Journal Name

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Supporting Information

Synthesis, structure and Hirshfeld surface analysis of three novel metal-tiron coordination complexes

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Bond Valence Sum Calculations

The bond valence sum calculated from the formula

$S = \exp[(R_o-R)/B]$

$V = \Sigma S$

For **1**

Where B = 0.37, R_o for Cd-O = 1.904 and R is Cd-O bond length

S1= exp[(1.904 -2.335)/0.37] = 0.3119

S2= exp[(1.904 -2.290)/0.37] = 0.3523

S3= exp[(1.904 -2.333)/0.37] = 0.3136

R_o for Cd-N = 1.96 and R is Cd-N bond length

S4= exp[(1.96 -2.333)/0.37] = 0.3649

S5= exp[(1.96-2.316)/0.37] = 0.3820

S6= exp[(1.96-2.358)/0.37] = 0.3410

And $V = \Sigma S$

V = S1+S2+S3+S4+S5+S6 = 2.0657

For **2**

Co1 Where B = 0.37, R_o for Co-O = 1.692 and R is Co-O bond length

S1= exp[(1.692 -2.000)/0.37] = 0.4349

S2= exp[(1.692 -2.000)/0.37] = 0.4349

S3= exp[(1.692 -2.203)/0.37] = 0.2513

S4= exp[(1.692 -2.203)/0.37] = 0.2513

S5= exp[(1.692 -2.121)/0.37] = 0.3136

S6= exp[(1.692 -2.121/0.37] = 0.3136

And $V = \Sigma S$

V = S1+S2+S3+S4+S5+S6 = 1.9996

Co2 Where B = 0.37, R_o for Co-O = 1.692 and R is Co-O bond length

S1= exp[(1.692 -2.142)/0.37] = 0.2963

S2= exp[(1.692 -2.057)/0.37] = 0.3728

S3= exp[(1.692 -2.130)/0.37] = 0.3061

S4= exp[(1.692 -2.062)/0.37] = 0.3678

S5= exp[(1.692 -2.103)/0.37] = 0.3292

R_o for Co-N = 1.790 and R is Co-N bond length

S6= exp[(1.790-2.174/0.37] = 0.3542

And V = ΣS

V = S1+S2+S3+S4+S5+S6 = 2.0264

For 3

Where B = 0.37, R_o for Ba-O = 2.285 and R is Ba-O bond length

S1= exp[(2.285-2.699)/0.37] = 0.3266

S2= exp[(2.285-2.724)/0.37] = 0.3052

S3= exp[(2.285-2.861)/0.37] = 0.2108

S4= exp[(2.285-2.864)/0.37] = 0.2091

S5= exp[(2.285-2.796)/0.37] = 0.2513

S6= exp[(2.285-2.877/0.37] = 0.2018

S7= exp[(2.285-2.831)/0.37] = 0.2286

S8= exp[(2.285-2.872)/0.37] = 0.2046

S9= exp[(2.285-2.878/0.37] = 0.2013

And V = ΣS

V = S1+S2+S3+S4+S5+S6+S7+S8+S9 = 2.1393

1. I. D. Brown and D. Altermatt, *Acta. Cryst.*, 1985, **B41**, 244-247.

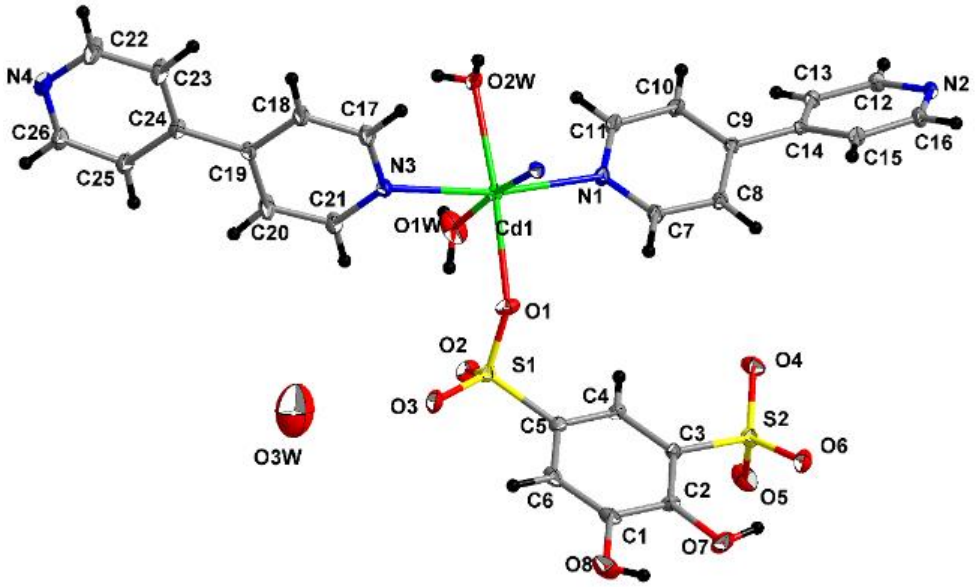

Fig. S1. Asymmetric unit of **1** with a 10 % thermal ellipsoidal probability drawn and unique atoms were labelled.

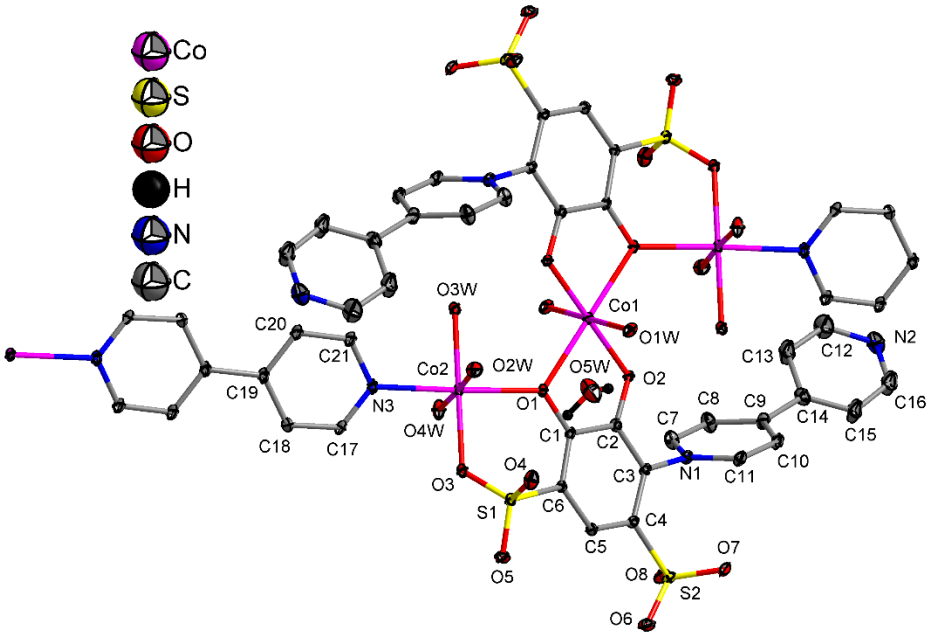

Fig. S2. Molecular unit presenting the coordination geometry of the Co(II) ions in **2**, where asymmetric units were labelled and thermal ellipsoidal probability drawn at 10 %.

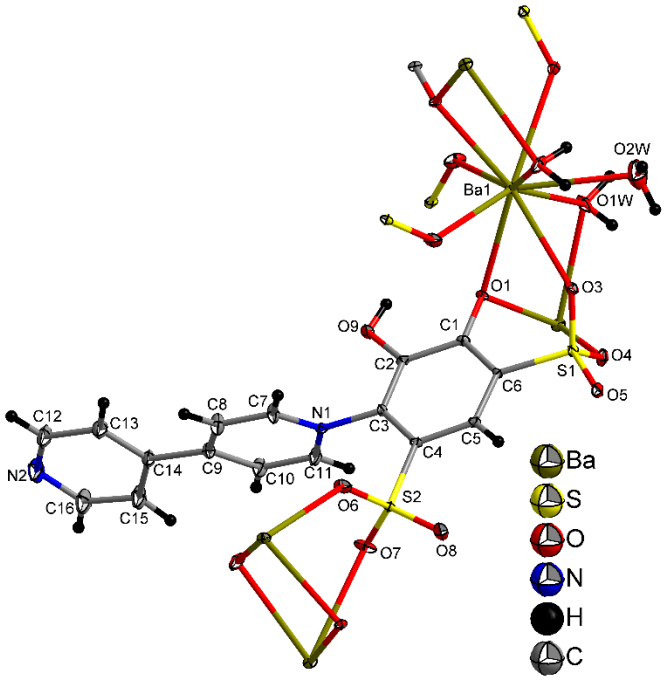

Fig. S3. Molecular unit of **3** where the asymmetric unit was labelled with 10 % thermal ellipsoidal probability and disorder bpy unit is shown by a ball and stick model.

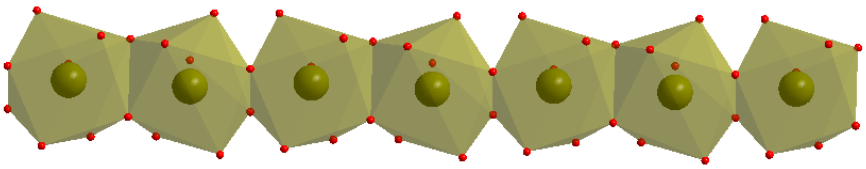

Fig. S4. A 1D Ba-O-Ba chain in **3** running along c-axis, formed between nona coordinated Ba(II) ions via edge-sharing.

