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Accessory Publication

Coordination Polymers with a Bulky Perylene-based Tetracarboxylate Ligand: Syntheses, Crystal Structures, and Luminescent Properties

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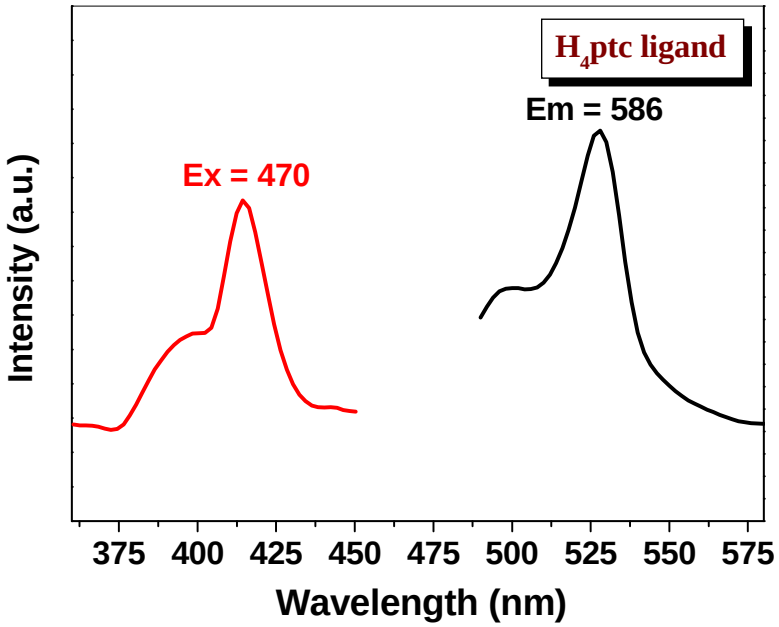
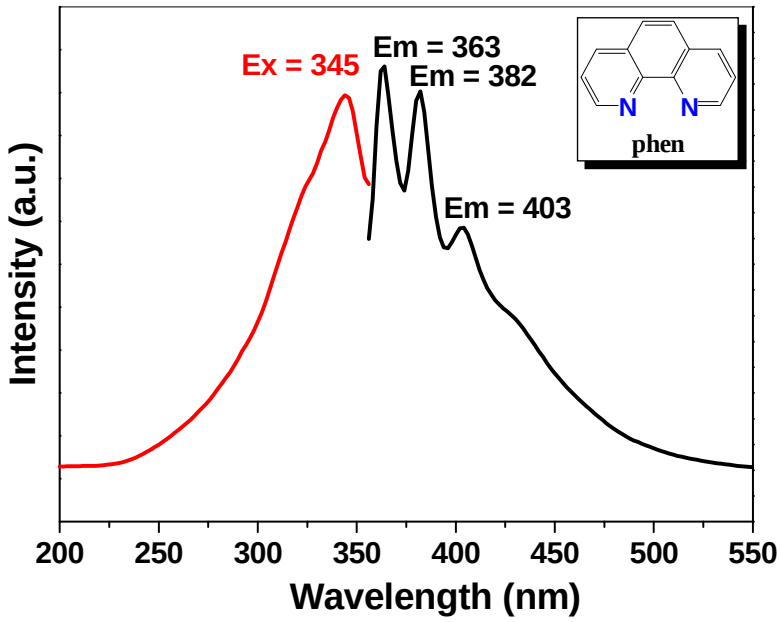


(a)



(b)

Fig. S1. Solid-state excitation/emission spectra of the free ligands at room temperature: (a) for perylene-3,4,9,10-tetracarboxylic acid (H_4**ptc**) and (b) for 1,10-phenanthroline (phen).

P.S. Perylene-3,4,9,10-tetracarboxylic acid (H_4**ptc**) was synthesized according to the method reported in the literature.[23a]

