Supporting Information

Organic-inorganic hybrid coordination polymers based on 5-oxyacetate isophthalic acid (H_3OABDC) ligand: syntheses, structures, magnetic and luminescent properties

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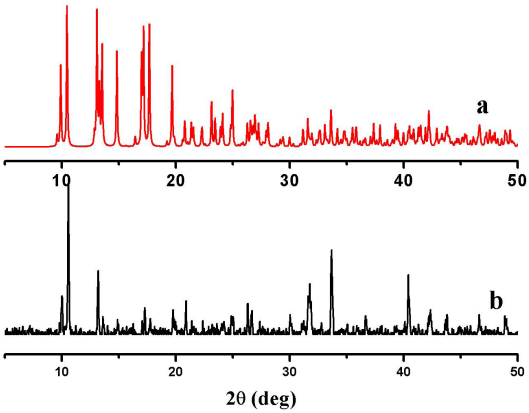

Fig. S1 PXRD patterns of $[Sm(OABDC)(H_2O)_5]_n \cdot 2nH_2O$ (**1**) (a) Simulated from single crystal structure data. (b) Experimental data of **1**.

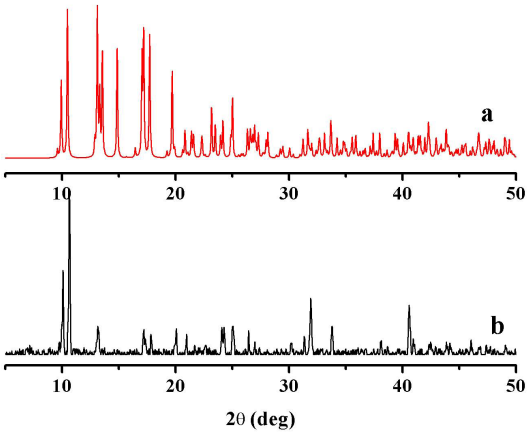

Fig. S2 PXRD patterns of $[Eu(OABDC)(H_2O)_5]_n \cdot 2nH_2O$ (**2**) (a) Simulated from single crystal structure data. (b) Experimental data of **2**.

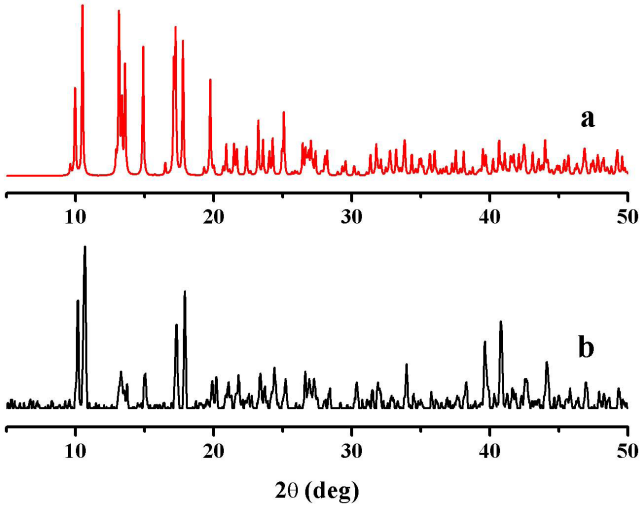

Fig. S3 PXRD patterns of $[Dy(OABDC)(H_2O)_5]_n \cdot 2nH_2O$ (**3**) (a) Simulated from single crystal structure data. (b) Experimental data of **3**.