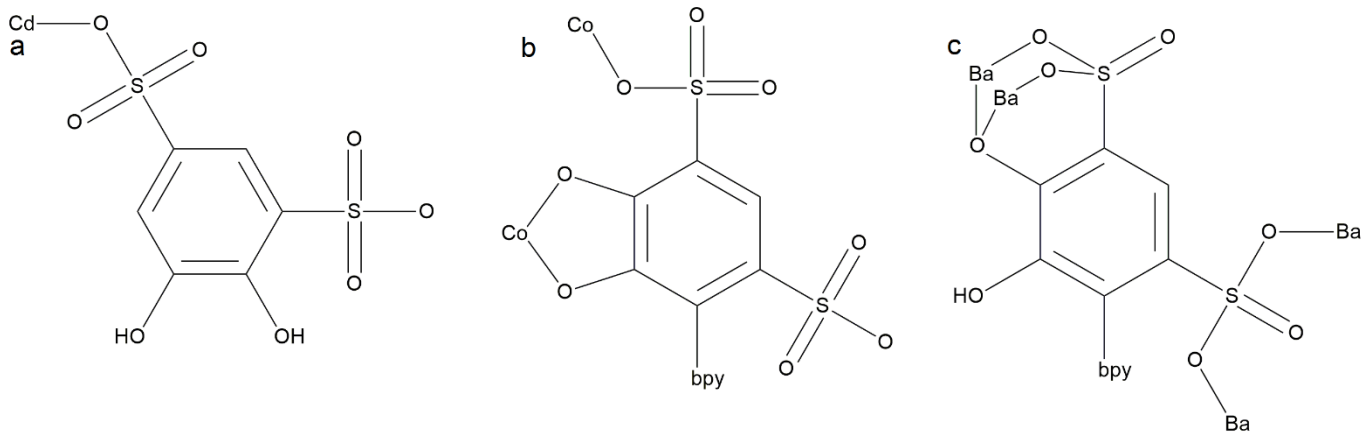

Fig. S5. Schematic representation of the coordination modes of the Metal-Tiron ligand a) for **1**, b) for **2** and c) for **3**.

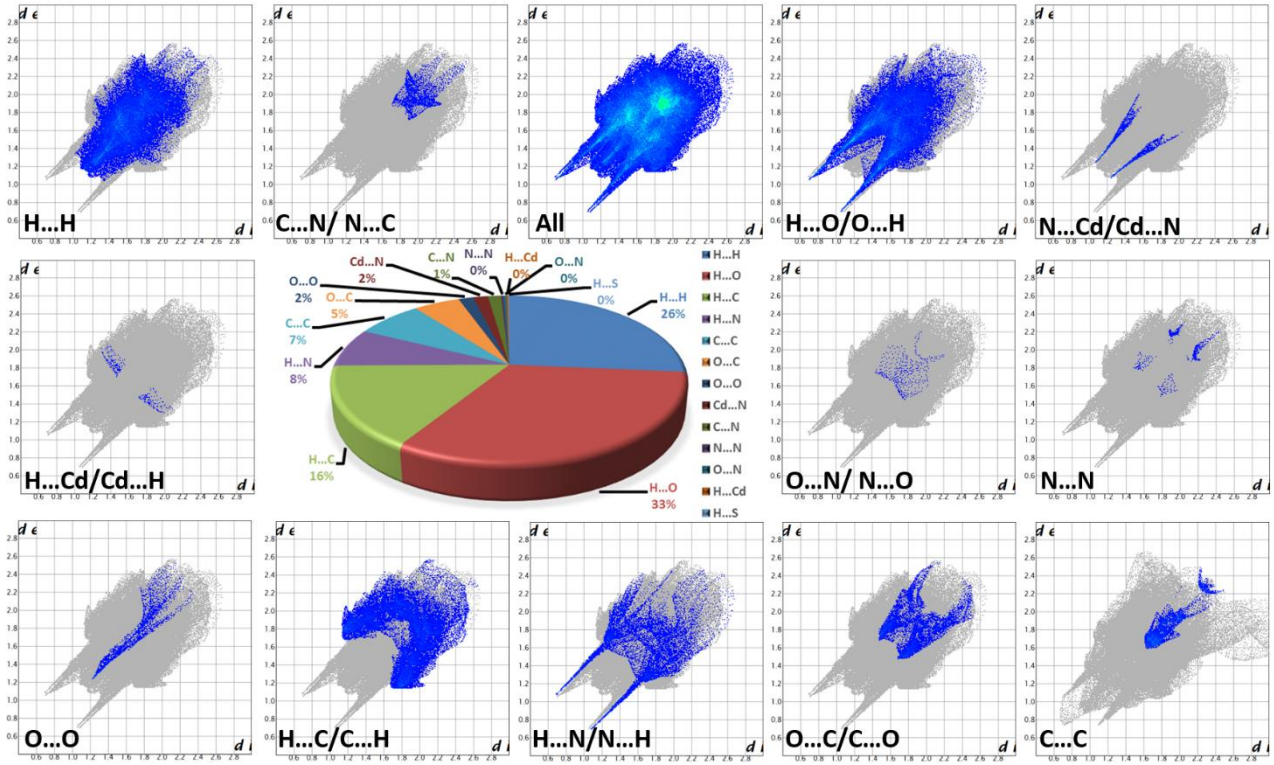

Fig. S6. The Percentage impact of different short intermolecular interaction in the crystal lattice of **1** along with the 2D fingerprint plots of short intermolecular interaction with their associate contributions to the Hirshfeld surface in the crystal lattice.

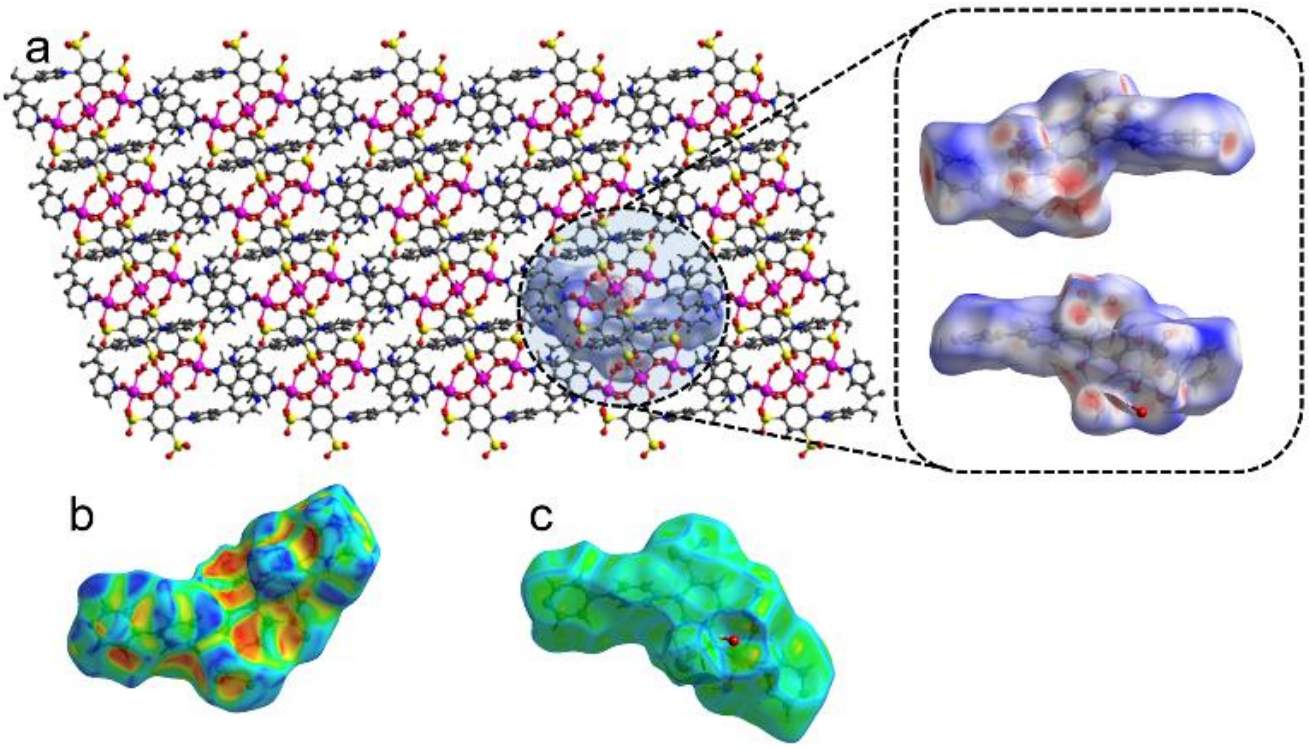

Fig. S7. (a) The perspective view of Hirshfeld surface in the crystal lattice of **2** which is highlighted in the circle and represented the d_{norm} plot in different direction of lattice, (b) the shape-index plot and (c) curvedness plot in the crystal lattice of **2**.