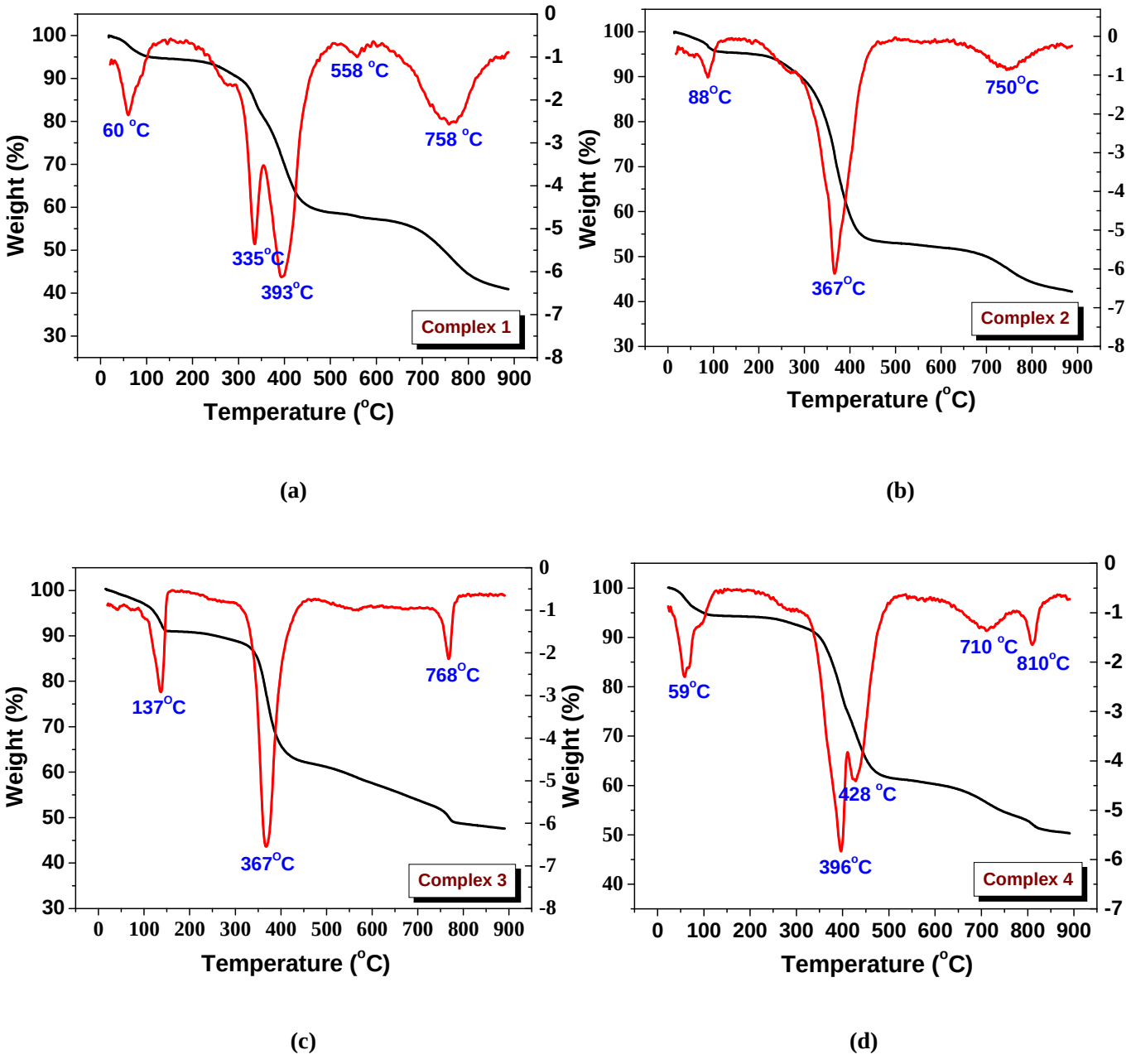


Fig. S2. Thermogravimetric (TG) analysis plots of (a) for **1**, (b) for **2**, (c) for **3**, and (d) for **4**.

