Supporting Information

Synthesis, Structure, and Spectroscopic Properties of Luminescent Coordination Polymers based on the 2,5-Dimethoxyterephthalate Linker

Aimée E. L. Cammiade,[a] Laura Straub,[a] David van Gerven,[a] Mathias S. Wickleder,[a] Uwe Ruschewitz*[a]

[a] A. E. L. Cammiade, Dr. L. Straub, Dr. D. van Gerven, Prof. Dr. M. S. Wickleder, Prof. Dr. U. Ruschewitz
Department of Chemistry
University of Cologne
Greinstraße 6, D-50939 Köln, Germany
E-mail: uwe.ruschewitz@uni-koeln.de

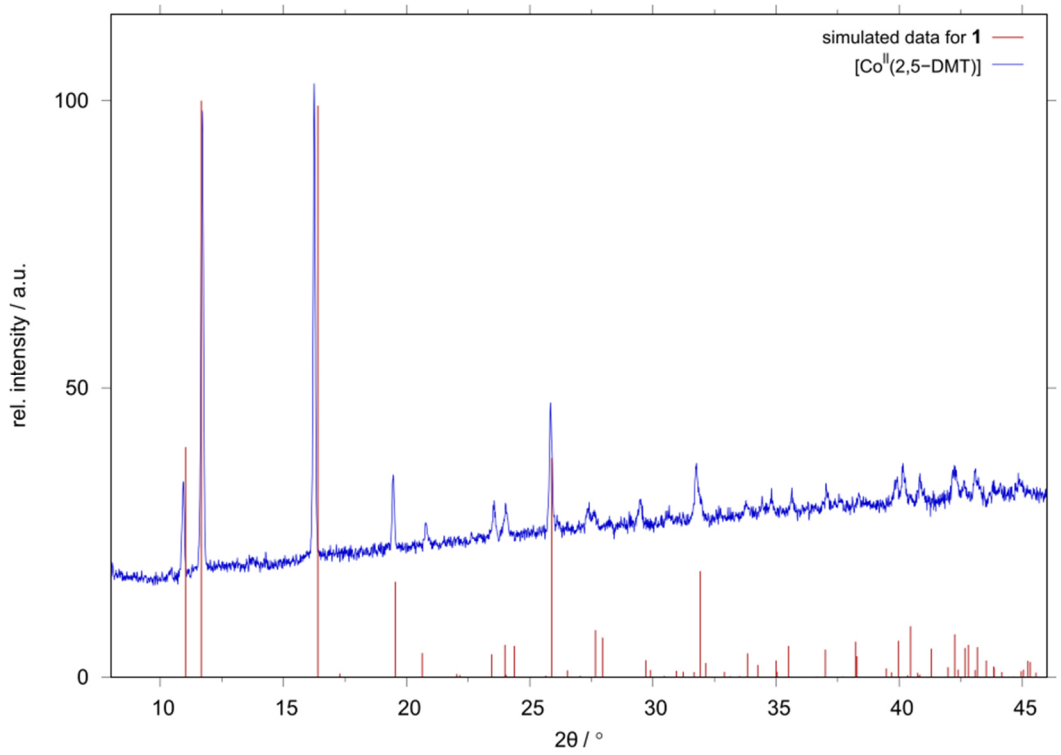


Figure S1. PXRD pattern of [Co^{II}(2,5-DMT)] (**1**), blue curve (Rigaku *Miniflex 600-C*, Cu Kα radiation, RT). A line diagram (red), simulated from the crystal structure of **1** (100 K), is given for comparison.

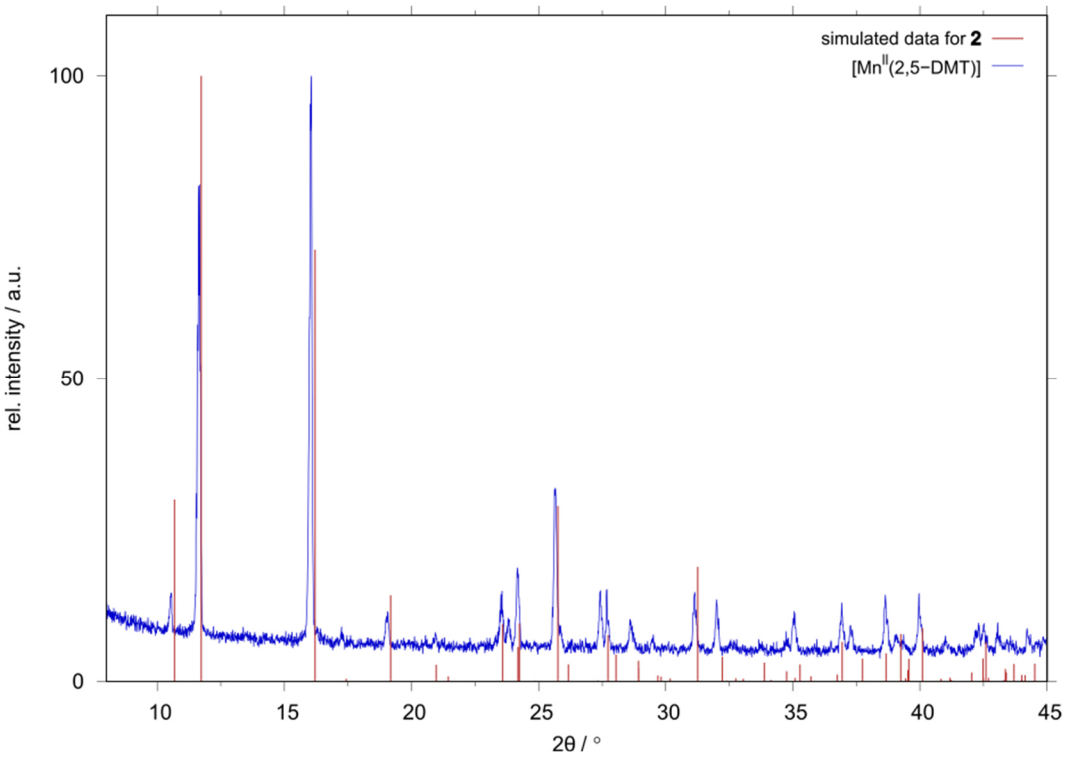


Figure S2. PXRD pattern of [Mn^{II}(2,5-DMT)] (**2**), blue curve (Rigaku *Miniflex 600-C*, Cu Kα radiation, RT). A line diagram (red), simulated from the crystal structure of **2** (153 K), is given for comparison.