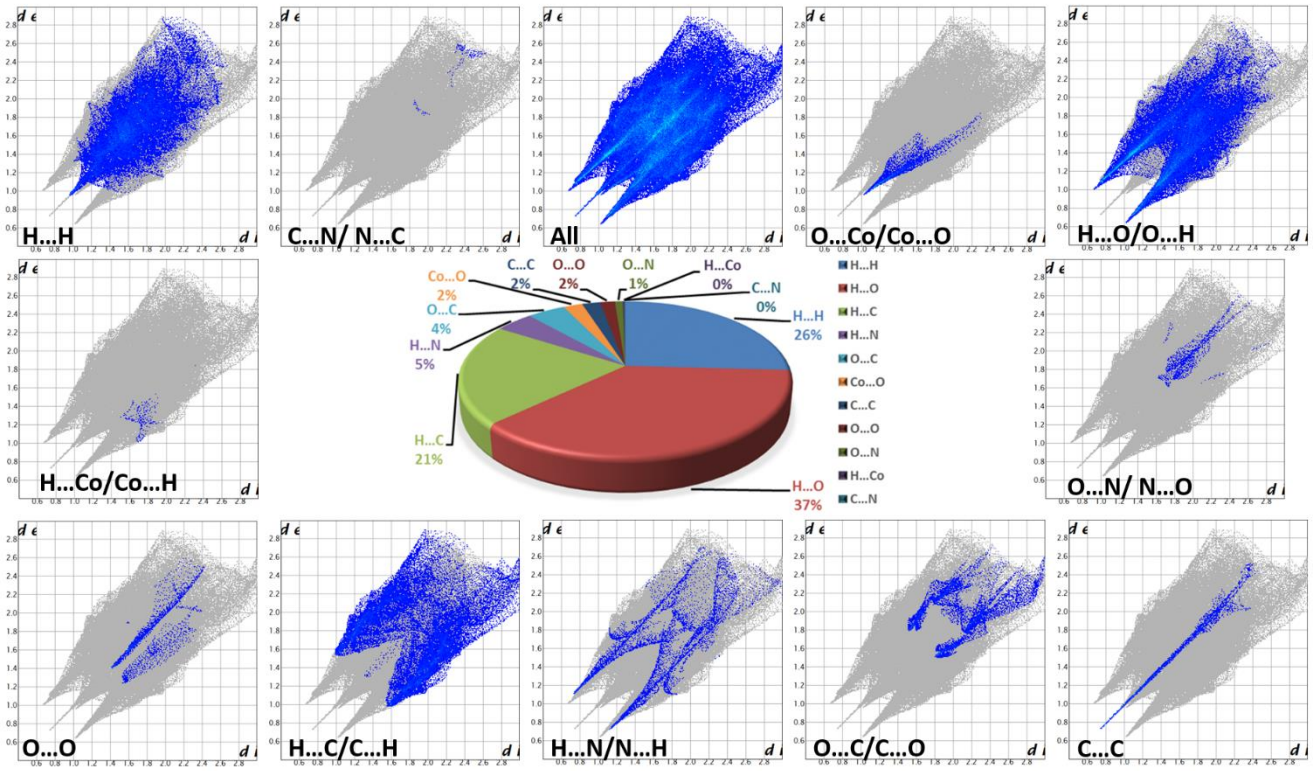

Fig. S8. The Percentage impact of different short intermolecular interaction in the crystal lattice of **2** along with the 2D fingerprint plots of short intermolecular interaction with their associate contributions to the Hirshfeld surface in the crystal lattice.

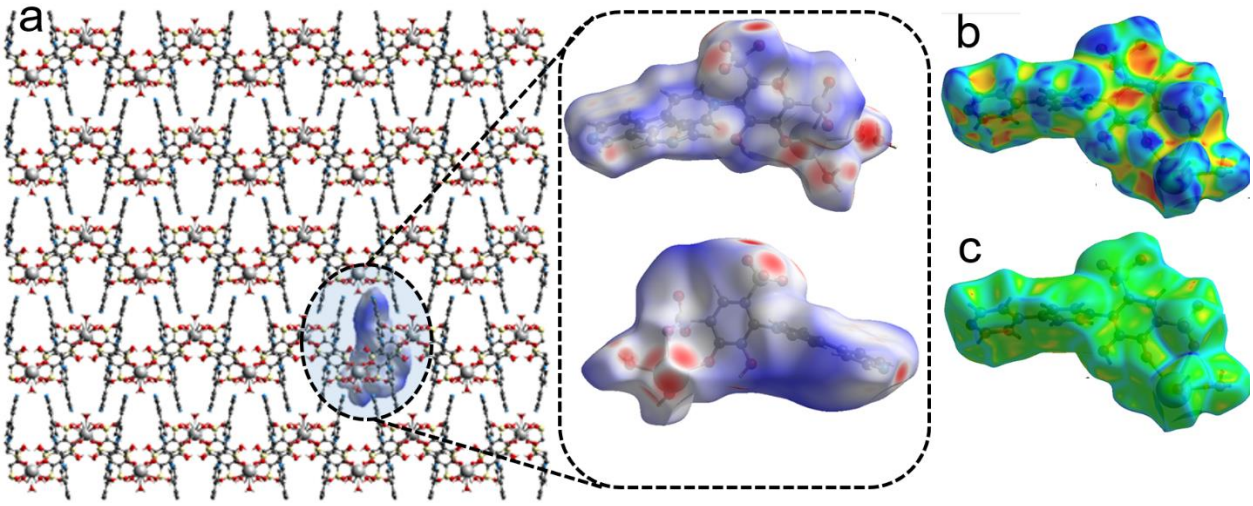

Fig. S9. (a) The perspective view of Hirshfeld surface in the crystal lattice of **3** which is highlighted in the circle and represented the d_{norm} plot in different direction of lattice, (b) the shape-index plot and (c) curvedness plot in the crystal lattice of **3**.

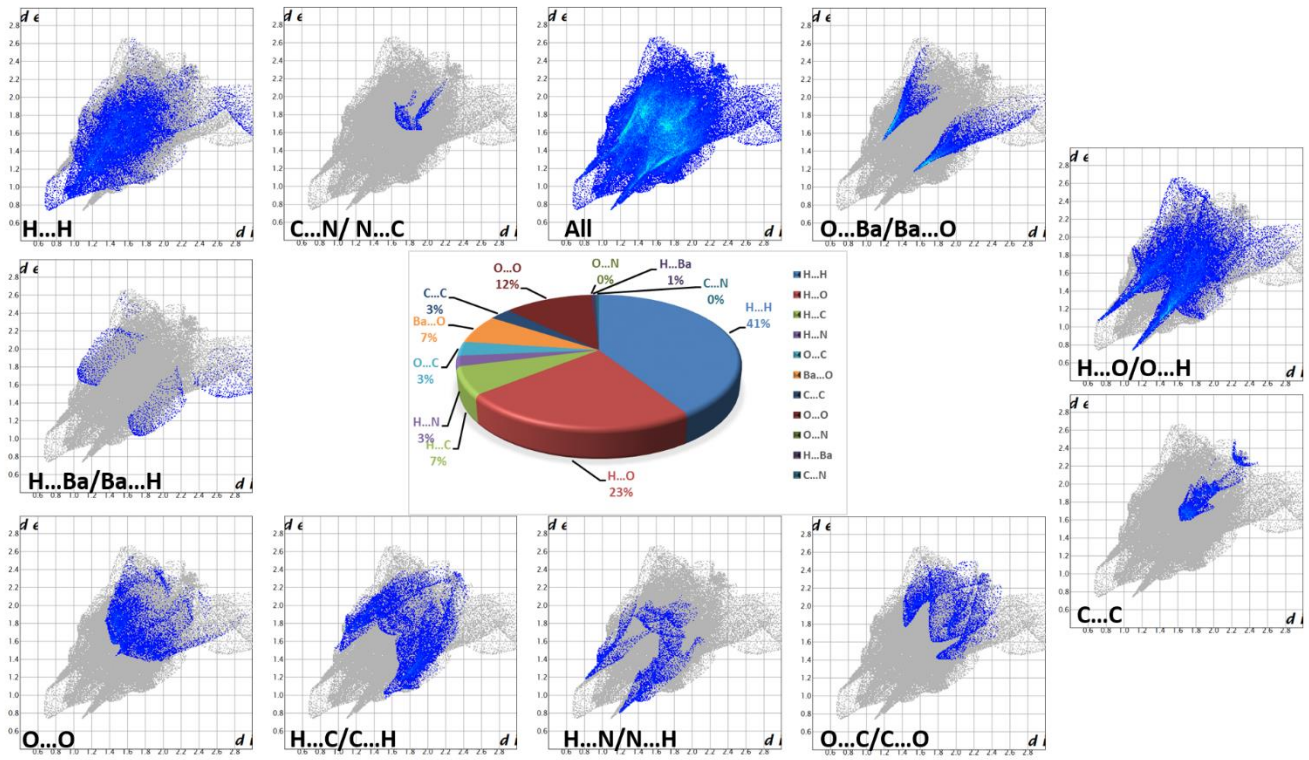

Fig. S10. The Percentage impact of different short intermolecular interaction in the crystal lattice of **3** along with the 2D fingerprint plots of short intermolecular interaction with their associate contributions to the Hirshfeld surface in the crystal lattice.

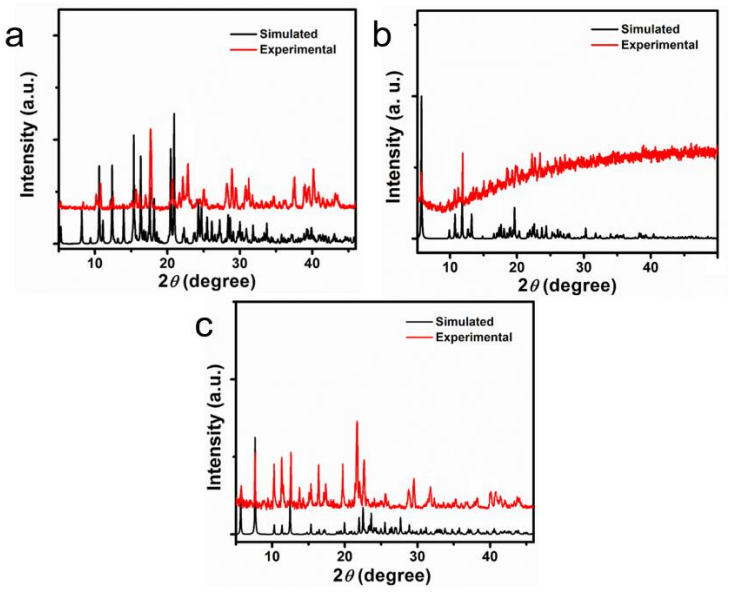

Fig. S11. PXRD pattern for a) $[Cd(tiron)(bpy)_2(H_2O)_2].0.5(H_2O)$, **1**, b) $[Co_3(tiron\text{-}bpy)_2(bpy)(H_2O)_8].(H_2O)_2$, **2**, and c) $[Ba_2(tiron\text{-}bpy)_2(H_2O)_4][Solvent]$, **3**.

