crystals

Coordination Polymers in Dicyanamido-Cadmium(II) with Diverse Network Dimensionalities

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Supplementary Materials

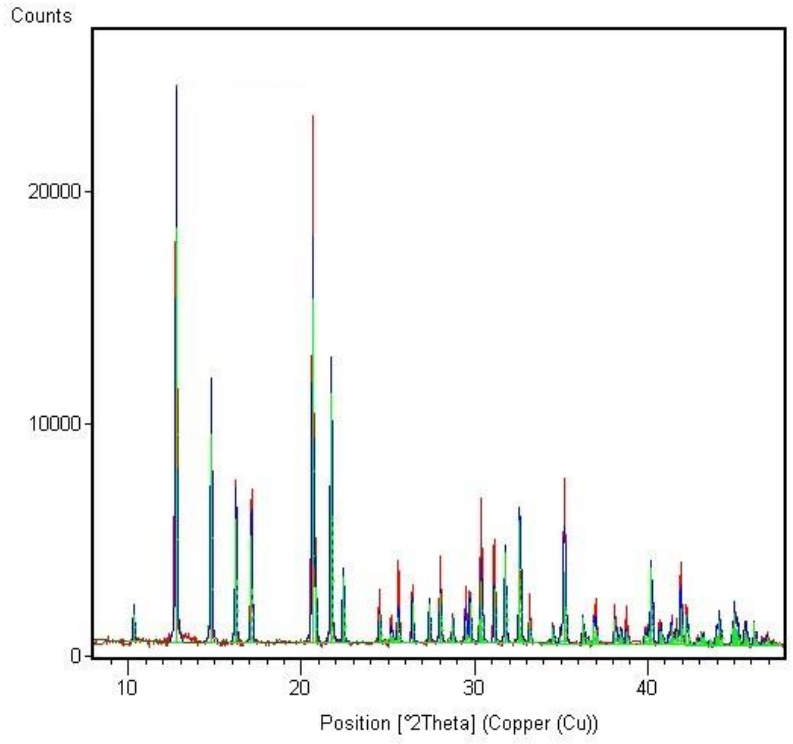

Figure S1. XRD pattern of **1**.

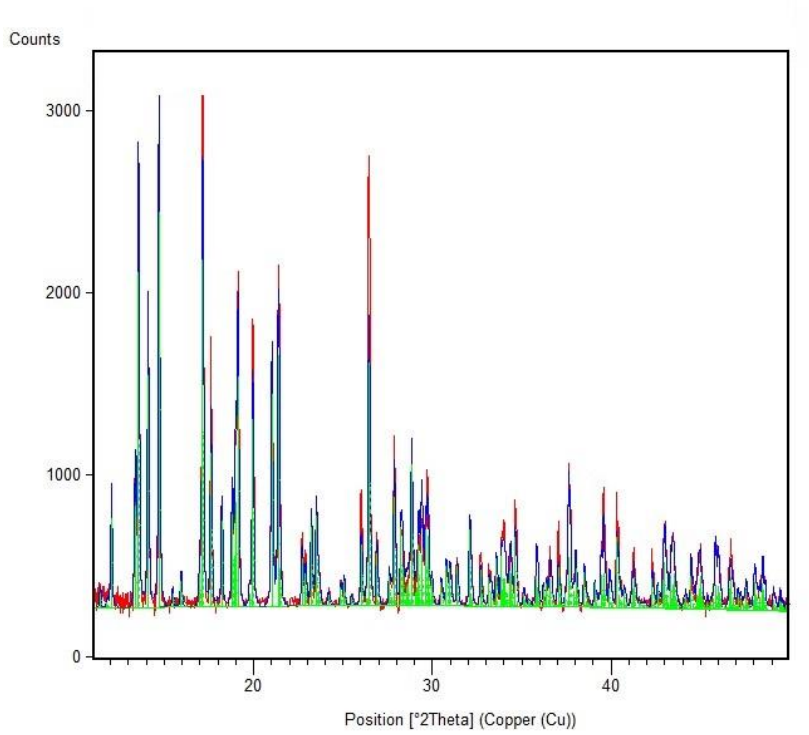

Figure S2. XRD pattern of **2** (observed intensities affected by preferred orientation).

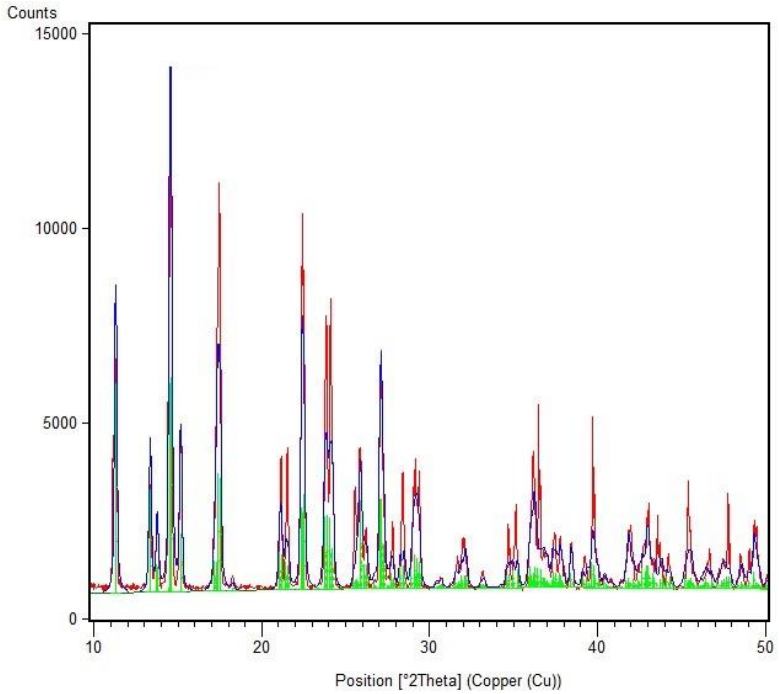

Figure S3. XRD pattern of **3** (observed intensities affected by preferred orientation).

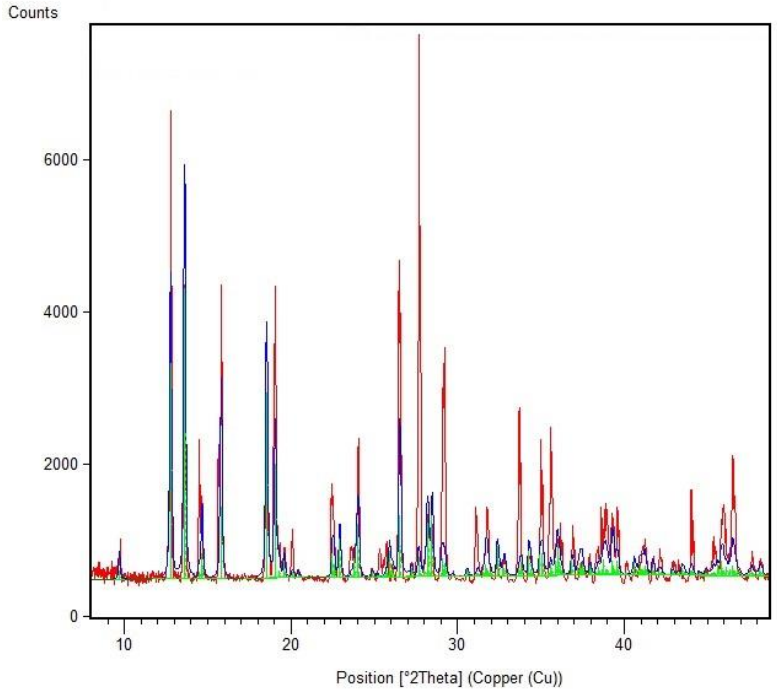

Figure S4. XRD pattern of **4** (observed intensities affected by preferred orientation).