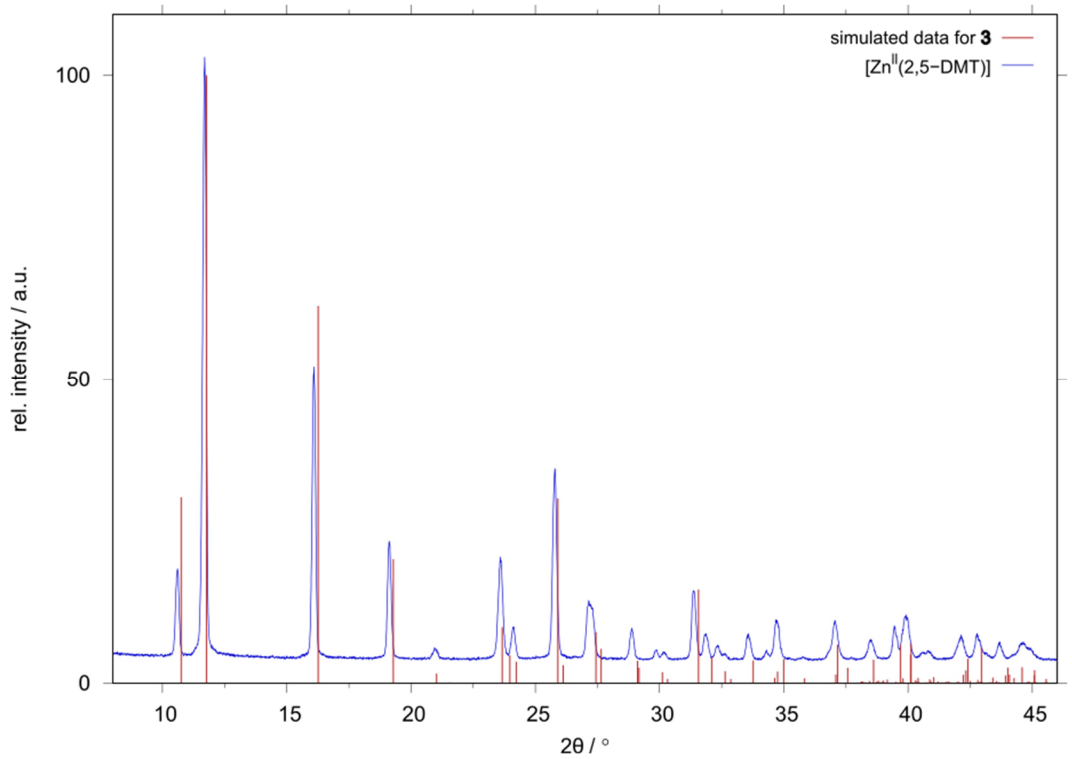


Figure S3. PXRD pattern of [Zn^{II}(2,5-DMT)] (**3**), blue curve (Rigaku *Miniflex 600-C*, Cu Kα radiation, RT). A line diagram (red), simulated from the crystal structure of **3** (153 K), is given for comparison

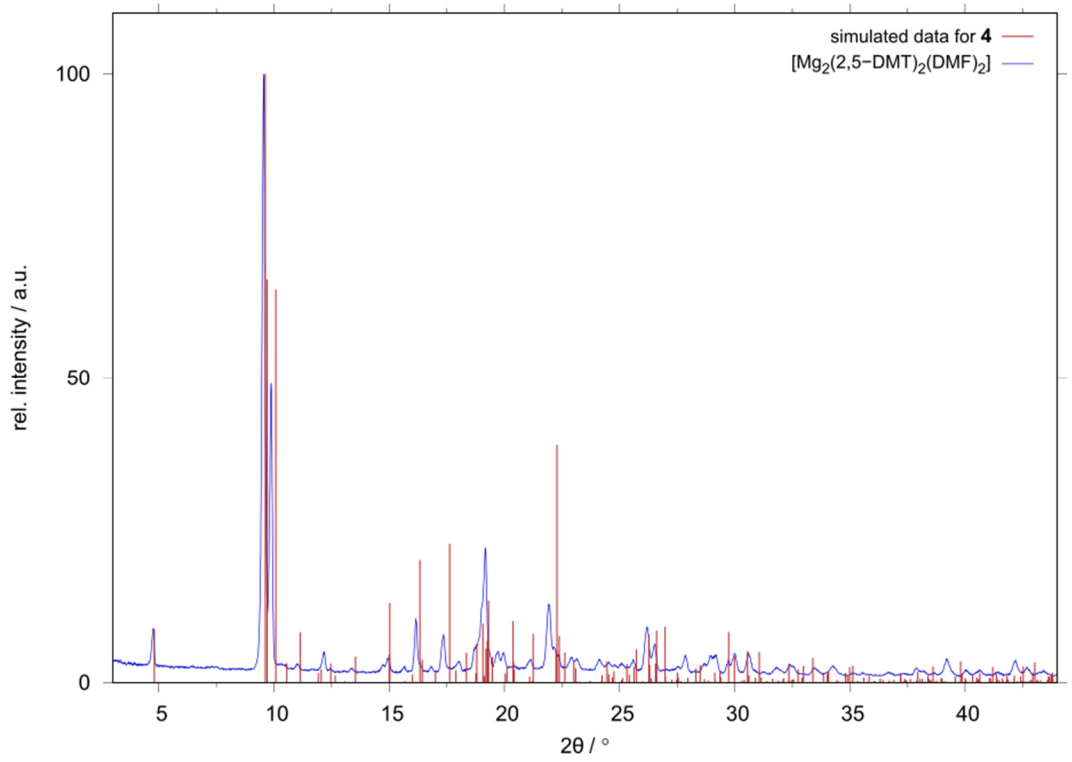


Figure S4. PXRD pattern of [Mg_2(2,5-DMT)$_2$(DMF)$_2$] (**4**), blue curve (Rigaku *Miniflex 600-C*, Cu Kα radiation, RT). A line diagram (red), simulated from the crystal structure of **4** (100 K), is given for comparison.

