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Supporting information for

Eight Zn(II) and Cd(II) complexes based on the aromatic C-centered triangular multicarboxylate and N-donor mixed ligands

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Table S1. Crystallographic data and structural refinement details for **1-8**.

Complexes	**1**	**2**	**3**	**4**
Formula	$C_{143}H_{123}O_{33}N_{13}Zn_8$	$C_{37}H_{29}N_3O_9Zn_2$	$C_{37}H_{27}N_3O_9Zn_2$	$C_{56}H_{40}N_2O_{16}Zn_3$
Formula weight	3074.50	790.37	788.36	1193.01
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P\bar{1}$
a (Å)	11.0265(16)	11.4877(12)	14.3130(18)	9.405(3)
b (Å)	13.461(2)	14.3195(14)	23.533(2)	13.541(3)
c (Å)	25.8071(19)	24.3237(15)	10.1409(13)	14.045(2)
α (°)	90.00	90.00	90.00	116.75(2)
β (°)	98.093(2)	99.615(2)	100.919(2)	90.123(10)
γ (°)	90.00	90.00	90.00	106.568(18)
V (Å^3)	3792.3(8)	3945.0(6)	3354.0(7)	1513.0(6)
Z	1	4	4	1
D_{calc} (g·cm^{-3})	1.346	1.331	1.561	1.309
μ (mm^{-1})	1.317	1.269	1.492	1.243
F (000)	1576	1616	1608	608
R_1, ωR_2 [$I > 2\sigma(I)$]	0.0553, 0.1463	0.0402, 0.1054	0.0361, 0.1058	0.0404, 0.1118
R_1, ωR_2 [all data]	0.0691, 0.1485	0.0844, 0.1248	0.0511, 0.1087	0.0712, 0.1186
GOF	1.019	1.052	1.012	1.004
Complexes	**5**	**6**	**7**	**8**
Formula	$C_{50}H_{44}Cd_3N_2O_{16}$	$C_{54}H_{34}Cd_3N_2O_{12}$	$C_{56}H_{36}Cd_3N_2O_{12}$	$C_{70}H_{56}N_6O_{16}Cd_3$
Formula weight	1266.07	1240.03	1266.07	1574.40
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	P_2/n	P_2/n	$P\bar{1}$	$P\bar{1}$
a (Å)	14.054(3)	13.3405(13)	9.3767(15)	13.179(2)
b (Å)	25.465(2)	9.3835(12)		13.630(2)
c (Å)	17.291(3)	23.3073(13)	14.0167(14)	13.915(2)
α (°)	90.00	90.00	63.182(3)	64.597(3)
β (°)	90.00	90.00	89.797(3)	79.867(4)
γ (°)	102.384(3)	94.221(3)	73.3358(14)	64.592(3)
V (Å^3)	6044.0(17)	2909.7(5)	1503.2(3)	2039.4(6)
Z	4	2	1	1
D_{calc} (g·cm^{-3})	1.391	1.415	1.399	1.282
μ (mm^{-1})	1.105	1.142	1.107	0.83
F (000)	2520	1224	626	790
R_1, ωR_2 [$I > 2\sigma(I)$]	0.0437, 0.1035	0.0462, 0.1262	0.0422, 0.0993	0.0532, 0.1116
R_1, ωR_2 [all data]	0.0568, 0.1058	0.0492, 0.1274	0.0524, 0.1030	0.0669, 0.1154
GOF	1.039	0.887	1.056	1.060

Table S2. Selected bond lengths (Å) and angles (°) for **1**-**8**.