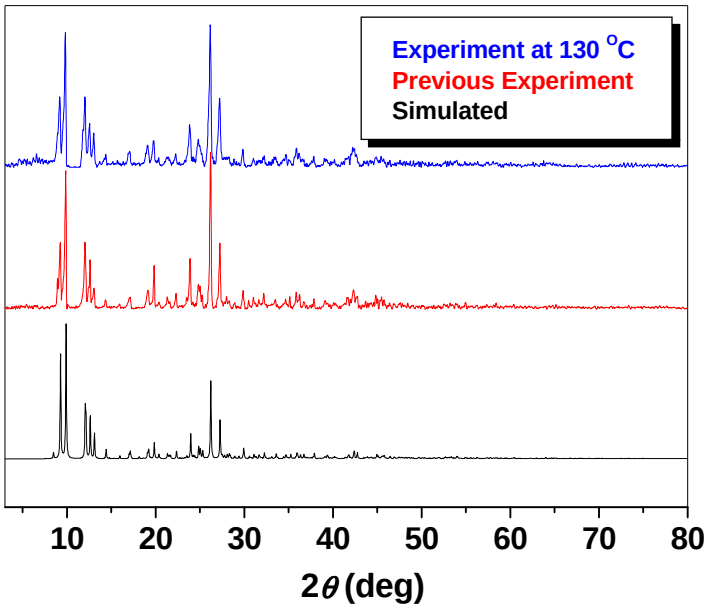


Fig. S3. XRPD pattern comparison for **3** based on the same sample (blue: experimental pattern based on the TG residue sample at 130°C; red: previous experimental pattern at room temperature; black: simulated pattern from the single crystal data).

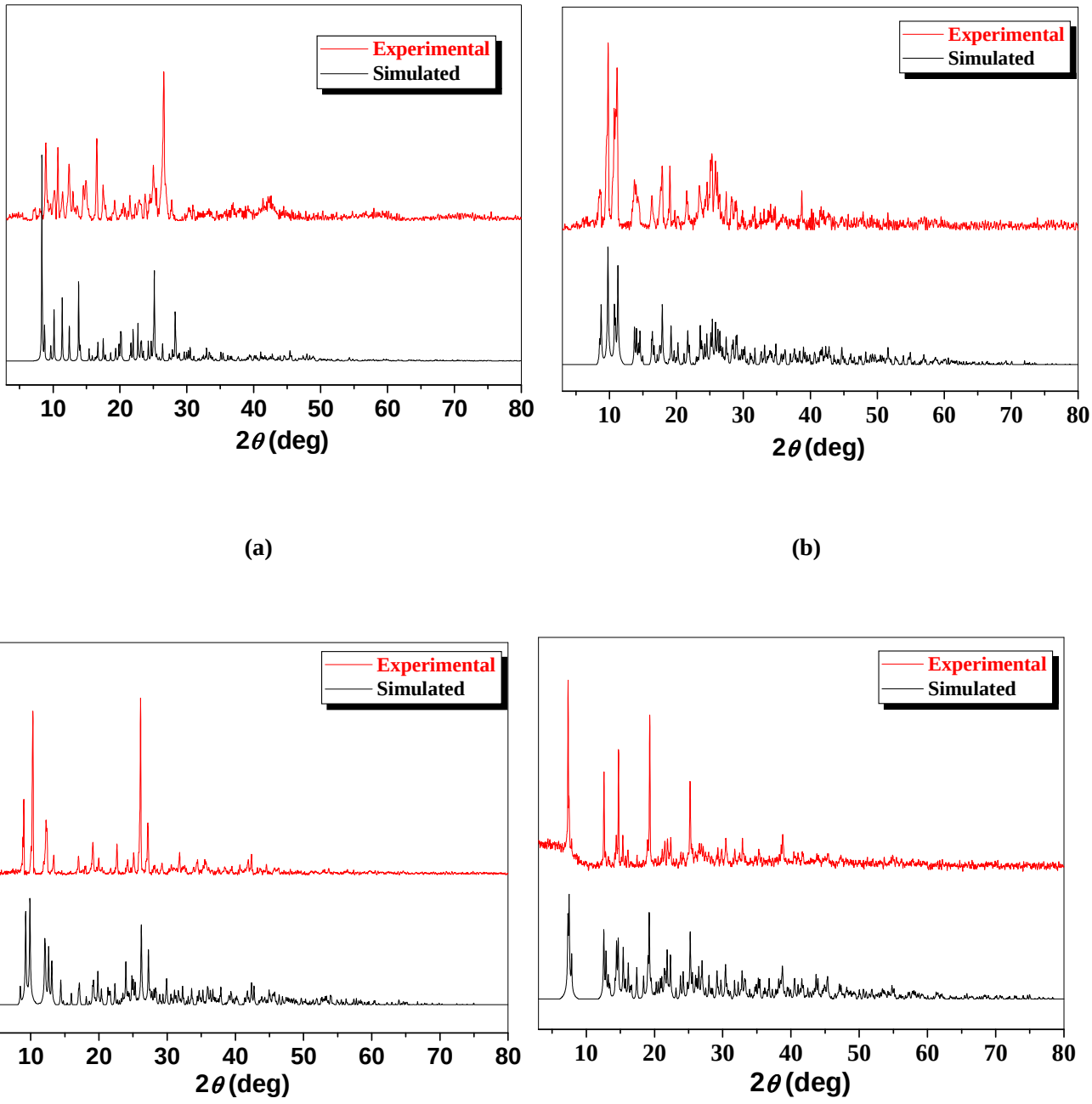
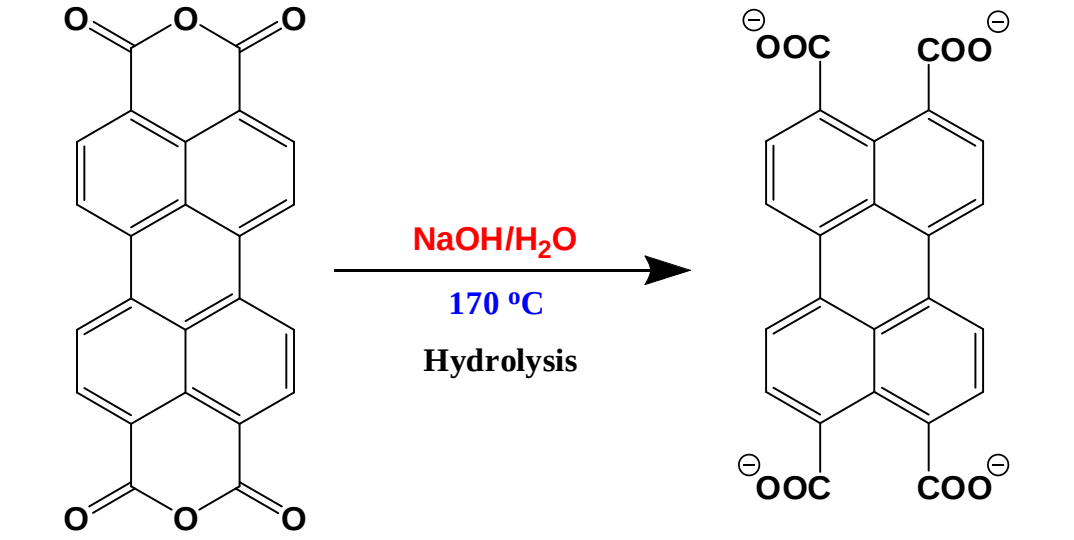