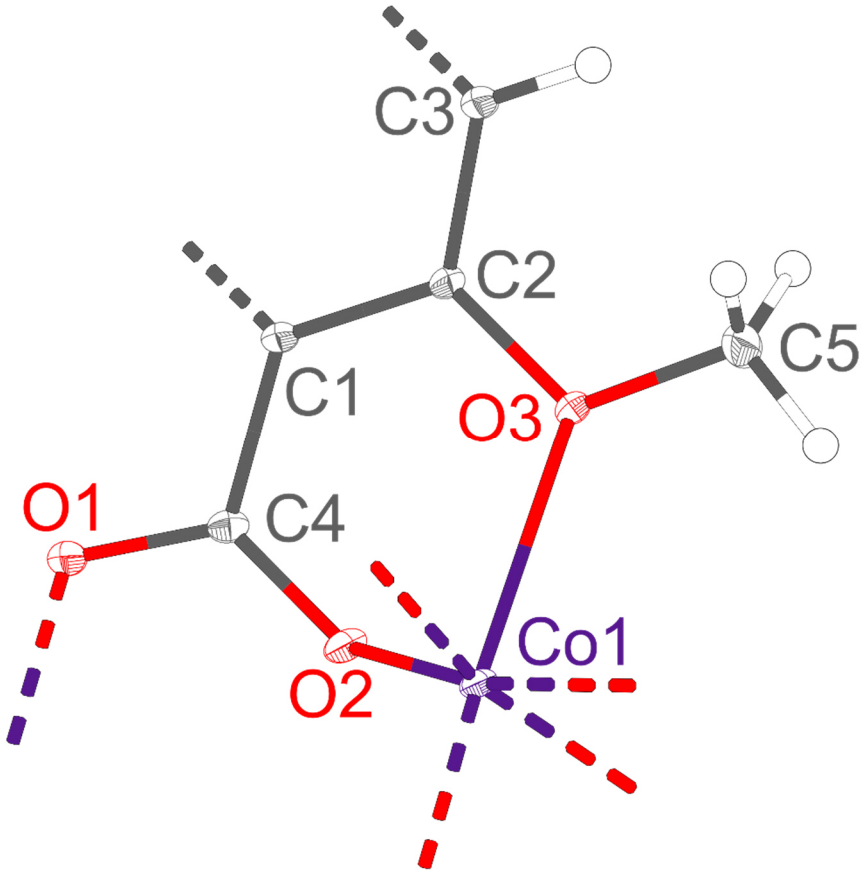


Figure S5. Asymmetric unit of [Co^{II}(2,5-DMT)] (**1**) with atomic numbering. Thermal ellipsoids are drawn with a 50% probability.

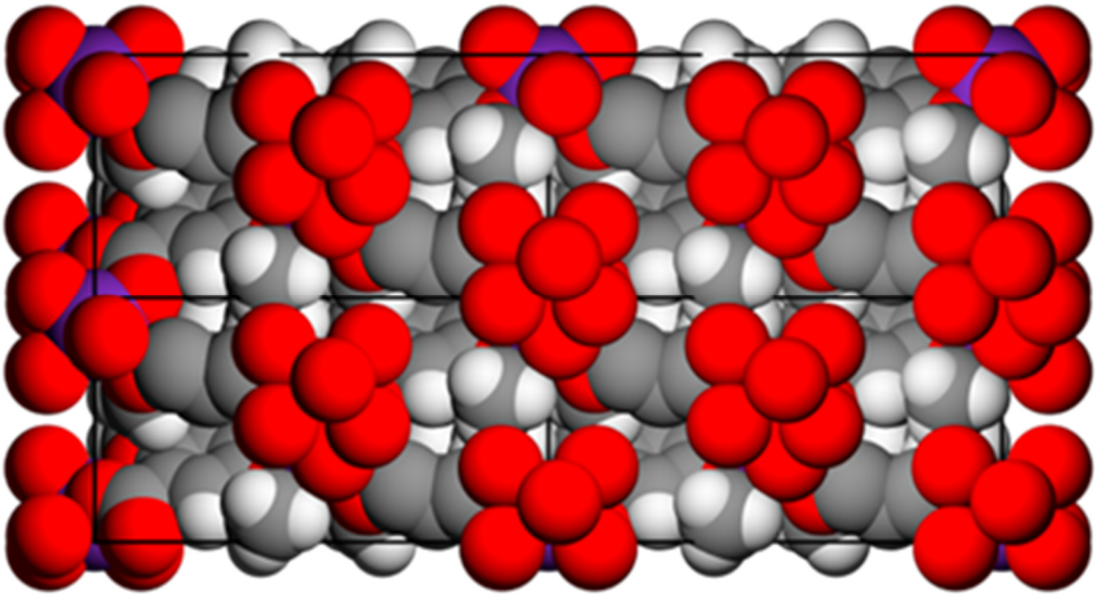


Figure S6. Space filling representation of the crystal structure of [Co^{II}(2,5-DMT)] (**1**) in a view along [001].

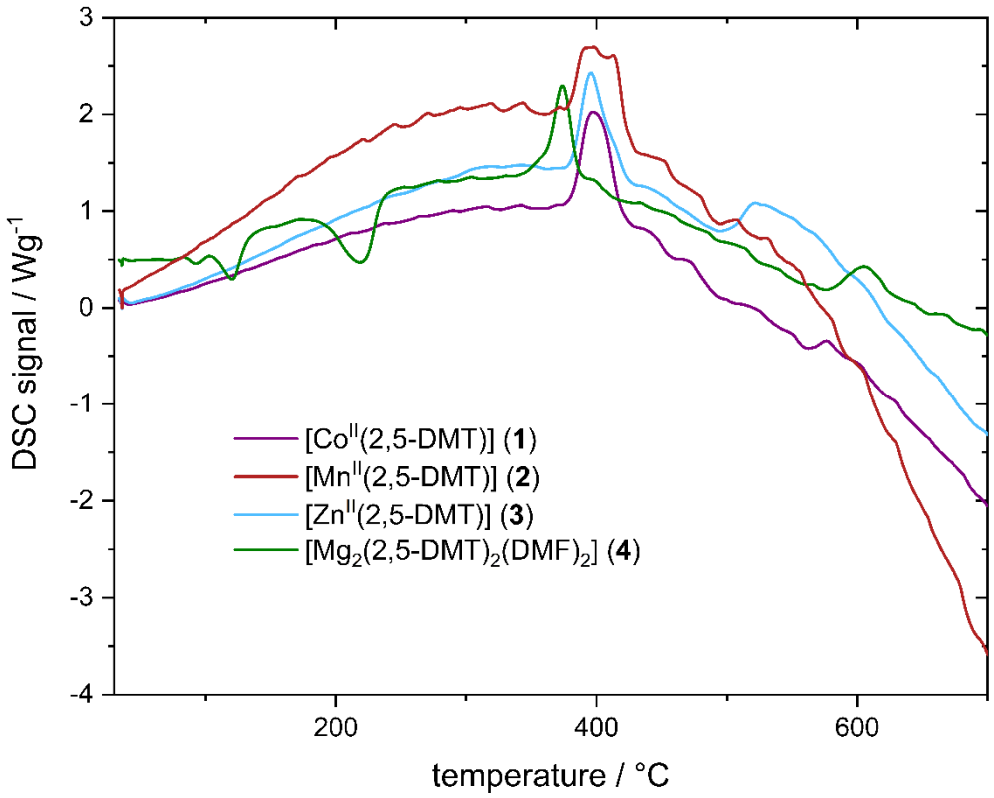


Figure S7: DSC measurements of compounds **1**-**4**.