1		**2**		**3**		**4**	
Zn1-O2	2.199(3)	Zn1-N1	2.198(3)	Zn1-N1	2.170(3)	Zn1-N1	2.298(3)
Zn1-O4	1.935(3)	Zn1-N2	2.129(3)	Zn1-N2	2.091(3)	Zn1-O1	2.432(3)
Zn1-O6^{vi}	1.935(2)	Zn1-O1	2.082(2)	Zn1-N3	2.155(3)	Zn1-O2	2.438(3)
Zn1-O7^{v}	2.111(3)	Zn1-O1^{i}	2.117(3)	Zn1-O1	1.916(2)	Zn1-O2^{ii}	2.468(3)
Zn2-O1	2.119(3)	Zn1-O2	2.119(3)	Zn1-O1^{w}	2.079(2)	Zn1-O3^{v}	2.204(3)
Zn2-O3	2.134(3)	Zn1- O4^{iv}	2.160(3)	Zn1-O7^{iii}	2.153(2)	Zn1-O6^{vi}	2.299(3)
Zn2-O7	2.077(3)	Zn2-O1	1.992(3)	Zn2-O1	1.930(2)	Zn2-O1	2.300(3)
Zn2-O7^{v}	2.111(3)	Zn2-O3	2.040(2)	Zn2-O2	2.043(2)	Zn2-O1^{viii}	2.300(3)
Zn2-N1	2.122(3)	Zn2-O5^{iv}	1.958(3)	N1-Zn1-N2	74.65(11)	Zn2-O4^{v}	2.245(3)
Zn2-N2	2.151(3)	Zn2-O7^{v}	1.932(3)	N1-Zn1-N3	149.90(11)	Zn2-O4^{vii}	2.245(3)
O2-Zn1-O4	106.97(12)	N1-Zn1-N2	78.98(12)	N1-Zn1-O1	105.95(10)	Zn2-O5^{ix}	2.326(3)
O2-Zn1-O6^{vi}	107.58(11)	N1-Zn1-O1	99.75(12)	N1-Zn1-O1^{w}	88.79(10)	Zn2-O5^{vi}	2.326(3)
O2-Zn1-O7	111.13(11)	N1-Zn1-O1^{i}	100.51(12)	N1-Zn1-O7^{iii}	88.23(10)	N1-Zn1-O1	103.63(12)
O4-Zn1-O6^{vi}	117.93(11)	N1-Zn1-O2	74.26(11)	N2-Zn1-N3	75.25(11)	N1-Zn1-O2	89.07(11)
O4-Zn1-O7	106.27(11)	N1-Zn1-O4^{iv}	166.74(11)	N2-Zn1-O1	176.72(10)	N1-Zn1-O3^{v}	139.79(13)
O6^{vi}-Zn1-O7	106.97(11)	N2-Zn1-O1	178.14(12)	N2-Zn1-O1^{w}	91.09(10)	N1-Zn1-O6^{vi}	83.09(11)
N1-Zn2-N2	77.87(13)	N2-Zn1-O1^{i}	96.65(11)	N2-Zn1-O7^{iii}	86.79(10)	O1-Zn1-O2	56.22(10)
N1-Zn2-O1	87.69(11)	N2-Zn1-O2	94.83(11)	N3-Zn1-O1	104.09(10)	O1-Zn1-O2^{ii}	124.96(9)
N1-Zn2-O3	91.93(11)	N2-Zn1-O4^{iv}	88.20(11)	N3-Zn1-O1^{w}	92.00(10)	O1-Zn1-O3^{v}	116.09(11)
N1-Zn2-O7	174.60(12)	O1-Zn1-O1^{i}	82.21(10)	N3-Zn1-O7^{iii}	89.89(10)	O1-Zn1-O6^{vi}	86.74(11)
N1-Zn2-O7^{v}	96.01(11)	O1-Zn1-O2	86.10(10)	O1-Zn1-O1^{w}	92.14(9)	O2-Zn1-O2^{ii}	70.64(11)
N2-Zn2-O1	81.16(12)	O1-Zn1-O4^{iv}	93.15(10)	O1-Zn1-O7^{iii}	90.00(8)	O2-Zn1-O3^{v}	117.51(11)
N2-Zn2-O3	166.78(12)	O1^{i}-Zn1-O2	166.22(10)	O1W-Zn1-O7^{iii}	176.72(9)	O2-Zn1-O6^{vi}	139.08(11)
N2-Zn2-O7	98.22(12)	O1^{i}-Zn1-O4^{iv}	84.18(10)	O1-Zn2-O2	105.71(9)	O3^{v}-Zn1-O6^{vi}	92.78(11)
N2-Zn2-O7^{v}	104.21(12)	O2-Zn1-O4^{iv}	103.80(10)	O1-Zn2-O4^{iv}	118.88(9)	O1-Zn2-O4^{v}	89.10(11)
O1-Zn2-O3	90.14(11)	O1-Zn2-O3	113.38(10)	O1-Zn2-O6^{iii}	110.32(9)	O1-Zn2-O4^{vii}	90.90(11)
O1-Zn2-O7	95.43(10)	O1-Zn2-O5^{iv}	110.66(11)	O2-Zn2-O4^{iv}	115.96(9)	O1-Zn2-O5i^{x}	87.31(10)
O1-Zn2-O7^{v}	174.00(10)	O1-Zn2-O7^{v}	110.65(12)	O2-Zn2-O6^{iii}	97.11(9)	O1^{viii}-Zn2-O4^{v}	90.89(11)
O3-Zn2-O7	92.47(10)	O3-Zn2-O5^{iv}	89.97(11)	O4^{iv}-Zn2-O6^{iii}	106.69(10)	O1^{v}-Zn2-O5^{vi}	87.31(10)
O3-Zn2-O7^{v}	85.02(11)	O3-Zn2-O7^{v}	122.95(12)			O4^{v}-Zn2-O5^{vi}	94.07(12)

