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Supplementary Material

Coordination Assemblies of the Cd^{II}-BDC/bpt Mixed-Ligand System: Positional Isomeric Effect, Structural Diversification and Luminescent Properties

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Table S1. Selected bond distances (Å) and angles (°) for the complexes 1-6

complex **1** [a]			
Cd1–O4	2.325 (10)	Cd2–O14	2.285 (12)
Cd1–N10A	2.325 (10)	Cd2–O15	2.370 (13)
Cd1–N1	2.335 (12)	Cd3–N5B	2.312 (11)
Cd1–O13	2.352 (13)	Cd3–N6	2.320 (11)
Cd1–O2	2.379 (11)	Cd3–O17	2.361 (11)
Cd1–O1	2.429 (12)	Cd3–O9	2.367 (9)
Cd1—O3	2.568 (12)	Cd3—O11	2.396 (13)
Cd2–O16	2.09 (2)	Cd3–O12	2.458 (14)
Cd2–O7	2.195 (14)	Cd3–O10	2.500 (11)
Cd2–O5	2.267 (10)		
O4–Cd1–N10A	140.4 (4)	O5–Cd2–O14	89.9 (4)
O4–Cd1–N1	88.5 (4)	O16–Cd2–O15	92.3 (8)
N10A–Cd1–N1	88.8 (4)	O7–Cd2–O15	92.5 (6)
O4–Cd1–O13	92.1 (4)	O5–Cd2–O15	172.3 (4)
N10A–Cd1–O13	88.9 (4)	O14–Cd2–O15	82.8 (4)
N1–Cd1–O13	177.0 (5)	N5B–Cd3–N6	90.3 (4)
O4–Cd1–O2	81.3 (4)	N5B–Cd3–O17	87.7 (4)
N10A–Cd1–O2	138.3 (4)	N6–Cd3–O17	173.7 (4)
N1–Cd1–O2	92.3 (4)	N5B–Cd3–O9	142.7 (4)
O13–Cd1–O2	90.7 (5)	N6–Cd3–O9	88.2 (4)
O4–Cd1–O1	134.6 (4)	O17–Cd3–O9	89.7 (4)
N10A–Cd1–O1	84.9 (4)	N5B–Cd3–O11	84.1 (5)
N1–Cd1–O1	91.9 (4)	N6–Cd3–O11	92.1 (5)
O13–Cd1–O1	89.8 (5)	O17–Cd3–O11	93.7 (5)
O2–Cd1–O1	53.3 (4)	O9–Cd3–O11	133.2 (4)
O4–Cd1–O3	53.2 (3)	N5B–Cd3–O12	136.9 (5)
N10A–Cd1–O3	87.7 (4)	N6–Cd3–O12	93.4 (4)