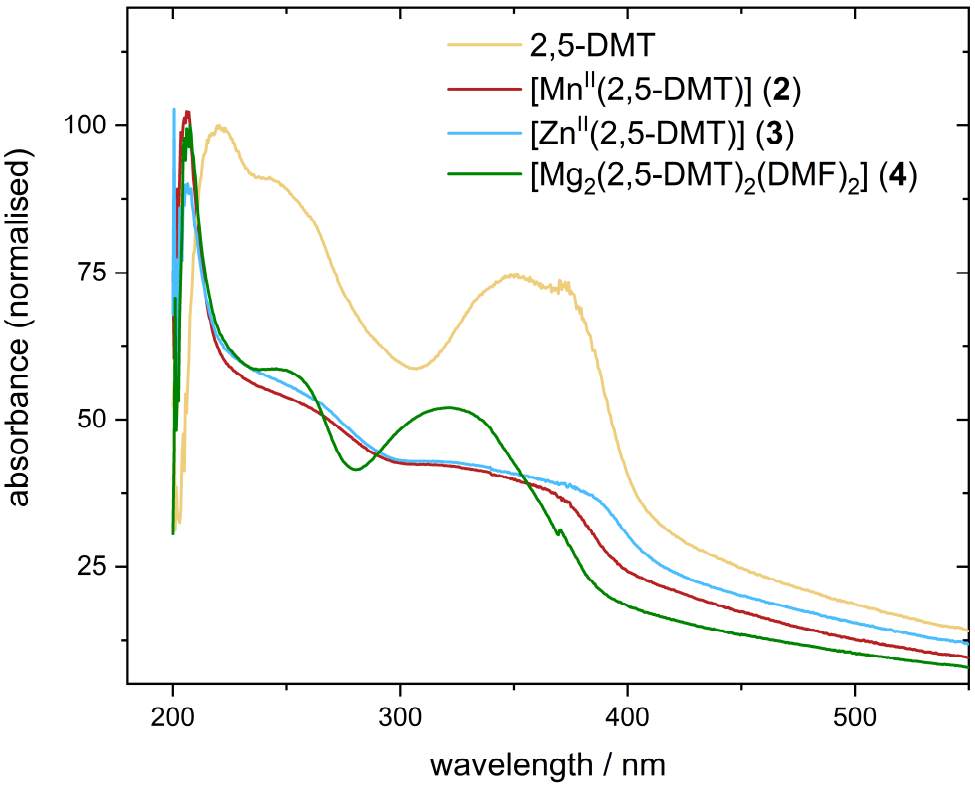
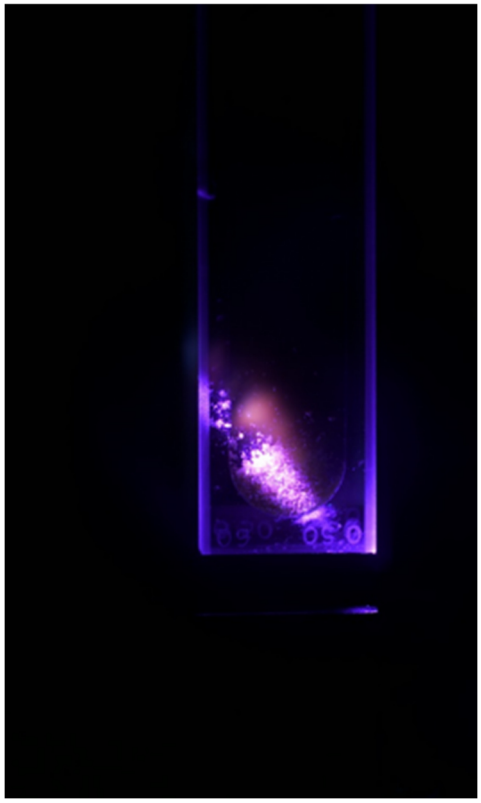


Figure S8. UV/vis measurements of 2,5-dimethoxy terephthalic acid (2,5-DMT) and compounds **2-4.**

1: [Co^{II}(2,5-DMT)]

2: [Mn^{II}(2,5-DMT)]



3: [Zn^{II}(2,5-DMT)]

4: [Mg_2(2,5-DMT)$_2$(DMF)$_2$]

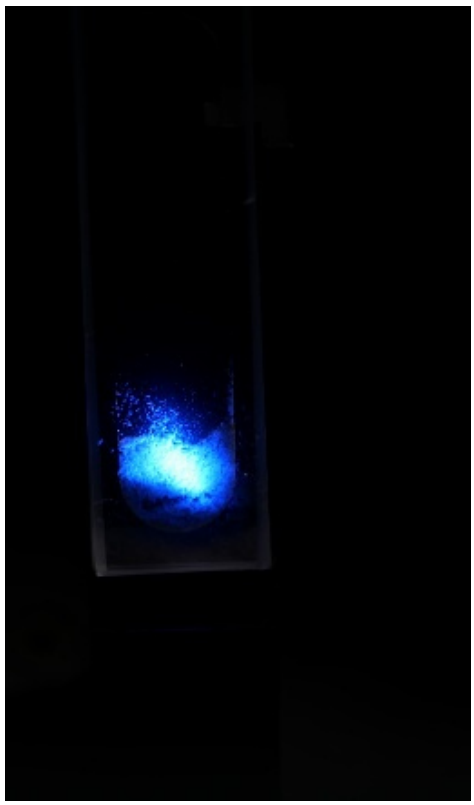


Figure S9: Photographs of fluorescence of compounds **1-4** upon blue light irradiation (λ = 405 nm).

Table S1. Crystal data and structure refinement details for [Co^{II}(2,5-DMT)] (**1**).

CCDC number	2225418
Empirical formula	$C_{10}H_8CoO_6$
Formula weight	283.09
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	*C*2/*c* (15)
a [Å]	16.1305(5)
b [Å]	8.6024(3)
c [Å]	7.3426(2)
α [°]	90
β [°]	96.425(1)
γ [°]	90
Volume [Å^3]	1012.47(5)
Z	4
ρ_{calc} [g·cm^{-3}]	1.857
μ [mm^{-1}]	0.889
F(000)	572
Crystal size [mm^3]	0.16×0.14×0.11
Crystal colour	clear pinkish violet
Crystal shape	block
Radiation	AgK_α (λ=0.56086 Å)
2Θ range [°]	4.24 to 52.90 (0.63 Å)
Index ranges	-25 ≤ h ≤ 25 -13 ≤ k ≤ 13 -11 ≤ l ≤ 11
Reflections collected	15620
Independent reflections	2133 R_{int} = 0.0298 R_{sigma} = 0.0180
Completeness to Θ = 19.665°	99.8 %
Data / Restraints / Parameters	2133/0/79
Goodness-of-fit on F^2	1.118
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0225 wR_2 = 0.0584
Final *R* indexes [all data]	R_1 = 0.0238 wR_2 = 0.0589
Largest peak/hole [eÅ^{-3}]	0.92/-0.38

Table S2. Atomic coordinates and U_{eq} [Å^2] for [Co^{II}(2,5-DMT)] (**1**).

