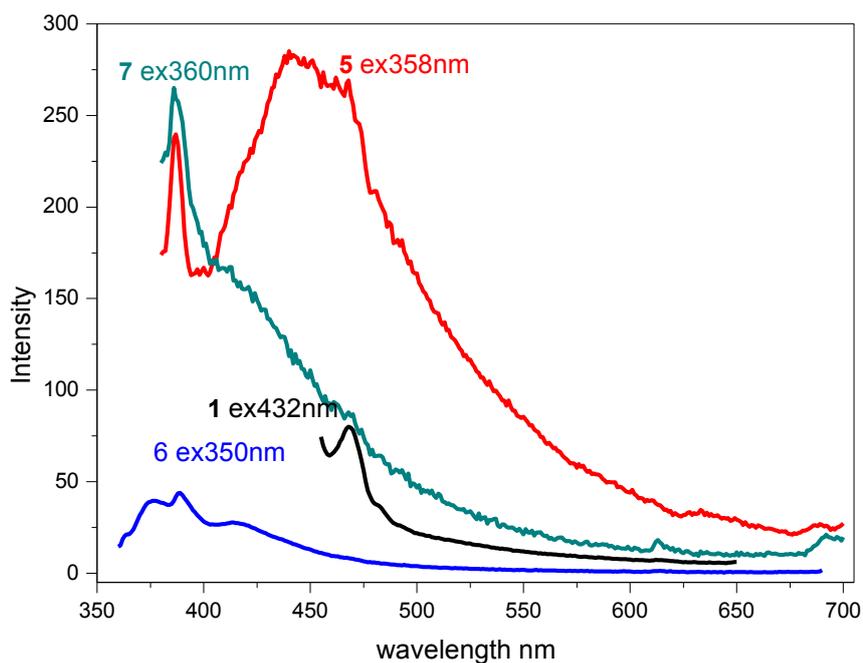


Fig. S115 Solid state fluorescence spectra of
 $\{[\text{Zn}_3(\mu_9\text{-L}^1)(\mu_2\text{-H}_2\text{O})_1(\mu_1\text{-H}_2\text{O})_7] \cdot (\text{H}_2\text{O})_5\}_n$ (**1**);
 $\{[\text{Zn}(\mu_3\text{-H}_4\text{L}^1)(4,4'\text{-bipy})(\mu_1\text{-H}_2\text{O})] \cdot (\text{H}_2\text{O})_2\}_n^2$ (**5**);
 $\{[\text{Zn}_2(\mu_4\text{-H}_3\text{L}^1)(1,10\text{-phen})_3 \cdot (\mu_1\text{-NO}_3)] \cdot \text{H}_2\text{O}\}_n^1$ (**6**);
 $\{[\text{Cd}_2(\mu_4\text{-H}_4\text{L}^1)_2(2,2'\text{-bipy})_2(\mu_1\text{-H}_2\text{O})_2] \cdot (2,2'\text{-bipy}) \cdot (\text{H}_2\text{O})_3\}_n^1$ (**7**).

Table S1. Bond lengths [Å] and angles [°] for complex **1-9**.