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N1–Cd1–O3	94.2 (4)	O17–Cd3–O12	92.1 (4)
O13–Cd1–O3	83.8 (5)	O9–Cd3–O12	80.4 (4)
O2–Cd1–O3	133.7 (4)	O11–Cd3–O12	52.8 (5)
O1–Cd1–O3	170.3 (4)	N5B–Cd3–O10	89.5 (4)
O16–Cd2–O7	138.3 (8)	N6–Cd3–O10	91.8 (4)
O16–Cd2–O5	89.3 (7)	O17–Cd3–O10	82.2 (4)
O7–Cd2–O5	91.3 (5)	O9–Cd3–O10	53.4 (3)
O16–Cd2–O14	120.4 (8)	O11–Cd3–O10	172.5 (4)
O7–Cd2–O14	101.2 (5)	O12–Cd3–O10	133.2 (4)
	complex **2** [b]		
Cd1–O4A	2.201 (3)	Cd1–N1	2.351 (3)
Cd1–O3	2.293 (2)	Cd1–O1	2.353 (2)
Cd1–N5B	2.297 (3)	Cd1–O2	2.440 (2)
O4A–Cd1–O3	126.59 (10)	N5B–Cd1–O1	92.64 (10)
O4A–Cd1–N5B	101.11 (11)	N1–Cd1–O1	83.66 (10)
O3–Cd1–N5B	86.50 (10)	O4A–Cd1–O2	88.83 (9)
O4A–Cd1–N1	87.30 (11)	O3–Cd1–O2	142.35 (9)
O3–Cd1–N1	84.09 (10)	N5B–Cd1–O2	99.94 (10)
N5B–Cd1–N1	169.98 (10)	N1–Cd1–O2	85.55 (10)
O4A–Cd1–O1	142.85 (9)	O1–Cd1–O2	54.65 (8)
O3–Cd1–O1	88.23 (9)		
	complex **3** [c]		
Cd1–O2	2.298 (5)	Cd2–O1	2.302 (6)
Cd1–O8A	2.332 (6)	Cd2–N6	2.329 (6)
Cd1–N5B	2.337 (6)	Cd2–O4B	2.333 (5)
Cd1–N1	2.341 (6)	Cd2–N10C	2.354 (6)
Cd1–O3B	2.371 (5)	Cd2–O5	2.359 (5)
Cd1–O7A	2.445 (6)	Cd2–O6	2.463 (5)
Cd1–O1	2.568 (6)	Cd2–O3B	2.495 (5)

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O2–Cd1–O8A	140.1 (2)	O1–Cd2–N6	83.5 (2)
O2–Cd1–N5B	99.1 (2)	O1–Cd2–O4B	126.81 (19)
O8A–Cd1–N5B	88.0 (2)	N6–Cd2–O4B	88.6 (2)
O2–Cd1–N1	89.4 (2)	O1–Cd2–N10C	95.4 (2)
O8A–Cd1–N1	90.2 (2)	N6–Cd2–N10C	176.8 (2)
N5B—Cd1—N1	168.8 (2)	O4B—Cd2—N10C	94.5 (2)
O2–Cd1–O3B	123.46 (19)	O1–Cd2–O5	95.57 (19)
O8A–Cd1–O3B	95.77 (19)	N6–Cd2–O5	88.5 (2)
N5B–Cd1–O3B	88.1 (2)	O4B–Cd2–O5	136.83 (19)
N1—Cd1—O3B	81.0 (2)	N10C—Cd2—O5	88.6 (2)
O2–Cd1–O7A	85.88 (19)	O1–Cd2–O6	149.54 (17)
O8A–Cd1–O7A	54.35 (19)	N6–Cd2–O6	93.6 (2)
N5B–Cd1–O7A	94.7 (2)	O4B–Cd2–O6	83.26 (18)
N1–Cd1–O7A	93.2 (2)	N10C–Cd2–O6	85.8 (2)
O3B–Cd1–O7A	149.76 (18)	O5–Cd2–O6	53.99 (17)
O2–Cd1–O1	53.02 (18)	O1–Cd2–O3B	73.99 (18)
O8A–Cd1–O1	166.80 (19)	N6–Cd2–O3B	91.4 (2)
N5B–Cd1–O1	88.0 (2)	O4B–Cd2–O3B	53.64 (18)
N1–Cd1–O1	91.3 (2)	N10C–Cd2–O3B	91.3 (2)
O3B–Cd1–O1	71.53 (17)	O5–Cd2–O3B	169.50 (17)
O7A–Cd1–O1	138.58 (18)	O6–Cd2–O3B	136.47 (16)
complex **4** [d]			
Cd1–O4A	2.245 (2)	Cd1–O2	2.342 (2)
Cd1–O5	2.317 (2)	Cd1–N1	2.350 (3)
Cd1–N5B	2.331 (3)	Cd1–O1	2.493 (2)
O4A–Cd1–O5	133.70 (8)	N5B–Cd1–N1	167.46(8)
O4A–Cd1–N5B	94.91 (10)	O2–Cd1–N1	90.89 (10)
O5–Cd1–N5B	85.45 (9)	O4A–Cd1–O1	139.59 (8)
O4A–Cd1–O2	85.78 (8)	O5–Cd1–O1	86.65 (8)