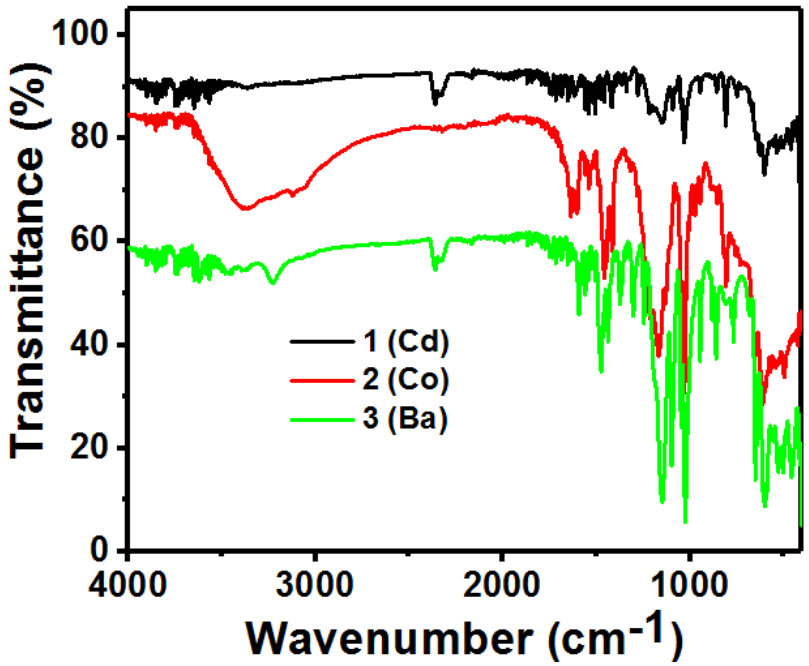

Fig. S12. FTIR profile diagram for a) $[Cd(tiron)(bpy)_2(H_2O)_2].0.5(H_2O)$, **1**, b) $[Co_3(tiron\text{-}bpy)_2(bpy)(H_2O)_8].(H_2O)_2$, **2**, and c) $[Ba_2(tiron\text{-}bpy)_2(H_2O)_4][Solvent]$, **3**.

Table S1. Hydrogen bonding table for complexes **1**-**3**.[#]

D–H···A	Symmetry of A	D–H	H···A	D–A	∠D–H···A
[Cd(tiron)(bpy)$_2$(H$_2$O)$_2$].0.5(H$_2$O), 1					
O1W–H1WA···O3W	x,y,-1+z	0.77	1.82(4)	2.541(8)	155(4)
O1W–H1WA···O3A	-1+x,y,-1+z	0.77	2.34(4)	2.944(11)	135(4)
O1W–H1WB···S1AA		0.80(5)	2.61(5)	3.21(3)	134(4)
O1W–H1WB···O2A	x,y,-1+z	0.80(5)	2.20(5)	2.945(12)	156(4)
O1W–H1WB···O2AA	x,y,-1+z	0.80(5)	1.82(5)	2.486(11)	140(5)
O2W–H2WA···N4	1-x, -y,1-z	0.79(3)	1.97(3)	2.738(5)	165(4)
O2W–H2WB···O5	x,y,1+z	0.81(4)	1.95(3)	2.725(4)	160(4)
O7–H7···O6		0.82	1.87	2.611(5)	151
O8–H8···O4	1+x,y,z	0.82	2.04	2.783(5)	151
O8–H8···O7		0.82	2.28	2.662(5)	109
C4–H4···O8	-1+x,y,z	0.93	2.44	3.318(6)	157
C4–H4···O2AA	x,y,-1+z	0.93	2.54	2.965(11)	108
C6–H6···O3A	x,y,-1+z	0.93	2.34	2.793(10)	109
C11–H11···O3W		0.93	2.48	3.100(5)	124
C15–H15···O5	x,1/2-y,1/2+z	0.93	2.59	3.438(5)	151
C20–H20···O2AA	1-x, -y,1-z	0.93	2.50	3.318(11)	148
[Co$_3$(tiron-bpy)$_2$(bpy)(H$_2$O)$_8$].(H$_2$O)$_2$, 2					
O1W–H1WA···O7	-x,1-y,1-z	0.86(13)	1.93	2.710(6)	150
O1W–H1WB···O8	x,-1+y,z	0.86(13)	1.94	2.800(6)	177
O2W–H2WB···O5W		0.79(11)	2.55(12)	3.140(14)	132(12)
O2W–H2WA···N2	x,y,-1+z	0.85	1.97	2.821(8)	176
O3W–H3WA···O6	1+x,-1+y,z	0.85	2.04	2.867(7)	162
O3W–H3WA···O7	1+x,-1+y,z	0.85	2.60	3.197(6)	129
O3W–H3WB···O2	1-x,-y,1-z	0.85	1.78	2.611(5)	165
O4W–H4WA···O8	1-x,1 -y,1-z	0.85	1.96	2.800(7)	169
O4W–H4WB···O5W	1+x,y,z	0.85	2.02	2.853(15)	166
O5W–H5WA···O4		0.85	2.04	2.850(13)	159
O5W–H5WB···O1W		0.85	2.26	2.972(11)	142
C5–H5···O5		0.93	2.44	2.859(7)	107
C5–H5···O7		0.93	2.49	2.886(6)	106
C8–H8···O5	1-x,1 -y,1-z	0.93	2.59	3.442(9)	153
C10–H10···O4	-x,1-y,1-z	0.93	2.54	3.385(8)	151
C11–H11···O6		0.93	2.53	2.890(8)	104
C18–H18···O5	1-x,1-y,-z	0.93	2.56	3.413(10)	153
C20–H20···O5	1+x,-1+y,z	0.93	2.51	3.287(10)	141
C21–H21···O3W		0.93	2.32	2.912(10)	121
[Ba$_2$(tiron-bpy)$_2$(H$_2$O)$_4$][Solvent], 3					
O1W–H1WA···N2	1+x,1/2-y,1/2+z	0.93	2.05	2.80(2)	136
O2W–H2WB···N2	1+x,y,1+z	0.84	2.46	3.27 (2)	161
O1W–H1WB···O2W	x,1/2-y,-1/2+z	0.81(5)	2.48(6)	3.146(18)	140(5)
C5–H5···O5		0.93	2.49	2.883(6)	106
C5–H54···O8		0.93	2.46	2.841(6)	105
C12–H12···O2W	1-x, 1/2+y,-1/2+z	0.93	2.58	3.093(11)	115

[#]Where 'D' is donor and 'A' is acceptor, the bond lengths are in (Å) and angles are in (°).

Table S2. Complete list of bond lengths [Å] and bond angles [◦] for complex **1-3**[#]