Complex 1					
Zn(1)-O(13)	2.065(2)	Zn(2)-O(12)#2	2.066(2)	Zn(3)-O(7)#3	2.079(2)
Zn(1)-O(15)	2.091(2)	Zn(2)-O(18)	2.094(3)	Zn(3)-O(19)	2.097(2)
Zn(1)-O(5)#1	2.094(2)	Zn(2)-O(16)	2.137(3)	Zn(3)-O(20)	2.116(3)
Zn(1)-O(14)	2.101(2)	Zn(2)-O(17)	2.174(3)	O(5)-Zn(1)#1	2.094(2)
Zn(1)-O(1)	2.116(2)	Zn(3)-O(10)	2.047(2)	O(6)-Zn(3)#4	2.072(2)
Zn(1)-O(15)#1	2.184(2)	Zn(3)-O(11)	2.070(2)	O(7)-Zn(3)#4	2.079(2)
Zn(2)-O(3)	2.020(2)	Zn(3)-O(6)#3	2.072(2)	O(12)-Zn(2)#2	2.066(2)
Zn(2)-O(2)	2.065(2)	O(13)-Zn(1)-O(15)	164.12(9)	O(13)-Zn(1)-O(5)#1	94.86(9)
O(15)-Zn(1)-O(5)#1	86.20(8)	O(2)-Zn(2)-O(12)#2	91.04(9)	O(11)-Zn(3)-O(6)#3	99.90(9)
O(13)-Zn(1)-O(14)	96.38(9)	O(3)-Zn(2)-O(18)	87.52(11)	O(10)-Zn(3)-O(7)#3	175.64(9)
O(15)-Zn(1)-O(14)	99.44(9)	O(2)-Zn(2)-O(18)	169.31(10)	O(11)-Zn(3)-O(7)#3	90.86(9)
O(5)#1-Zn(1)-O(14)	91.05(9)	O(12)#2-Zn(2)-O(18)	99.64(10)	O(6)#3-Zn(3)-O(7)#3	89.05(9)
O(13)-Zn(1)-O(1)	90.87(9)	O(3)-Zn(2)-O(16)	176.50(12)	O(10)-Zn(3)-O(19)	90.03(9)
O(15)-Zn(1)-O(1)	86.94(8)	O(2)-Zn(2)-O(16)	90.55(11)	O(11)-Zn(3)-O(19)	86.23(9)
O(5)#1-Zn(1)-O(1)	172.42(8)	O(12)#2-Zn(2)-O(16)	85.28(11)	O(6)#3-Zn(3)-O(19)	172.10(9)
O(14)-Zn(1)-O(1)	93.23(9)	O(18)-Zn(2)-O(16)	90.70(13)	O(7)#3-Zn(3)-O(19)	85.86(9)
O(13)-Zn(1)-O(15)#1	84.35(9)	O(3)-Zn(2)-O(17)	92.67(11)	O(10)-Zn(3)-O(20)	85.66(10)
O(15)-Zn(1)-O(15)#1	79.84(9)	O(2)-Zn(2)-O(17)	85.96(10)	O(11)-Zn(3)-O(20)	172.00(10)
O(5)#1-Zn(1)-O(15)#1	88.32(8)	O(12)#2-Zn(2)-O(17)	168.96(12)	O(6)#3-Zn(3)-O(20)	87.36(10)
O(14)-Zn(1)-O(15)#1	179.07(9)	O(18)-Zn(2)-O(17)	83.61(11)	O(7)#3-Zn(3)-O(20)	92.65(10)
O(1)-Zn(1)-O(15)#1	87.33(8)	O(16)-Zn(2)-O(17)	84.13(12)	O(19)-Zn(3)-O(20)	86.85(11)
O(3)-Zn(2)-O(2)	90.64(9)	O(10)-Zn(3)-O(11)	90.32(9)	Zn(1)-O(15)-Zn(1)#1	100.16(9)
O(3)-Zn(2)-O(12)#2	97.99(10)	O(10)-Zn(3)-O(6)#3	94.88(9)		
Symmetry codes: #1 -x+1,-y+1,-z+1, #2 -x,-y+1,-z+1, #3 x-1/2,-y+1/2,z-1/2, #4 x+1/2,-y+1/2,z+1/2.					
Complex 2					
Co(1)-O(7)#1	2.106(4)	Co(1)-O(11)	2.092(4)	Co(1)-O(13)	2.073(4)
Co(1)-O(14)	2.117(4)	Co(1)-O(15)	2.089(4)	Co(1)-O(15)#1	2.150(4)
Co(2)-O(6)#2	2.102(4)	Co(2)-O(8)	2.065(4)	Co(2)-O(9)	2.012(4)
Co(2)-O(16)	2.109(5)	Co(2)-O(17)	2.096(4)	Co(2)-O(18)	2.156(5)
Co(3)-O(1)	2.068(4)	Co(3)-O(4)#3	2.051(4)	Co(3)-O(5)#3	2.068(4)
Co(3)-O(12)	2.075(4)	Co(3)-O(19)	2.117(4)	Co(3)-O(20)	2.090(4)
O(7)#1-Co(1)-O(14)	92.34(15)	O(7)#1-Co(1)-O(15)#1	87.86(14)	O(11)-Co(1)-O(7)#1	173.35(14)
O(11)-Co(1)-O(14)	90.34(14)	O(11)-Co(1)-O(15)#1	89.34(14)	O(13)-Co(1)-O(7)#1	91.07(15)
O(13)-Co(1)-O(11)	94.74(15)	O(13)-Co(1)-O(14)	95.15(16)	O(13)-Co(1)-O(15)	166.61(15)
O(13)-Co(1)-O(15)#1	85.91(15)	O(14)-Co(1)-O(15)#1	178.92(15)	O(15)-Co(1)-O(7)#1	87.51(14)
O(15)-Co(1)-O(11)	86.09(14)	O(15)-Co(1)-O(13)	98.21(15)	O(15)-Co(1)-O(15)#1	80.74(14)
O(6)#2-Co(2)-O(16)	85.76(18)	O(6)#2-Co(2)-O(18)	171.1(2)	O(8)-Co(2)-O(6)#2	90.19(15)
O(8)-Co(2)-O(16)	91.34(17)	O(8)-Co(2)-O(17)	171.74(17)	O(8)-Co(2)-O(18)	171.74(17)
O(9)-Co(2)-O(6)#2	86.98(17)	O(9)-Co(2)-O(8)	95.88(17)	O(9)-Co(2)-O(16)	89.74(15)
O(9)-Co(2)-O(17)	178.0(2)	O(9)-Co(2)-O(18)	87.91(19)	O(16)-Co(2)-O(18)	85.8(2)
O(17)-Co(2)-O(6)#2	97.92(17)	O(17)-Co(2)-O(16)	90.8(2)	O(17)-Co(2)-O(18)	85.22(18)

O(1)-Co(3)-O(5)#3	91.54(15)	O(1)-Co(3)-O(12)	88.80(14)	O(1)-Co(3)-O(19)	91.88(17)
O(1)-Co(3)-O(20)	86.29(16)	O(4)#3-Co(3)-O(1)	175.73(15)	O(4)#3-Co(3)-O(5)#3	90.32(14)
O(4)#3-Co(3)-O(12)	94.69(15)	O(4)#3-Co(3)-O(19)	85.85(16)	O(4)#3-Co(3)-O(20)	89.99(16)
O(5)#3-Co(3)-O(12)	99.38(15)	O(5)#3-Co(3)-O(19)	172.83(17)	O(5)#3-Co(3)-O(20)	86.48(16)
O(12)-Co(3)-O(19)	86.99(17)	O(12)-Co(3)-O(20)	172.46(16)	O(20)-Co(3)-O(19)	87.46(18)
O(4)#3-Co(3)-O(1)	175.73(15)	O(4)#3-Co(3)-O(5)#3	90.32(14)	O(4)#3-Co(3)-O(12)	94.69(15)

Symmetry codes: #1 -x,-y,-z+2, #2 -x+1,-y,-z+2, #3 x-1/2,-y+1/2,z-1/2, #4 x+1/2,-y+1/2,z+1/2.