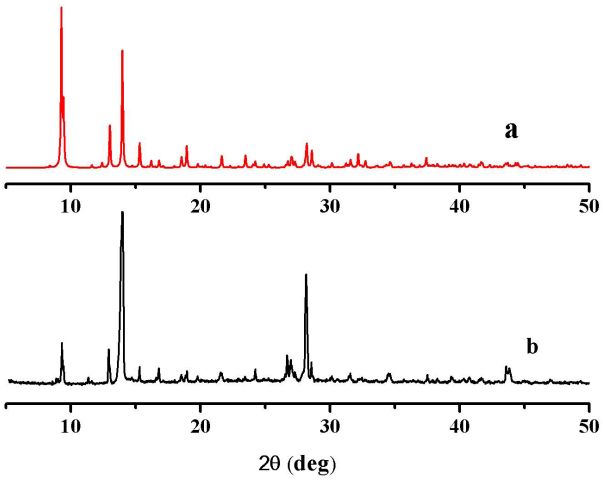

Fig. S4 PXRD patterns of $[Ni_4(OABDC)_2(OH)_2(H_2O)_4]_n \cdot 4nH_2O$ (**4**) (a) Simulated from single crystal structure data. (b) Experimental data of **4**.

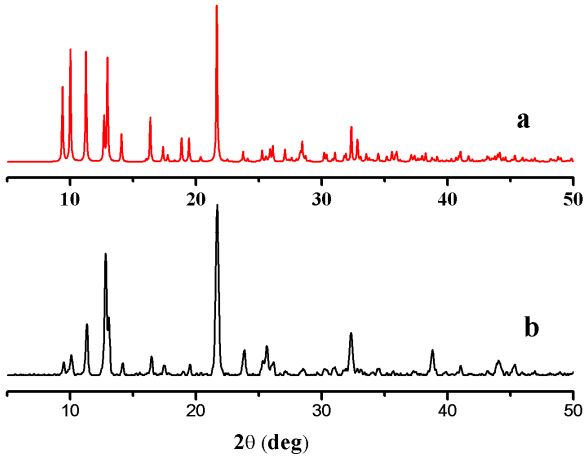

Fig. S5 PXRD patterns of $[Cu_2(OABDC)_{0.5}(4,4'\text{-bpy})(OH)]_n$ (**5**) (a) Simulated from single crystal structure data. (b) Experimental data of **5**.