[Cd(tiron)(bpy)$_2$(H$_2$O)$_2$].0.5(H$_2$O), 1							
Cd1-O1	2.335(3)	S1A-O3	1.432(14)	N2-C12	1.333(5)	C9-C14	1.487(5)
Cd1-O1W	2.290(3)	S1A-O3A	1.90(3)	N2-C16	1.345(5)	C10-C11	1.378(5)
Cd1-O2W^b	2.333(3)	S1A-C5	1.874(15)	N3-C17	1.329(5)	C12-C13	1.380(5)
Cd1-N1	2.333(3)	S2-O4	1.441(3)	N3-C21	1.326(5)	C13-C14	1.382(5)
Cd1-N2^a	2.316(3)	S2-O5	1.442(3)	N4-C22	1.315(6)	C14-C15	1.393(5)
Cd1-N3	2.358(3)	S2-O6	1.453(3)	N4-C26	1.315(6)	C15-C16	1.364(5)
S1-S1A	0.553(9)	S2-C3	1.783(4)	C1-C6	1.384(6)	C17-C18	1.377(6)
S1-O1	1.445(7)	O2-O2A	0.951(8)	C1-C2	1.388(6)	C18-C19	1.379(5)
S1-O2	1.460(18)	O2-O3A	1.501(12)	C2-C3	1.394(5)	C19-C20	1.378(6)
S1-O2A	1.99(2)	O3-O3A	1.067(10)	C3-C4	1.394(5)	C19-C24	1.482(5)
S1-O3	1.45(2)	O3W-O3W^c	1.598(12)	C4-C5	1.373(6)	C20-C21	1.379(6)
S1-O3A	1.269(11)	O7-C2	1.340(5)	C5-C6	1.390(6)	C22-C23	1.383(6)
S1-C5	1.728(6)	O8-C1	1.354(5)	C7-C8	1.374(5)	C23-C24	1.368(6)
S1A-O1	1.498(13)	N1-C7	1.334(5)	C8-C9	1.379(5)	C24-C25	1.381(6)
S1A-O2	1.02(2)	N1-C11	1.332(5)	C9-C10	1.384(5)	C25-C26	1.388(6)
S1A-O2A	1.44(3)						
O1-Cd1-O1W	86.45(14)	O3A-S1-C5	121.0(7)	S1A-O2-O3A	66.0(11)	S1-C5-C4	125.0(8)
O1-Cd1-O2W^b	174.79(10)	S1-S1A-O1	73.8(19)	O2A-O2-O3A	158.4(10)	S1-C5-C6	113.1(8)
O1-Cd1-N1	97.14(11)	S1-S1A-O2	133.8(15)	S1-O2A-S1A	1.8(4)	S1A-C5-C4	110.0(7)
O1-Cd1-N2^a	87.21(10)	S1-S1A-O2A	173.5(15)	S1-O2A-O2	43.5(6)	S1A-C5-C6	128.7(8)
O1-Cd1-N3	93.36(11)	S1-S1A-O3	29.2(10)	S1A-O2A-O2	44.9(7)	C4-C5-C6	121.3(4)
O1W-Cd1-O2W^b	89.16(14)	S1-S1A-O3A	61.9(12)	S1-O3-S1A	10.8(3)	C1-C6-C5	119.2(4)
O1W-Cd1-N1	90.51(14)	S1-S1A-C5	66.3(15)	S1-O3-O3A	58.4(8)	N1-C7-C8	123.4(4)
O1W-Cd1-N2^a	173.59(14)	O1-S1A-O2	140.3(16)	S1A-O3-O3A	48.1(8)	C7-C8-C9	120.0(4)
O1W-Cd1-N3	89.93(14)	O1-S1A-O2A	112.7(11)	S1-O3A-S1A	22.6(3)	C8-C9-C10	117.0(3)
O2W^b-Cd1-N1	85.72(11)	O1-S1A-O3	88.9(12)	S1-O3A-O2	62.9(10)	C8-C9-C14	122.1(3)
O2W^b-Cd1-N2^a	97.12(11)	O1-S1A-O3A	114.8(14)	S1-O3A-O3	75.9(13)	C10-C9-C14	120.9(3)
O2W^b-Cd1-N3	83.80(11)	O2-S1A-O2A	41.1(11)	S1A-O3A-O2	40.7(11)	C9-C10-C11	119.3(4)
N1-Cd1-N2^a	91.21(11)	O2-S1A-O3	107.0(8)	S1A-O3A-O3	98.2(14)	N1-C11-C10	123.8(4)
N1-Cd1-N3	169.50(11)	O2-S1A-O3A	73.3(7)	O2-O3A-O3	138.8(9)	N2-C12-C13	123.8(4)
N2^a-Cd1-N3	89.50(11)	O2A-S1A-O3A	113.9(14)	Cd1-N1-C7	122.9(3)	C12-C13-C14	119.4(3)
S1A-S1-O1	84.6(17)	O3-S1A-O2A	147.4(8)	Cd1-N1-C11	120.3(2)	C9-C14-C13	121.7(3)
S1A-S1-O2	30.3(11)	O3-S1A-O3A	33.7(7)	C7-N1-C11	116.5(3)	C9-C14-C15	121.5(3)
S1A-S1-O2A	4.7(11)	O1-S1A-C5	98.6(10)	Cd1^d-N2-C12	123.3(3)	C13-C14-C15	116.8(3)
S1A-S1-O3	140.0(13)	O2-S1A-C5	117.7(7)	Cd1^d-N2-C16	120.1(2)	C14-C15-C16	120.2(4)
S1A-S1-O3A	95.5(13)	O2A-S1A-C5	111.4(8)	C12-N2-C16	116.7(3)	N2-C16-C15	123.1(4)
S1A-S1-C5	96.7(16)	O3-S1A-C5	87.7(11)	Cd1-N3-C17	118.6(3)	N3-C17-C18	123.7(4)
O1-S1-O2	109.7(12)	O3A-S1A-C5	103.9(12)	Cd1-N3-C21	122.3(3)	C17-C18-C19	120.3(4)
O1-S1-O2A	89.3(10)	O4-S2-O5	113.0(2)	C17-N3-C21	116.2(4)	C18-C19-C20	115.7(4)
O1-S1-O3	112.3(10)	O4-S2-O6	113.4(2)	C22-N4-C26	116.0(4)	C18-C19-C24	121.8(4)
O1-S1-O3A	130.8(5)	O5-S2-O6	112.4(2)	O8-C1-C2	120.4(4)	C20-C19-C24	122.5(4)
O2-S1-O2A	26.6(5)	O4-S2-C3	106.68(18)	O8-C1-C6	120.3(4)	C19-C20-C21	120.6(4)
O2-S1-O3	112.0(5)	O5-S2-C3	105.73(19)	C2-C1-C6	119.3(4)	N3-C21-C20	123.3(4)
O2-S1-O3A	66.3(7)	O6-S2-C3	104.68(18)	O7-C2-C1	116.1(4)	N4-C22-C23	123.6(5)
O2A-S1-O3	137.8(6)	Cd1-O1-S1	142.1(6)	O7-C2-C3	124.2(4)	C22-C23-C24	120.7(5)
O2A-S1-O3A	92.5(10)	Cd1-O1- S1A	124.2(10)	C1-C2-C3	119.7(4)	C19-C24-C23	122.4(4)
O3-S1-O3A	45.7(7)	S1-O1-S1A	21.6(2)	S2-C3-C2	119.9(3)	C19-C24-C25	121.7(4)
O1-S1-C5	107.8(4)	S1-O2-S1A	15.9(6)	S2-C3-C4	120.1(3)	C23-C24-C25	115.9(4)
O2-S1-C5	104.0(8)	S1-O2-O2A	109.8(10)	C2-C3-C4	120.0(4)	C24-C25-C26	119.3(4)
O2A-S1-C5	95.0(8)	S1A-O2-O2A	94.0(14)	C3-C4-C5	119.3(4)	N4-C26-C25	124.5(4)
O3-S1-C5	110.7(10)	S1-O2-O3A	50.7(7)	S1-C5-S1A	17.05(17)		
[Co$_3$(tiron-bpy)$_2$(bpy)(H$_2$O)$_8$].(H$_2$O)$_2$, 2							
Co1-O1	2.203(3)	S1-O4	1.433(4)	N2-C12	1.347(14)	C9-C10	1.377(9)
Co1-O1^e	2.203(3)	S1-O5	1.443(4)	N2-C16	1.291(13)	C9-C14	1.474(9)
Co1-O2	2.000(3)	S1-C6	1.793(5)	N3-C17	1.295(9)	C10-C11	1.366(8)
Co1-O2^e	2.001(3)	S2-O6	1.432(4)	N3-C21	1.340(9)	C12-C13	1.362(13)
Co1-O1W	2.121(4)	S2-O7	1.454(4)	C1-C2	1.447(7)	C13-C14	1.388(12)
Co1-O1W^e	2.121(4)	S2-O8	1.449(4)	C1-C6	1.405(6)	C14-C15	1.350(11)

Co2-O1	2.142(3)	S2-C4	1.773(5)	C2-C3	1.398(7)	C15-C16	1.366(14)
Co2-O3	2.058(4)	O1-C1	1.308(6)	C3-C4	1.403(7)	C17-C18	1.378(10)
Co2-O2W	2.132(4)	O2-C2	1.310(6)	C4-C5	1.361(7)	C18-C19	1.372(10)
Co2-O3W	2.062(4)	N1-C3	1.441(6)	C5-C6	1.378(7)	C19-C20	1.356(10)
Co2-O4W	2.104(5)	N1-C7	1.345(7)	C7-C8	1.366(9)	C19-C19^{f}	1.491(11)
Co2-N3	2.174(4)	N1-C11	1.356(7)	C8-C9	1.396(9)	C20-C2)	1.362(10)
S1-O3	1.465(4)						
O1-Co1-O1^{e}	180	O3W-Co2-N3	87.15(16)	C7-N1-C11	120.5(5)	N1-C7-C8	121.2(6)
O1-Co1-O2	79.05(12)	O4W-Co2-N3	87.16(19)	C12-N2-C16	116.2(8)	C7-C8-C9	119.7(6)
O1-Co1- O2^{e}	100.95(12)	O3-S1-O4	112.4(3)	Co2-N3-C17	125.9(4)	C8-C9-C10	117.4(6)
O1-Co1-O1 W	84.51(15)	O3-S1-O5	111.6(3)	Co2-N3-C21	119.1(4)	C8-C9-C14	120.1(6)
O1-Co1-O1W^{e}	95.49(15)	O4-S1-O5	113.4(3)	C17-N3-C21	114.5(5)	C10-C9-C14	122.5(6)
O2-Co1-O2^{e}	180	O3-S1-C6	106.9(2)	O1-C1-C2	116.4(4)	C9-C10-C11	121.8(5)
O2-Co1-O1W	93.68(14)	O4-S1-C6	105.8(2)	O1-C1-C6	127.7(4)	N1-C11-C10	119.3(5)
O2-Co1-O1W^{e}	86.32(14)	O5-S1-C6	106.0(2)	C2-C1-C6	115.9(4)	N2-C12-C13	122.5(10)
O1W^{e}-Co1-O1W	180	O6-S2-O7	112.0(3)	O2-C2-C1	119.8(4)	C12-C13-C14	119.9(10)
O1-Co2-O3	89.90(14)	O6-S2-O8	113.1(3)	O2-C2-C3	120.7(4)	C9-C14-C13	119.0(7)
O1-Co2-N3	90.96(16)	O6-S2-C4	107.0(2)	C1-C2-C3	119.5(4)	C9-C14-C15	124.3(7)
O1-Co2-O2W	177.18(15)	O7-S2-O8	112.5(3)	N1-C3-C2	115.0(4)	C13-C14-C15	116.5(7)
O1-Co2-O3W	90.39(14)	O7-S2-C4	106.0(2)	N1-C3-C4	123.6(4)	C14-C15-C16	119.9(9)
O1-Co2-O4W	91.56(16)	O8-S2-C4	105.6(2)	C2-C3-C4	121.4(4)	N2-C16-C15	124.9(10)
O3-Co2-O2W	90.67(17)	C1-O1-Co1	108.9(3)	S2-C4- C3	120.5(4)	N3-C17-C18	125.2(6)
O3-Co2-O3W	177.81(17)	Co1-O1-Co2	123.92(15)	S2-C4- C5	120.3(4)	C19-C18-C17	119.5(6)
O3-Co2-O4W	89.8(2)	Co2-O1-C1	124.6(3)	C3-C4-C5	119.1(4)	C18-C19-C19^{f}	122.9(7)
O3-Co2-N3	92.61(16)	Co1-O2-C2	113.8(3)	C4-C5-C6	120.9(4)	C18-C19-C20	115.5(6)
O2W-Co2-O3W	87.15(17)	Co2-O3-S1	125.6(2)	S1-C6-C1	119.3(4)	C19^{f}-C19-C20	121.3(7)
O2W-Co2-O4W	177.44(18)	C3-N1-C7	117.4(4)	S1-C6-C5	117.7(4)	C19-C20-C21	120.9(7)
O2W-Co2-N3	90.30(19)	C3-N1-C11	121.9(4)	C1-C6-C5	123.0(4)	N3-C21-C20	123.8(7)
O3W-Co2-O4W	92.3(2)						