Fig. S4. XRPD patterns of (a) for **1**, (b) for **2**, (c) for **3**, and (d) for **4**.



Perylene-3,4,9,10-tetracarboxylic dianhydride

ptcd

Perylene-3,4,9,10-tetracarboxylate

ptc

Scheme S1. Reaction process for the synthesis of **ptc** ligand.

Table S1. Selected bond lengths [Å] and angles [°] for complex 1[A]

Zn(1)–O(4)$^{\#1}$	1.941(3)	Zn(1)–O(1)	1.953(3)
Zn(1)–N(1)	2.104(4)	Zn(1)–N(2)	2.123(4)
O(4)$^{\#1}$–Zn(1)–O(1)	130.06(13)	O(4)$^{\#1}$–Zn(1)–N(1)	105.64(14)
O(1)–Zn(1)–N(1)	112.13(14)	O(4)$^{\#1}$–Zn(1)–N(2)	100.05(14)
O(1)–Zn(1)–N(2)	118.21(14)	N(1)–Zn(1)–N(2)	78.53(16)

[A]Symmetry transformation codes: #1 $-x + 1, -y, -z + 1$.

Table S2. Selected hydrogen–bonding geometry [Å, °] for complex 1[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
O(1W)–H(1WA)···O(2)[a]	0.85	2.13	2.837(7)	140
O(1W)–H(1WA)···O(4)[b]	0.85	2.52	2.885(5)	107
O(1W)–H(1WB)···O(3)	0.85	1.96	2.676(6)	141
O(2W)–H(2WA)···O(1)	0.85	1.99	2.839(7)	177
O(2W)–H(2WB)···O(4W)[b]	0.85	1.98	2.815(8)	167
O(3W)–H(3WA)···O(1W)	0.85	2.32	3.068(7)	147
O(3W)–H(3WB)···O(5W)[c]	0.85	2.05	2.792(8)	145
O(4W)–H(4WA)···O(3W)	0.85	2.14	2.983(8)	170
O(4W)–H(4WB)···O(2W)[d]	0.85	2.03	2.872(7)	174
O(5W)–H(5WA)···O(2W)[c]	0.85	2.39	2.929(8)	122
O(5W)–H(5WB)···O(2W)[c]	0.85	2.22	2.929(8)	140
C(7)–H(7A)···O(3)[b]	0.93	2.56	3.337(7)	141
C(13)–H(13A)···O(1W)	0.93	2.42	3.022(7)	122
C(15)–H(15A)···O(4)[e]	0.93	2.55	3.365(9)	146