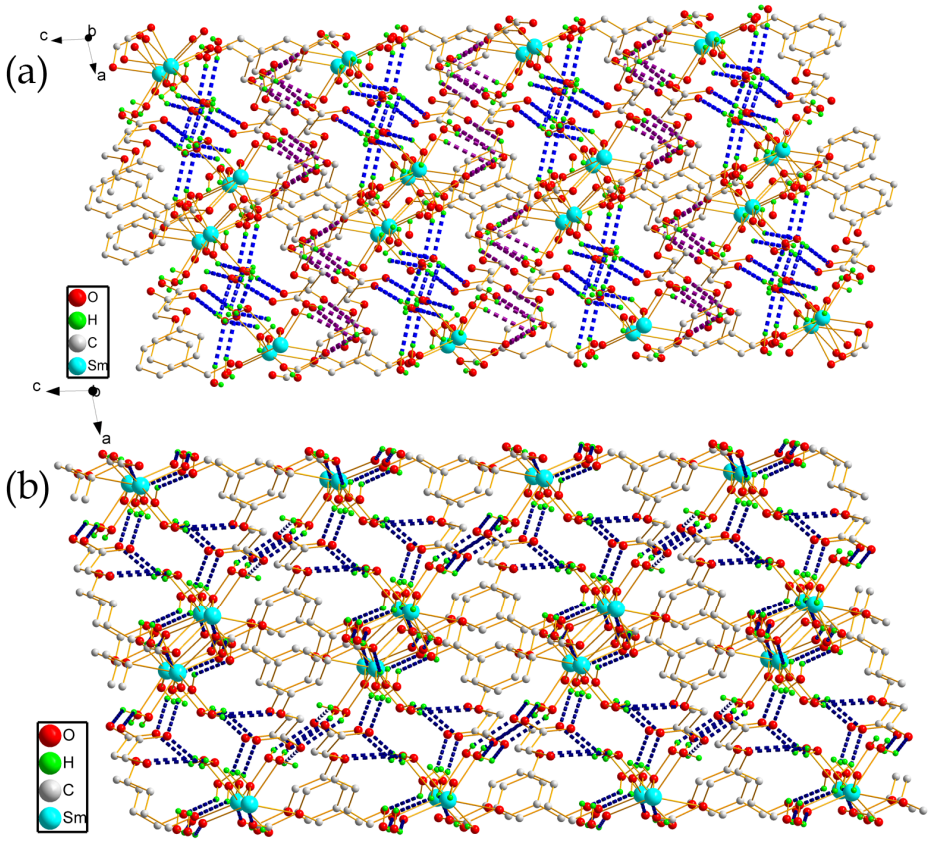

Fig. S6 In order to facilitate viewing, hydrogen bonds have been divided into two categories. One is obtained by lattice water (a) (purple and blue dotted lines represent hydrogen bonds obtained by different lattice water); the other one is obtained by the remaining water molecules (b) (blue dotted lines).

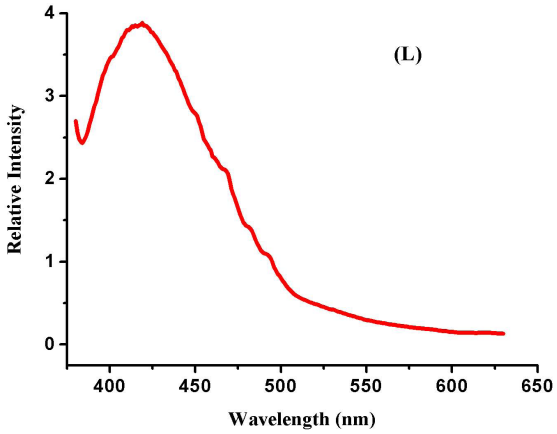

Fig. S7 Fluorescent emission spectra of ligand (H_3OABDC) in the solid state at room temperature.

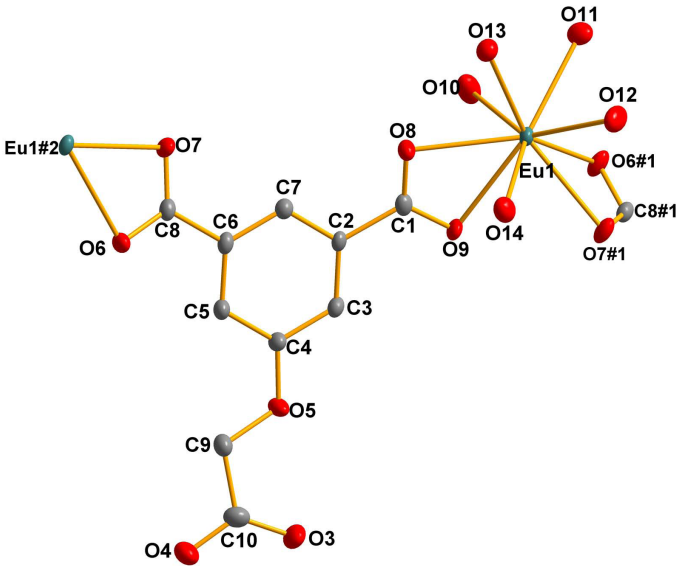

Fig. S8 An ORTEP drawing of **2** showing 50% ellipsoid probability (hydrogen atoms and lattice water molecules are omitted for clarity). Symmetry codes: #1= *x*, 1/2-*y*, -1/2+*z*; #2 = *x*, 1/2-*y*, 1/2+*z*.