Complex 3

Cu(1)-O(2W)	1.941(3)	Cu(1)-O(1)#1	1.9461(19)	Cu(1)-O(1)	1.9461(19)
Cu(1)-O(1W)	1.951(3)	Cu(1)-O(3W)	2.404(2)	Cu(1)-O(3W)#1	2.404(2)
Cu(2)-O(3)	1.910(2)	Cu(2)-O(2)	1.918(2)	Cu(2)-O(4W)	1.963(2)
Cu(2)-O(5)#2	1.965(2)	Cu(3)-O(11)	1.935(2)	Cu(3)-O(10)	1.942(2)
Cu(3)-O(12)#3	1.9665(19)	Cu(3)-O(5W)	1.988(2)	Cu(3)-O(6W)	2.342(2)
O(5)-Cu(2)#2	1.965(2)	O(12)-Cu(3)#4	1.9665(19)	O(2W)-Cu(1)-O(1)#1	85.69(7)
O(2W)-Cu(1)-O(1)	85.69(7)	O(1)#1-Cu(1)-O(1)	171.38(13)	O(2W)-Cu(1)-O(1W)	180.000(1)
O(1)#1-Cu(1)-O(1W)	94.31(7)	O(2W)-Cu(1)-O(3W)	98.17(6)	O(1)#1-Cu(1)-O(3W)	95.15(8)
O(1)-Cu(1)-O(1W)	94.31(7)	O(1)-Cu(1)-O(3W)	86.08(8)	O(1W)-Cu(1)-O(3W)	81.83(6)
O(2W)-Cu(1)-O(3W)#1	98.17(6)	O(1)#1-Cu(1)-O(3W)#1	86.08(8)	O(1)-Cu(1)-O(3W)#1	95.15(8)
O(1W)-Cu(1)-O(3W)#1	81.83(6)	O(3W)-Cu(1)-O(3W)#1	163.66(11)	O(3)-Cu(2)-O(2)	94.37(9)
O(3)-Cu(2)-O(4W)	176.77(10)	O(2)-Cu(2)-O(4W)	85.38(9)	O(3)-Cu(2)-O(5)#2	86.08(9)
O(2)-Cu(2)-O(5)#2	169.31(10)	O(4W)-Cu(2)-O(5)#2	94.77(9)	O(11)-Cu(3)-O(10)	94.50(8)
O(11)-Cu(3)-O(12)#3	160.39(9)	O(10)-Cu(3)-O(12)#3	96.37(9)	O(11)-Cu(3)-O(5W)	83.68(8)
O(10)-Cu(3)-O(5W)	171.08(9)	O(12)#3-Cu(3)-O(5W)	87.93(8)	O(11)-Cu(3)-O(6W)	103.42(8)
O(10)-Cu(3)-O(6W)	88.00(8)	O(12)#3-Cu(3)-O(6W)	93.25(8)	O(5W)-Cu(3)-O(6W)	83.94(9)

Symmetry codes: #1 -x+1,y,-z+3/2 #2 -x+1,-y,-z+1 #3 -x+3/2,y-1/2,-z+3/2 #4 -x+3/2,y+1/2,-z+3/2

Complex 4

Ni(1)-O(4)#1	2.044(4)	Ni(1)-O(1W)	2.067(4)	O(2)-Ni(1)#6	2.080(4)
Ni(1)-O(1)	2.047(4)	Ni(1)-O(2W)	2.074(4)	O(3)-Ni(1)#2	2.061(4)
Ni(1)-O(3)#2	2.061(4)	Ni(1)-O(2)#3	2.081(4)	O(4)-Ni(1)#7	2.045(4)
O(4)#1-Ni(1)-O(1)	90.82(16)	O(3)#2-Ni(1)-O(1W)	104.12(17)	O(4)#1-Ni(1)-O(2)#3	91.69(15)
O(4)#1-Ni(1)-O(3)#2	168.53(16)	O(4)#1-Ni(1)-O(2W)	81.75(16)	O(1)-Ni(1)-O(2)#3	173.88(16)
O(1)-Ni(1)-O(3)#2	89.84(15)	O(1)-Ni(1)-O(2W)	99.79(16)	O(3)#2-Ni(1)-O(2)#3	88.80(15)
O(4)#1-Ni(1)-O(1W)	87.35(17)	O(3)#2-Ni(1)-O(2W)	86.85(16)	O(1W)-Ni(1)-O(2)#3	86.36(16)
O(1)-Ni(1)-O(1W)	88.18(16)	O(1W)-Ni(1)-O(2W)	166.54(17)	O(2W)-Ni(1)-O(2)#3	86.10(16)

Symmetry codes: #1 y,-x+y+1,-z+2 #2 -x+4/3, -y+5/3,-z+5/3 #3 x-y+4/3,x+2/3,-z+5/3 #4 -y+1,x-y+1,z #5 -x+y,-x+1,z #6 y-2/3,-x+y+2/3,-z+5/3 #7 x-y+1,x,-z+2

