Supporting Information

Syntheses, Structures and Magnetic Properties of Nine Coordination Polymers Based on Terphenyl-Tetracarboxylic Acid Ligand

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Table S1. Selected bond lengths (Å) and bond angles (º) for **1**.

Mn1-O1	2.172(1)	Mn1-O5i	2.178(1)
Mn1-O6	2.107(1)	Mn1-O10	2.196(1)
Mn1-N1	2.308(1)	Mn1-N2	2.280(1)
C13-O1	1.249(2)	C13-O2	1.274(2)
C20-O3	1.204 (2)	C20-O4	1.343(2)
C25-O5	1.254 (2)	C25-O6	1.258(2)
C34-O7	1.321(2)	C34-O8	1.229(2)
C35-O9	1.280(2)	C35-O10	1.243(2)
C45-O11	1.238(2)	C45-O12	1.306(2)
O6-Mn1-O1	87.44(4)	O5i-Mn1-N2	85.98(4)
O6-Mn1-O5i	105.49(4)	O10-Mn1-N2	85.91(4)
O1-Mn1-O5i	111.64(4)	O6-Mn1-N1	92.03(4)
O6-Mn1-O10	173.23(4)	O1-Mn1-N1	90.39(4)
O1-Mn1-O10	94.66(4)	O5i-Mn1-N1	152.03(4)
O5i-Mn1-O10	79.74(4)	O10-Mn1-N1	81.53(4)
O6-Mn1-N2	90.13(4)	N2-Mn1-N1	72.09(4)

O1-Mn1-N2	162.22(4)			
D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
O(2)–H(9A)···O(9)	1.158	1.296	2.436(1)	165.91(6)

Symmetry code: i = 1 – *x*, –*y*, –*z*.

Table S2. Selected bond lengths (Å) and bond angles (º) for **2**.

Ni1-O1	2.031(4)	Ni1-O2i	2.004(4)
Ni1-O3ii	2.050(4)	Ni1-O5	2.088(3)
Ni1-N1	2.115(5)	Ni1-N2	2.054(6)
O2i-Ni1-O1	97.8(2)	N2-Ni1-O5	175.1(2)
O2i-Ni1-O3ii	171.7(2)	O2i-Ni1-N1	87.9(2)
O1-Ni1-O3ii	89.2(2)	O1-Ni1-N1	169.6(2)
O2i-Ni1-N2	89.9(2)	O3ii-Ni1-N1	84.5(2)
O1-Ni1-N2	90.1(2)	N2-Ni1-N1	81.1(2)
O3ii-Ni1-N2	85.7(2)	O5-Ni1-N1	94.9(2)
O2i-Ni-1O5	92.7(1)	Ni1-O5-Ni1i	113.6(2)
O1-Ni1-O5	93.6(1)	O3ii-Ni1-O5	91.2(2)

Symmetry codes: i = –*x*, *y*, 1.5 – *z*; ii = 0.5 + *x*, –0.5 + *y*, *z*.

Table S3. Selected bond lengths (Å) and bond angles (º) for **3**.

Mn1-O1	2.157(4)	Mn2-O2	2.155(4)
Mn1-O3	2.154(3)	Mn2-O4	2.198(3)
Mn1-O5	2.161(4)	Mn2-O6	2.133(4)
Mn1-O8	2.134(4)	Mn2-O7	2.184(4)
Mn1-N1	2.346(6)	Mn2-N3	2.358(5)
Mn1-N2	2.316(6)	Mn2-N4	2.305(5)
O8-Mn1-O3	162.78(2)	O6-Mn2-O2	157.7(2)
O8-Mn1-O1	85.9(2)	O6-Mn2-O7	81.9(2)
O3-Mn1-O1	86.0(2)	O2-Mn2-O7	93.8(2)
O8-Mn1-O5	83.2(2)	O6-Mn2-O4	83.4(2)
O3-Mn1-O5	91.8(2)	O2-Mn2-O4	83.0(2)
O1-Mn1-O5	135.1(2)	O7-Mn2-O4	130.5(2)
O8-Mn1-N2	111.6(2)	O6-Mn2-N4	86.5(2)
O3-Mn1-N2	83.9(2)	O2-Mn2-N4	109.2(2)
O1-Mn1-N2	141.6(2)	O7-Mn2-N4	142.0(2)
O5-Mn1-N2	82.3(2)	O4-Mn2-N4	83.2(2)
O8-Mn1-N1	76.5(2)	O6-Mn2-N3	109.2(2)
O3-Mn1-N1	117.5(2)	O2-Mn2-N3	91.4(2)
O1-Mn1-N1	83.2(2)	O7-Mn2-N3	79.9(2)