5		**6**		**7**		**8**	
Cd1-O1	2.246(3)	Cd1-O4^{ii}	2.185(3)	Cd1-O1	2.222(3)	Cd1-O1	2.224(3)
Cd1-O5^{iv}	2.290(3)	Cd1-O2^{iii}	2.275(4)	Cd1-N1	2.243(3)	Cd1-O3^{ii}	2.165(3)
Cd1-O11^{i}	2.207(4)	Cd1-N1	2.327(4)	Cd1-O3^{ii}	2.279(3)	Cd1-O6^{vi}	2.271(3)
Cd2-O1W	2.319(4)	Cd1-O7^{iv}	2.384(4)	Cd1-O4^{iii}	2.400(3)	Cd2-O1	2.360(3)
Cd2-O3	2.373(3)	Cd1-O2	2.505(3)	Cd1-O4^{iv}	2.414(2)	Cd2-O2	2.416(3)
Cd2-O4	2.406(3)	Cd1-O6^{iv}	2.512(3)	Cd1-O5^{v}	2.533(3)	Cd2-N1	2.302(4)
Cd2-O7	2.258(3)	Cd1-O3	2.525(3)	Cd2-O6^{iii}	2.204(2)	Cd2-N2	2.246(4)
Cd2-O9^{vi}	2.158(3)	Cd2-O7^{iv}	2.203(4)	Cd2-O2	2.248(3)	Cd2-O4^{iii}	2.174(3)
Cd2-O13	2.257(4)	Cd2-O5^{ii}	2.204(4)	Cd2-O3^{vii}	2.379(2)	Cd1-O5^{vi}	2.279(3)
O1-Cd1-O5^{iv}	89.64(11)	Cd2-O3	2.336(3)	Cd2-O3^{iii}	2.379(2)	Cd2-O6^{vi}	2.526(3)
O1-Cd1-O11^{i}	173.43(13)	N1-Cd1-O2	103.90(16)	N1-Cd1-O1	138.34(13)	O1-Cd1-O1^{iv}	180.00(15)
O1^{iii}-Cd1-O11^{ii}	82.14(11)	N1-Cd1-O2^{iii}	92.71(14)	N1-Cd1-O6^{iiii}	91.93(12)	O1-Cd1-O3^{ii}	85.55(10)
O1^{iii}-Cd1-O5^{v}	89.64(11)	N1-Cd1-O4^{ii}	171.56(15)	O1-Cd1-O6	84.64(11)	O1-Cd1-O6^{v}	100.84(11)
O5^{iv}-Cd1-O5^{v}	173.53(17)	N1-Cd1-O7^{iv}	84.76(15)	O1-Cd1-O3^{iii}	119.40(10)	O1-Cd2-O2	54.58(10)
O1W-Cd2-O7	80.63(13)	O2-Cd1-O4^{ii}	84.39(12)	O3^{iii}-Cd1-O6^{ii}	86.26(10)	N1-Cd2-O1	157.81(12)
O1W-Cd2-O9^{vi}	143.14(14)	O2-Cd1-O2^{iii}	79.92(12)	N1-Cd1-O3^{iii}	101.83(12)	N1-Cd2-O2	147.32(12)
O1W-Cd2-O13	98.69(14)	O3-Cd1-O4^{ii}	98.80(11)	N1-Cd1-O4^{iii}	91.61(11)	N2-Cd2-O1	131.05(12)
O3-Cd2-O7	90.81(11)	O2^{iii}-Cd1-O3	129.67(12)	O3^{iii}-Cd1-O4^{iii}	52.83(9)	N2-Cd2-O2	86.31(13)
O3-Cd2-O13	156.15(13)	O2-Cd1-O3	51.47(11)	O2-Cd2-O5^{v}	86.79(11)	N1-Cd2-N2	67.80(14)
O4-Cd2-O7	132.22(10)	O3-Cd2-O5^{v}	79.72(12)	O2-Cd2-O5^{ii}	93.21(11)	O1-Cd2-O4^{iii}	95.10(11)
O3-Cd2-O4	54.73(11)	O3^{i}-Cd2-O5^{i}	100.28(12)	O2-Cd2-O2^{vi}	180.0	O1-Cd2-O5^{vi}	80.65(10)
O1W-Cd2-O4	73.97(12)	O3^{i}-Cd2-O7^{v}	87.43(13)	O3^{vii}-Cd2-O5^{v}	93.27(9)	O2-Cd2-O4^{iii}	93.94 (12)
O1W-Cd2-O3	98.09(12)	O5^{ii}-Cd2-O7^{iv}	92.57(13)	O3^{vii}-Cd2-O5^{ii}	86.73(9)	O2-Cd2-O5^{vi}	115.45(10)
O4-Cd2-O9^{vi}	90.32(12)	O5^{ii}-Cd2-O7^{v}	91.52(14)	O5^{ii}-Cd2-O5^{v}	180.0(2)	O2-Cd2-O6^{vi}	126.10(10)

Symmetry codes for **1**: (v) $-x+1, -y, -z+1$; (vi) $x, y-1, z$. **2**: (i) $-x, -y, -z$; (iv) $x, -y+1/2, z-1/2$; (v) $x, y-1, z$. **3**: (iii) $x-1, y, z$; (iv) $-x+1, y-1/2, -z+3/2$. **4**: (ii) $-x+1, -y, -z$; (v) $x, y, z-1$; (vi) $x, y-1, z-1$; (vii) $-x+2, -y, -z+1$; (viii) $-x+2, -y, -z$; (ix) $-x+2, -y+1, -z+1$. **5**: (i) $-x, -y+2, -z+1$; (ii) $x+1/2, -y+2, z-1/2$; (iii) $-x+1/2, y, -z+1/2$; (iv) $x-1/2, -y+2, z+1/2$; (v) $-x+1, -y+2, -z$; (vi) $x+1/2, -y+1, z-1/2$. **6**: (i) $-x+3/2, y, -z+1/2$; (ii) $x+1, y, z$; (iii) $-x+2, -y+1, -z+1$; (iv) $x+1/2, -y, z-1/2$; (v) $-x+3/2, y, -z+3/2$. **7**: (ii) $x, y-1, z$; (iii) $x, y, z-1$; (iv) $-x+1, -y, -z+1$; (v) $-x, -y+1, -z$; (vi) $-x, -y, -z$; (vii) $-x, -y, -z+1$. **8**: (i) $x, y-1, z$; (ii) $-x, -y+2, -z+1$; (iii) $x+1, y, z$; (iv) $-x+1, -y+2, -z+1$; (v) $-x+1, -y+1, -z+1$; (vi) $x, y+1, z$.