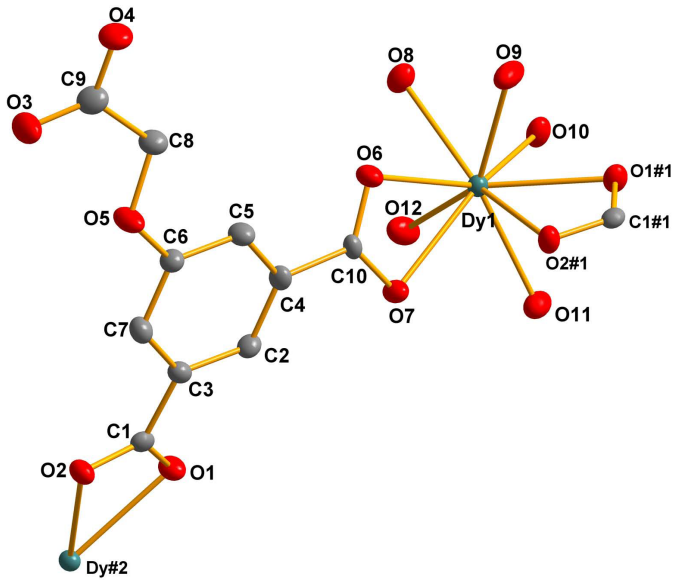

Fig. S9 An ORTEP drawing of **3** showing 50% ellipsoid probability (hydrogen atoms and lattice water molecules are omitted for clarity). Symmetry codes: #1= *x*, 3/2-*y*, 1/2+*z*; #2 = *x*, 3/2-*y*, -1/2+*z*.

Table S1 Selected bond distances (Å) and angles (°)

Complex **1**

Sm1─O1	2.456(4)	Sm1─O8	2.473(4)
Sm1─O2	2.552(4)	Sm1─O9	2.432(4)
Sm1[a]─O3	2.489(4)	Sm1─O10	2.434(4)
Sm1[a]─O4	2.496(4)	O11─Sm1	2.454(4)
Sm1─C1	2.881(6)	Sm1─O12	2.437(4)
Sm1[a]─C10	2.866(5)		

O11─Sm1─O4[a]	74.11(14)	O9─Sm1─O2	123.91(12)
O1─Sm1─O4[a]	128.02(14)	O10─Sm1─O2	139.58(14)
O8─Sm1─O4[a]	125.26(13)	O12─Sm1─O2	74.89(15)
O3[a]─Sm1─O4[a]	52.04(13)	O11─Sm1─O2	142.90(14)
O9─Sm1─O10	75.18(14)	O1─Sm1─O2	51.60(12)
O9─Sm1─O12	91.49(16)	O8─Sm1─O2	74.16(14)
O10─Sm1─O12	144.63(15)	O3[a]─Sm1─O2	76.31(13)
O9─Sm1─O11	71.96(14)	O4[a]─Sm1─O2	83.87(14)
O10─Sm1─O11	73.57(15)	O9─Sm1─O8	84.39(14)
O12─Sm1─O11	71.15(14)	O10─Sm1─O8	72.94(14)
O9─Sm1─O1	72.67(13)	O12─Sm1─O8	139.26(13)
O10─Sm1─O1	134.14(15)	O11─Sm1─O8	142.88(15)
O12─Sm1─O1	67.97(14)	O1─Sm1─O8	72.16(14)
O11─Sm1─O1	124.07(13)	O9─Sm1─O3[a]	145.20(14)
O10─Sm1─O3[a]	72.57(14)	O8─Sm1─O3[a]	74.02(13)
O12─Sm1─O3[a]	122.65(15)	O10─Sm1─O4[a]	96.47(14)
O11─Sm1─O3[a]	110.27(13)	O12─Sm1─O4[a]	76.36(14)
O1─Sm1─O3[a]	123.46(14)	O9─Sm1─O4[a]	146.04(14)

Complex **2**

Eu1[a]─O6	2.478(4)	Eu1─O11	2.433(4)
Eu1[a]─O7	2.478(3)	Eu1─O12	2.427(4)
Eu1─O8	2.451(3)	Eu1─O13	2.425(4)
Eu1─O9	2.545(3)	Eu1─O14	2.451(4)
Eu1─O10	2.433(4)	Eu1[a]─C8	2.857(5)

O13─Eu1─O12	74.87(14)	O13─Eu1─O6[a]	145.82(13)
O13─Eu1─O11	71.81(13)	O12─Eu1─O6[a]	96.18(14)
O12─Eu1─O11	73.46(14)	O11─Eu1─O6[a]	74.02(13)
O13─Eu1─O10	92.10(14)	O10─Eu1─O6[a]	75.88(13)
O12─Eu1─O10	144.14(14)	O14─Eu1─O6[a]	125.24(12)
O11─Eu1─O10	70.73(14)	O8─Eu1─O6[a]	128.32(12)
O13─Eu1─O14	84.51(13)	O7[a]─Eu1─O6[a]	52.14(11)
O12─Eu1─O14	73.57(12)	O13─Eu1─O9	124.24(11)
O11─Eu1─O14	143.34(14)	O12─Eu1─O9	139.78(12)