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O5–Cd1–O2	140.50 (8)	N5B–Cd1–O1	84.65 (8)
N5B–Cd1–O2	90.41 (10)	O2–Cd1–O1	53.85 (7)
O4A–Cd1–N1	97.63 (10)	N1–Cd1–O1	85.84 (8)
O5–Cd1–N1	85.61 (9)		
complex **5** [e]			
Cd1–N1	2.320 (5)	Cd1–O5	2.415 (5)
Cd1–N5A	2.330 (5)	Cd1–O4B	2.478 (5)
Cd1–O1	2.338 (5)	Cd1–O2	2.506 (5)
Cd1-O3B	2.368 (4)		
N1–Cd1–N5A	164.86 (18)	N5A–Cd1–O4B	87.63 (17)
N1–Cd1–O1	89.52 (18)	O1–Cd1–O4B	142.54 (15)
N5A–Cd1–O1	96.76 (18)	O3B–Cd1–O4B	53.50 (15)
N1–Cd1–O3B	93.65 (17)	O5–Cd1–O4B	76.88 (16)
N5A–Cd1–O3B	100.18 (17)	N1–Cd1–O2	88.81 (17)
O1–Cd1–O3B	89.22 (16)	N5A–Cd1–O2	83.81 (17)
N1–Cd1-O5	83.67 (18)	O1–Cd1–O2	54.13 (15)
N5A–Cd1–O5	82.74 (18)	O3B–Cd1–O2	143.27 (16)
O1–Cd1–O5	140.57 (17)	O5–Cd1–O2	86.84 (17)
O3B–Cd1–O5	129.86 (17)	O4B–Cd1–O2	162.46 (14)
N1–Cd1–O4B	95.76 (18)		
complex 6 [f]			
Cd1–N5A	2.318 (14)	Cd1–O6	2.417 (14)
Cd1–N1	2.322 (13)	Cd1–O2	2.470 (12)
Cd1–O4B	2.386 (14)	Cd1–O3B	2.640 (17)
Cd1–O1	2.397 (12)		
N5A–Cd1–N1	173.1 (5)	N1–Cd1–O2	93.6 (4)
N5A–Cd1–O4B	86.9 (5)	O4B–Cd1–O2	165.6 (4)
N1–Cd1–O4B	91.7 (5)	O1–Cd1–O2	53.3 (4)
N5A–Cd1–O1	94.5 (5)	O6–Cd1–O2	97.8 (4)

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N1–Cd1–O1	90.9 (5)	N5A–Cd1–O3B	99.1 (5)
O4B–Cd1–O1	140.0 (5)	N1–Cd1–O3B	85.2 (5)
N5A–Cd1–O6	88.5 (5)	O4B–Cd1–O3B	51.4 (5)
N1–Cd1–O6	84.7 (5)	O1–Cd1–O3B	89.1 (5)
O4B–Cd1–O6	69.4 (5)	O6–Cd1–O3B	119.4 (5)
O1–Cd1–O6	150.5 (5)	O2–Cd1–O3B	142.4 (4)
N5A–Cd1–O2	86.2 (5)		

[a] Symmetry codes: (A) -*x*+1, -*y*+2, -*z*+2; (B) -*x*+1, -*y*+2, -*z*+1. [b] Symmetry codes: (A) -*x*+1, -*y*+2, -*z*+1; B) *x*+1, *y*, *z*+1. [c] Symmetry codes: (A) *x*+1, -*y*+1/2, *z*+1/2; (B) *x*, -*y*+1/2, *z*+1/2; (C) *x*, -*y*+1/2, *z*-1/2. [d] Symmetry codes: (A) *x*-1, *y*+1, *z*; (B) -*x*, -*y*, -*z*+1. [e] Symmetry codes: A: −*x*+2, −*y*, −*z*+2; B: −*x*+3/2, *y*−1/2, −*z*+3/2. [f] Symmetry codes: (A) -*x*, *y*+1/2, -*z*+1/2; (B) *x*, -*y*+1/2, *z*+1/2.