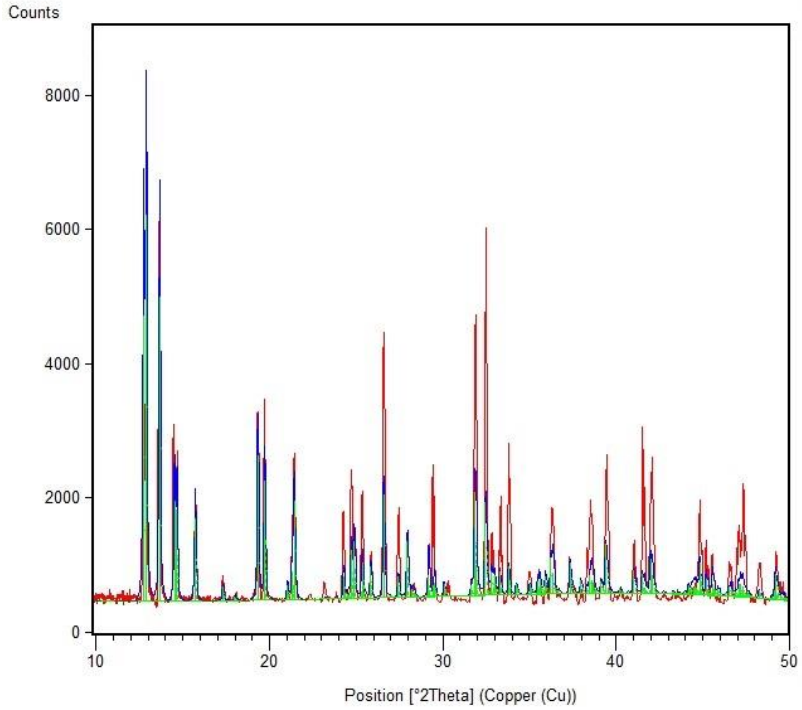

Figure S5. XRD pattern of **5** (observed intensities affected by preferred orientation).

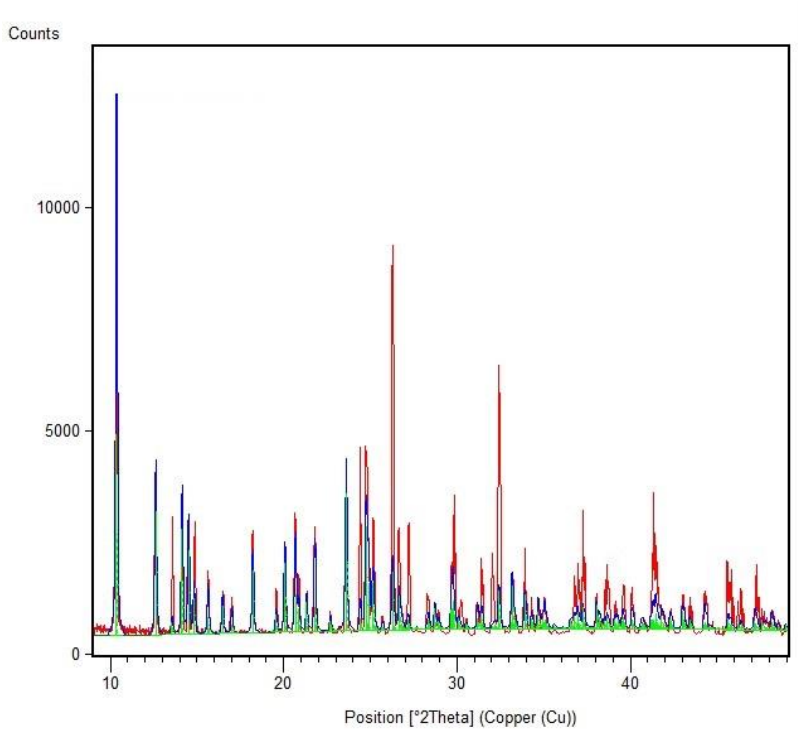

Figure S6. XRD pattern of **6** (observed intensities affected by preferred orientation).

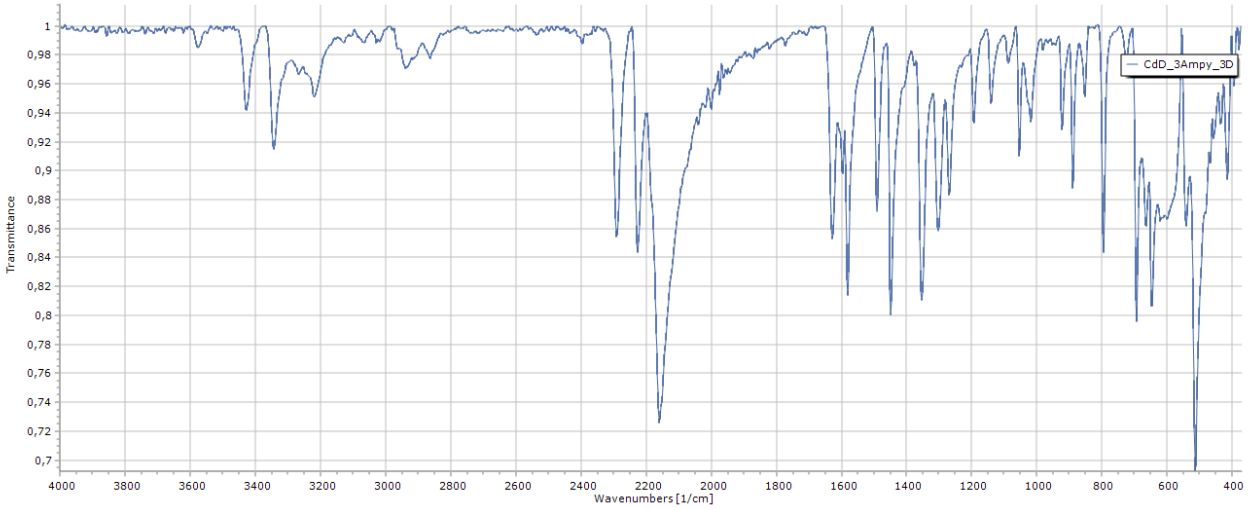

Figure S7. IR spectrum of *catena*-[Cd($\mu_{1,3}$-dca)($\mu_{1,5}$-dca)(3-ampy)] (**1**).