[Ba$_2$(tiron-bpy)$_2$(H$_2$O)$_4$][Solvent], 3

Ba1-O1	2.699(3)	S2-O6	1.430(4)	C1-C2	1.428(7)	C13-C14	1.358(9)
Ba1-O1^{g}	2.724(3)	S2-O7	1.451(4)	C1-C6	1.396(7)	C14-C15	1.362(10)
Ba1-O3	2.861(4)	S2-O8	1.427(4)	C2-C3	1.366(7)	C15-C16	1.374(10)
Ba1-O4^{g}	2.864(4)	S1-C6	1.768(5)	C3-C4	1.400(7)		
Ba1-O6^{h}	2.796(4)	S2-C4	1.763(5)	C4-C5	1.392(7)		
Ba1-O7^{i}	2.877(4)	O1-C1	1.309(6)	C5-C6	1.390(7)		
Ba1-O1W	2.831(4)	O2-C2	1.348(6)	C7-C8	1.359(9)		
Ba1-O1W^{g}	2.872(4)	N1-C3	1.465(6)	C8-C9	1.389(8)		
Ba1-O2W	2.878(7)	N1-C7	1.327(7)	C9-C10	1.372(8)		
S1-O3	1.454(4)	N1-C11	1.338(7)	C9-C14	1.496(8)		
S1-O4	1.457(4)	N2-C12	1.302(10)	C10-C11	1.363(8)		
S1-O5	1.448(4)	N2-C16	1.328(10)	C12-C13	1.392(10)		
O1-Ba1-O1^{g}	127.04(13)	O6^{h}-Ba1-O7^{i}	112.61(14)	Ba1^{j}-O4-S1	128.7(2)	C8-C9-C14	123.6(6)
O1-Ba1-O3	66.22(10)	O6^{h}-Ba1-O1W	147.40(12)	Ba1^{h}-O6- S2	136.8(2)	C10-C9-C14	120.1(6)
O1^{g}-Ba1-O3	134.75(10)	O6^{h}-Ba1-O1W^{g}	64.97(15)	Ba1^{k}-O7-S2	128.0(2)	C9-C10-C11	121.3(6)
O1-Ba1-O4^{g}	146.97(10)	O6^{h}-Ba1-O2W	121.87(17)	Ba1-O1W-Ba1^{j}	103.36(13)	N1-C11-C10	120.4(6)
O1^{g}-Ba1-O4^{g}	66.27(10)	O7^{i}-Ba1-O1W	64.31(15)	C11-N1-C3	117.3(5)	N2-C12-C13	124.2(8)
O1-Ba1-O6^{h}	75.28(11)	O7^{i}-Ba1- O1W^{g}	152.83(11)	C7-N1-C11	120.3(5)	C14-C13-C12	119.4(8)
O1^{g}-Ba1-O6^{h}	71.42(10)	O7^{i}-Ba1-O2W	125.32(17)	C12-N2-C16	115.7(7)	C9-C14-C13	120.4(7)
O1-Ba1-O7^{i}	74.47(11)	O1W-Ba1-O1W^{g}	133.3(2)	O1-C1-C2	118.2(4)	C9-C14-C15	122.8(6)
O1^{g}-Ba1-O7^{i}	81.80(10)	O1W-Ba1-O2W	67.5(2)	O1-C1-C6	125.2(5)	C13-C14-C15	116.8(7)
O1-Ba1-O1W	72.74(11)	O1W^{g}-Ba1-O2W	65.78(19)	C2-C1-C6	116.6(4)	C14-C15-C16	120.0(8)
O1-Ba1-O1W^{g}	126.84(13)	O3-S1-O4	111.6(2)	O2-C2-C1	119.8(4)	N2-C16-C15	123.7(8)
O1^{g}-Ba1-O1W	135.16(13)	O3-S1-O5	112.3(2)	O2-C2-C3	119.7(5)		
O1^{g}-Ba1-O1W^{g}	71.73(10)	O4-S1-O5	112.7(2)	C1-C2-C3	120.3(5)		
O1-Ba1-O2W	113.89(19)	O3-S1-C6	107.3(2)	C2-C3-C4	123.0(5)		
O3-Ba1-O4^{g}	129.77(11)	O4-S1-C6	106.3(2)	N1-C3-C2	114.2(5)		
O3-Ba1-O6^{h}	72.27(12)	O5-S1-C6	106.1(2)	N1-C3-C4	122.8(5)		
O3-Ba1-O7^{i}	137.74(11)	O6-S2-O7	110.9(3)	C3-C4-C5	116.8(5)		
O3-Ba1-O1W	89.05(14)	O6-S2-O8	114.9(3)	S2-C4-C5	120.2(4)		

O3-Ba1-O1W^{g}	68.95(11)	O7-S2-O8	112.3(3)	C6-C5-C4	121.1(5)
O3-Ba1-O2W	62.66(16)	O7-S2-C4	106.7(2)	S1-C6-C1	117.3(4)
O4^{g}-Ba1-O6^{h}	133.99(11)	O8-S2-C4	104.8(2)	C1-C6-C5	120.6(4)
O4^{g}-Ba1-O7^{i}	78.74(13)	Ba1-O1-Ba1^{j}	111.21(11)	C1-C6-C5	122.0(5)
O4^{g}-Ba1-O1W	78.46(12)	Ba1-O1-C1	123.3(3)	N1-C7-C8	120.7(6)
O4^{g}-Ba1-O1W^{g}	84.96(13)	Ba1^{j}-O1-C1	114.6(3)	C7-C8-C9	121.0(6)
O4^{g}-Ba1-O2W	67.64(17)	Ba1-O3-S1	128.6(2)	C8-C9-C10	116.2(6)

#Symmetry transformations used to generate equivalent atoms:

(*a*) x-1,-y+3/2,z-1/2; (*b*) -x+1,-y+1,-z+1; (*c*) -x,-y+1,-z+1; (*d*) x+1,-y+3/2,z+1/2; (*e*) -x+1,-y+2,-z+1; (*f*) -x,-y+2,-z+2; (*g*) x,-y+3/2,z-1/2; (*h*) -x+1,-y+1,-z; (*i*) -x+1, y+1/2,-z+1/2; (*j*) x,-y+3/2,z+1/2; (*k*) -x+1,y-1/2,-z+1/2;

Table S3. Filtering fingerprint by element type. Surface area included (as percentage of the total surface area) for close contacts between atoms inside and outside the surface for complex **1-3**.

Inside Atom	**Outside Atom**						
[Cd(tiron)(bpy)$_2$(H$_2$O)$_2$].0.5(H$_2$O), 1							
Atom	Cd	S	O	N	H	C	All
C	.	0.0	2.7	0.7	8.6	7.2	19.2
Cd	.	.	.	0.8	0.1	.	0.9
H	0.1	0.0	17.0	3.3	26.4	7.3	54.1
N	0.8	.	0.2	0.3	4.1	0.7	6.1
O	.	.	1.6	0.2	15.6	2.2	19.6
S	.	.	.	.	0.0	0.0	0.0
All	0.9	0.0	21.4	5.3	54.9	17.4	
[Co$_3$(tiron-bpy)$_2$(bpy)(H$_2$O)$_8$].(H$_2$O)$_2$, 2							
Atom	Co	S	O	N	H	C	All
C	.	0.0	2.6	0.1	11.8	2.1	16.5
Co	.	.	2.2	.	0.2	.	2.4
H	.	0.0	18.2	1.9	25.9	9.3	55.3
N	.	.	0.4	.	2.5	0.1	3.0
O	.	.	1.7	0.4	19.0	1.8	22.9
S	.	.	.	.	0.0	0.0	0.0
All	0.0	0.0	25.0	2.4	59.3	13.3	
[Ba$_2$(tiron-bpy)$_2$(H$_2$O)$_4$][Solvent], 3							
Atom	Ba	S	O	N	H	C	All
Ba	.	.	5.5	.	0.9	0.1	6.5
C	0.0	.	3.0	0.8	6.8	4.0	14.7
H	0.5	0.0	12.1	2.2	24.1	5.3	44.1
N	.	.	.	.	2.6	0.3	2.9
O	4.2	0.0	8.1	.	16.6	2.8	31.7
S	.	.	0.1	.	0.0	.	0.1
All	4.7	0.1	28.7	3.0	51.0	12.5	