O10─Eu1─O14	139.41(12)	O11─Eu1─O9	142.77(13)
O13─Eu1─O8	72.88(12)	O10─Eu1─O9	75.03(13)
O12─Eu1─O8	134.16(14)	O14─Eu1─O9	73.83(12)
O11─Eu1─O8	124.01(13)	O8─Eu1─O9	51.71(11)
O10─Eu1─O8	68.67(13)	$O7^{a}$─Eu1─O9	76.04(11)
O14─Eu1─O8	71.73(12)	$O6^{a}$─Eu1─O9	83.98(12)
O13─Eu1─$O7^{a}$	145.02(12)	O10─Eu1─$O7^{a}$	122.18(14)
O12─Eu1─$O7^{a}$	72.80(13)	O14─Eu1─$O7^{a}$	73.89(12)
O11─Eu1─$O7^{a}$	110.62(12)	O8─Eu1─$O7^{a}$	123.19(12)

Complex**3**

$Dy1^{b}$─O1	2.427(3)	Dy1─O9	2.390(3)
$Dy1^{b}$─O2	2.512(3)	Dy1─O10	2.382(3)
Dy1─O6	2.452(3)	Dy1─O11	2.423(3)
Dy1─O7	2.448(3)	Dy1─O12	2.401(3)
Dy1─O8	2.399(3)		

O10─Dy1─O9	92.45(12)	O10─Dy1─O6	146.01(11)
O10─Dy1─O8	72.36(11)	O9─Dy1─O6	76.05(12)
O9─Dy1─O8	71.14(12)	O8─Dy1─O6	73.66(11)
O10─Dy1─O12	74.48(12)	O12─Dy1─O6	96.35(12)
O9─Dy1─O12	144.50(12)	O11─Dy1─O6	125.87(10)
O8─Dy1─O12	73.45(12)	$O1^{b}$─Dy1─O6	128.73(10)
O10─Dy1─O11	83.46(11)	O7─Dy1─O6	52.86(10)
O9─Dy1─O11	139.30(12)	O10─Dy1─$O2^{b}$	124.51(10)
O8─Dy1─O11	142.75(11)	O9─Dy1─$O2^{b}$	75.13(12)
O12─Dy1─O11	73.02(11)	O8─Dy1─$O2^{b}$	142.96(11)
O10─Dy1─$O1^{b}$	72.49(10)	O12─Dy1─$O2^{b}$	139.37(11)
O9─Dy1─$O1^{b}$	68.45(12)	O11─Dy1─$O2^{b}$	74.24(10)
O8─Dy1─$O1^{b}$	124.08(11)	$O1^{b}$─Dy1─$O2^{b}$	52.46(9)
O12─Dy1─$O1^{b}$	133.66(12)	O7─Dy1─$O2^{b}$	75.56(10)
O11─Dy1─$O1^{b}$	71.75(11)	O6─Dy1─$O2^{b}$	83.87(10)
O10─Dy1─O7	144.21(11)	O12─Dy1─O7	72.68(11)
O9─Dy1─O7	122.80(11)	O11─Dy1─O7	73.72(10)
O8─Dy1─O7	110.75(11)	$O1^{b}$─Dy1─O7	123.21(10)

Complex **4**

Ni1─O9	2.015(3)	Ni2─O17	2.025(3)
Ni1─O20	2.045(3)	$Ni2^{d}$─O10	2.035(3)
Ni1─O17	2.070(3)	$Ni2^{d}$─O4	2.052(3)
Ni1─O15	2.088(3)	Ni2─O20	2.068(3)
$Ni1^{e}$─O6	2.094(3)	Ni2─O16	2.109(3)
$Ni1^{c}$─O14	2.114(3)	Ni2─O3	2.135(3)
Ni3─O17	2.012(3)	Ni4─O8	1.991(3)