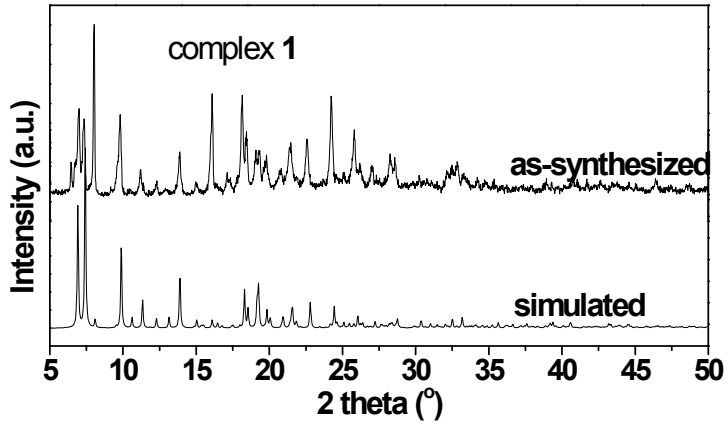

Fig. S1 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **1**.

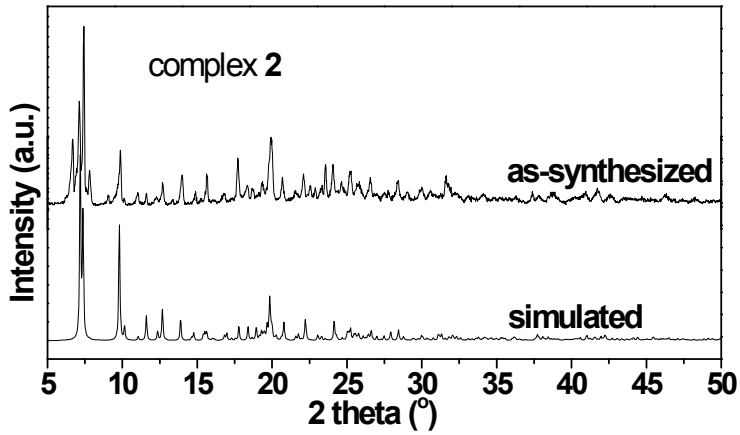

Fig. S2 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **2**.

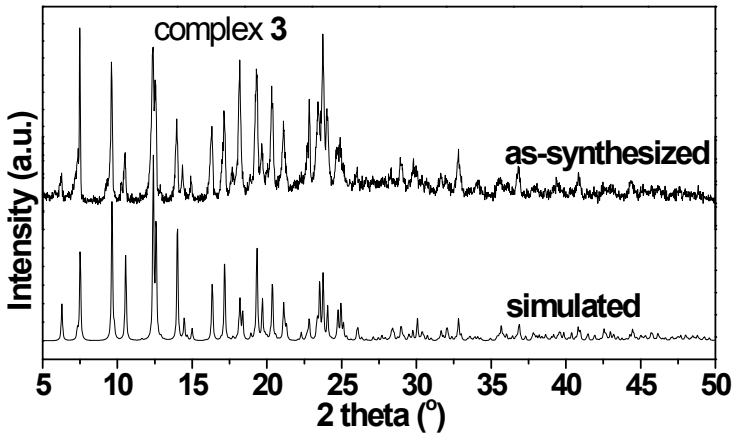

Fig. S3 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **3**.

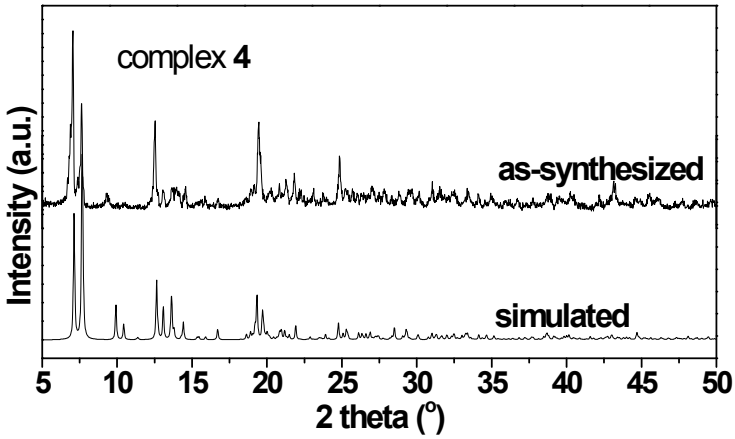

Fig. S4 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **4**.

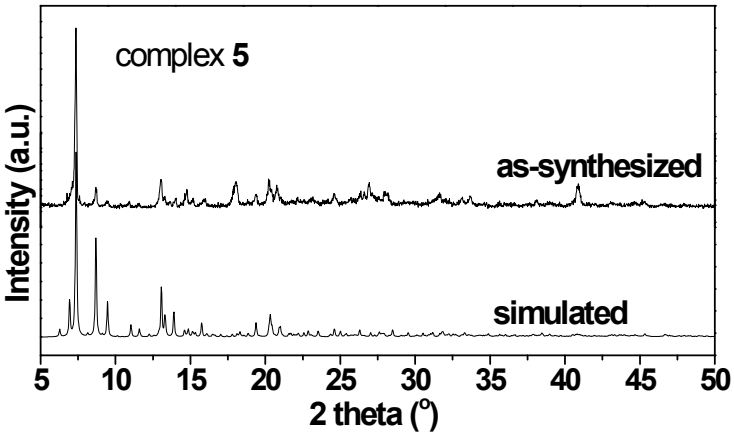

Fig. S5 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **5**.