[A]Symmetry codes for **1**: a $-x + 1, -y, -z + 1$; b $x + 1, y, z$; c $-x + 1, -y + 1, -z + 1$; d $-x + 1, -y + 1, -z + 2$; e $x, y, z + 1$

Table S3. Selected bond lengths [Å] and angles [°] for complex 2[A]

Zn(1)–O(5)	1.951(5)	Zn(1)–O(5)$^{\#1}$	1.951(5)
Zn(1)–O(1)$^{\#1}$	1.973(5)	Zn(1)–O(1)	1.973(5)
Zn(2)–O(5)	1.923(5)	Zn(2)–N(1)	2.039(5)
Zn(2)–N(2)	2.050(6)	Zn(2)–O(3)$^{\#1}$	2.107(5)
Zn(2)–O(4)$^{\#1}$	2.211(6)		
O(5)–Zn(1)–O(5)$^{\#1}$	111.3(3)	O(5)–Zn(1)–O(1)$^{\#1}$	106.7(2)
O(5)$^{\#1}$–Zn(1)–O(1)$^{\#1}$	113.3(2)	O(5)–Zn(1)–O(1)	113.3(2)
O(5)$^{\#1}$–Zn(1)–O(1)	106.7(2)	O(1)$^{\#1}$–Zn(1)–O(1)	105.5(3)
O(5)–Zn(2)–N(1)	108.8(2)	O(5)–Zn(2)–N(2)	101.0(2)
N(1)–Zn(2)–N(2)	80.8(3)	O(5)–Zn(2)–O(3)$^{\#1}$	102.0(2)
N(1)–Zn(2)–O(3)$^{\#1}$	108.5(2)	N(2)–Zn(2)–O(3)$^{\#1}$	150.7(3)
O(5)–Zn(2)–O(4)$^{\#1}$	113.3(2)	N(1)–Zn(2)–O(4)$^{\#1}$	137.8(2)
N(2)–Zn(2)–O(4)$^{\#1}$	93.8(2)	O(3)$^{\#1}$–Zn(2)–O(4)$^{\#1}$	60.3(2)

[A]Symmetry transformation codes: #1 $-x + 1, y, -z + 3/2$

Table S4. Selected hydrogen–bonding geometry [Å, °] for complex 2[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
O(1W)–H(1WB)···O(2)	0.85	1.93	2.747(9)	161
O(2W)–H(2WB)···O(4)[a]	0.85	1.96	2.781(2)	161
O(2W)–H(2WA)···O(1W)[b]	0.85	1.96	2.785(2)	164
O(5)–H(5)···O(2)	0.85	2.34	2.929(1)	127

[A]Symmetry codes for **2**: a x –1/2, $–y$ +1/2, z – 1/2; b $–x$ + 1, $– y$, $–z$ + 1

Table S5. Selected bond lengths [Å] and angles [°] for complex 3[A]

Mn(1)–O(3)$^{\#1}$	2.139(3)	Mn(1)–O(1)	2.139(3)
Mn(1)–O(1W)	2.180(3)	Mn(1)–O(2W)	2.252(4)
Mn(1)–N(2)	2.253(4)	Mn(1)–N(1)	2.293(4)
O(3)$^{\#1}$–Mn(1)–O(1)	85.69(12)	O(3)$^{\#1}$–Mn(1)–O(1W)	89.66(13)
O(1)–Mn(1)–O(1W)	93.41(13)	O(3)$^{\#1}$–Mn(1)–O(2W)	170.71(13)
O(1)–Mn(1)–O(2W)	85.62(13)	O(1W)–Mn(1)–O(2W)	94.10(14)
O(3)$^{\#1}$–Mn(1)–N(2)	85.24(13)	O(1)–Mn(1)–N(2)	98.23(14)
O(1W)–Mn(1)–N(2)	166.89(13)	O(2W)–Mn(1)–N(2)	92.78(14)
O(3)$^{\#1}$–Mn(1)–N(1)	100.55(13)	O(1)–Mn(1)–N(1)	168.57(13)
O(1W)–Mn(1)–N(1)	96.18(14)	O(2W)–Mn(1)–N(1)	87.50(13)
N(2)–Mn(1)–N(1)	72.99(14)		