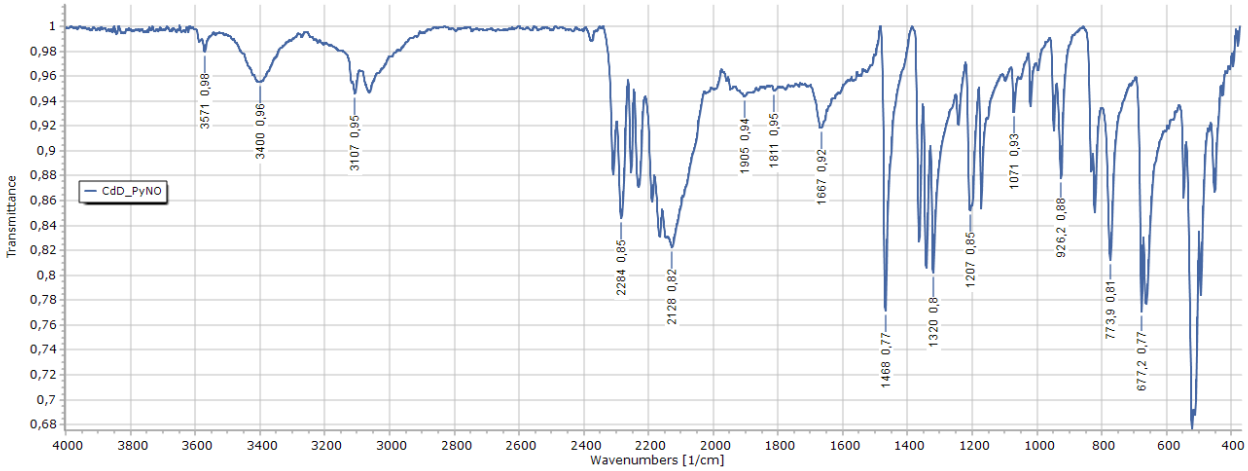

Figure S8. IR spectrum of *catena*-[$Cd_3(\mu_{1,3,5}\text{-dca})_2(\mu_{1,5}\text{-dca})_4(pyNO)_2(H_2O)_2$] (**2**).

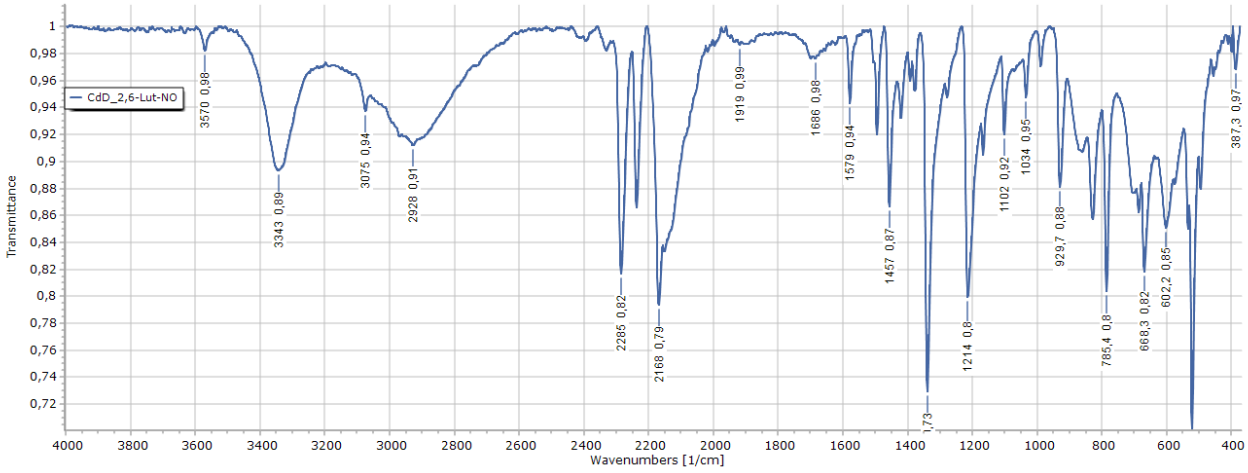

Figure S9. IR spectrum of *catena*-{$Cd(H_2O)_2(\mu_{1,5}\text{-dca})_2$](2,6-lut-NO)} (**3**).

Table S1. Selected bond distances (Å) and bond angles (°) of **1**–**6**.

Compound 1			
Cd1-N3	2.297(3)	Cd1-N5c	2.309(3)
Cd1-N6	2.319(3)	Cd1-N1	2.323(3)
Cd1-N2a	2.375(4)	Cd1-N7b	2.392(4)
N3-C6	1.155(5)	N4-C7	1.305(5)
N4-C6	1.305(5)	N5-C7	1.150(5)
N6-C8	1.160(5)	N7-C8	1.308(5)
N7-C9	1.332(6)	N8-C9	1.158(6)
N3-Cd1-N5c	176.85(13)	N3-Cd1-N6	92.82(12)
N5c-Cd1-N6	85.52(12)	N3-Cd1-N1	91.19(12)
N5c-Cd1-N1	90.34(12)	N6-Cd1-N1	175.15(12)
N3-Cd1-N2a	88.21(12)	N5-Cd1-N2a	94.38(13)
N6-Cd1-N2a	87.50(13)	N1-Cd1-N2a	95.36(12)
N3-Cd1-N7b	86.55(12)	N5-Cd1-N7b	90.71(13)
N6-Cd1-N7b	87.74(12)	N1-Cd1-N7b	89.78(12)
N2-Cd1-N7b	172.74(12)	C6-N3-Cd1	159.1(3)
C7-N4-C6	123.6(4)	C7-N5-Cd1d	160.2(3)
C8-N6-Cd1	149.8(3)	N3-C6-N4	172.1(4)
C8-N7-C9	119.4(4)	C8-N7-Cd1e	212.9(3)

C9-N7-Cd1e	116.4(3)	N5-C7-N4	172.3(4)
N6-C8-N4	173.5(5)	N8-C9-N7	174.4(5)
Compound 2			
Cd1-O1	2.2916(16)	Cd1-O2	2.2930(16)
Cd1-N6a	2.303(2)	Cd1-N1	2.307(2)
Cd1-N4	2.312(2)	Cd1-N3b	2.332(2)
Cd2-N7c	2.274(2)	Cd2-N7	2.274(2)
Cd2-N9d	2.3041(19)	Cd2-N9	2.3041(19)
Cd2-N5c	2.3858(19)	Cd2-N5	2.3858(19)
N4-C3	1.153(3)	C4-N6	1.150(3)
C4-N5	1.320(3)	C3-N5	1.316(3)
C5-N7	1.155(3)	C5-N8	1.304(3)
C8-C7	1.373(3)	C8-C9	1.396(4)
N8-C6	1.301(3)	C7-N10	1.348(3)
C6-N9	1.160(3)		
O1-Cd1-O2	178.17(6)	O1-Cd1-N6a	91.78(7)
O2-Cd1-N6	87.92(7)	O1-Cd1-N1	94.36(7)
O2-Cd1-N1	83.83(7)	N6-Cd1-N1	87.16(8)
O1-Cd1-N4	91.15(6)	O2-Cd1-N4	90.68(7)
N6-Cd1-N4a	96.38(7)	N1-Cd1-N4	173.37(7)
O1-Cd1-N3	89.93(7)	O2-Cd1-N3b	90.36(7)
N6a-Cd1-N3b	178.23(7)	N1-Cd1-N3b	92.24(8)
N4-Cd1-N3	84.05(8)	N7-Cd2-N7c	180
N7c-Cd2-N9d	93.54(7)	N7-Cd2-N9	86.46(7)
N7-Cd2-N9d	86.46(7)	N7c-Cd2-N9d	93.54(7)
N9-Cd2-N9	180	N7-Cd2-N5	88.70(7)
N7-Cd2-N5	91.30(7)	N9c-Cd2-N5	87.20(7)
N9-Cd2-N5	92.80(7)	N7c-Cd2-N5c	91.30(7)
N7c-Cd2-N5	88.70(7)	N9a-Cd2-N5	92.80(7)
N9-Cd2-N5	87.20(7)	N5-Cd2-N5	180
N1-C1-N2	173.4(2)	C1-N1-Cd1a	136.64(18)
N10-O1-Cd1	116.19(12)	N3-C2-N2	172.7(3)
C1-N2-C2	121.0(2)	C3-N4-Cd1	154.75(18)
N6-C4-N5	174.4(2)	C2-N3-Cd1	147.3(2)
N4-C3-N5	174.0(2)	C3-N5-C4	119.17(19)
C3-N5-Cd2	119.32(14)	C4-N5-Cd2	121.49(14)
N7-C5-N8	173.1(2)	C7-C8-C9	120.2(2)
C6-N8-C5	120.2(2)	C5-N7-Cd2	148.21(18)
C4-N6-Cd1b	159.13(19)	N9-C6-N8	174.3(2)
C6-N9-Cd2b	143.49(17)		
Compound 3			
Cd1-O1	2.279(3)	Cd1-N1a	2.323(3)
Cd1-N3b	2.331(3)	C1-N1	1.154(5)
C1-N2	1.314(4)	Cd2-O2c	2.284(3)
Cd2-N4c	2.314(3)	Cd2-N6d	2.325(3)
C2-N3	1.150(5)	C2-N2	1.315(4)
C3-N4	1.154(5)	C3-N5	1.311(4)
C4-N6	1.149(5)	C4-N5	1.319(4)