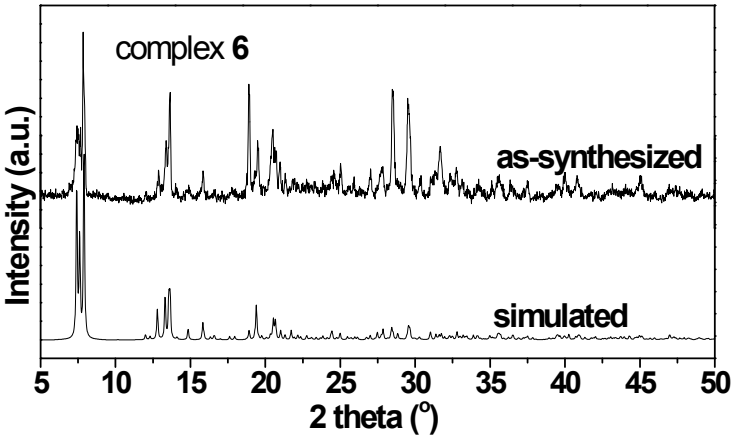

Fig. S6 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **6**.

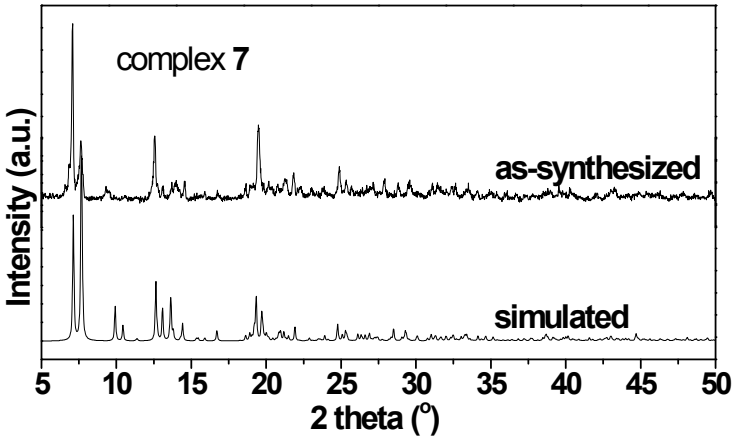

Fig. S7 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **7**.

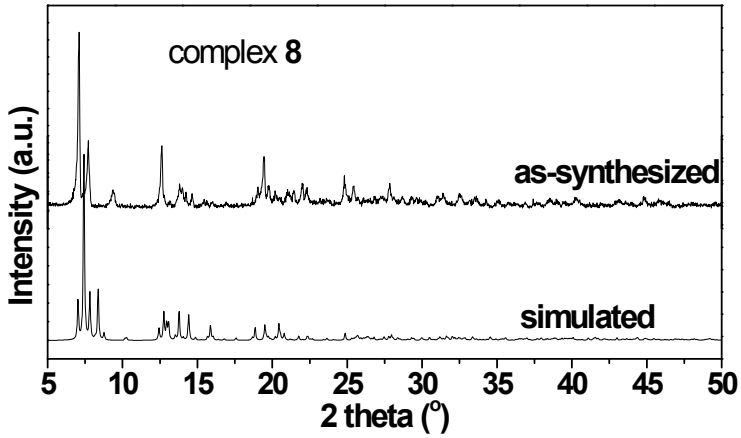

Fig. S8 Powder XRD patterns of as-synthesized and simulated from single-crystal diffraction data of **8**.

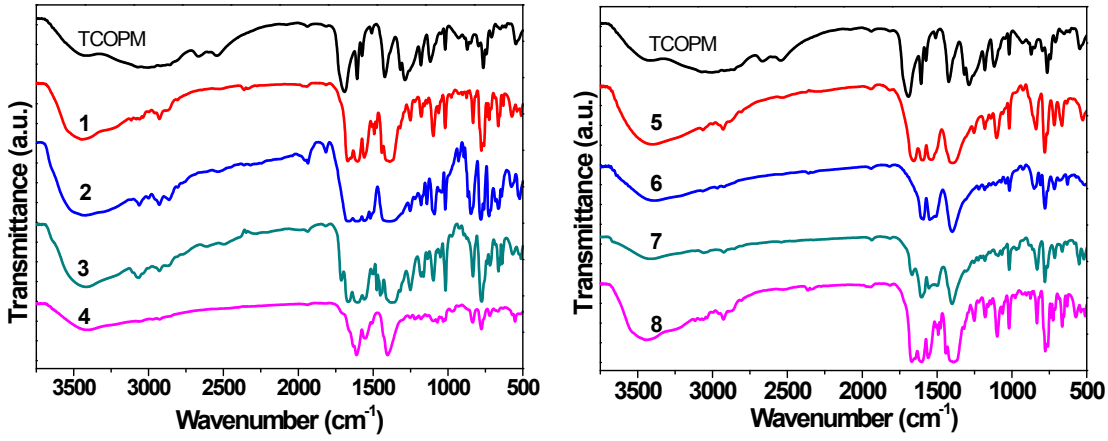

Fig. S9 FT-IR spectra of **1**-**8** and the free TCOPM ligand.