Table S2. Selected geometrical parameters of hydrogen bonds in the complexes 2, 3, 5, 6.

D—*H*···*A*	*D*—*H*	*H*···*A*	*D*···*A*	*D*—*H*···*A*
Complex **2**				
N3—H3A···O2^{i}	0.94(6)	1.82(6)	2.739(4)	166(5)
Symmetry codes：(i): -*x*+1, -*y*+2, -*z*.				
Complex **3**				
N3—H3A···O11^{i}	0.78	2.02	2.776 (11)	165
N8—H8A···O6^{ii}	0.89	1.89	2.756 (8)	165
O9—H9A···O12	0.85	2.55	3.38 (6)	164
O10—H10A···O4^{iii}	0.85	2.17	3.018(19)	178
O10—H10B···O13^{iv}	0.79	2.22	2.81 (7)	132
O11—H11A···O7^{ii}	0.83	1.97	2.796(12)	179
O11—H11B···N3^{v}	0.83	1.95	2.796(11)	180
O12—H12B···O13	0.71	2.33	2.84 (9)	131
O14—H14A···O2	0.91	1.86	2.77 (3)	176

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Symmetry codes: (i) *x*, *y*-1, *z*-1; (ii) -*x*, -*y*, -*z*; (iii) *x*+1, *y*, *z*+1; (iv) -*x*+1, -*y*-1, -*z*+1; (v) *x*, *y*+1, *z*+1.

Complex **5**				
N3—H3···O4^{i}	0.92	1.83	2.687 (7)	155
O5—H5*A*···O6^{ii}	0.85	2.13	2.758 (9)	130
O5—H5*B*···N4^{iii}	0.86	2.44	2.910 (7)	115
O6—H6*A*···O2^{iv}	0.85	1.94	2.785 (7)	178
O6—H6*B*···N2^{v}	0.87	2.17	3.042 (9)	180
O7—H7*A*···N9^{vi}	0.86	2.10	2.959 (10)	179
O7—H7*B*···N7	0.85	2.10	2.953 (9)	179
N8—H8···O8	0.96	1.73	2.674 (9)	169
O8-H8*A*···N6^{vii}	0.86	1.91	2.775 (11)	178
O8—H8*B*···O4^{vi}	0.87	2.46	3.315 (10)	167
O9—H9*A*···O6^{vii}	0.85	2.07	2.924 (17)	180
O9—H9*B*···O7^{vi}	0.85	2.21	3.065 (17)	179

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) *x*, *y*−1, *z*; (iv) −*x*+3/2, *y*+1/2, −*z*+5/2; (v) *x*−1, *y*, *z*; (vi) −*x*, −*y*, −*z*+1; (vii) *x*, *y*+1, *z*.

Complex **6**				
N3—H3···O5^{i}	0.89	1.85	2.75(2)	179
O5—H5*C*···O1^{ii}	0.85	1.95	2. 80 (2)	180
O5—H5*D*···O2	0.85	1.89	2.74 (2)	180

Symmetry codes: (i) -*x*+1, *y*+1/2, -*z*+3/2; (ii) *x*+1, *y*, *z*.