Complex 5

Zn(1)-O(9)#1	2.048(2)	Zn(1)-O(1W)	2.057(2)	N(2)-Zn(1)#3	2.159(3)
Zn(1)-N(1)	2.147(3)	Zn(1)-N(2)#2	2.159(3)	O(9)-Zn(1)#4	2.048(2)
Zn(1)-O(1)	2.287(2)	Zn(1)-O(2)	2.308(2)		
O(9)#1-Zn(1)-O(1W)	121.80(9)	C(13)-N(1)-Zn(1)	124.6(2)	O(1W)-Zn(1)-O(1)	145.43(9)
O(1W)-Zn(1)-N(1)	93.56(9)	C(21)-N(2)-Zn(1)#3	123.8(2)	N(2)#2-Zn(1)-O(1)	90.82(9)
O(1W)-Zn(1)-N(2)#2	86.42(10)	C(1)-O(1)-Zn(1)	92.1(2)	O(1W)-Zn(1)-O(2)	88.91(9)
O(9)#1-Zn(1)-O(1)	92.39(9)	C(11)-O(9)-Zn(1)#4	117.2(2)	N(2)#2-Zn(1)-O(2)	92.75(9)

N(1)-Zn(1)-O(1)	90.79(9)	Zn(1)-O(1W)-H(1WA)	124.5	C(17)-N(1)-Zn(1)	118.1(2)
O(9)#1-Zn(1)-O(2)	149.18(9)	O(9)#1-Zn(1)-N(1)	90.58(9)	C(21)-N(2)-C(20)	116.5(3)
N(1)-Zn(1)-O(2)	90.06(9)	O(9)#1-Zn(1)-N(2)#2	87.04(9)	C(20)-N(2)-Zn(1)#3	119.7(2)
O(1)-Zn(1)-O(2)	56.78(8)	N(1)-Zn(1)-N(2)#2	177.18(10)	C(1)-O(2)-Zn(1)	90.1(2)
Zn(1)-O(1W)-H(1WB)	109.5				

Symmetry codes: #1 x-1,y,z; #2 x,y+1,z; #3 x,y-1,z; #4 x+1,y,z

Complex 6

Zn(1)-O(1)	1.985(2)	Zn(1)-O(6)#1	2.024(2)	Zn(1)-O(13)	2.058(4)
Zn(1)-N(1)	2.157(3)	Zn(1)-N(2)	2.091(3)	Zn(2)-O(9)	2.402(2)
Zn(2)-O(10)	2.037(2)	Zn(2)-N(4)	2.072(3)	Zn(2)-N(5)	2.160(3)
Zn(2)-N(6)	2.094(3)	Zn(2)-N(7)	2.155(3)	O(6)-Zn(1)#2	2.024(2)
O(1)-Zn(1)-O(13)	90.70(15)	O(6)#1-Zn(1)-O(13)	99.32(16)	O(1)-Zn(1)-O(6)#1	94.01(10)
O(6)#1-Zn(1)-N(1)	165.41(10)	O(13)-Zn(1)-N(1)	93.11(16)	O(1)-Zn(1)-N(1)	93.44(10)
O(6)#1-Zn(1)-N(2)	89.11(10)	O(13)-Zn(1)-N(2)	122.53(15)	O(1)-Zn(1)-N(2)	145.67(10)
O(10)-Zn(2)-O(9)	58.35(8)	O(10)-Zn(2)-N(4)	104.55(10)	N(2)-Zn(1)-N(1)	77.72(10)
O(10)-Zn(2)-N(6)	151.83(11)	O(10)-Zn(2)-N(7)	92.91(11)	O(10)-Zn(2)-N(5)	92.92(10)
N(5)-Zn(2)-O(9)	93.18(9)	N(6)-Zn(2)-O(9)	94.77(10)	N(4)-Zn(2)-O(9)	160.97(9)
N(4)-Zn(2)-N(5)	78.55(10)	N(4)-Zn(2)-N(6)	103.21(11)	N(7)-Zn(2)-O(9)	91.12(10)
N(6)-Zn(2)-N(5)	97.20(13)	N(6)-Zn(2)-N(7)	78.24(14)	N(4)-Zn(2)-N(7)	98.55(11)
N(7)-Zn(2)-N(5)	173.99(11)				