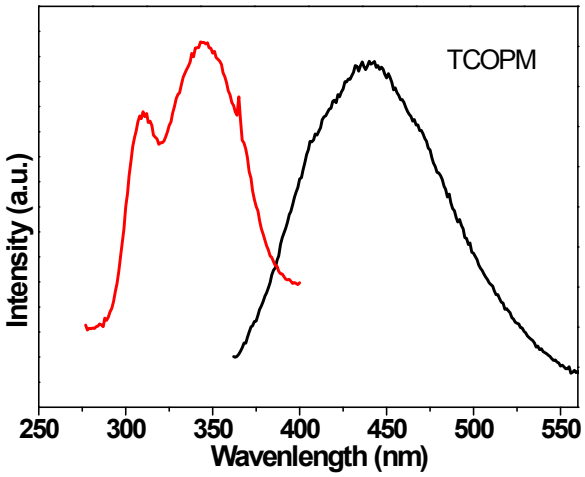

Fig. S10 Solid-state, room-temperature photoemission (excitation wavelength λ_{ex} = 344 nm, and emission wavelength λ_{em} = 446 nm) spectra for the free TCOPM.

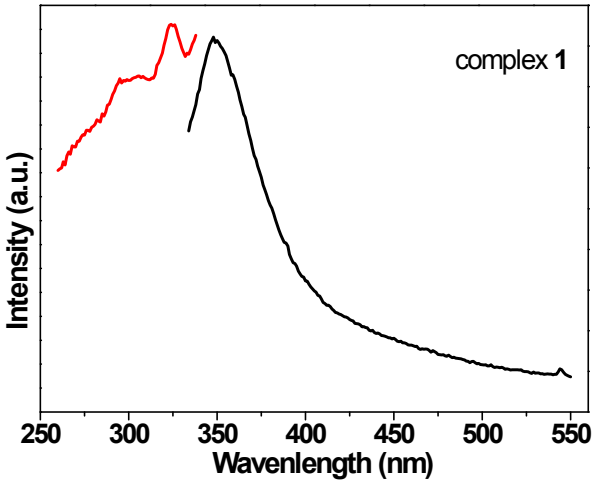

Fig. S11 Solid-state, room-temperature photoemission (excitation wavelength λ_{ex} = 324 nm, and emission wavelength λ_{em} = 348 nm) spectra for **1**.

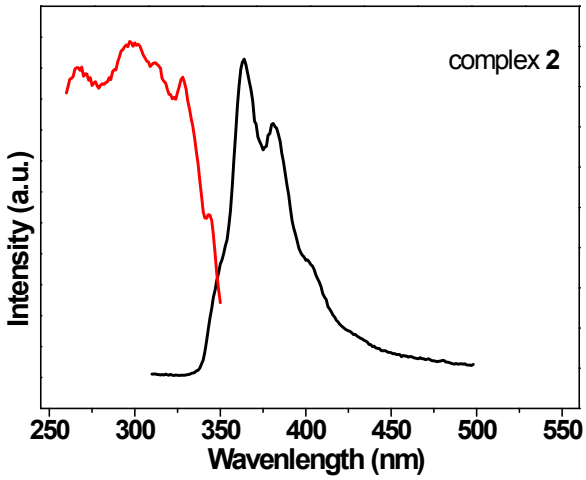

Figure S12. Solid-state, room-temperature photoemission (excitation wavelength λ_{ex} = 270 nm, and emission wavelength λ_{em} = 364 nm) spectra for **2**.

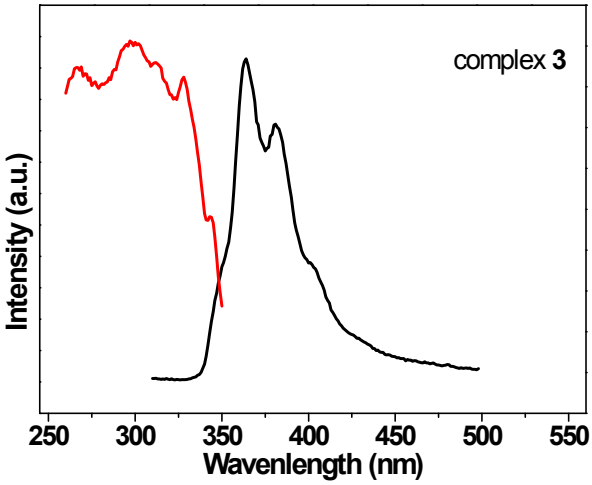

Figure S13. Solid-state, room-temperature photoemission (excitation wavelength λ_{ex} = 298 nm, and emission wavelength λ_{em} = 357 nm) spectra for **3**.

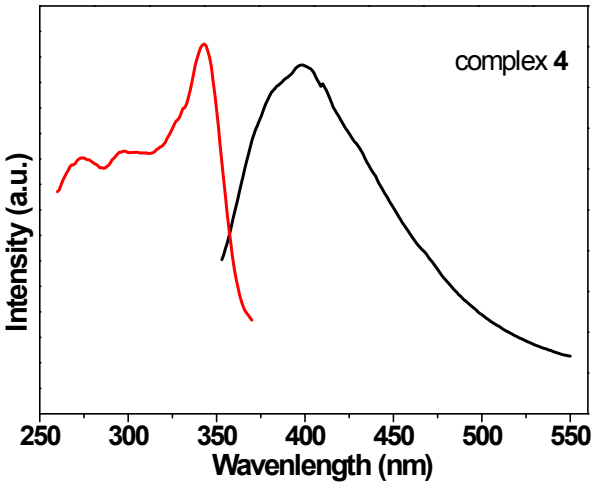

Figure S14. Solid-state, room-temperature photoemission (excitation wavelength λ_{ex} = 343 nm and emission wavelength λ_{em} = 398 nm) spectra for **4**.