O5-Mn1-N1	135.1(2)	O4-Mn2-N3	149.3(2)
N2-Mn1-N1	69.2(2)	N4-Mn2-N3	70.1(2)

Table S4. Selected bond lengths (Å) and bond angles (º) for **4**.

Co1-O2	2.0837(17)	Co1-O2i	2.0837(17)
Co1-O3ii	2.0104(18)	Co1-O3iii	2.0104(18)
Co1-O5	2.1880(18)	Co1-O5i	2.1880(18)
Co2-O1	2.0424(17)	Co2-O1iv	2.0424(17)
Co2-O4ii	2.0906(18)	Co2-O4v	2.0906(18)
Co2-O5	2.1789(18)	Co2-O5iv	2.1789(18)
O3ii-Co1-O3iii	180.00(10)	O3ii-Co1-O2	93.50(7)
O3iii-Co1-O2	86.50(7)	O3ii-Co1-O2i	86.50(7)
O3iii-Co1-O2i	93.50(7)	O2-Co1-O2i	180.0
O3ii-Co1-O5i	91.09(8)	O3iii-Co1-O5i	88.91(8)
O2-Co1-O5i	84.36(7)	O2i-Co1-O5i	95.64(7)
O3ii-Co1-O5	88.91(8)	O3iii-Co1-O5	91.09(8)
O2-Co1-O5	95.64(7)	O2i-Co1-O5	84.36(7)
O5-Co1-O5i	180.0	O1-Co2-O1iv	180.0
O1-Co2-O4ii	94.62(7)	O1iv-Co2-O4ii	85.38(7)
O1-Co2-O4v	85.38(7)	O1iv-Co2-O4v	94.62(7)
O4ii-Co2-O4v	180.00(8)	O1-Co2-O5iv	88.15(8)
O1iv-Co2-O5iv	91.85(8)	O4ii-Co2-O5iv	87.51(7)
O4v-Co2-O5iv	92.49(7)	O1-Co2-O5	91.85(8)
O1iv-Co2-O5	88.15(8)	O4ii-Co2-O5	92.49(7)
O4v-Co2-O5	87.51(7)	O5-Co2-O5iv	180.000(1)

Symmetry codes: i = $-x$, $2-y$, $1-z$; ii = $-x$, y, $1.5-z$; iii = x, $2-y$, $-0.5+z$; iv = $-x$, $1-y$, $1-z$; v = x, $1-y$, $-0.5+z$.

Table S5. Selected bond lengths (Å) and bond angles (º) for **5**.

Co1-O1	2.154(2)	Co1-O1i	2.142(2)
Co1-O3ii	2.050(2)	Co1-O5	2.150(2)
Co1-N1	2.125(2)	Co1-N2	2.122(2)
O3ii-Co1-N2	167.83(9)	O1i-Co1-O5	167.74(7)
O3ii-Co1-N1	90.99(8)	O3ii-Co1-O1	94.64(7)
N2-Co1-N1	78.31(9)	N2-Co1-O1	96.06(8)
O3ii-Co1-O1i	90.30(7)	N1-Co1-O1	174.36(8)
N2-Co1-O1i	97.60(8)	O1i-Co1-O1	77.83(7)
N1-Co1-O1i	102.44(8)	O5-Co1-O1	89.92(7)
O3ii-Co1-O5	90.19(7)	N2-Co1-O5	84.06(8)

N1-Co1-O5	89.80(8)	Co1-O1-Co1i	102.17(7)

Symmetry codes: i = –*x*, –*y*, –*z*; ii = *x*, –1 + *y*, *z*.

Table S6. Selected bond lengths (Å) and bond angles (º) for **6** and **7**.