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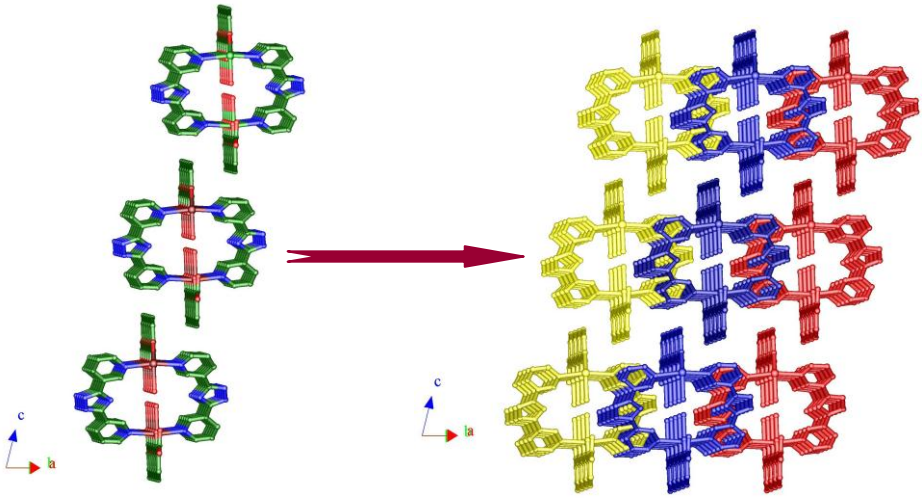

Figure **S1.** Molecular packing by $\pi\cdots\pi$ interaction viewed in the *ac* plane.

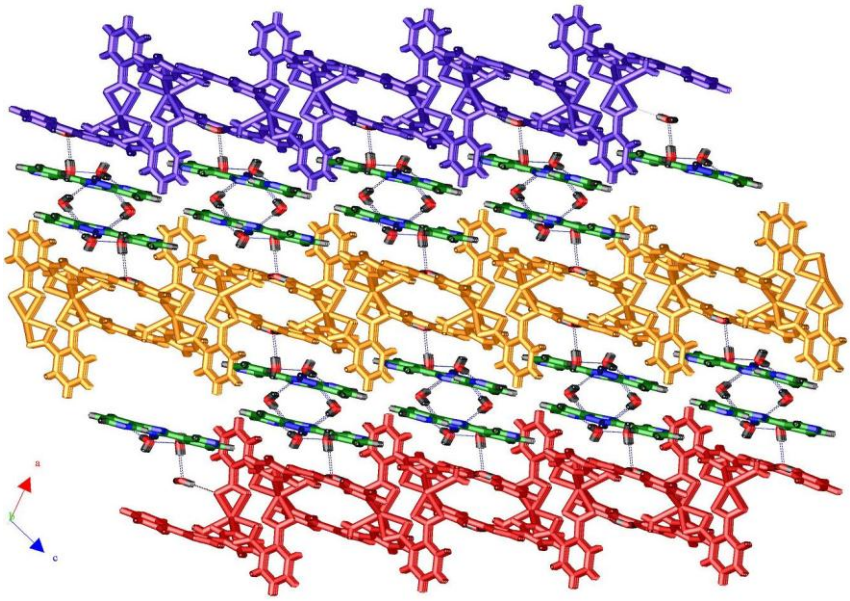

Figure **S2.** The 3D supra-molecular network along the *ac* plane.

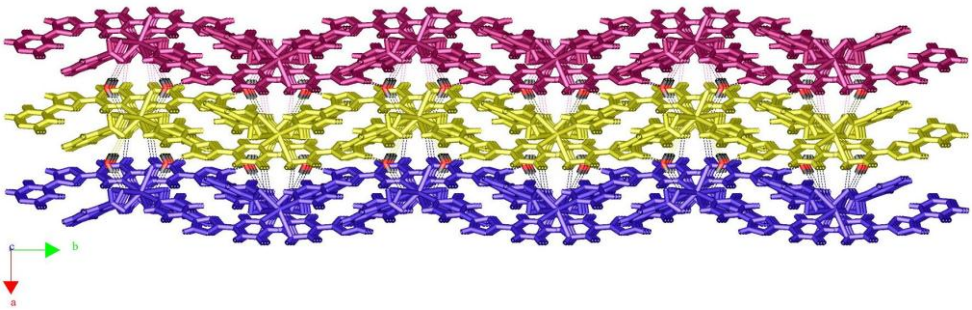

Figure **S3.** The extended 3D network viewed along the *ab* plane.