O1a-Cd1-N1a	90.25(11)	O1-Cd1-N3	92.51(11)
N1-Cd1-N3	94.51(12)	N1-C1-N2	173.0(4)
N1-C1-Cd1	164.1(3)	O2-Cd2-N4	92.66(11)
O2c-Cd2-N6d	90.31(11)	N4c-Cd2-Nd6	93.87(13)
N4-Cd2-N6	86.13(13)	N3-C2-N2	173.4(4)
C1-N2-C2	120.2(3)	C2-N3-Cd1e	140.2(3)
N4-C3-N5	173.9(4)	C3-N4-Cd2	142.5(3)
N6-C4-N5	174.6(4)	C3-N5-C4	120.6(3)
C4-N6-Cd2f	160.6(3)		
Compound 4			
Cd1-N6	2.2916(11)	Cd1-N1	2.2938(11)
Cd1-N5a	2.3264(11)	Cd1-N3	2.3344(11)
Cd1-Nb8	2.3545(12)	Cd1-N2	2.4523(10)
N3-C5	1.1550(17)	N4-C6	1.2958(16)
N4-C5	1.3097(16)	N5-C6	1.1668(16)
N6-C7	1.1571(16)	N7-C7	1.3040(15)
N7-C8	1.3084(15)	N8-C8	1.1553(16)
N6-Cd1-N1	98.56(4)	N6-Cd1-Na5	97.61(5)
N1-Cd1-N5a	163.82(4)	N6-Cd1-N3	91.63(4)
N1-Cd1-N3	89.01(4)	N5-Cd1-N3	89.97(4)
N6-Cd1-N8	86.01(4)	N1-Cd1-N8b	93.67(4)
N5-Cd1-N8	88.02(4)	N3-Cd1-N8b	176.67(4)
N6-Cd1-N2	173.82(4)	N1-Cd1-N2	77.25(4)
N5-Cd1-N2	86.68(4)	N3-Cd1-N2	92.82(4)
N8-Cd1-N2	89.71(4)	C5-N3-Cd1	161.76(10)
C6-N4-C5	121.36(11)	C6-N5-Cd1c	126.04(9)
C7-N6-Cd1	161.34(10)	C7-N-C8	119.49(11)
C8-N8-Cd1b	161.30(10)	N3-C5-N4	172.64(14)
N5-C6-N4	173.37(13)	N6-C7-N7	174.28(13)
N8-C8-N7	173.79(13)		
Compound 5			
Cd1-N1	2.321(2)	Cd1-N3a	2.350(3)
Cd1-N4	2.351(9)	Cd1-N7	2.3906(16)
Cd1-N7b	2.3906(16)	C1-N1	1.150(4)
C1-N2	1.305(3)	N2-C2	1.300(3)
C2-N3	1.149(4)	N4-C3	1.144(10)
C3-N5	1.307(6)	N5-C4	1.311(6)
C4-N6	1.142(10)		
N1-Cd1-N3a	175.49(9)	N1-Cd1-N7	93.65(6)
N3a-Cd1-N4	89.9(2)	N3-Cd1-N7	89.87(7)
N4-Cd1-N7	88.04(17)	N4-Cd1-N7	165.38(17)
N7-Cd1-N7b	77.34(8)	N1-C1-N2	173.2(3)
C1-N1-Cd1	168.5(2)	C2-N2-C1	121.2(2)
N3-C2-N2	173.4(3)	C2-N3-Cd1c	162.6(3)
C3-N4-Cd1	175.1(8)	N4-C3-N5	171.6(6)
C3-N5-C4	120.8(5)	N6-C4-N5	172.0(7)
Compound 6			

Cd1-N1	2.3051(9)	Cd1-N5	2.3565(10)
Cd1-N2	2.3655(9)	N2-C12	1.1608(13)
N3-C12	1.3075(13)	N3-C13	1.3196(13)
N4-C13	1.1588(14)		
N1-Cd1-N5	105.81(3)	N1-Cd1-N2	91.80(3)
N5-Cd1-N2a	93.09(3)	C12-N2-Cd1	162.29(8)
C12-N3-C13	121.82(9)	N2-C12-N3	172.70(11)
N4-C13-N3	172.23(11)		

Symmetry codes for **1**: (a) x, −y, −1/2 + z; (b) x, 1 − y,1/2 + z; (c) −1/2 + x, 1/2 + y, z; (d) 1/2 + x, −1/2 + y, z; and (e) x, 1 − y, −1/2 + z. Symmetry codes for **2**: (a) x, y − 1, z; (b) x, y + 1, z; (c) 2 − x, 2 − y, 1 − z; and (d) 2 − x, 3 − y, 1 − z. Symmetry codes for **3**: (a) 1 − x, 1 − y, 1 − z; (b) 2 − x, −y, 1 − z; (c) −x, 1 − y, 2 − z; (d) −x, 2 − y, 2 − z; (e) x + 1, y − 1, x; and (f) x, y + 1, z. Symmetry codes for **4**: (a) x + 1, y, z; (b) 2 − x,1 − y,1 − z; and (c) x − 1, y, z. Symmetry codes for **5**: (a) x − 1/2, y, −z + 3/2; (b) x, −y + 1/2, z; and (c) x + 1/2, y, −z + 3/2. Symmetry code for **6**: (a) 1 − x, 1 − y, 1 − x.

Table S2. Possible hydrogen bonds of compounds **1–4** and **6**.