Atom	***x***	***y***	***z***	U_{eq}
Co1	½	0.61097(2)	¼	0.00744(5)
O1	0.60171(4)	0.52493(9)	0.7255(1)	0.0107(1)
O2	0.52456(4)	0.66173(8)	0.51402(9)	0.0095(1)
O3	0.60474(4)	0.80245(9)	0.2654(1)	0.0112(1)
C1	0.67322(5)	0.6906(1)	0.5410(1)	0.0081(1)
C2	0.67697(5)	0.7774(1)	0.3802(1)	0.0084(1)
C4	0.59436(5)	0.6213(1)	0.5964(1)	0.0083(1)
C3	0.75368(5)	0.8355(1)	0.3422(1)	0.0091(1)
H3	0.756398	0.894597	0.233704	0.011
C5	0.61164(7)	0.8929(2)	0.1037(2)	0.0215(2)
H5A	0.649021	0.840157	0.027163	0.032
H5B	0.634240	0.995706	0.138642	0.032
H5C	0.556381	0.904534	0.034626	0.032

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S3. Atomic displacement parameters (Å^2) for [Co^{II}(2,5-DMT)] (**1**).

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.0059(3)	0.0092(3)	0.0089(3)	−0.0014(2)	−0.0003(2)	0.0004(3)
C2	0.0062(3)	0.0091(3)	0.0094(3)	−0.0010(3)	−0.0014(3)	0.0008(3)
C3	0.0067(3)	0.0112(4)	0.0092(3)	−0.0017(3)	−0.0006(3)	0.0015(3)
C4	0.0067(3)	0.0095(3)	0.0085(3)	−0.0011(3)	0.0005(3)	−0.0016(3)
C5	0.0149(4)	0.0268(5)	0.0205(5)	−0.0084(4)	−0.0074(4)	0.0149(4)
Co1	0.00448(7)	0.01072(8)	0.00697(8)	0	−0.00002(5)	0
O1	0.0078(3)	0.0133(3)	0.0109(3)	−0.0020(2)	−0.0002(2)	0.0029(2)
O2	0.0059(2)	0.0130(3)	0.0093(3)	0.0005(2)	−0.0003(2)	−0.0007(2)
O3	0.0068(3)	0.0137(3)	0.0121(3)	−0.0024(2)	−0.0033(2)	0.0051(2)

Table S4. Bond lengths and angles for [Co^{II}(2,5-DMT)] (**1**).

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
Co1–O1$^{\#1}$	2.0389(7)	O1–Co1–O1	110.02(4)
Co1–O1$^{\#2}$	2.0389(7)	O1–Co1–O3	167.84(3)
Co1–O2	1.9834(7)	O1–Co1–O3	167.84(3)
Co1–O2$^{\#3}$	1.9834(7)	O1–Co1–O3	79.93(3)
Co1–O3	2.3533(7)	O1–Co1–O3	79.93(3)
Co1–O3$^{\#3}$	2.3532(7)	O2–Co1–O1	97.93(3)
O1–C4	1.254(1)	O2–Co1–O1	96.58(3)
O2–C4	1.266(1)	O2–Co1–O1	97.93(3)
O3–C2	1.376(1)	O2–Co1–O1	96.58(3)
O3–C5	1.435(1)	O2–Co1–O2	154.56(4)
C1–C2	1.404(1)	O2–Co1–O3	74.63(3)
C1–C4	1.502(1)	O2–Co1–O3	87.52(3)
C1–C3$^{\#4}$	1.397(1)	O2–Co1–O3	87.52(3)
C2–C3	1.391(1)	O2–Co1–O3	74.63(3)
C3–H3	0.9500	O3–Co1–O3	91.15(4)
C5–H5A	0.9800	C4–O1–Co1	115.89(6)
C5–H5B	0.9800	C4–O2–Co1	118.44(6)
C5–H5C	0.9800	C2–O3–Co1	118.29(6)
		C2–O3–C5	116.94(8)
		C5–O3–Co1	117.48(6)
		C2–C1–C4	123.81(8)
		C3–C1–C2	119.29(8)
		C3–C1–C4	116.90(8)
		O3–C2–C1	119.01(8)
		O3–C2–C3	122.13(8)
		C3–C2–C1	118.86(8)
		O1–C4–O2	123.12(8)
		O1–C4–C1	117.11(8)
		O2–C4–C1	119.76(8)
		C1–C3–H3	119.1
		C2–C3–C1	121.85(8)
		C2–C3–H3	119.1
		O3–C5–H5A	109.5
		O3–C5–H5B	109.5
		O3–C5–H5C	109.5
		H5A–C5–H5B	109.5
		H5A–C5–H5C	109.5
		H5B–C5–H5C	109.5

Symmetry transformations used to generate equivalent atoms:
#1: 1-x, 1-y, 1-z; #2: +x, 1-y, -0.5+z; #3: 1-x, +y, 0.5-z; #4: 1.5-x, 1.5-y, 1-z

Table S5. Torsion angles for [Co^{II}(2,5-DMT)] (**1**).

Atom–Atom–Atom–Atom	Torsion Angle [°]
Co1$^{\#1}$–O1–C4–O2	17.1(1)
Co1$^{\#1}$–O1–C4–C1	−163.34(6)
Co1–O2–C4–O1	−116.13(9)
Co1–O2–C4–C1	64.3(1)
Co1–O3–C2–C1	−31.1(1)
Co1–O3–C2–C3	149.04(7)
O3–C2–C3–C1$^{\#2}$	−179.85(9)
C1–C2–C3–C1$^{\#2}$	0.3(2)
C2–C1–C4–O1	168.07(9)
C2–C1–C4–O2	−12.3(1)
C4–C1–C2–O3	0.5(1)
C4–C1–C2–C3	−179.65(8)
C3$^{\#2}$–C1–C2–O3	179.85(8)
C3$^{\#2}$–C1–C2–C3	−0.2(2)
C3$^{\#2}$–C1–C4–O1	−11.3(1)
C3$^{\#2}$–C1–C4–O2	168.25(9)
C5–O3–C2–C1	179.47(9)
C5–O3–C2–C3	−0.4(1)

Symmetry transformations used to generate equivalent atoms:
#1: 1-x, 1-y, 1-z; #2: 1.5-x, 1.5-y, 1-z

Table S6. Crystal data and structure refinement details for $[Mg_2(2,5\text{-DMT})_2(DMF)_2]$ (**4**).

CCDC number	2225419
Empirical formula	$C_{26}H_{30}Mg_2N_2O_{14}$
Formula weight	643.14
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	8.833(3)
b [Å]	9.691(3)
c [Å]	18.674(6)
α [°]	98.274(7)
β [°]	93.31(1)
γ [°]	107.308(9)
Volume [Å^3]	1501.6(8)
Z	2
ρ_{calc} [g·cm^{-3}]	1.422
μ [mm^{-1}]	0.152
F(000)	672
Crystal size [mm^3]	0.110×0.110×0.070
Crystal colour	colourless
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	4.43 to 50.78 (0.83 Å)
Index ranges	-10 ≤ h ≤ 10 -11 ≤ k ≤ 11 0 ≤ l ≤ 22
Reflections collected	5584
Independent reflections	5584 R_{int} = 0.0992 R_{sigma} = 0.0954
Completeness to Θ = 25.242°	100.0 %
Data / Restraints / Parameters	5584/0/407
Goodness-of-fit on F^2	1.032
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0744 wR_2 = 0.1448
Final *R* indexes [all data]	R_1 = 0.1208 wR_2 = 0.1659
Largest peak/hole [eÅ^{-3}]	1.36/-0.80
Extinction coefficient	0.009(2)

Table S7. Atomic coordinates and U_{eq} [Å^2] for [Mg_2(2,5-DMT)$_2$(DMF)$_2$] (**4**).