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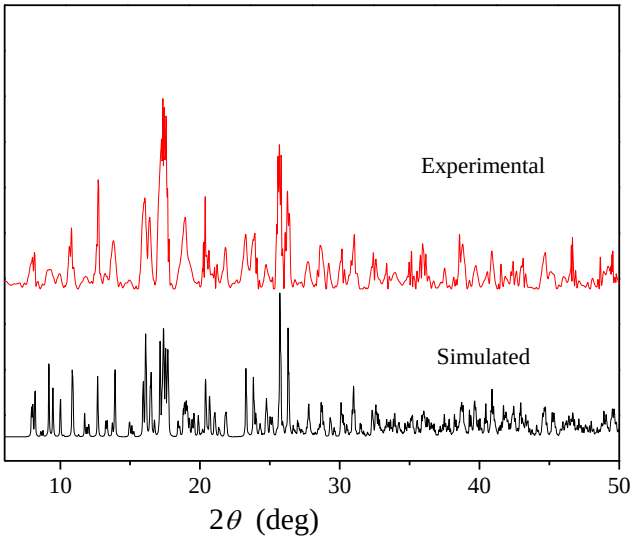

Figure **S4.** Measured and calculated powder X-ray diffraction (PXRD) pattern of **1**.

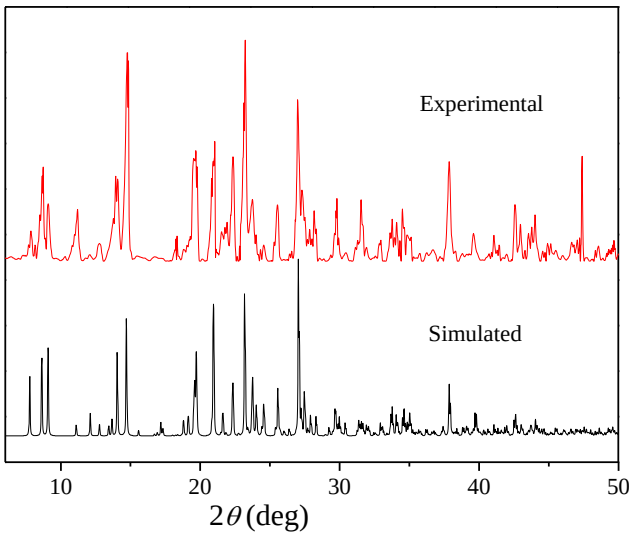

Figure **S5.** Measured and calculated powder X-ray diffraction (PXRD) pattern of **2**.

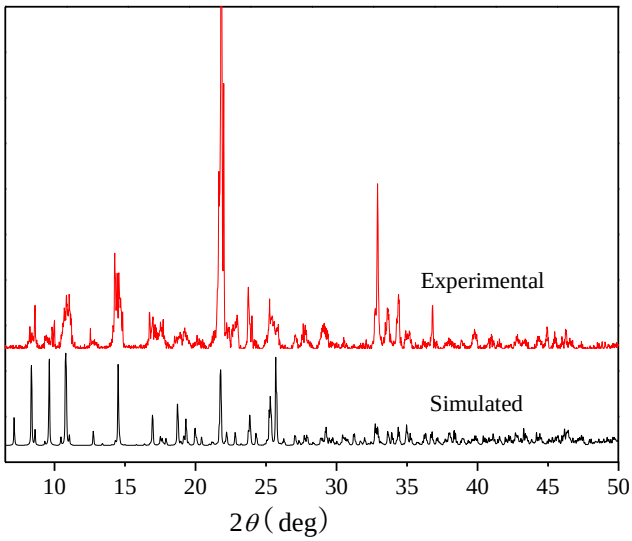

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Figure **S6.** Measured and calculated powder X-ray diffraction (PXRD) pattern of **3**.