Symmetry codes: #1 -x+1/2, y+1/2, -z+1/2; #2 -x+1/2, y-1/2, -z+1/2

Complex 7

Cd(1)-O(1W)	2.269(8)	Cd(1)-O(2)	2.587(6)	Cd(2)-O(9)	2.324(7)
Cd(1)-O(1)	2.317(6)	Cd(1)-O(22)#1	2.596(7)	Cd(2)-N(4)	2.326(9)
Cd(1)-N(2)	2.319(8)	Cd(2)-O(13)	2.271(7)	Cd(2)-O(10)	2.547(6)
Cd(1)-O(21)#1	2.348(8)	Cd(2)-O(2W)	2.300(9)	O(21)-Cd(1)#2	2.348(8)
Cd(1)-N(1)	2.325(8)	Cd(2)-N(3)	2.325(8)	O(22)-Cd(1)#2	2.596(7)
O(1W)-Cd(1)-O(1)	95.8(3)	N(2)-Cd(1)-O(2)	96.6(2)	O(13)-Cd(2)-O(9)	87.6(3)
O(1W)-Cd(1)-N(2)	164.8(3)	O(21)#1-Cd(1)-O(2)	134.7(2)	O(2W)-Cd(2)-O(9)	89.0(3)
O(1)-Cd(1)-N(2)	92.2(3)	N(1)-Cd(1)-O(2)	90.4(2)	N(3)-Cd(2)-O(9)	141.1(3)
O(1W)-Cd(1)-O(21)#1	96.4(3)	O(1W)-Cd(1)-O(22)#1	84.4(3)	O(13)-Cd(2)-N(4)	110.5(3)
O(1)-Cd(1)-O(21)#1	83.8(2)	O(1)-Cd(1)-O(22)#1	135.2(2)	O(2W)-Cd(2)-N(4)	154.1(3)
N(2)-Cd(1)-O(21)#1	97.4(3)	N(2)-Cd(1)-O(22)#1	99.0(3)	N(3)-Cd(2)-N(4)	71.8(3)
O(1W)-Cd(1)-N(1)	94.5(3)	O(21)#1-Cd(1)-O(22)#1	51.9(3)	O(9)-Cd(2)-N(4)	97.9(3)
O(1)-Cd(1)-N(1)	138.2(3)	N(1)-Cd(1)-O(22)#1	86.0(3)	O(13)-Cd(2)-O(10)	141.2(2)
N(2)-Cd(1)-N(1)	71.0(3)	O(2)-Cd(1)-O(22)#1	161.9(2)	O(2W)-Cd(2)-O(10)	84.6(3)
O(21)#1-Cd(1)-N(1)	134.9(3)	O(13)-Cd(2)-O(2W)	94.6(3)	N(3)-Cd(2)-O(10)	87.6(3)
O(1W)-Cd(1)-O(2)	78.3(2)	O(13)-Cd(2)-N(3)	131.2(3)	O(9)-Cd(2)-O(10)	53.6(2)
O(1)-Cd(1)-O(2)	52.8(2)	O(2W)-Cd(2)-N(3)	87.3(4)	N(4)-Cd(2)-O(10)	79.6(3)

Symmetry codes: #1 x+1,y,z; #2 x-1,y,z.

Complex 8

Co(1)-O(1W)	2.069(2)	Co(1)-O(1)	2.086(2)	Co(1)-O(10)#1	2.103(2)
Co(1)-O(2W)	2.134(2)	Co(1)-N(3)	2.161(3)	Co(1)-N(1)	2.171(3)
Co(2)-O(6)#2	2.070(2)	Co(2)-O(6)	2.070(2)	Co(2)-O(3W)	2.132(2)

Co(2)-O(3W)#2	2.132(2)	Co(2)-N(5)	2.153(3)	Co(2)-N(5)#2	2.153(3)
O(10)-Co(1)#1	2.103(2)	O(1W)-Co(1)-O(1)	90.28(9)	O(1W)-Co(1)-O(10)#1	176.60(9)
O(1)-Co(1)-O(10)#1	86.32(8)	O(1W)-Co(1)-O(2W)	89.93(9)	O(1)-Co(1)-O(2W)	179.77(9)
O(10)#1-Co(1)-O(2W)	93.47(9)	O(1W)-Co(1)-N(3)	90.28(11)	O(1)-Co(1)-N(3)	89.10(10)
O(10)#1-Co(1)-N(3)	89.75(10)	O(2W)-Co(1)-N(3)	90.83(10)	O(1W)-Co(1)-N(1)	93.94(11)
O(1)-Co(1)-N(1)	93.67(10)	O(10)#1-Co(1)-N(1)	86.20(10)	O(2W)-Co(1)-N(1)	86.39(10)
N(3)-Co(1)-N(1)	174.93(11)	O(6)#2-Co(2)-O(6)	179.999(1)	O(6)#2-Co(2)-O(3W)	91.48(9)
O(6)-Co(2)-O(3W)	88.52(9)	O(6)#2-Co(2)-O(3W)#2	88.52(9)	O(6)-Co(2)-O(3W)#2	91.48(9)
O(3W)-Co(2)-O(3W)#2	80.000(1)	O(6)#2-Co(2)-N(5)	92.23(10)	O(6)-Co(2)-N(5)	87.77(10)
O(3W)-Co(2)-N(5)	90.93(11)	O(3W)#2-Co(2)-N(5)	89.07(11)	O(6)#2-Co(2)-N(5)#2	87.77(10)
O(6)-Co(2)-N(5)#2	92.23(10)	O(3W)-Co(2)-N(5)#2	89.07(11)	O(3W)#2-Co(2)-N(5)#2	90.93(11)
N(5)-Co(2)-N(5)#2	180.000(1)				
Symmetry codes: #1 -x+2,-y,-z+1		#2 -x+2,-y+1,-z+2.			

Complex 9

Mn(1)-O(2W)	2.128(4)	Mn(1)-N(4)	2.265(4)	Mn(1)-O(1W)	2.138(3)
Mn(1)-N(1)	2.275(4)	Mn(1)-N(2)	2.228(4)	Mn(1)-N(3)	2.303(4)
O(2W)-Mn(1)-O(1W)	92.15(14)	N(2)-Mn(1)-N(1)	73.89(16)	O(2W)-Mn(1)-N(2)	92.04(15)
O(2W)-Mn(1)-N(2)	92.04(15)	O(1W)-Mn(1)-N(2)	102.31(15)	O(2W)-Mn(1)-N(3)	94.03(15)
O(2W)-Mn(1)-N(4)	96.85(14)	O(1W)-Mn(1)-N(3)	163.16(15)	O(1W)-Mn(1)-N(4)	91.09(14)
N(2)-Mn(1)-N(3)	93.12(15)	N(2)-Mn(1)-N(4)	163.63(15)	N(4)-Mn(1)-N(3)	72.63(15)
O(2W)-Mn(1)-N(1)	165.45(14)	N(1)-Mn(1)-N(3)	83.28(16)	O(1W)-Mn(1)-N(1)	94.45(16)
Symmetry codes: none.					