Atom	*x*	*y*	*z*	U_{eq}
C1	1.4920(5)	0.5866(4)	0.7513(2)	0.0131(9)
C10	1.7393(6)	0.3037(5)	0.6680(3)	0.028(1)
C11	1.0241(5)	0.5970(5)	0.5661(2)	0.0140(9)
C12	0.9717(5)	0.6347(5)	0.5015(2)	0.0143(9)
C13	1.0546(6)	0.4639(5)	0.5638(2)	0.0145(9)
C14	1.0529(6)	0.6971(5)	0.6389(2)	0.014(1)
C15	1.0769(6)	0.9719(5)	0.9383(2)	0.016(1)
C16	0.9143(6)	0.9026(5)	0.9391(2)	0.018(1)
C17	0.8375(6)	0.9275(5)	1.0006(2)	0.017(1)
C18	1.1534(5)	0.9256(5)	0.8740(2)	0.0130(9)
C19	0.5810(8)	0.790(1)	0.9393(3)	0.082(3)
C2	1.3380(5)	0.5274(5)	0.7707(2)	0.0119(9)
C20	0.7758(6)	1.1318(5)	0.8145(2)	0.018(1)
C21	0.6065(7)	1.2492(6)	0.8809(3)	0.037(1)
C22	0.8802(7)	1.2748(5)	0.9344(3)	0.026(1)
C23	0.6919(7)	0.8480(6)	0.6022(3)	0.029(1)
C24	0.4817(8)	0.7024(7)	0.5088(3)	0.049(2)
C25	0.4542(7)	0.9205(6)	0.5866(3)	0.033(1)
C26	0.9078(7)	0.8147(5)	0.4403(2)	0.027(1)
C3	1.2665(6)	0.3761(5)	0.7577(2)	0.0140(9)
C4	1.3455(6)	0.2814(5)	0.7272(2)	0.0154(9)
C5	1.4997(6)	0.3404(5)	0.7091(2)	0.017(1)
C6	1.5713(6)	0.4912(5)	0.7205(2)	0.017(1)
C7	1.5840(6)	0.7476(5)	0.7624(2)	0.0133(9)
C8	1.2618(6)	0.1184(4)	0.7218(2)	0.0131(9)
C9	1.1254(7)	0.5577(6)	0.8392(3)	0.039(2)
H10A	1.781862	0.223881	0.650535	0.043
H10B	1.799690	0.359054	0.714187	0.043
H10C	1.748715	0.369104	0.631930	0.043
H13	1.093827	0.439560	0.607149	0.017
H16	0.854963	0.837360	0.897116	0.022
H19A	0.469899	0.755559	0.949903	0.124
H19B	0.611617	0.706477	0.915661	0.124
H19C	0.592279	0.862387	0.906834	0.124
H20	0.688917	1.092511	0.777427	0.022
H21A	0.627013	1.355640	0.890158	0.055
H21B	0.556955	1.206872	0.921612	0.055
H21C	0.534723	1.206527	0.835919	0.055
H22A	0.907147	1.381842	0.945045	0.039
H22B	0.975420	1.248105	0.922177	0.039
H22C	0.841239	1.233288	0.977161	0.039
H23	0.744683	0.777617	0.588264	0.034
H24A	0.377863	0.643924	0.520540	0.073
H24B	0.552741	0.641560	0.503658	0.073
H24C	0.467853	0.737801	0.463052	0.073
H25A	0.346367	0.859528	0.592085	0.050
H25B	0.449145	0.978485	0.548161	0.050
H25C	0.500881	0.986399	0.632579	0.050

H26A	0.892490	0.911296	0.451341	0.041
H26B	0.807946	0.742725	0.416545	0.041
H26C	0.991633	0.819435	0.407690	0.041
H3	1.161207	0.336589	0.769972	0.017
H6	1.675823	0.530282	0.707255	0.020
H9A	1.147751	0.490368	0.869751	0.058
H9B	1.037712	0.503458	0.801525	0.058
H9C	1.095264	0.634760	0.869412	0.058
Mg1	1.2871(2)	0.8424(2)	0.76918(7)	0.0123(3)
Mg2	0.9230(2)	0.9240(2)	0.73244(7)	0.0126(3)
N1	0.7570(5)	1.2173(4)	0.8733(2)	0.0211(9)
N2	0.5516(5)	0.8277(4)	0.5674(2)	0.0241(9)
O1	1.5079(4)	0.8396(3)	0.7668(2)	0.0161(7)
O10	1.2937(4)	0.9218(3)	0.8815(2)	0.0190(7)
O11	1.0725(4)	0.8789(3)	0.8114(2)	0.0141(7)
O12	0.6802(4)	0.8540(4)	1.0044(2)	0.0257(8)
O13	0.9013(4)	1.0999(3)	0.8050(2)	0.0205(7)
O14	0.7620(4)	0.9522(3)	0.6523(2)	0.0192(7)
O2	1.7320(4)	0.7788(3)	0.7656(2)	0.0142(7)
O3	1.1154(4)	0.0756(3)	0.7033(2)	0.0178(7)
O4	1.3446(4)	0.0415(3)	0.7401(2)	0.0196(7)
O5	1.2646(4)	0.6227(3)	0.8057(2)	0.0159(7)
O6	1.5759(4)	0.2441(3)	0.6786(2)	0.0232(8)
O7	1.1808(4)	0.7121(3)	0.6764(2)	0.0181(7)
O8	0.9484(4)	0.7534(3)	0.6577(2)	0.0163(7)
O9	0.9535(4)	0.7717(3)	0.5064(2)	0.0223(8)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table S8. Atomic displacement parameters (Å^2) for [Mg_2(2,5-DMT)$_2$(DMF)$_2$] (**4**).