	6	**7**		**6**	**7**
M1-O2	2.0272(19)	2.081(3)	M1-O2i	2.0272(19)	2.081(3)
M1-O7vi	2.0130(19)	2.067(3)	M1-O7vii	2.0130(19)	2.067(3)
M1-O9	2.119(2)	2.206(3)	M1-O9i	2.119(2)	2.206(3)
M2-O1	2.0135(19)	2.040(3)	M2-O3ii	2.0348(19)	2.060(3)
M2-O6v	2.0190(18)	2.039(3)	M2-O8vi	2.0185(19)	2.053(3)
M2-O9	2.119(2)	2.184(3)	M2-O10	2.140(2)	2.234(3)
M3-O4ii	2.0130(19)	2.048(3)	M3-O4iii	2.0130(19)	2.048(3)
M3-O5iv	2.0545(17)	2.067(3)	M3-O5v	2.0545(17)	2.067(3)
M3-O10	2.089(2)	2.142(3)	M3-O10viii	2.089(2)	2.142(3)
O7vi-M1-O7vii	180.00(15)	180.00(15)	O7vii-M1-O2	89.65(8)	90.88(13)
O7vi-M1-O2	90.35(8)	89.12(13)	O7vii-M1-O2i	90.35(8)	89.12(13)
O7vi-M1-O2i	89.65(8)	90.88(13)	O2-M1-O2i	180.0	180.0(3)
O7vii-M1-O9	89.95(8)	91.00(11)	O7vi-M1-O9	90.05(8)	89.00(11)
O2-M1-O9	93.71(8)	93.97(12)	O2i-M1-O9	86.29(8)	86.03(12)
O7vii-M1-O9i	90.05(8)	89.00(11)	O7vi-M1-O9i	89.95(8)	91.00(11)
O2-M1-O9i	86.29(8)	86.03(12)	O2i-M1-O9i	93.70(8)	93.97(12)
O9-M1-O9i	180.0	180.00(15)	O1-M2-O8vi	96.42(8)	95.65(13)
O1-M2-O6v	172.22(8)	167.37(13)	O8vi-M2-O6v	87.68(8)	91.22(13)
O1-M2-O3ii	87.67(8)	85.48(14)	O8vi-M2-O3ii	174.85(7)	176.65(12)
O6v-M2-O3ii	88.63(8)	88.27(13)	O1-M2-O9	95.82(8)	98.92(12)
O8vi-M2-O9	86.36(8)	86.23(11)	O6v-M2-O9	91.03(8)	92.09(12)
O3ii-M2-O9	90.12(8)	90.48(12)	O1-M2-O10	82.57(8)	79.35(12)
O8vi-M2-O10	86.61(8)	86.37(11)	O6v-M2-O10	91.09(8)	90.54(11)
O3ii-M2-O10	97.05(8)	96.94(12)	O9-M2-O10	172.57(8)	172.20(10)
O4ii-M3-O4iii	180.0	180.00(12)	O4ii-M3-O5v	95.27(8)	95.61(13)
O4iii-M3-O5v	84.73(8)	84.39(13)	O4ii-M3-O5iv	84.73(8)	84.39(13)
O4iii-M3-O5iv	95.27(8)	95.61(13)	O5iv-M3-O5v	180.00(15)	180.0
O4ii-M3-O10viii	90.41(8)	91.05(12)	O4iii-M3-O10viii	89.59(8)	88.95(12)
O5v-M3-O10viii	86.95(8)	86.34(11)	O5iv-M3-O10viii	93.05(8)	93.66(11)
O4ii-M3-O10	89.59(8)	88.95(12)	O4iii-M3-O10	90.41(8)	91.05(12)
O5v-M3-O10	93.05(8)	93.66(11)	O5iv-M3-O10	86.95(8)	86.34(11)
O10-M3-O10viii	180.0	180.00(7)	M2-O9-M1	115.30(9)	113.02(12)
M3-O10-M2	114.37(9)	112.78(12)			

Symmetry codes: i = –*x*, –*y*, –*z*; ii = –0.5 + *x*, 0.5 – *y*, –0.5 + *z*; iii = 0.5 – *x*, 0.5 + *y*, 0.5 – *z*; iv = 1.5 – *x*, 0.5 + *y*, 0.5 – *z*; v = –1.5 + *x*, 0.5 – *y*, –0.5 + *z*; vi = –1 + *x*, *y*, *z*; vii = 1 – *x*, –*y*, –*z*; viii = –*x*, 1 – *y*, –*z*.