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å \times 10^3$) for **1-3** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
[Cd(tiron)(bpy)$_2$(H$_2$O)$_2$].0.5(H$_2$O), 1									
Cd1	5408.0(4)	6256.1(2)	4232.4(2)	26.41(9)	C4	4029(6)	6384.6(12)	8171(3)	31.9(9)
S1	2860(30)	5891.2(14)	6258(7)	32.3(19)	C5	2653(6)	6152.8(12)	7485(3)	36.8(10)
S1A	3620(40)	5863(3)	6404(9)	33(3)	C6	843(6)	6152.4(12)	7640(4)	39.4(10)
S2	5378.5(15)	6919.5(3)	9962.2(9)	36.7(2)	C7	6959(6)	6940.5(12)	6198(4)	35.8(10)
O1	3379(4)	6173.0(9)	5460(2)	42.9(7)	C8	8100(6)	7232.3(12)	6813(4)	36.2(10)
O2	4408(17)	5615(3)	6699(6)	49(3)	C9	9874(5)	7286.7(11)	6650(3)	26.5(8)
O2A	5558(18)	5758(3)	6881(7)	41(3)	C10	10428(6)	7032.6(13)	5869(4)	37.7(10)
O3	1146(14)	5682(3)	5735(7)	55(3)	C11	9194(6)	6748.6(13)	5284(4)	37.7(10)
O3A	2400(20)	5525(3)	6125(9)	64(4)	C12	14165(6)	7863.9(11)	8157(3)	32.4(9)
O4	6668(4)	7033.1(10)	9275(3)	50.1(8)	C13	13051(5)	7554.3(11)	7609(3)	30.4(9)
O5	6209(5)	6663.6(11)	10935(3)	67.1(11)	C14	11138(5)	7607.2(11)	7264(3)	25.0(8)
O6	4392(4)	7256.9(10)	10310(3)	56.1(9)	C15	10447(5)	7977.7(12)	7505(4)	32.8(9)
O7	1221(4)	6872.1(11)	9954(3)	59.1(10)	C16	11644(5)	8271.0(12)	8033(4)	33.5(9)
O8	-1349(4)	6397.1(11)	8639(4)	59.8(10)	C17	3386(6)	5925.0(12)	1677(4)	41.9(11)
O1W	7037(5)	5722.9(11)	5197(4)	70.7(11)	C18	2942(6)	5658.2(12)	760(4)	41.7(11)
O2W	7474(4)	6276.2(9)	3013(2)	36.6(7)	C19	2799(5)	5255.0(11)	973(3)	30.4(9)
O3W	9124(10)	5126(2)	5088(8)	198(3)	C20	3045(8)	5148.7(13)	2131(4)	56.9(14)
N1	7469(4)	6699.8(9)	5425(3)	30.3(7)	C21	3497(8)	5432.8(13)	3003(4)	54.5(13)
N2	13507(4)	8220.6(9)	8369(3)	27.5(7)	C22	2012(8)	4772.4(15)	-1996(4)	63.0(15)
N3	3696(5)	5818.5(10)	2796(3)	34.5(8)	C23	2274(8)	5061.1(14)	-1130(4)	58.9(14)
N4	1909(5)	4386.9(12)	-1793(3)	46.2(9)	C24	2447(6)	4956.4(12)	14(3)	34.0(9)
C1	415(5)	6396.4(13)	8489(4)	37.4(10)	C25	2329(7)	4552.2(13)	230(4)	51.0(12)
C2	1778(5)	6637.8(12)	9178(3)	31.5(9)	C26	2063(8)	4284.3(14)	-696(4)	57.2(14)
C3	3598(5)	6627.4(11)	9032(3)	28.3(8)					
[Co$_3$(tiron-bpy)$_2$(bpy)(H$_2$O)$_8$].(H$_2$O)$_2$, 2									
Co1	5000	10000	5000	30(1)	C2	6378(5)	6949(5)	5187(3)	31(1)
Co2	3938(1)	8611(1)	7275(1)	35(1)	C3	7165(5)	5595(5)	4994(3)	31(1)
S1	6956(2)	5536(1)	7829(1)	38(1)	C4	7832(5)	4257(5)	5650(3)	32(1)
S2	8766(1)	2549(1)	5388(1)	37(1)	C5	7724(6)	4284(5)	6492(3)	35(1)
O1	5350(4)	8264(4)	6211(2)	36(1)	C6	6939(6)	5599(5)	6703(3)	33(1)
O2	5800(4)	8194(3)	4570(2)	32(1)	C7	5752(7)	6091(8)	3627(4)	54(2)
O3	5298(5)	6452(4)	7966(2)	44(1)	C8	5626(8)	6353(9)	2748(4)	60(2)
O4	8090(5)	6119(5)	7988(3)	57(1)	C9	6993(8)	6228(7)	2309(4)	50(1)
O5	7444(6)	4002(4)	8296(3)	58(1)	C10	8447(7)	5747(7)	2801(4)	47(1)
O6	9303(6)	1406(4)	6188(3)	55(1)	C11	8542(7)	5503(6)	3680(4)	44(1)
O7	10114(5)	2624(5)	4909(3)	61(1)	C12	5312(15)	8344(16)	30(6)	118(4)
O8	7523(5)	2473(4)	4863(3)	51(1)	C13	5439(13)	7858(14)	909(6)	107(4)
O1W	7370(4)	9717(4)	5388(3)	46(1)	C14	6834(9)	6669(8)	1355(4)	56(2)
O2W	5555(6)	9311(5)	7803(3)	53(1)	C15	8022(13)	6078(13)	874(6)	102(4)
O3W	2631(5)	10799(4)	6608(2)	45(1)	C16	7808(13)	6647(15)	-5(7)	108(4)
O4W	2271(6)	7955(6)	6795(3)	61(1)	C17	2321(13)	8059(8)	8972(6)	90(3)
O5W	9042(13)	8422(12)	7184(6)	124(3)	C18	1464(12)	8355(8)	9664(6)	89(3)
N1	7179(5)	5689(4)	4084(3)	37(1)	C19	501(8)	9794(7)	9645(4)	51(1)
N2	6505(10)	7720(10)	-438(4)	85(2)	C20	637(12)	10838(8)	8976(5)	93(3)
N3	2406(6)	9048(5)	8310(3)	44(1)	C21	1599(12)	10448(8)	8345(5)	85(3)
C1	6181(5)	6970(5)	6079(3)	29(1)					
[Ba$_2$(tiron-bpy)$_2$(H$_2$O)$_4$][Solvent], 3									
Ba1	3116(1)	7555(1)	-869(1)	31(1)	C3	5425(3)	5404(3)	2656(5)	28(1)
S1	2561(1)	5685(1)	1300(2)	31(1)	C4	4923(3)	4730(3)	2461(5)	27(1)
S2	5358(1)	3790(1)	2796(2)	31(1)	C5	4044(3)	4829(3)	1991(6)	29(1)
O1	3888(2)	6951(2)	1816(4)	28(1)	C6	3685(3)	5567(3)	1782(5)	22(1)
O2	5611(2)	6757(2)	2605(5)	48(1)	C7	6909(4)	5270(4)	2303(7)	53(2)
O3	2386(2)	6117(2)	-121(4)	45(1)	C8	7764(4)	5358(5)	2817(8)	66(2)
O4	2306(2)	6121(2)	2543(4)	45(1)	C9	8075(4)	5589(4)	4303(7)	46(2)
O5	2204(2)	4909(2)	1150(4)	42(1)	C10	7477(4)	5678(5)	5224(7)	68(2)
O6	5861(3)	3649(2)	1648(5)	56(1)	C11	6624(4)	5584(5)	4675(7)	63(2)
O7	5892(3)	3804(2)	4295(4)	60(1)	C12	10404(5)	6063(5)	4512(11)	87(3)
O8	4632(3)	3293(2)	2734(7)	75(2)	C13	9553(4)	5879(5)	3931(9)	73(2)
O1W	2394(3)	8292(3)	1434(5)	58(1)	C14	8999(4)	5759(4)	4902(8)	58(2)
O2W	1275(5)	7445(4)	-1399(10)	135(3)	C15	9329(5)	5802(6)	6415(9)	86(3)

N1	6351(3)	5391(2)	3219(5)	31(1)	C16	10177(5)	5986(6)	6893(11)	95(3)
N2	10717(4)	6135(5)	5954(9)	87(2)					
C1	4185(3)	6240(3)	1967(5)	26(1)					
C2	5089(3)	6133(3)	2383(6)	29(1)					