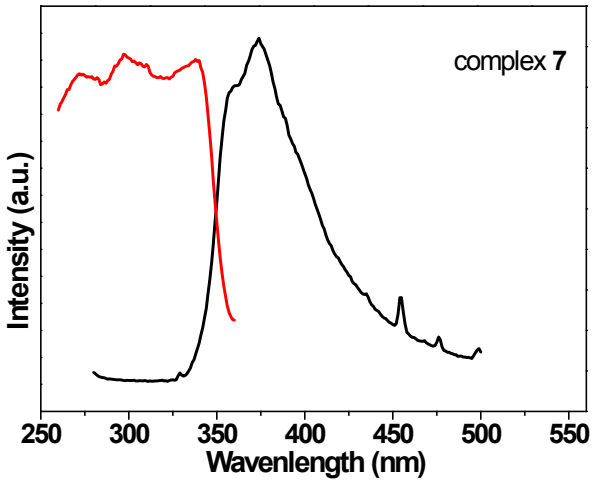

Figure S15. Solid-state, room-temperature photoemission (excitation wavelength λ_{ex} = 270 nm and emission wavelength λ_{em} = 374 nm) spectra for **7**.

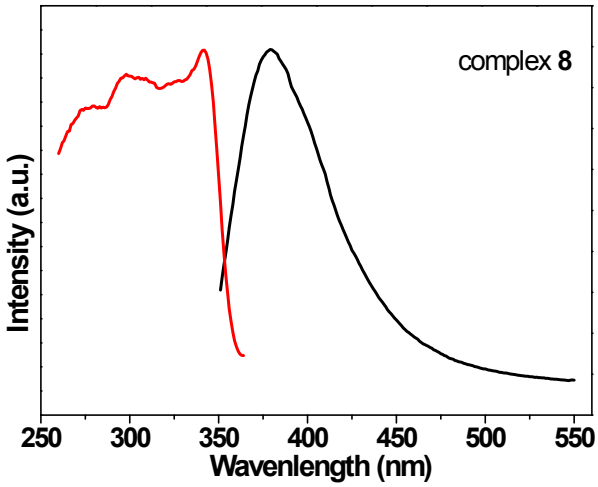

Figure S16. Solid-state, room-temperature photoemission (excitation wavelength, λ_{ex} = 341 nm and emission wavelength λ_{em} = 378 nm) spectra for **8**.

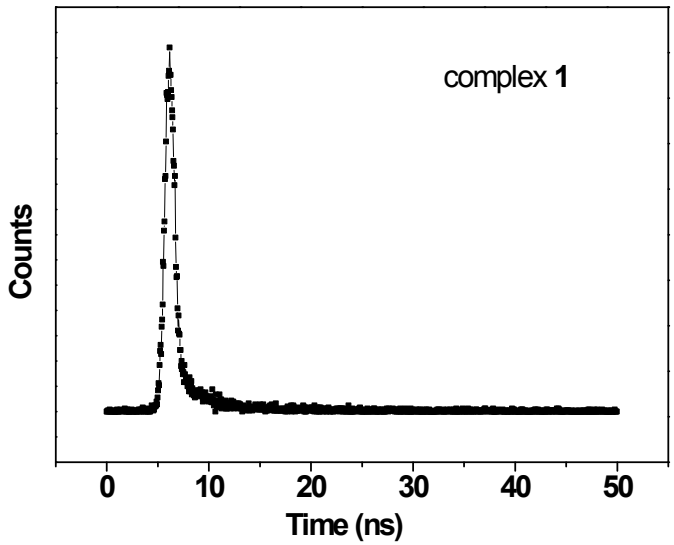

Figure S17. The emission decay lifetime of **1**.

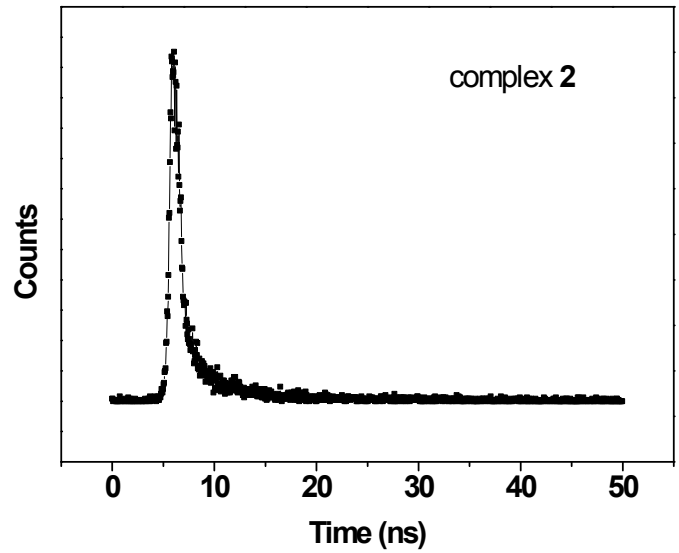

Figure S18. The emission decay lifetime of **2**.