Table S7. Selected bond lengths (Å) and bond angles (º) for **8**.

Ni1-O2i	2.020(2)	Ni1-O4	2.007(2)
Ni1-O5	2.0321(19)	Ni1-O9	2.117(2)
Ni1-O12	2.050(2)	Ni1-O13	2.039(2)
Ni2-O3	2.040(2)	Ni2-O6	2.024(2)
Ni2-O8ii	2.059(2)	Ni2-O10	2.042(2)
Ni2-O13	2.023(2)	Ni2-O14	2.128(2)
O4-Ni1-O2i	91.31(9)	O4-Ni1-O5	93.49(9)
O2i-Ni1-O5	171.77(8)	O4-Ni1-O13	89.84(8)
O2i-Ni1-O13	91.13(8)	O5-Ni1-O13	95.56(8)
O4-Ni1-O12	178.14(8)	O2i-Ni1-O12	87.29(9)
O5-Ni1-O12	87.75(9)	O13-Ni1-O12	91.42(8)
O4-Ni1-O9	85.71(9)	O2i-Ni1-O9	86.77(9)
O5-Ni1-O9	86.93(8)	O13-Ni1-O9	175.04(8)
O12-Ni1-O9	92.97(9)	O13-Ni2-O6	96.60(8)
O13-Ni2-O3	89.48(8)	O6-Ni2-O3	94.55(9)
O13-Ni2-O10	175.81(8)	O6-Ni2-O10	87.07(9)
O3-Ni2-O10	88.22(9)	O13-Ni2-O8ii	92.30(8)
O6-Ni2-O8ii	92.43(9)	O3-Ni2-O8ii	172.56(9)
O10-Ni2-O8ii	89.54(9)	O13-Ni2-O14	88.13(9)
O6-Ni2-O14	175.02(9)	O3-Ni2-O14	87.01(10)
O10-Ni2-O14	88.24(10)	O8ii-Ni2-O14	85.83(10)

Symmetry codes: i = 1 + *x*, *y*, *z*; ii = *x*, 1 + *y*, *z*.

Table S8. Selected bond lengths (Å) and bond angles (º) for **9**.

Ni1-O2i	2.201(4)	Ni1-O2ii	2.201(4)
Ni1-O3	1.992(4)	Ni1-O3iii	1.992(4)
Ni1-O9	2.036(4)	Ni1-O9iii	2.036(4)
Ni2-O2i	2.113(4)	Ni2-O4	2.035(4)
Ni2-O9	2.082(4)	Ni2-O10	2.084(4)
Ni2-O6iv	1.998(5)	Ni2-O8v	2.066(4)
Ni3-O5iv	2.007(4)	Ni3-O5vi	2.007(4)
Ni3-O10	2.084(4)	Ni3-O10vii	2.084(4)
Ni3-O11	2.048(4)	Ni3-O11vii	2.048(4)
O3-Ni1-O3iii	180.000(1)	O3iii-Ni1-O9	85.29(16)
O3-Ni1-O9	94.71(16)	O3iii-Ni1-O9iii	94.71(16)