D-H..A*	**Symmetry of A**	**D…A (Å)**	**D-H…A (°)**
Compound **1**			
N2-H11…N4	[−1/2 + x, −1/2 + y, z]	3.096(5)	175
N2-H12…N8	[x, −1 + y, z]	3.166(5)	164
Compound **2**			
O2-H1… N2	[2 − x, −y,2 − z]	2.869(3)	168
O2-H2… O1	[1 + x, y, z]	2.672(2)	176
Compound **3**			
O1-H1… N2	[−1 + x, y, z]	2.859(4)	174
O1-H2 …O3		2.626(5)	168
O2-H3 …N5	[1 + x, −1 + y,z]	2.859(5)	172
O2-H4 …O3		2.634(6)	163
Compound **4**			
N1-H1A…N7	[1 − x, 1 − y, 1 − z]	3.2046(16)	160
N1-H1B…N5	[1 + x, 1/2 − y, −1/2 + z]	3.1402(15)	151
Compound **6**			
N1-H1A…N4	[−1/2 + x, 3/2 − y, 1/2 + z]	3.0440(13)	156
N1-H1B…N3	[−1 + x, y, z]	3.0534(13)	165
N5-H5A…N3	[2 − x, 1 − y, 1 − z]	3.2013(14)	157
N5-H5B…N4	[−1/2 + x, 3/2 − y, 1/2 + z]	3.2200(15)	144

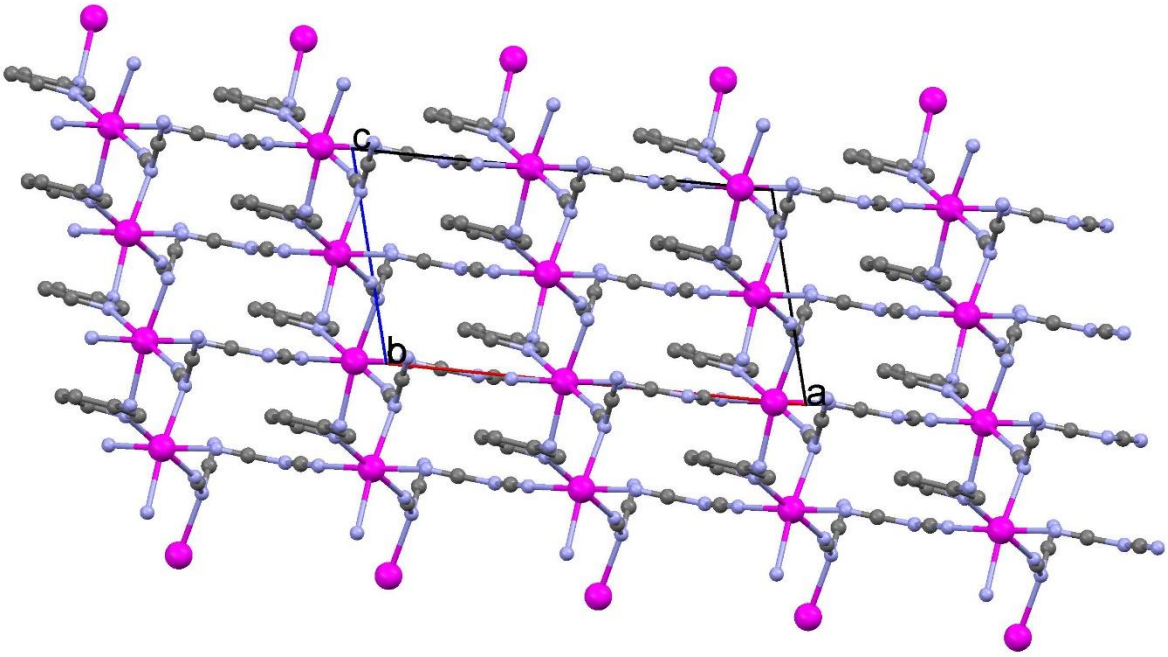

Figure S10. Packing plot of **1**.

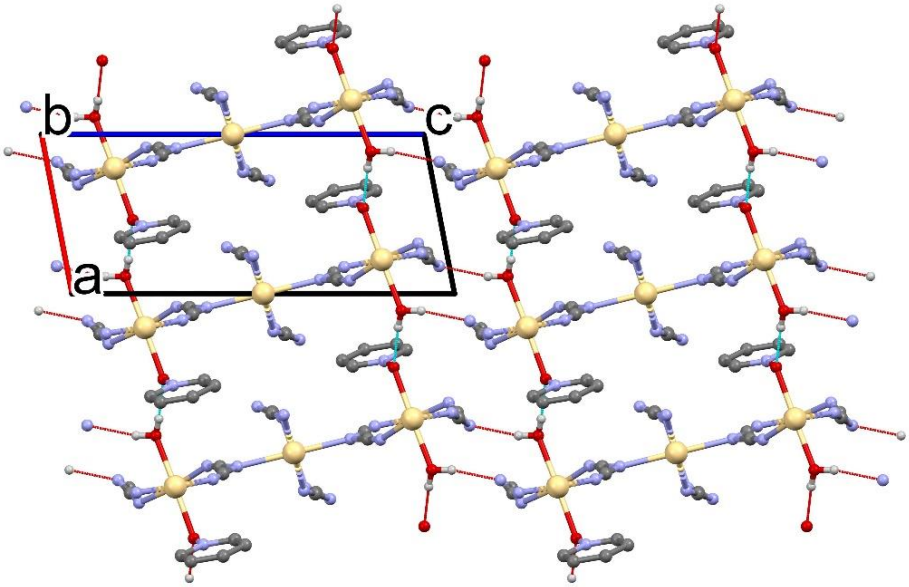

Figure S11. Packing plot of **2**.

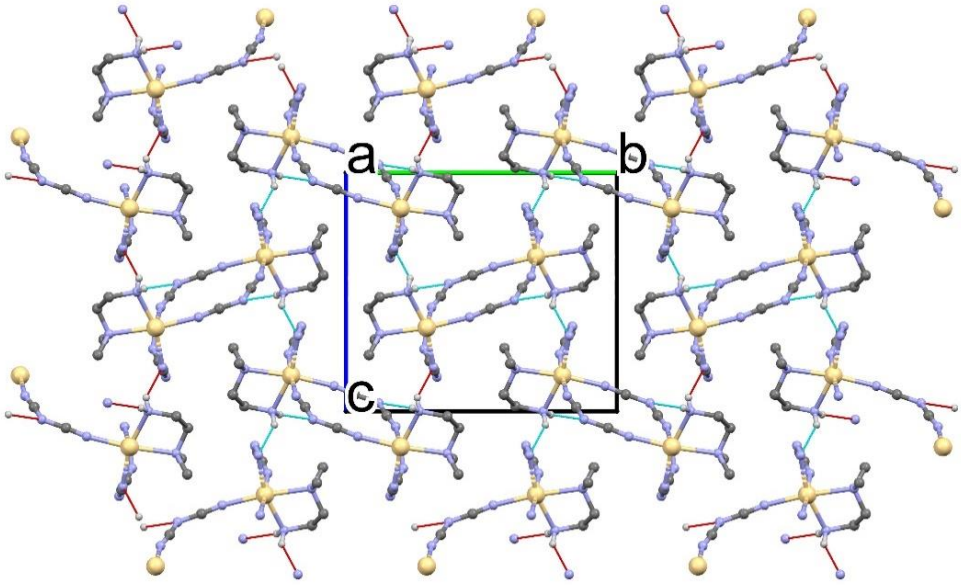

Figure S12. Packing plot of **4**.