Table S2 .Hydrogen bonds for complex 1-9 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Complex 1				
O(25)-H(25B)...O(3)	0.85	2.27	2.824(4)	122.9
O(21)-H(21B)...O(2)	0.84	2.53	3.106(4)	126.6
O(21)-H(21B)...O(12)#2	0.84	2.50	3.187(4)	139.3
O(21)-H(21B)...O(16)	0.84	2.43	3.160(5)	144.5
O(23)-H(23B)...O(4)	0.86	1.92	2.772(4)	168.5
O(24)-H(24B)...O(9)#5	0.85	1.90	2.735(4)	167.6
O(22)-H(22B)...O(23)#6	0.85	2.12	2.863(6)	146.1
O(25)-H(25A)...O(21)#2	0.85	1.98	2.811(4)	164.1
O(21)-H(21A)...O(14)	0.85	1.96	2.799(4)	168.9
O(15)-H(15A)...O(9)#1	0.84	1.71	2.540(3)	168.6
O(17)-H(17B)...O(22)	0.84	1.93	2.756(5)	166.3
O(20)-H(20B)...O(22)#1	0.84	2.06	2.878(5)	161.6
O(19)-H(19B)...O(25)#2	0.84	1.96	2.803(4)	174.3
O(18)-H(18B)...O(23)#6	0.84	2.04	2.875(4)	169.8
O(14)-H(14B)...O(8)#7	0.85	1.88	2.692(3)	158.6
O(16)-H(16B)...O(24)#8	0.85	1.91	2.733(4)	165.4
O(15)-H(15B)...O(2)	0.85	1.74	2.573(3)	165.9
O(13)-H(13B)...O(10)	0.85	1.90	2.742(3)	169.5

O(20)-H(20A)...O(24)#9	0.82	2.00	2.802(4)	166.7
O(19)-H(19A)...O(7)#7	0.82	2.17	2.878(3)	145.1
O(18)-H(18A)...O(7)#8	0.82	2.39	3.031(4)	135.8
O(18)-H(18A)...O(11)#2	0.82	2.10	2.778(3)	139.7
O(17)-H(17A)...O(13)#1	0.82	2.15	2.827(4)	140.3
O(16)-H(16A)...O(4)#8	0.82	2.15	2.869(4)	145.8
O(14)-H(14A)...O(6)#1	0.82	1.84	2.588(3)	150.9
O(13)-H(13A)...O(8)#7	0.82	1.90	2.687(3)	159.8

Symmetry codes: #1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z+1 #3 x-1/2,-y+1/2,z-1/2 #4
x+1/2,-y+1/2,z+1/2 #5 x-1/2,-y+1/2,z+1/2 #6 -x+1,-y+1,-z+2 #7 -x+1/2,y+1/2,-z+1/2 #8
-x+1/2,y+1/2,-z+3/2 #9 x,y,z-1

Complex 2

O(13)-H(13A)...O(4)#1	0.85	1.96	2.756(5)	155
O(13)-H(13B)...O(2)#3	0.82	1.88	2.671(6)	161
O(14)-H(14A)...O(12)	0.82	1.84	2.593(5)	151.6
O(14)-H(14B)...O(2)#3	0.86	1.86	2.716(6)	175.1
O(15)-H(15A)...O(3)	0.85	1.71	2.538(5)	165.2
O(15)-H(15B)...O(8)#1	0.85	1.86	2.572(5)	140.1
O(15)-H(15B)...O(18)#1	0.85	2.56	3.255(6)	139.5
O(16)-H(16A)...O(25)#6	0.82	1.96	2.711(7)	152.6
O(16)-H(16B)...O(10)#7	0.85	2.03	2.862(6)	165.1
O(17)-H(17B)...O(23)#8	0.82	2.1	2.875(8)	157.4
O(17)-H(17A)...O(1)#7	0.86	2.2	3.034(6)	162.2
O(18)-H(18A)...O(13)	0.82	2.17	2.809(6)	135
O(18)-H(18B)...O(21)#9	0.82	2.02	2.776(9)	152.3
O(19)-H(19A)...O(25)#10	0.82	2.01	2.806(7)	165.5
O(19)-H(19B)...O(21)#7	0.85	2.1	2.872(9)	151.9
O(20)-H(20A)...O(24)#11	0.85	1.97	2.807(7)	165.9
O(20)-H(20B)...O(2)#12	0.85	2.19	3.021(6)	166.9
O(20)-H(20B)...O(1)#12	0.85	2.39	2.869(5)	116.2
O(22)-H(22A)...O(6)	0.86	2.44	3.200(7)	147.7
O(22)-H(22A)...O(8)#2	0.86	2.45	3.103(7)	133.3
O(22)-H(22A)...O(16)#2	0.86	2.57	3.168(8)	127.9
O(22)-H(22B)...O(14)#13	0.86	1.97	2.782(7)	157.7
O(23)-H(23A)...O(10)	0.86	1.94	2.775(8)	163.4
O(23)-H(23B)...O(23)#8	0.86	2.6	3.290(14)	138.1
O(24)-H(24A)...O(22)#14	0.85	2	2.818(8)	160.7
O(24)-H(24B)...O(9)#14	0.85	2	2.841(7)	173.5
O(25)-H(25A)...O(24)	0.85	1.87	2.692(7)	162.5
O(25)-H(25B)...O(3)#15	0.86	1.9	2.727(6)	158.7