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C1	0.013(3)	0.010(2)	0.015(2)	0.002(2)	−0.002(2)	0.000(2)
C10	0.015(3)	0.021(3)	0.050(3)	0.004(2)	0.011(2)	0.005(2)
C11	0.014(3)	0.017(2)	0.010(2)	0.005(2)	0.003(2)	−0.003(2)
C12	0.014(3)	0.014(2)	0.016(2)	0.008(2)	0.001(2)	0.001(2)
C13	0.018(3)	0.016(2)	0.010(2)	0.008(2)	−0.001(2)	0.001(2)
C14	0.020(3)	0.009(2)	0.012(2)	0.002(2)	0.001(2)	0.001(2)
C15	0.023(3)	0.016(2)	0.010(2)	0.007(2)	0.003(2)	0.001(2)
C16	0.021(3)	0.021(2)	0.011(2)	0.008(2)	−0.002(2)	−0.004(2)
C17	0.014(3)	0.023(2)	0.013(2)	0.004(2)	0.004(2)	0.006(2)
C18	0.009(3)	0.013(2)	0.017(2)	0.003(2)	0.001(2)	0.001(2)
C19	0.026(4)	0.163(9)	0.028(4)	−0.010(5)	−0.005(3)	0.004(4)
C2	0.012(2)	0.014(2)	0.013(2)	0.009(2)	0.001(2)	0.003(2)
C20	0.024(3)	0.011(2)	0.017(2)	0.001(2)	0.003(2)	0.001(2)
C21	0.026(3)	0.051(4)	0.034(3)	0.019(3)	0.004(2)	−0.008(3)
C22	0.033(3)	0.024(3)	0.021(2)	0.014(2)	−0.003(2)	−0.004(2)
C23	0.031(3)	0.032(3)	0.024(3)	0.014(3)	0.004(2)	0.000(2)
C24	0.052(5)	0.047(4)	0.044(4)	0.025(3)	−0.018(3)	−0.015(3)
C25	0.033(4)	0.036(3)	0.034(3)	0.014(3)	0.008(2)	0.006(2)
C26	0.047(4)	0.023(3)	0.017(2)	0.021(3)	−0.004(2)	0.005(2)
C3	0.011(2)	0.014(2)	0.017(2)	0.002(2)	0.003(2)	0.005(2)
C4	0.012(3)	0.013(2)	0.020(2)	0.001(2)	0.002(2)	0.003(2)
C5	0.016(3)	0.011(2)	0.025(2)	0.004(2)	0.004(2)	0.001(2)
C6	0.009(3)	0.014(2)	0.026(2)	0.000(2)	0.002(2)	0.004(2)
C7	0.015(3)	0.013(2)	0.011(2)	0.003(2)	0.003(2)	0.001(2)
C8	0.013(3)	0.010(2)	0.016(2)	0.002(2)	0.002(2)	0.002(2)
C9	0.039(4)	0.017(3)	0.064(4)	0.008(3)	0.037(3)	0.008(2)
Mg1	0.0116(9)	0.0120(7)	0.0125(7)	0.0032(6)	0.0019(6)	−0.0001(5)
Mg2	0.0121(8)	0.0114(7)	0.0132(7)	0.0027(6)	0.0014(6)	0.0003(5)
N1	0.020(2)	0.023(2)	0.019(2)	0.006(2)	0.004(2)	0.000(2)
N2	0.022(3)	0.025(2)	0.025(2)	0.009(2)	−0.002(2)	−0.002(2)
O1	0.016(2)	0.013(2)	0.021(2)	0.006(1)	0.004(1)	0.003(1)
O10	0.018(2)	0.025(2)	0.014(2)	0.009(2)	0.002(1)	−0.002(1)
O11	0.014(2)	0.014(2)	0.011(2)	0.002(1)	0.002(1)	−0.001(1)
O12	0.014(2)	0.036(2)	0.018(2)	−0.002(2)	0.003(1)	−0.005(1)
O13	0.022(2)	0.015(2)	0.024(2)	0.007(2)	0.001(1)	−0.001(1)
O14	0.024(2)	0.017(2)	0.017(2)	0.007(2)	0.001(1)	0.002(1)
O2	0.007(2)	0.014(2)	0.019(2)	0.001(1)	0.000(1)	0.002(1)
O3	0.017(2)	0.017(2)	0.017(2)	0.000(1)	0.000(1)	0.005(1)
O4	0.019(2)	0.012(2)	0.028(2)	0.004(1)	0.004(1)	0.004(1)
O5	0.015(2)	0.014(2)	0.021(2)	0.006(1)	0.007(1)	0.004(1)
O6	0.016(2)	0.013(2)	0.041(2)	0.006(1)	0.013(2)	0.003(1)
O7	0.019(2)	0.019(2)	0.016(2)	0.010(1)	−0.004(1)	−0.002(1)
O8	0.013(2)	0.019(2)	0.015(2)	0.007(1)	0.000(1)	−0.003(1)
O9	0.039(2)	0.016(2)	0.015(2)	0.016(2)	−0.005(1)	0.000(1)

Table S9. Bond lengths and angles for $[Mg_2(2,5\text{-DMT})_2(DMF)_2]$ (**4**).

Atom–Atom	Length [Å]	Atom–Atom	Length [Å]
C10–H10A	0.9800	Mg1–Mg2	3.585(2)
C10–H10B	0.9800	Mg1–O1	1.961(3)
C10–H10C	0.9800	Mg1–O10	2.118(3)
C11–C12	1.402(6)	Mg1–O11	2.198(3)
C11–C13	1.390(6)	Mg1–O4$^{\#1}$	2.007(3)
C13–C12$^{\#4}$	1.398(6)	Mg1–O5	2.284(3)
C13–H13	0.9500	Mg1–O7	1.989(3)
C14–C11	1.512(6)	Mg2–O11	2.100(3)
C15–C18	1.490(6)	Mg2–O13	2.082(3)
C16–C15	1.395(7)	Mg2–O14	2.107(3)
C16–C17	1.394(6)	Mg2–O2$^{\#2}$	2.042(4)
C16–H16	0.9500	Mg2–O3$^{\#1}$	2.048(4)
C17–C15$^{\#3}$	1.402(6)	Mg2–O8	2.080(3)
C19–H19A	0.9800	N1–C20	1.326(6)
C19–H19B	0.9800	N1–C21	1.462(6)
C19–H19C	0.9800	N1–C22	1.453(6)
C1–C2	1.400(6)	N2–C23	1.312(7)
C1–C6	1.398(6)	N2–C24	1.464(7)
C20–H20	0.9500	N2–C25	1.443(6)
C21–H21A	0.9800	O10–C18	1.251(5)
C21–H21B	0.9800	O11–C18	1.282(5)
C21–H21C	0.9800	O12–C17	1.371(6)
C22–H22A	0.9800	O12–C19	1.402(7)
C22–H22B	0.9800	O13–C20	1.251(6)
C22–H22C	0.9800	O14–C23	1.253(6)
C23–H23	0.9500	O1–C7	1.264(5)
C24–H24A	0.9800	O2–C7	1.247(5)
C24–H24B	0.9800	O3–C8	1.245(5)
C24–H24C	0.9800	O4–C8	1.256(5)
C25–H25A	0.9800	O5–C2	1.390(5)
C25–H25B	0.9800	O5–C9	1.429(6)
C25–H25C	0.9800	O6–C10	1.423(6)
C26–H26A	0.9800	O6–C5	1.383(5)
C26–H26B	0.9800	O7–C14	1.253(5)
C26–H26C	0.9800	O8–C14	1.247(5)
C2–C3	1.392(6)	O9–C12	1.375(5)
C3–C4	1.389(6)	O9–C26	1.432(5)
C3–H3	0.9500		
C4–C5	1.394(7)		
C4–C8	1.518(6)		
C5–C6	1.388(6)		
C6–H6	0.9500		
C7–C1	1.506(6)		
C9–H9A	0.9800		
C9–H9B	0.9800		
C9–H9C	0.9800		
Mg1–C18	2.501(4)		