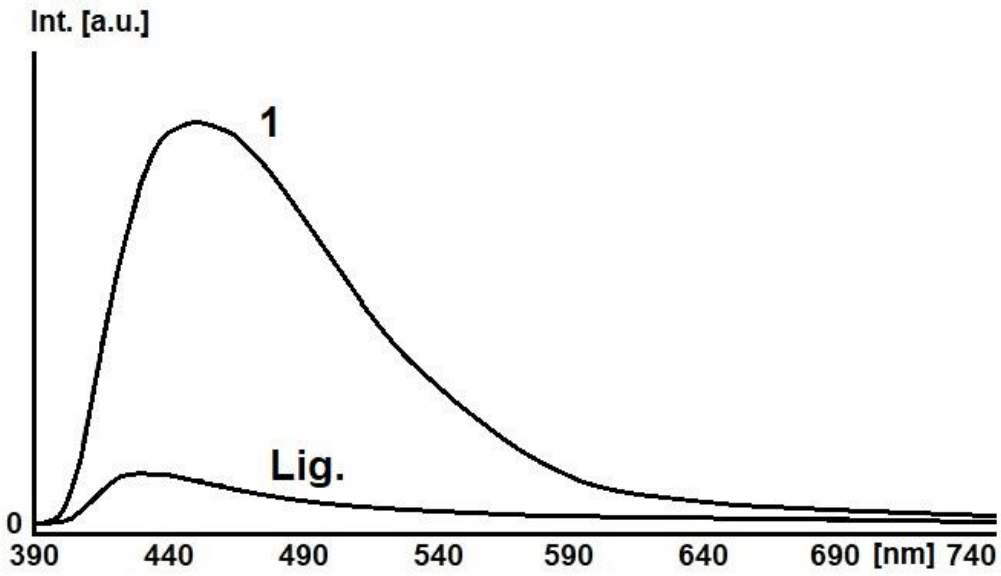

Figure S13. Emission spectra of **1** and 3-ampy (Lig) with excitation wavelength at 366 nm. (Maximum intensity of **1** at 460 nm and of 3-ampy Lig. at 429 nm.)

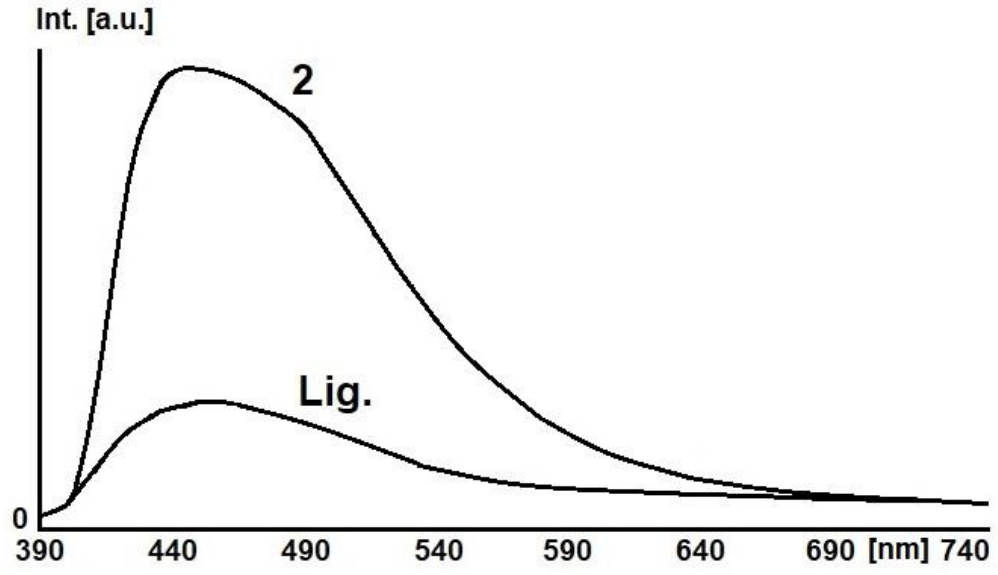

Figure S14. Emission spectra of **2** and pyNO (Lig) with excitation wavelength at 366 nm. (Maximum intensity of **2** at 445 nm and of pyNO Lig. at 454 nm.)

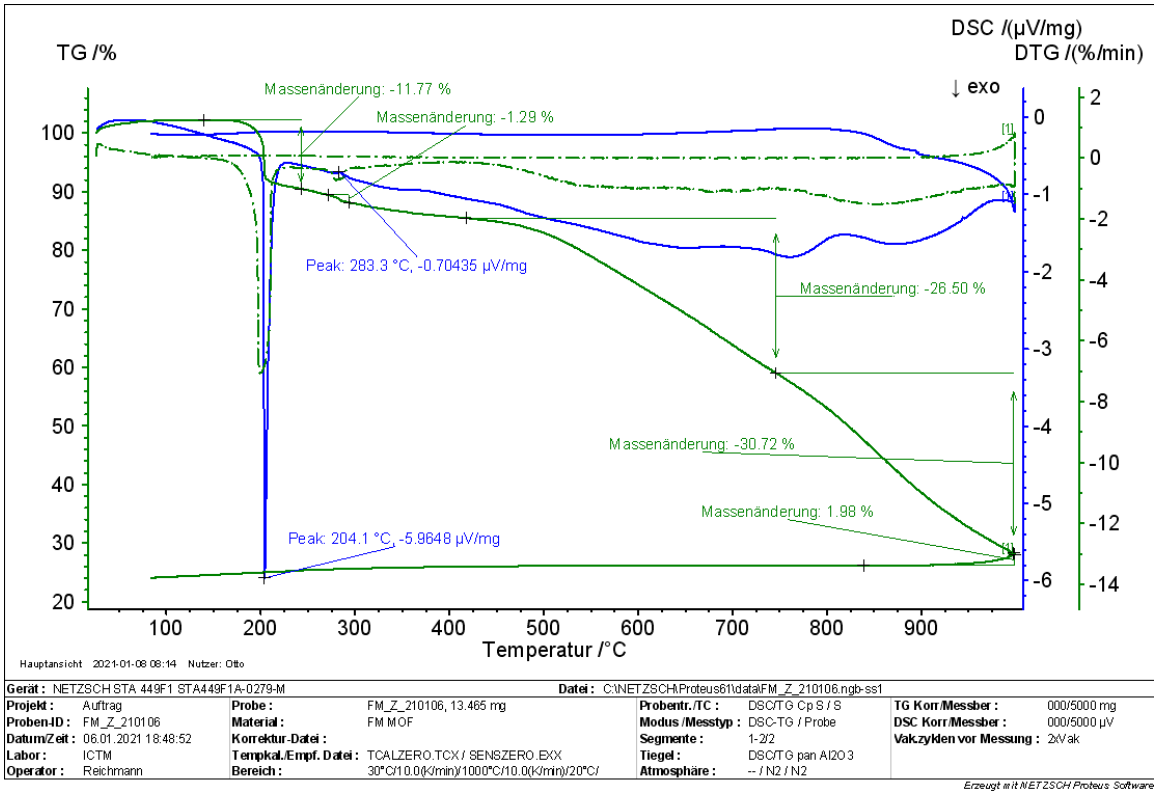

Figure S15. Thermal analysis plot of **1**.