Symmetry codes: #1 -x,-y,-z+2, #2 -x+1,-y,-z+2, #3 x-1/2,-y+1/2,z-1/2, #4
x+1/2,-y+1/2,z+1/2, #5 -x-1/2,y-1/2,-z+3/2, #6 -x+1,-y,-z+1, #7 -x+1/2,y-1/2,-z+3/2, #8
-x,-y,-z+1, #9 x-1,y-1,z, #10 x-1,y,z+1, #11 -x+1,-y+1,-z+1, #12 -x,-y+1,-z+2, #13 x+1,y,z,
#14 x+1/2,-y+1/2,z-1/2, #15 x+1,y,z-1.

Complex 3

O(1W)-H(1WA)···O(10)#3	0.82	1.93	2.716(2)	161.2
O(1W)-H(1WA)···O(9)#3	0.82	2.66	3.215(2)	126.5
O(2W)-H(2WA)···O(5W)#5	0.82	1.98	2.727(3)	151.2
O(3W)-H(3WB)···O(8)#6	0.82	1.84	2.652(3)	171.4
O(4W)-H(4WB)···O(6)#2	0.82	1.88	2.609(3)	148.2
O(5W)-H(5WB)···O(7W)#7	0.82	2.28	3.057(4)	159.4
O(6W)-H(6WB)···O(4)	0.82	1.94	2.752(3)	173.5
O(6W)-H(6WA)···O(3W)#8	0.85	1.88	2.704(3)	163.4
O(3W)-H(3WA)···O(2)	0.85	1.96	2.753(3)	154.9
O(3W)-H(3WA)···O(4W)	0.85	2.62	3.154(3)	121.7
O(5W)-H(5WA)···O(9)#9	0.85	1.97	2.792(3)	162.1
O(4W)-H(4WA)···O(7)#6	0.85	2.00	2.827(3)	163.7
O(8W)-H(8WB)···O(6)#10	0.85	2.54	3.248(6)	141.5
O(7W)-H(7WB)···O(3)#11	0.85	2.11	2.879(4)	149.1
O(7)-H(7)···O(6)	0.82	1.72	2.508(3)	161.5

Symmetry codes: #1 -x+1,y,-z+3/2 #2 -x+1,-y,-z+1 #3 -x+3/2,y-1/2,-z+3/2 #4
-x+3/2,y+1/2,-z+3/2 #5 -x+1,y+1,-z+3/2 #6 x-1/2,y+1/2,z #7 x,y-1,z #8
x+1/2,y-1/2,z #9 x-1/2,y-1/2,z #10 -x+3/2,-y+1/2,-z+1 #11 x,y+1,z

Complex 4

O(1W)-H(1WA)...O(3W)#8	0.82	1.67	2.136(12)	113.7
O(1W)-H(1WA)...O(3)#1	0.82	2.08	2.790(6)	145.1
O(1W)-H(1WA)...O(2)#8	0.82	2.25	2.788(6)	123.0
O(1W)-H(1WB)...O(1W)#7	0.87	2.00	2.856(4)	168.0
O(2W)-H(2WA)...O(3W)	0.85	1.19	1.855(12)	130.1
O(2W)-H(2WA)...O(1)#9	0.85	2.09	2.899(5)	158.4
O(2W)-H(2WB)...O(2W)#6	0.85	2.26	3.086(5)	164.5
O(2W)-H(2WB)...O(2)	0.85	2.41	2.906(6)	118.1
O(3W)-H(3WA)...O(4)#9	0.85	1.70	2.357(13)	132.1

Symmetry codes: #1 y,-x+y+1,-z+2 #2 -x+4/3,-y+5/3,-z+5/3 #3
x-y+4/3,x+2/3,-z+5/3 #4 -y+1,x-y+1,z #5 -x+y,-x+1,z #6 y-2/3,-x+y+2/3,-z+5/3 #7
x-y+1,x,-z+2 #8 -y+5/3,x-y+4/3,z+1/3 #9 -x+y+1/3,-x+5/3,z-1/3.

Complex 5

O(1W)-H(1WB)...O(10)#5	0.82	1.95	2.703(3)	151.2
O(12)-H(12)...O(2)	0.82	1.87	2.660(3)	161.5
O(8)-H(8)...O(9)	0.82	1.75	2.557(3)	167.8
O(6)-H(6A)...O(3W)	0.82	1.81	2.593(4)	159.2
O(4)-H(4A)...O(5)	0.82	1.86	2.641(4)	158.2
O(1W)-H(1WA)...O(2W)#6	0.85	1.95	2.795(4)	172.2
O(2W)-H(2WA)...O(2)#7	0.85	2.10	2.939(3)	166.8
O(3W)-H(3WA)...O(2W)#8	0.85	2.02	2.779(4)	149.0
O(3W)-H(3WB)...O(6)#7	0.85	2.49	3.226(4)	144.8
O(3W)-H(3WB)...O(12)#9	0.85	2.38	2.921(4)	122.1
O(2W)-H(2WB)...O(7)#9	0.85	2.08	2.853(4)	150.1