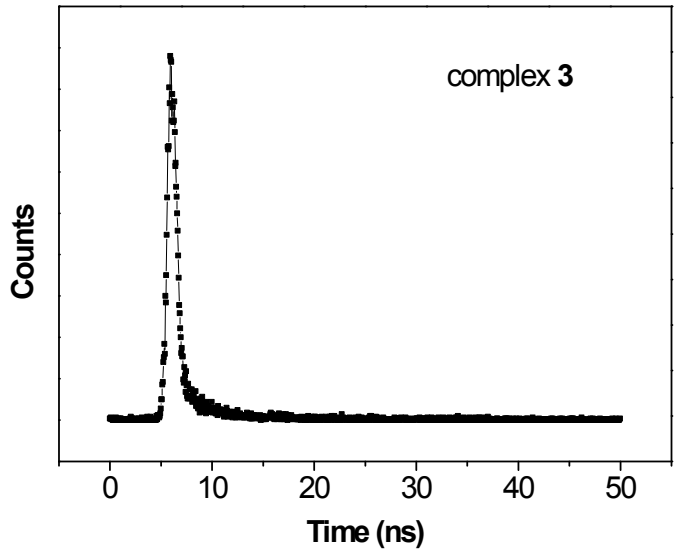

Figure S19. The emission decay lifetime of **3**.

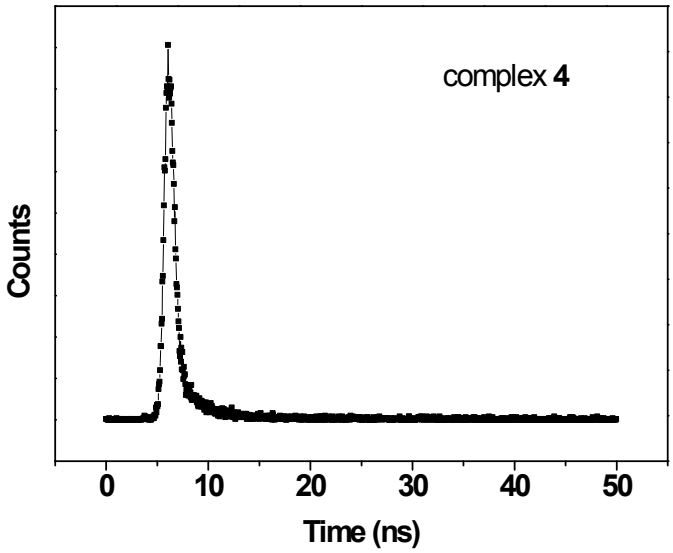

Figure S20. The emission decay lifetime of **4**.

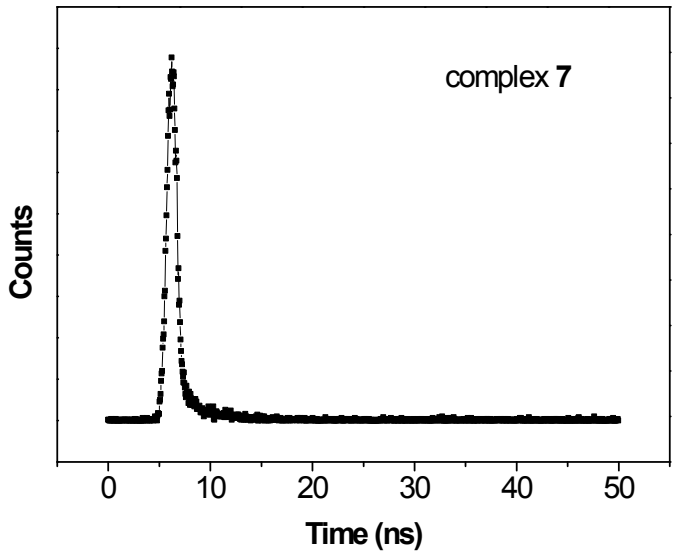

Figure S21. The emission decay lifetime of **7**.

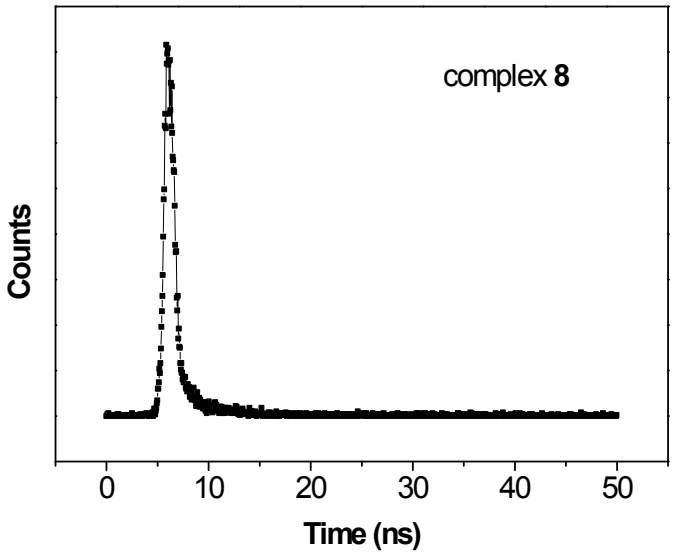

Figure S22. The emission decay lifetime of **8**.