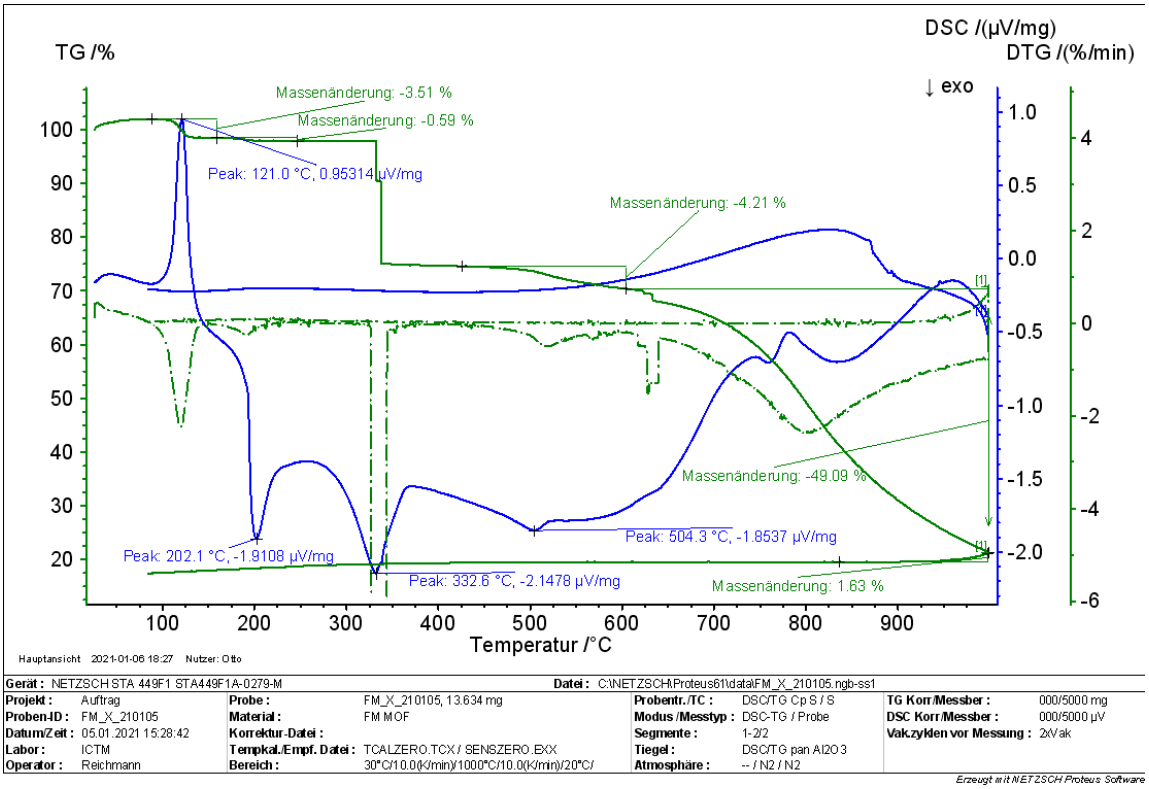

Figure S16. Thermal analysis plot of **2**.

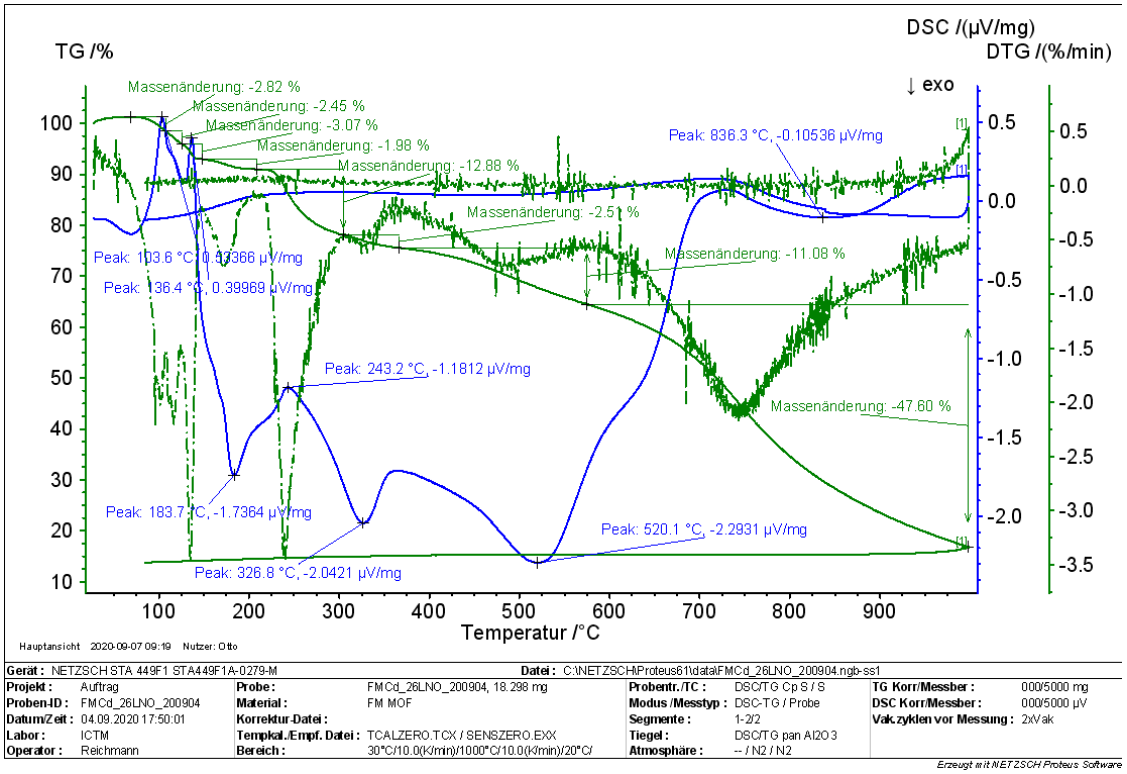

Figure S17. Thermal analysis plot of **3**.

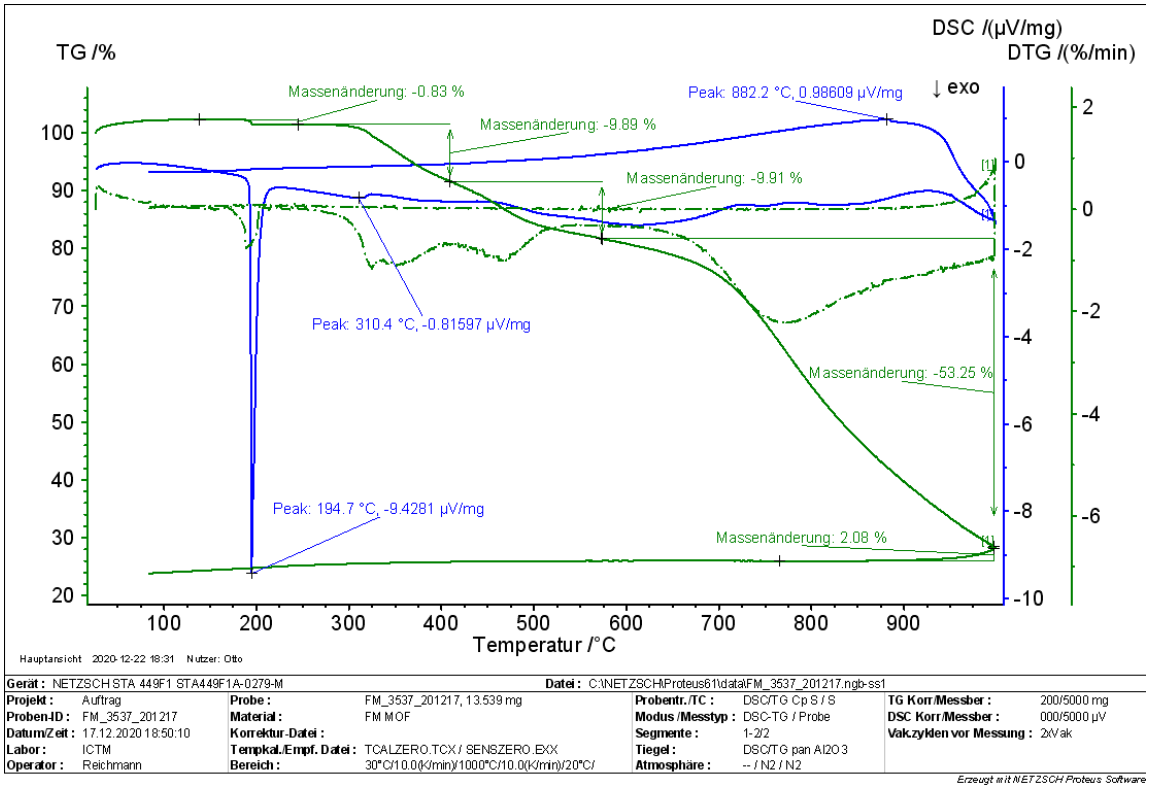

Figure S18. Thermal analysis plot of **4**.