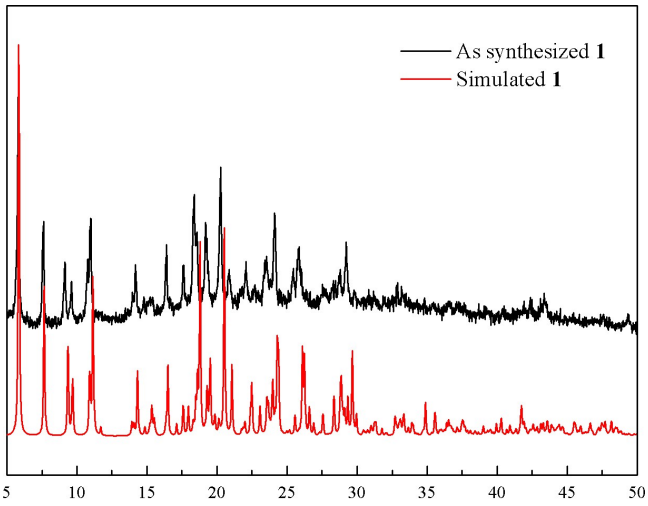
O3-Ni1-O9iii	85.29(16)	O9-Ni1-O9iii	180.0(2)
O3iii-Ni1-O2i	90.27(16)	O3-Ni1-O2i	89.73(16)
O9-Ni1-O2i	79.71(15)	O9iii-Ni1-O2i	100.29(15)
O3iii-Ni1-O2ii	89.73(16)	O3-Ni1-O2ii	90.27(16)
O9-Ni1-O2ii	100.29(15)	O9iii-Ni1-O2ii	79.71(15)
O2i-Ni1-O2ii	180.000(1)	O6-Ni2-O4	175.76(19)
O6-Ni2-O8	89.31(19)	O4-Ni2-O8	87.23(17)
O6-Ni2-O9	87.52(18)	O4-Ni2-O9	90.28(17)
O8-Ni2-O9	94.01(16)	O6-Ni2-O10	97.80(18)
O4-Ni2-O10	84.72(17)	O8-Ni2-O10	91.10(16)
O9-Ni2-O10	172.67(17)	O6-Ni2-O2	90.38(18)
O4-Ni2-O2	92.84(17)	O8-Ni2-O2	174.79(16)
O9-Ni2-O2	80.78(15)	O10-Ni2-O2	94.10(16)
O5iv-Ni3-O5vi	180.000(2)	O5iv-Ni3-O11vii	88.1(2)
O5vi-Ni3-O11vii	91.9(2)	O5iv-Ni3-O11	91.9(2)
O5vi-Ni3-O11	88.1(2)	O11-Ni3-O11vii	180.000(1)
O5iv-Ni3-O10vii	86.60(17)	O5vi-Ni3-O10vii	93.40(17)
O11vii-Ni3-O10vii	87.71(17)	O11-Ni3-O10vii	92.29(17)
O5iv-Ni3-O10	93.40(17)	O5vi-Ni3-O10	86.60(17)
O11vii-Ni3-O10	92.29(17)	O11-Ni3-O10	87.71(17)
O10-Ni3-O10vii	180.000(1)		

Symmetry codes: i = –1 + *x*, –1 + *y*, *z*; ii = 2 – *x*, 2 – *y*, 1 – *z*; iii = 1 – *x*, 1 – *y*, 1 – *z*; iv = *x*, –1 + *y*, *z*; v = 1 + *x*, *y*, *z*; vi = 2 – *x*, 2 – *y*, 2 – *z*; vii = 2 – *x*, 1 – *y*, 2 – *z*.

Table S9. Crystallographic data for $H_4L \cdot 2DMA \cdot 0.5H_2O$.

$H_4L \cdot 2DMA \cdot 0.5H_2O$			
Empirical formula	$C_{60}H_{66}N_4O_{21}$	*Z*	2
Formula weight	1179.17	ρ_{calc} g/cm^3	1.338
Crystal system	Monoclinic	μ/mm^{-1}	0.102
Space group	*C*2/*c*	*F*(000)	1244
a/Å	25.461(12)	Reflections collected	5638
b/Å	6.279(2)	Unique reflections	2401
c/Å	19.834(6)	*GOF* (F^2)	1.011
β/°	112.59(2)	$R_1{}^a$, $wR_2{}^b$, (I>2σ(I))	0.0595, 0.1302
V/Å^3	2927.6(19)	$R_1{}^a$, $wR_2{}^b$, (all data)	0.1627, 0.1923