Table S5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1-3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12		U11	U22	U33	U23	U13	U12
[Cd(tiron)(bpy)$_2$(H$_2$O)$_2$].0.5(H$_2$O), 1													
Cd1	28(1)	25(1)	26(1)	-2(1)	4(1)	0(1)	C4	34(2)	34(2)	31(2)	-2(2)	14(2)	-1(2)
S1	37(5)	29(1)	34(2)	-3(1)	15(2)	6(2)	C5	53(3)	33(2)	28(2)	2(2)	15(2)	-3(2)
S1A	37(7)	36(2)	30(2)	-3(2)	15(3)	-3(3)	C6	40(2)	38(2)	34(2)	6(2)	-5(2)	-15(2)
S2	35(1)	40(1)	32(1)	0(1)	2(1)	-8(1)	C7	28(2)	37(2)	42(2)	-10(2)	9(2)	-7(2)
O1	45(2)	53(2)	35(2)	11(1)	18(1)	11(1)	C8	35(2)	37(2)	39(2)	-11(2)	14(2)	-3(2)
O2	65(8)	35(4)	51(4)	14(3)	23(4)	31(5)	C9	30(2)	25(2)	24(2)	0(2)	4(2)	-1(2)
O2A	45(6)	42(5)	40(4)	-4(3)	16(4)	12(4)	C10	28(2)	47(3)	40(2)	-14(2)	12(2)	-6(2)
O3	53(6)	56(5)	61(5)	-31(4)	21(4)	-15(4)	C11	35(2)	45(3)	34(2)	-16(2)	7(2)	-3(2)
O3A	72(10)	47(6)	80(7)	-25(5)	35(7)	-26(6)	C12	30(2)	31(2)	34(2)	0(2)	5(2)	1(2)
O4	33(2)	59(2)	61(2)	3(2)	15(2)	-12(2)	C13	31(2)	25(2)	37(2)	-2(2)	11(2)	4(2)
O5	67(2)	65(2)	52(2)	20(2)	-19(2)	-20(2)	C14	27(2)	28(2)	20(2)	1(2)	6(2)	-1(2)
O6	63(2)	53(2)	55(2)	-24(2)	20(2)	-12(2)	C15	24(2)	32(2)	41(2)	-7(2)	7(2)	1(2)
O7	48(2)	80(3)	58(2)	-23(2)	30(2)	-2(2)	C16	30(2)	26(2)	44(2)	-7(2)	7(2)	-1(2)
O8	26(2)	63(2)	91(3)	5(2)	16(2)	-5(2)	C17	58(3)	26(2)	39(2)	1(2)	6(2)	-2(2)
O1W	55(3)	47(2)	98(3)	20(2)	-6(2)	14(2)	C18	63(3)	31(2)	28(2)	-1(2)	5(2)	-5(2)
O2W	171(7)	159(7)	251(9)	-44(6)	27(6)	50(5)	C19	33(2)	27(2)	29(2)	-1(2)	3(2)	-2(2)
O3W	42(2)	39(2)	30(2)	-8(1)	11(1)	-3(2)	C20	103(4)	26(2)	34(2)	2(2)	1(3)	-8(3)
N1	26(2)	33(2)	29(2)	-7(1)	2(1)	-3(1)	C21	97(4)	36(3)	26(2)	2(2)	5(2)	-18(3)
N2	30(2)	23(2)	30(2)	-4(1)	7(1)	-3(1)	C22	105(5)	49(3)	29(3)	-6(2)	4(3)	11(3)
N3	43(2)	29(2)	31(2)	-3(1)	7(2)	-6(2)	C23	101(4)	33(3)	36(3)	-4(2)	4(3)	5(3)
N4	53(2)	45(2)	40(2)	-13(2)	10(2)	2(2)	C24	38(2)	31(2)	32(2)	-3(2)	5(2)	2(2)
C1	25(2)	43(2)	42(3)	11(2)	5(2)	-2(2)	C25	85(4)	32(2)	39(3)	-3(2)	22(3)	-1(2)
C2	29(2)	37(2)	30(2)	2(2)	11(2)	2(2)	C26	92(4)	34(3)	53(3)	-12(2)	32(3)	-4(3)
C3	27(2)	31(2)	26(2)	0(2)	5(2)	-3(2)							
[Co$_3$(tiron-bpy)$_2$(bpy)(H$_2$O)$_8$].(H$_2$O)$_2$, 2													
Co1	36(1)	28(1)	21(1)	-10(1)	6(1)	-7(1)	C2	29(2)	37(2)	23(2)	-8(2)	0(2)	-10(2)
Co2	40(1)	36(1)	20(1)	-10(1)	8(1)	-7(1)	C3	31(2)	32(2)	28(2)	-13(2)	5(2)	-10(2)
S1	45(1)	37(1)	23(1)	-9(1)	5(1)	-7(1)	C4	27(2)	27(2)	35(3)	-8(2)	1(2)	-6(2)
S2	39(1)	30(1)	42(1)	-17(1)	5(1)	-9(1)	C5	40(3)	33(2)	30(3)	-9(2)	6(2)	-12(2)
O1	50(2)	33(2)	23(2)	-12(1)	10(1)	-11(2)	C6	37(2)	28(2)	27(2)	-9(2)	9(2)	-8(2)
O2	41(2)	26(1)	23(2)	-8(1)	5(1)	-7(1)	C7	46(3)	78(4)	41(3)	-11(3)	3(2)	-30(3)
O3	50(2)	42(2)	26(2)	-8(2)	11(2)	-8(2)	C8	55(4)	93(5)	37(3)	-15(3)	0(3)	-38(3)
O4	53(2)	79(3)	46(2)	-30(2)	3(2)	-28(2)	C9	60(4)	55(3)	40(3)	-23(3)	9(3)	-23(3)
O5	77(3)	38(2)	32(2)	-1(2)	4(2)	-3(2)	C10	45(3)	55(3)	34(3)	-19(2)	8(2)	-8(2)
O6	72(3)	36(2)	50(3)	-15(2)	1(2)	-13(2)	C11	39(3)	50(3)	39(3)	-20(2)	6(2)	-9(2)
O7	48(2)	45(2)	90(4)	-32(2)	32(2)	-12(2)	C12	105(8)	149(11)	52(5)	-6(6)	-11(5)	-17(7)
O8	56(2)	46(2)	54(3)	-25(2)	1(2)	-19(2)	C13	84(6)	144(9)	50(5)	-24(5)	6(4)	-7(6)
O1W	39(2)	39(2)	60(3)	-22(2)	6(2)	-12(2)	C14	72(4)	67(4)	33(3)	-16(3)	1(3)	-32(3)
O2W	61(3)	52(2)	46(2)	-18(2)	1(2)	-20(2)	C15	86(6)	131(8)	46(5)	-30(5)	9(4)	2(6)
O3W	46(2)	44(2)	28(2)	-3(2)	7(2)	-4(2)	C16	89(7)	140(10)	61(6)	-34(6)	11(5)	-11(6)
O4W	60(3)	88(3)	50(3)	-33(3)	13(2)	-36(3)	C17	125(7)	41(3)	85(6)	-24(4)	70(6)	-11(4)
O5W	150(8)	145(7)	99(6)	-25(6)	36(6)	-89(6)	C18	121(7)	48(3)	70(5)	-7(3)	65(5)	-13(4)
N1	38(2)	36(2)	36(2)	-15(2)	8(2)	-13(2)	C19	57(3)	53(3)	33(3)	-16(2)	18(3)	-11(3)
N2	104(6)	113(6)	39(3)	-22(4)	1(3)	-45(5)	C20	123(8)	53(4)	54(5)	-8(3)	50(5)	7(4)
N3	48(3)	52(3)	24(2)	-12(2)	13(2)	-10(2)	C21	113(7)	48(3)	51(4)	-8(3)	44(4)	6(4)
C1	31(2)	30(2)	24(2)	-13(2)	7(2)	-9(2)							
[Ba$_2$(tiron-bpy)$_2$(H$_2$O)$_4$][Solvent], 3													
Ba1	42(1)	28(1)	26(1)	3(1)	10(1)	3(1)	C3	23(3)	27(3)	32(3)	1(2)	3(2)	5(2)
S1	27(1)	28(1)	38(1)	1(1)	4(1)	0(1)	C4	30(3)	16(3)	36(3)	1(2)	7(2)	3(2)
S2	34(1)	20(1)	41(1)	3(1)	9(1)	5(1)	C5	35(3)	20(3)	34(3)	1(2)	10(2)	2(2)
O1	32(2)	15(2)	37(2)	0(1)	8(2)	5(2)	C6	22(3)	18(3)	27(2)	-1(2)	6(2)	3(2)
O2	34(2)	20(2)	88(3)	2(2)	7(2)	-2(2)	C7	37(4)	75(5)	47(4)	-15(3)	11(3)	3(3)
O3	38(2)	49(3)	43(2)	15(2)	-5(2)	0(2)	C8	41(4)	98(6)	61(4)	-18(4)	15(3)	-9(4)
O4	38(2)	43(2)	58(2)	-9(2)	19(2)	1(2)	C9	31(3)	53(4)	52(4)	3(3)	1(3)	-1(3)
O5	27(2)	33(2)	61(3)	1(2)	-1(2)	-8(2)	C10	43(4)	115(7)	42(4)	10(4)	-4(3)	-14(4)
O6	82(3)	42(3)	53(3)	8(2)	36(2)	30(2)	C11	37(4)	115(6)	36(3)	9(4)	9(3)	-11(4)
O7	94(3)	41(3)	38(2)	4(2)	-4(2)	28(2)	C12	45(5)	115(8)	104(7)	6(6)	17(5)	-27(5)
O8	40(3)	21(2)	163(5)	17(3)	16(3)	0(2)	C13	48(4)	103(7)	68(5)	4(4)	9(4)	-7(4)
O1W	48(3)	74(3)	51(3)	0(2)	7(2)	29(3)	C14	33(4)	74(5)	67(5)	6(4)	9(3)	-7(4)
O2W	76(5)	126(7)	196(9)	-27(5)	1(5)	-5(4)	C15	43(4)	138(9)	71(5)	-10(5)	-3(4)	-22(5)

N1	30(2)	24(2)	38(2)	8(2)	3(2)	3(2)	C16	58(5)	125(8)	95(6)	-17(6)	-1(5)	-24(5)
N2	48(4)	116(6)	90(5)	-13(5)	-7(4)	-23(4)							
C1	37(3)	23(3)	20(2)	-1(2)	5(2)	4(2)							
C2	35(3)	15(3)	38(3)	1(2)	8(2)	-4(2)							