Ni3─O19	2.027(3)	Ni4^{d}─O11	2.005(3)
Ni3^{e}─O7	2.029(3)	Ni4─O20	2.023(3)
Ni3^{d}─O5	2.031(3)	Ni4─O3	2.044(3)
Ni3^{c}─O14	2.042(3)	Ni4─O18	2.086(3)
Ni3^{c}─O12	2.179(3)	Ni4─O1	2.210(3)

O9─Ni1─O20	95.81(13)	O17─Ni2─O10^{d}	178.27(13)
O9─Ni1─O17	96.50(13)	O17─Ni2─O4^{d}	98.61(12)
O20─Ni1─O17	83.13(12)	O10^{d}─Ni2─O4^{d}	81.30(13)
O9─Ni1─O15	97.08(15)	O17─Ni2─O20	83.64(12)
O20─Ni1─O15	92.12(13)	O10^{d}─Ni2─O20	98.09(12)
O17─Ni1─O15	166.00(13)	O4^{d}─Ni2─O20	95.46(12)
O9─Ni1─O6^{e}	80.86(13)	O17─Ni2─O16	91.72(13)
O20─Ni1─O6^{e}	176.63(13)	O10^{d}─Ni2─O16	86.56(13)
O17─Ni1─O6^{e}	97.74(12)	O4^{d}─Ni2─O16	91.66(13)
O15─Ni1─O6^{e}	87.77(13)	O20─Ni2─O16	172.01(13)
O9─Ni1─O14^{c}	165.23(13)	O17─Ni2─O3	92.51(12)
O20─Ni1─O14^{c}	96.84(12)	O10^{d}─Ni2─O3	87.82(13)
O17─Ni1─O14^{c}	77.53(12)	O4^{d}─Ni2─O3	166.38(12)
O15─Ni1─O14^{c}	90.04(13)	O20─Ni2─O3	77.91(12)
O6^{e}─Ni1─O14^{c}	86.53(13)	O16─Ni2─O3	95.86(13)
O17─Ni3─O19	101.48(15)	O8─Ni4─O11^{d}	163.33(13)
O17─Ni3─O7^{e}	93.72(13)	O8─Ni4─O20	97.81(13)
O19─Ni3─O7^{e}	82.83(13)	O11^{d}─Ni4─O20	94.23(13)
O17─Ni3─O5^{d}	99.11(13)	O8─Ni4─O3	99.38(13)
O19─Ni3─O5^{d}	85.86(13)	O11^{d}─Ni4─O3	93.83(13)
O7^{e}─Ni3─O5^{d}	164.35(13)	O20─Ni4─O3	81.08(12)
O17─Ni3─O14^{c}	80.53(12)	O8─Ni4─O18	81.89(14)
O19─Ni3─O14^{c}	177.29(15)	O11^{d}─Ni4─O18	83.31(13)
O7─Ni3─O14^{c}	95.26(13)	O20─Ni4─O18	109.04(13)
O5─Ni3─O14^{c}	95.65(13)	O3─Ni4─O18	169.61(14)
O17─Ni3─O12^{c}	156.80(12)	O8─Ni4─O1	86.68(13)
O19─Ni3─O12^{c}	101.66(14)	O11^{d}─Ni4─O1	86.61(13)
O7─Ni3─O12^{c}	87.61(13)	O20─Ni4─O1	157.39(12)
O5─Ni3─O12^{c}	84.12(12)	O3─Ni4─O1	76.32(12)
O14─Ni3─O12^{c}	76.29(12)	O18─Ni4─O1	93.51(13)

Complex **5**

Cu1─O6	1.929(6)	Cu2^{i}─O2	1.936(5)
Cu1^{f}─O1	1.949(5)	Cu2─O5	1.959(5)
Cu1^{g}─O7	1.973(5)	Cu2─O7	1.969(5)
Cu1─O7	2.001(5)	Cu2─N1	2.023(6)
Cu1^{h}─O3	2.152(5)	Cu2^{h}─O4	2.152(5)
Cu1^{g}─Cu1	3.0213(17)		