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2{}^b = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)]^{1/2}$.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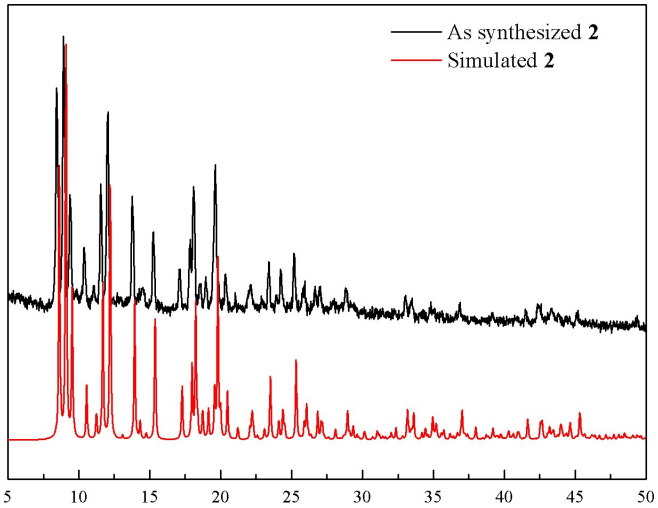
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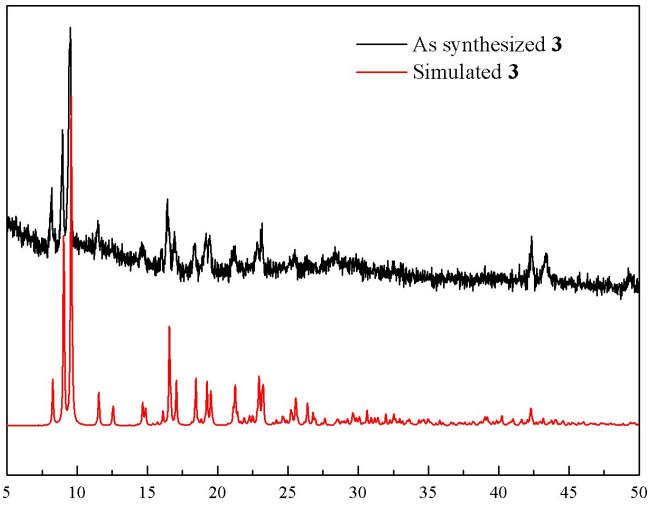
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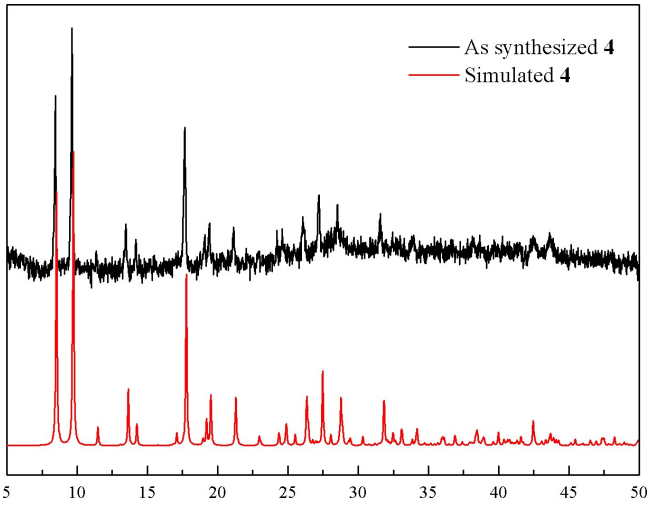
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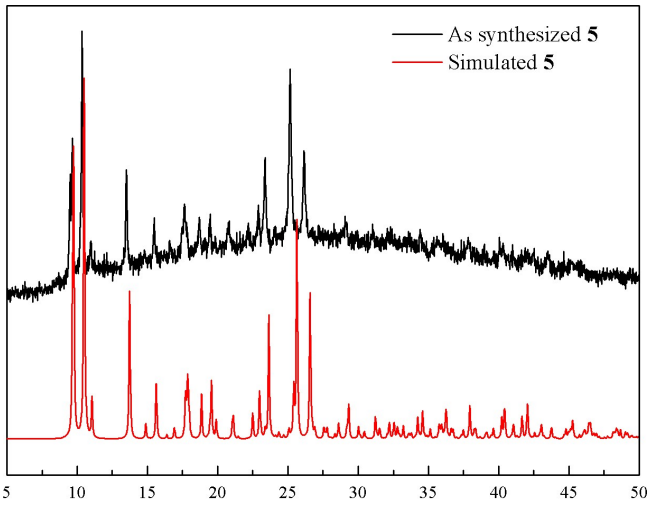
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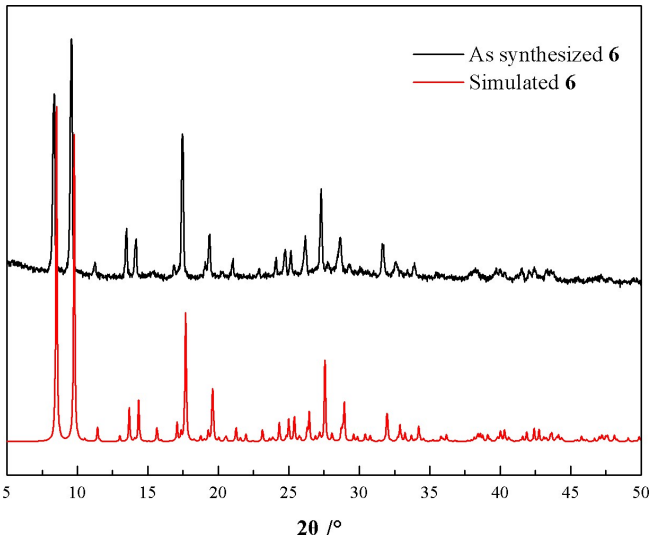
50
2θ /°