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

Table S6. Selected hydrogen–bonding geometry [Å, °] for complex 3[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
O(1W)–H(1WA)···O(4W)	0.85	2.22	2.987(1)	150
O(1W)–H(1WB)···O(4)	0.85	2.10	2.712(4)	129
O(2W)–H(2WB)···O(2)	0.85	2.32	2.815(8)	118
O(3W)–H(3WA)···O(3)	0.85	2.51	3.031(9)	120
O(3W)–H(3WA)···O(4)	0.85	2.09	2.930(6)	168
O(3W)–H(3WB)···O(1)[a]	0.85	2.37	2.999(6)	131

[A]Symmetry codes for **3**: a $-x + 3/2$, $y - 1/2$, $-z + 3/2$

Table S7. Selected bond lengths [Å] and angles [°] for complex 4[A]

Co(1)–O(2)	2.089(2)	Co(1)–O(3)	2.098(2)
Co(1)–O(6)$^{\#1}$	2.104(2)	Co(1)–N(1)	2.123(3)
Co(1)–N(2)	2.131(3)	Co(1)–O(4)	2.141(3)
Co(1)$^{\#2}$–O(6)	2.104(2)		
O(2)–Co(1)–O(3)	93.03(9)	O(2)–Co(1)–O(6)$^{\#1}$	90.65(8)
O(3)–Co(1)–O(6)$^{\#1}$	90.83(9)	O(2)–Co(1)–N(1)	93.56(10)
O(3)–Co(1)–N(1)	87.23(10)	O(6)$^{\#1}$–Co(1)–N(1)	175.45(10)
O(2)–Co(1)–N(2)	172.05(9)	O(3)–Co(1)–N(2)	86.78(10)
O(6)$^{\#1}$–Co(1)–N(2)	97.30(9)	N(1)–Co(1)–N(2)	78.49(10)
O(2)–Co(1)–O(4)	91.57(11)	O(3)–Co(1)–O(4)	174.21(9)
O(6)$^{\#1}$–Co(1)–O(4)	92.64(9)	N(1)–Co(1)–O(4)	88.97(10)
N(2)–Co(1)–O(4)	88.18(11)		

[A]Symmetry transformation codes: #1 $-x + 1, y, z$; #2 $-x + 1, y, z$

Table S8. Selected hydrogen–bonding geometry [Å, °] for complex 4[A]

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	D–H···A
O(1W)–H(1WB)···O(3W)	0.85	2.35	2.945(1)	127
O(3)–H(3C)···O(1)	0.85	2.12	2.622(4)	117
O(2W)–H(2WB)···O(5)[a]	0.85	1.97	2.764(5)	155
O(4)–H(4C)···O(1W)	0.85	2.11	2.665(8)	122
O(3W)–H(3WB)···O(2)	0.85	1.99	2.822(6)	167
C(21)–H(21A)···Cg(1)[b,c]	0.93	2.68	3.430(6)	138
C(20)–H(20A)···Cg(2)[b,c]	0.93	2.91	3.596(6)	131
C(8)–H(8A)···Cg(3)[d]	0.93	3.04	3.601(7)	121
C(9)–H(9A)···Cg(4)[d]	0.93	3.12	3.833(8)	135

Symmetry codes for **4**: a –*x*, –*y* + 1, –*z* + 1; b –*x*, –*y* + 2, –*z*; c *x* – 1, *y* + 1, *z*; d –*x* + 1, –*y* + 2, –*z*

Cg(1), Cg(2), Cg(3), and Cg(4) are the centroids of the C(6)–C(11) phenyl ring of **ptc** ligand, the C(5)–C(7)/C(5)[e]–C(7)[e] phenyl ring of **ptc** ligand [symmetry code for e = –*x* + 1, –*y* + 1, –*z*], the C(16)–C(19)/C(23)–C(24) phenyl ring of phen ligand, and the C(19)–C(23)/N(2) pyridyl ring of phen ligand, respectively.