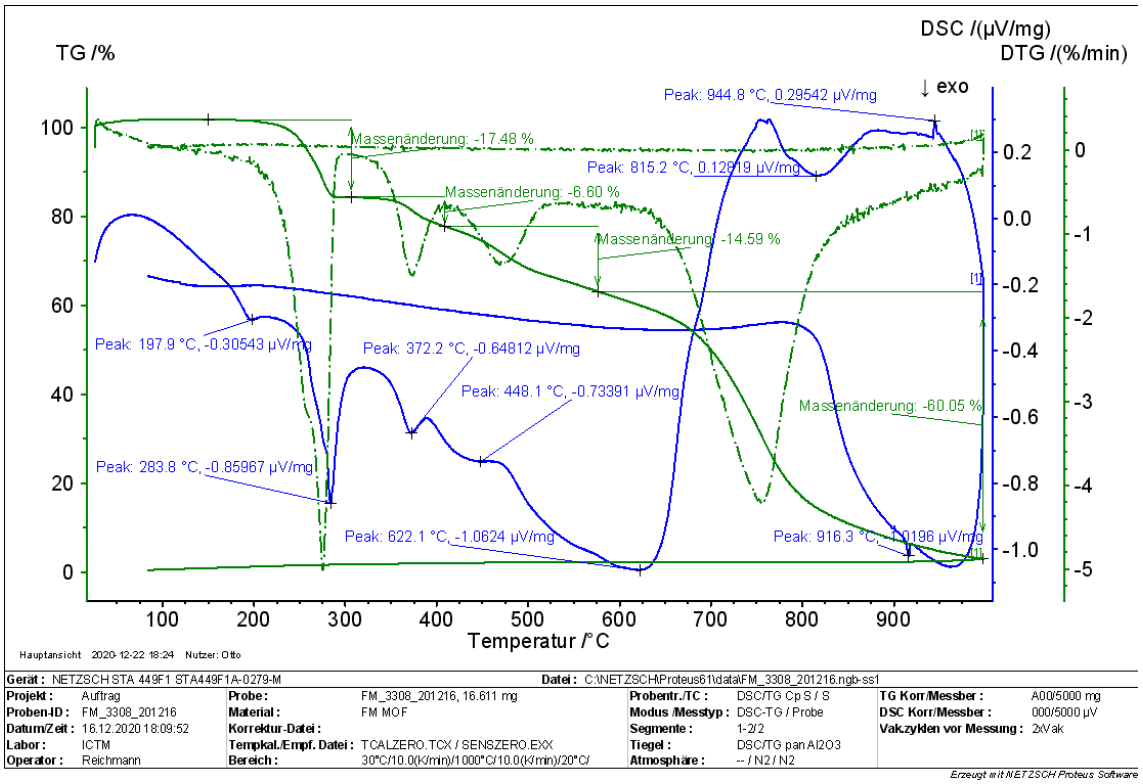

Figure S19. Thermal analysis plot of **5**.

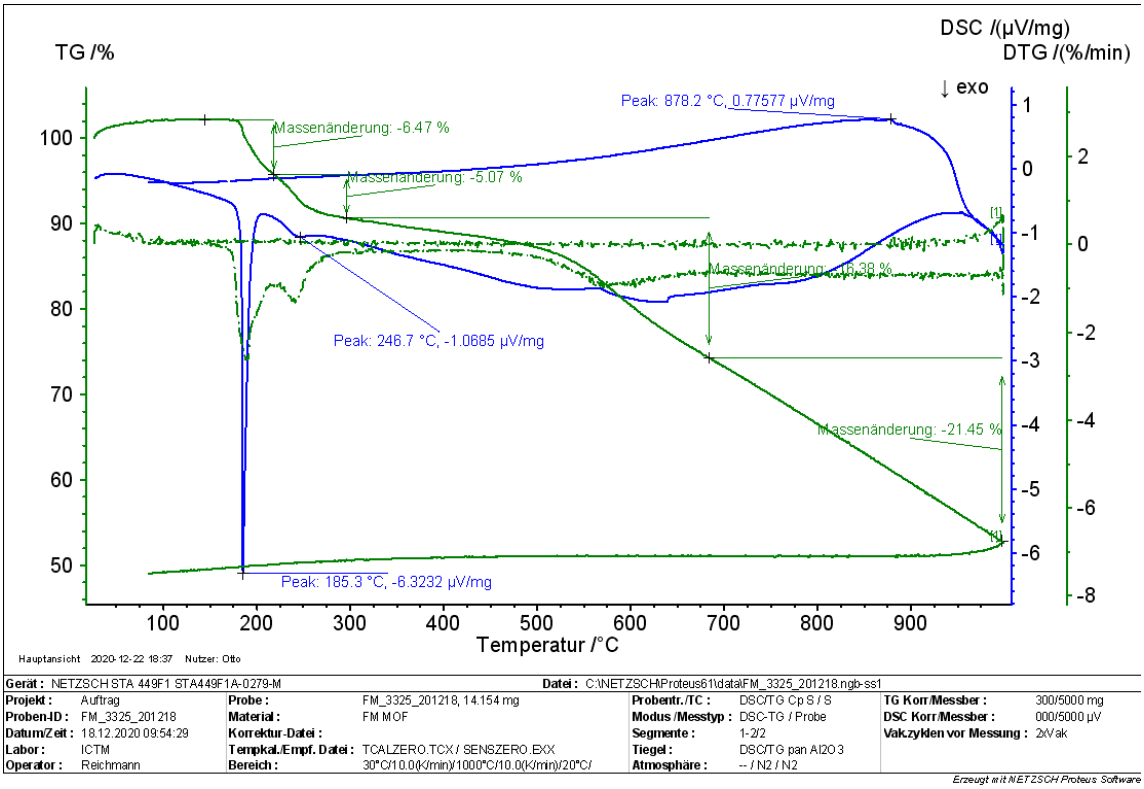

Figure S20. Thermal analysis plot of **6**.

Supplementary Materials: Supplementary data: bond parameters (Table S1), hydrogen bond systems (Table S2), and XRD powder pattern (Figures S1–S6) for compounds **1–6**, respectively; IR spectra (Figures S7–S9) for **1–3**; packing plots (Figures S10–S12) for **1**, **2**, and **4**; luminescence spectra (Figures S13 and S14) for compounds **1** and **2,** and thermal analysis plots (Figures S15–S20) for compounds **1–6**, respectively.

Author Contributions: F.A.M., R.C.F., and A.T. performed the X-ray structural analysis. S.S.M., P.V.J., M.M.H., F.R.L., and N.M.H.S. contributed to the synthesis and spectral characterization of the designed compounds. F.A.M. and R. K. contributed to studying the thermal and luminescence properties of the complexes. F.A.M., S.S.M., F.R.L., K.J.G., and N.M.H.S. contributed to the writing of the manuscript. All authors have read and agreed to the published version of the manuscript.

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