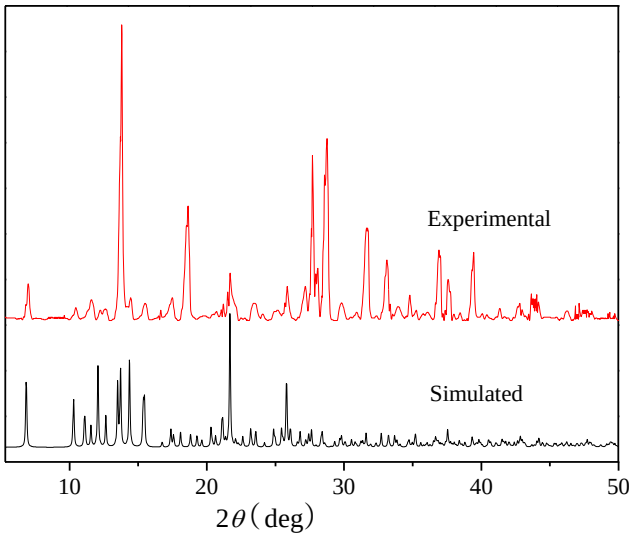

Figure **S7.** Measured and calculated powder X-ray diffraction (PXRD) pattern of **4**.

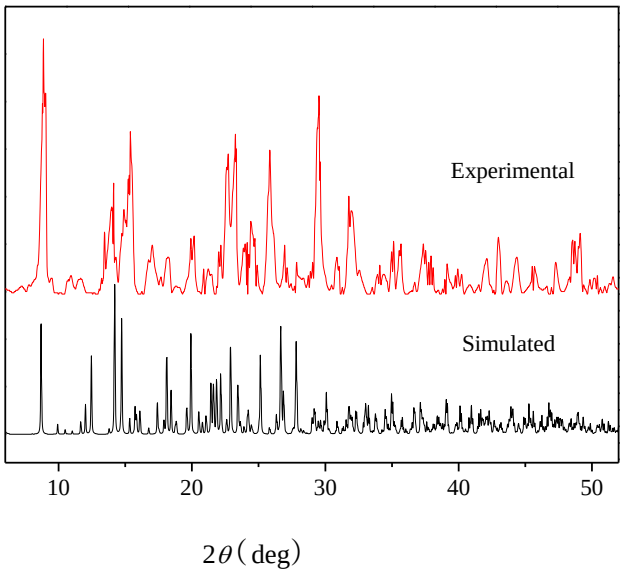

Figure **S8.** Measured and calculated powder X-ray diffraction (PXRD) pattern of **5**.

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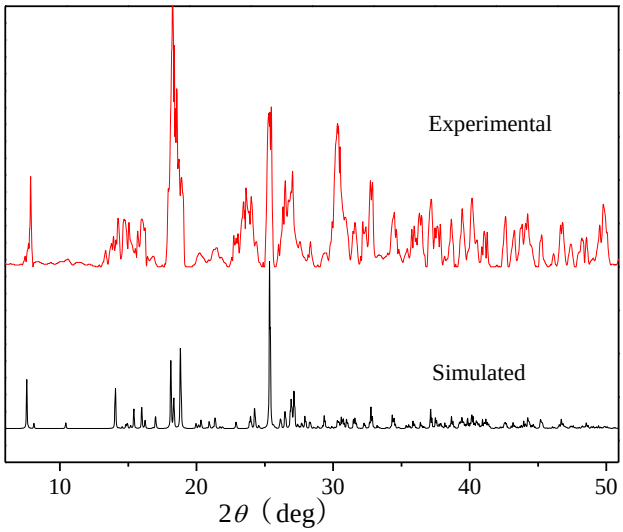

Figure **S9.** Measured and calculated powder X-ray diffraction (PXRD) pattern of **6**.