O6─Cu1─O1^{f}	84.2(2)	O2^{i}─Cu2─O5	161.8(3)
O6─Cu1─O7	95.2(2)	O2^{i}─Cu2─O7	92.9(2)
O1^{f}─Cu1─O7	161.8(2)	O5─Cu2─O7	93.7(2)
O7^{g}─Cu1─O7	81.0(2)	O2^{i}─Cu2─N1	85.7(2)
O6─Cu1─O3^{h}	94.4(2)	O5─Cu2─N1	83.3(2)
O1^{f}─Cu1─O3^{h}	98.2(2)	O7─Cu2─N1	164.2(2)
O7─Cu1─O3^{h}	99.9(2)	O2^{i}─Cu2─O4^{h}	99.9(2)
O6─Cu1─Cu1^{g}	135.23(18)	O5─Cu2─O4^{h}	96.6(2)
O1^{f}─Cu1─Cu1^{g}	135.88(16)	O7─Cu2─O4^{h}	93.0(2)
O7─Cu1─Cu1^{g}	40.17(15)	N1─Cu2─O4^{h}	102.8(2)
O3^{h}─Cu1─Cu1^{g}	97.22(13)		

Symmetry codes: a = *x*, -*y*+1/2, z-1/2, b = *x*, -*y*+3/2, *z*+1/2, c = 1-*x*, *y*-1/2, -*z*+3/2, D = 2-*x*, *y*-1/2, -*z*+3/2, e = *x*-1, *y*, *z*, f = -*x*, *y*+5/2, -*z*+3/2, g = -*x*, *y*+3/2, -*z*+5/2, h = 1-*x*, *y*+3/2, -z+3/2, i= *x*, *y*-1, *z*+1

Table S2 Hydrogen bonds in the crystal structures

Complex **1**

D─H···A	D···A	□D─H···A
O13─H13C···O10	2.833(6)	125.9
O11─H11B···O2^{a}	2.743(6)	133.0
O11─H11C···O7^{b}	2.717(6)	148.1
O10─H10A···O5^{a}	3.129(6)	116.9
O10─H10C···O7^{a}	2.848(6)	128.9
O8─H8C···O13^{e}	2.772(6)	135.6
O8─H8E···O4^{c}	2.786(6)	151.0
O12─H12A···O3^{g}	2.763(6)	152.5
O12─H12B···O13^{f}	3.127(7)	160.5
O14─H14A···O6^{d}	3.060(6)	133.2
O14─H14C···O1^{h}	2.862(6)	156.4
O9─H9B···O6^{b}	2.649(6)	129.8
O9─H9B···O14^{i}	3.335(6)	147.2
O9─H9C···O6^{c}	2.826(6)	127.5

Symmetry codes: a = -*x*, *y*+1/2, 3/2-*z*, b = *x*+1, *y*+1, *z*, c = -*x*, -*y*, 2-*z*, d = *x*+1, 1/2-*y*, *z*-1/2, e = 1-*x*, *y*-1/2, 3/2-*z*, f = *x*-1, *y*, *z*, g = -*x*, 1-*y*, 2-*z*, h = *x*, 3/2-*y*, *z*-1/2, i = *x*, 3/2-*y*, *z*+1/2.

Complex **2**

D─H···A	D···A	□D─H···A
O2─H2B···O3^{f}	2.921(8)	114.7
O2─H2B···O11^{g}	3.393(7)	157.2
O2─H2C···O1a	3.226(6)	134.8
O14─H14A···O2^{j}	2.786(6)	136.9
O14─H14C···O6^{h}	2.792(5)	151.0