Symmetry codes: #1 $x-1, y, z$; #2 $x, y+1, z$; #3 $x, y-1, z$; #4 $x+1, y, z$; #5 $-x, -y+1, -z$; #6 $x-1, y, z-1$; #7 $-x+1, -y+1, -z+1$; #8 $x-1/2, -y+3/2, z-1/2$; #9 $x+1/2, -y+3/2, z+1/2$

Complex 6

C(2)-H(2)...O(8)#3	0.93	2.44	3.207(5)	139.5
O(1W)-H(1A)...O(5)	0.85	2.06	2.887(4)	164.5
O(4)-H(4)...O(5)	0.82	1.75	2.556(4)	165.5
O(8)-H(8A)...O(9)	0.82	1.78	2.591(3)	170.6
O(12)-H(12)...O(1)	0.82	1.81	2.605(3)	162.1

Symmetry codes: #1 $-x+1/2, y+1/2, -z+1/2$ #2 $-x+1/2, y-1/2, -z+1/2$ #3 $x, -y+1, z+1/2$

Complex 7

O(23)-H(23)...O(22)	0.82	1.73	2.541(11)	169.0
O(19)-H(19A)...O(14)#3	0.82	2.00	2.815(9)	175.2
O(15)-H(15A)...O(13)	0.82	1.88	2.620(10)	150.1
O(11)-H(11)...O(10)	0.82	1.81	2.610(10)	165.9
O(7)-H(7A)...O(6)	0.82	1.84	2.616(11)	157.5
O(5)-H(5A)...O(4W)	0.82	1.91	2.692(16)	158.7
O(3)-H(3A)...O(1)	0.82	1.76	2.567(9)	167.8

Symmetry codes: #1 $x+1, y, z$ #2 $x-1, y, z$ #3 $-x, y+1/2, -z+3/2$.

Complex 8

O(7W)-H(7WB)...O(9)#3	0.88	2.00	2.833(7)	157.9
O(4W)-H(4WB)...O(5W)	0.86	2.28	2.778(11)	117.0
O(8W)-H(8WB)...O(8)#4	0.82	2.02	2.807(5)	162.3
O(6W)-H(6WA)...O(4)#5	0.84	1.98	2.799(5)	166.9
O(8W)-H(8WA)...O(4W)#3	0.87	2.10	2.918(10)	154.9
O(4W)-H(4WA)...O(12)#5	0.83	2.02	2.799(5)	154.6
O(3W)-H(3WA)...O(7W)#6	0.85	2.48	3.152(13)	136.9
O(3W)-H(3WA)...O(9W)#7	0.85	2.32	3.118(17)	156.8
O(2W)-H(2WA)...O(10)#1	0.84	2.68	3.085(3)	111.2
O(2W)-H(2WA)...O(9)#1	0.84	1.91	2.711(4)	159.4
O(5W)-H(5WA)...O(6W)	0.87	2.36	2.785(12)	110.0
O(1W)-H(1WA)...O(5)#8	0.88	1.90	2.743(3)	158.5
O(3W)-H(3WB)...O(5)#2	0.82	1.97	2.699(3)	147.9
O(2W)-H(2WB)...N(4)#9	0.82	1.95	2.759(4)	169.0
O(1W)-H(1WB)...O(2)	0.82	1.91	2.659(3)	151.0
O(11)-H(11)...O(10)	0.82	1.81	2.603(3)	160.9
O(7)-H(7)...O(6)	0.82	1.75	2.551(3)	167.0
O(3)-H(3A)...O(2)	0.82	1.74	2.527(4)	161.0

Symmetry codes: #1 $-x+2, -y, -z+1$; #2 $-x+2, -y+1, -z+2$; #3 $x-1, y, z$; #4 $x-1, y+1, z$; #5 $x, y+1, z$
#6 $x+1, y, z$; #7 $x+1, y, z+1$; #8 $-x+1, -y, -z+1$; #9 $-x+1, -y, -z$

Complex 9

O(2)-H(2A)...O(6W)	0.82	1.75	2.568(6)	174.8
O(3)-H(3A)...O(5W)	0.82	1.88	2.701(6)	174.6
O(7)-H(7)...O(6)	0.82	1.72	2.536(5)	170.1
O(1W)-H(1WA)...O(7W)#1	0.85	1.88	2.700(5)	161.2

O(1W)-H(1WB)...O(1)#2	0.85	2.10	2.776(5)	136.2
O(2W)-H(2WB)...O(5)#3	0.85	1.88	2.685(5)	159.5
O(4W)-H(4WA)...O(8)#4	0.87	2.41	3.167(8)	145.9
O(4W)-H(4WA)...O(7)#4	0.87	2.56	3.386(7)	159.0
O(5W)-H(5WB)...O(8)#4	0.86	2.66	3.101(6)	113.3
O(5W)-H(5WB)...O(11)#4	0.86	2.64	3.107(6)	114.8
O(6W)-H(6WB)...O(9)#5	0.99	1.82	2.764(6)	157.8
O(7W)-H(7WA)...O(5)#6	0.85	2.11	2.900(5)	154.7
O(3W)-H(3WA)...O(12)#4	0.85	2.54	3.339(12)	156.3
O(4W)-H(4WB)...O(3W)	0.88	2.07	2.874(12)	151.9

Symmetry codes: #1 x,y-1,z; #2 x,-y+1/2,z+1/2; #3 x,y,z+1; #4 -x+1,y+1/2,-z+1/2; #5 x,y+1,z; #6 -x,-y+1,-z+1.