As synthesized 6
Simulated 6
5
10
15
20
25
30
35
40
45
50
2θ /°

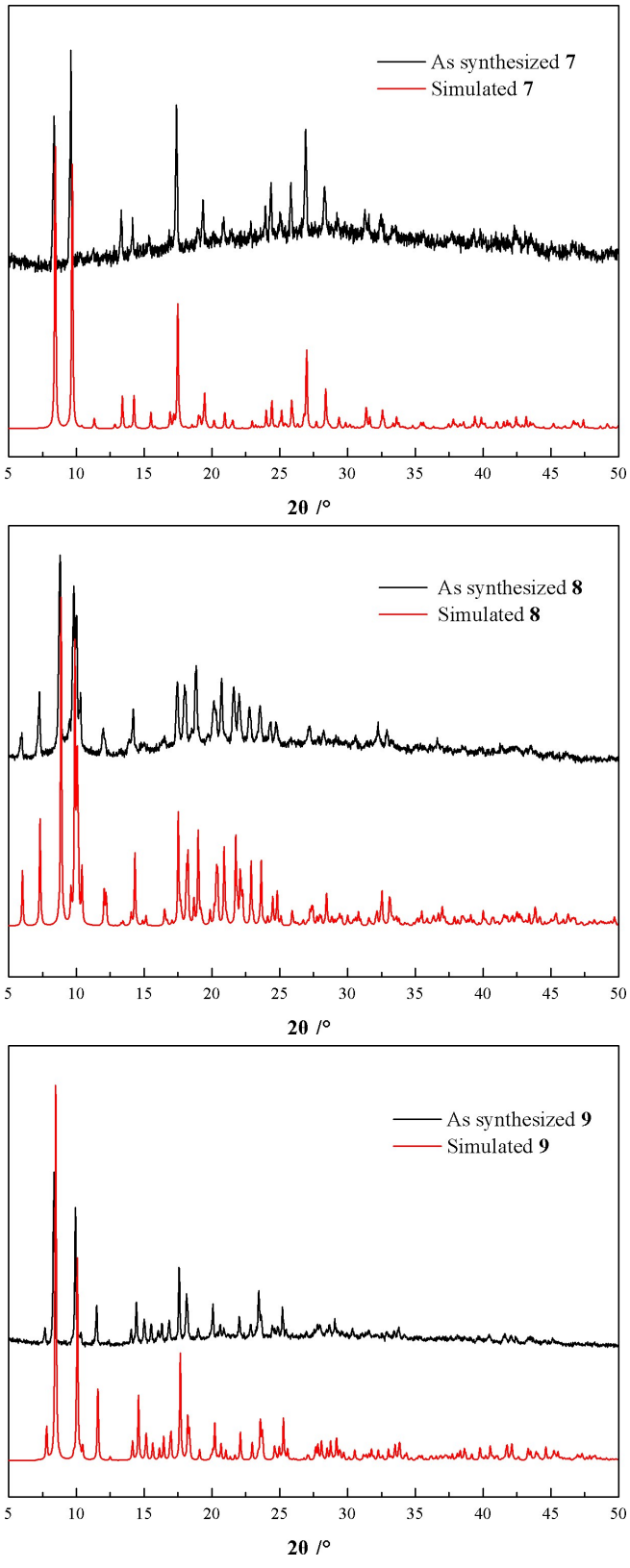


Fig. S1 The simulated and as-synthesized powder X-ray diffraction patterns of **1-9**.