O11─H11B···O9[b]	2.745(5)	132.3
O11─H11C···O3[e]	2.721(6)	147.1
O13─H13B···O4[e]	2.650(6)	130.0
O13─H13B···O1[c]	3.343(5)	146.9
O13─H13C···O4[h]	2.821(5)	127.6
O12─H12B···O2[g]	2.792(7)	111.0
O12─H12C···O3[b]	2.851(5)	130.3
O10─H10A···O7[i]	2.752(5)	152.7
O1─H1D···O8[b]	2.874(6)	170.7
O1─H1C···O4[d]	3.068(5)	152.4

Symmetry codes: a=1-*x*, *y*-1/2, -*z*+1/2, b=1-*x*, *y*+1/2, -z+3/2, c=1-*x*, *y*-1/2, -*z*+3/2, d=-*x*, *y*+3/2, -*z*+3/2, e= *x*+1, *y*+1, *z*, f=*1*-*x*, -*y*, 1-*z*, g=*2*-*x*, 1-*y*, 1-*z*, h=1-*x*, -*y*, 2-*z*, i=1-*x*, 1-*y*, 2-*z*, j= *x*, -y+1/2, *z*+1/2.

Complex **3**

D─H···A	D···A	□D─H···A
O13─H13B···O12[a]	2.792(5)	119.6
O13─H13A···O14[b]	3.231(6)	160.2
O14─H14C···O1[c]	2.853(5)	153.6
O14─H14A···O4[d]	3.056(5)	156.4
O9─H9C···O13[e]	3.174(5)	141.6
O9─H9C···O14[f]	2.733(5)	118.8
O9─H9B···O7[g]	2.764(5)	153.3
O12─H12C···O5[e]	3.122(5)	128.2
O12─H12B···O3[e]	2.859(5)	130.4
O11─H11C···O13[h]	2.780(5)	149.2
O11─H11B···O6[i]	2.807(4)	160.0
O10─H10C···O3[j]	3.294(5)	170.6
O10─H10C···O4[j]	2.670(5)	130.4
O10─H10A···O14[k]	3.356(5)	145.7
O10─H10A···O4[i]	2.819(4)	118.4
O8─H8E···O7[g]	3.387(5)	146.5
O8─H8E···O2[e]	2.755(4)	131.7
O8─H8C···O3[j]	2.723(4)	148.6

Symmetry codes: a = 1-*x*, 2-*y*, 1-*z*, b = *x*, *y*+1, z, c = *x*, -*y*+1/2, *z*-1/2, d = 1+*x*, -*y* +3/2, *z*-1/2, e = -*x*, 2-*y*, 1-*z*, f = -*x*, 1-*y*, 1-*z* , g = -*x*, *y*+1/2, -*z*+3/2, h = *x*, -*y*+3/2, *z*+1/2, i = -*x*, *y*-1/2, -*z*+3/2, j = *x*-1, -*y*+5/2, *z*+1/2, k = *x*, *y*+1, *z*+1.

Complex **4**

D─H···A	D···A	□D─H···A
O15─H15B···O13[a]	2.860(5)	139.2bb
O15─H15C···O22[g]	3.036(7)	148.1
O16─H16C···O21	3.280(7)	141.2
O16─H16B···O23[e]	3.250(7)	166.3

O17─H17C···O19[c]	3.296(5)	149.3
O18─H18A···O24[d]	2.781(5)	146.8
O18─H18C···O13[f]	2.817(5)	144.7
O19─H19A···O2[c]	2.836(5)	113.2
O19─H19C···O16[c]	3.334(5)	173.7
O20─H20C···O24	3.017(5)	148.4
O21─H21A···O9[c]	2.882(6)	147.1
O21─H21D···O19	2.738(6)	167.8
O22─H22B···O21	2.926(9)	145.4
O22─H22C···O6[b]	2.951(7)	131.5

Symmetry codes: a = 1-*x*, *y*-1/2, 3/2-*z*, b = 2-*x*, *y*-1/2, 3/2-*z*, c = 1-*x*, 1-*y*, 1-*z*, d = 2-*x*, 1-*y*, 2-*z*, e = *x*, 1/2-*y*, *z*+1/2, f = 1+*x*, 3/2-*y*, *z*+1/2, g = 1-*x*, *y*+1/2, 3/2-*z*.