Atom–Atom–Atom	Angle [°]	Atom–Atom–Atom	Angle [°]
C11–C13–C12	120.8(4)	C7–O2–Mg2	140.0(3)
C11–C13–H13	119.6	C8–O3–Mg2	135.2(3)
C12–C11–C14	122.7(4)	C8–O4–Mg1	132.4(3)
C12–C13–H13	119.6	C9–O5–Mg1	117.4(3)
C12–O9–C26	117.4(3)	H10A–C10–H10B	109.5
C13–C11–C12	119.3(4)	H10A–C10–H10C	109.5
C13–C11–C14	117.9(4)	H10B–C10–H10C	109.5
C13–C12–C11	119.8(4)	H19A–C19–H19B	109.5
C14–O7–Mg1	132.4(3)	H19A–C19–H19C	109.5
C14–O8–Mg2	139.6(3)	H19B–C19–H19C	109.5
C15–C16–H16	119.5	H21A–C21–H21B	109.5
C15–C18–Mg1	177.7(3)	H21A–C21–H21C	109.5
C16–C15–C17	119.2(4)	H21B–C21–H21C	109.5
C16–C15–C18	117.5(4)	H22A–C22–H22B	109.5
C16–C17–C15	119.7(4)	H22A–C22–H22C	109.5
C17–C15–C18	123.1(4)	H22B–C22–H22C	109.5
C17–C16–C15	121.1(4)	H24A–C24–H24B	109.5
C17–C16–H16	119.5	H24A–C24–H24C	109.5
C17–O12–C19	118.6(4)	H24B–C24–H24C	109.5
C18–Mg1–Mg2	61.2(1)	H25A–C25–H25B	109.5
C18–O10–Mg1	92.2(3)	H25A–C25–H25C	109.5
C18–O11–Mg1	87.7(3)	H25B–C25–H25C	109.5
C18–O11–Mg2	145.3(3)	H26A–C26–H26B	109.5
C1–C6–H6	119.5	H26A–C26–H26C	109.5
C20–N1–C21	120.9(4)	H26B–C26–H26C	109.5
C20–N1–C22	121.7(4)	H9A–C9–H9B	109.5
C20–O13–Mg2	126.4(3)	H9A–C9–H9C	109.5
C22–N1–C21	117.3(4)	H9B–C9–H9C	109.5
C23–N2–C24	120.9(4)	Mg2–O11–Mg1	113.0(1)
C23–N2–C25	122.7(4)	N1–C20–H20	118.1
C23–O14–Mg2	119.9(3)	N1–C21–H21A	109.5
C25–N2–C24	116.3(4)	N1–C21–H21B	109.5
C2–C1–C7	125.4(4)	N1–C21–H21C	109.5
C2–C3–H3	119.2	N1–C22–H22A	109.5
C2–O5–C9	116.5(3)	N1–C22–H22B	109.5
C2–O5–Mg1	120.3(3)	N1–C22–H22C	109.5
C3–C2–C1	119.6(4)	N2–C23–H23	117.2
C3–C4–C5	118.8(4)	N2–C24–H24A	109.5
C3–C4–C8	116.9(4)	N2–C24–H24B	109.5
C4–C3–C2	121.6(4)	N2–C24–H24C	109.5
C4–C3–H3	119.2	N2–C25–H25A	109.5
C5–C4–C8	124.1(4)	N2–C25–H25B	109.5
C5–C6–C1	121.0(4)	N2–C25–H25C	109.5
C5–C6–H6	119.5	O10–C18–C15	120.4(4)
C5–O6–C10	117.4(4)	O10–C18–Mg1	57.8(2)
C6–C1–C2	118.8(4)	O10–C18–O11	119.2(4)
C6–C1–C7	115.8(4)	O10–Mg1–C18	30.0(1)
C6–C5–C4	120.2(4)	O10–Mg1–Mg2	90.5(1)
C7–O1–Mg1	138.9(3)	O10–Mg1–O11	60.8(1)

Atom–Atom–Atom	Angle [°]	Atom–Atom–Atom	Angle [°]
O10–Mg1–O5	84.7(1)	O4–Mg1–O10	94.8(1)
O11–C18–C15	120.2(4)	O4–Mg1–O11	89.3(1)
O11–C18–Mg1	61.4(2)	O4–Mg1–O5	170.8(2)
O11–Mg1–C18	30.8(1)	O5–C2–C1	118.2(4)
O11–Mg1–Mg2	32.61(8)	O5–C2–C3	122.1(4)
O11–Mg1–O5	98.4(1)	O5–C9–H9A	109.5
O11–Mg2–Mg1	34.34(9)	O5–C9–H9B	109.5
O11–Mg2–O14	175.6(2)	O5–C9–H9C	109.5
O12–C17–C15	118.1(4)	O5–Mg1–C18	92.6(1)
O12–C17–C16	122.2(4)	O5–Mg1–Mg2	116.6(1)
O12–C19–H19A	109.5	O6–C10–H10A	109.5
O12–C19–H19B	109.5	O6–C10–H10B	109.5
O12–C19–H19C	109.5	O6–C10–H10C	109.5
O13–C20–H20	118.1	O6–C5–C4	117.8(4)
O13–C20–N1	123.9(4)	O6–C5–C6	122.0(4)
O13–Mg2–Mg1	113.4(1)	O7–C14–C11	115.6(4)
O13–Mg2–O11	90.8(1)	O7–Mg1–C18	126.7(2)
O13–Mg2–O14	91.8(1)	O7–Mg1–Mg2	74.2(1)
O14–C23–H23	117.2	O7–Mg1–O10	152.3(2)
O14–C23–N2	125.5(5)	O7–Mg1–O11	97.3(1)
O14–Mg2–Mg1	146.2(1)	O7–Mg1–O4	102.1(1)
O1–C7–C1	118.8(4)	O7–Mg1–O5	82.0(1)
O1–Mg1–C18	129.2(2)	O8–C14–C11	118.8(4)
O1–Mg1–Mg2	161.7(1)	O8–C14–O7	125.6(4)
O1–Mg1–O10	99.3(1)	O8–Mg2–Mg1	66.6(1)
O1–Mg1–O11	160.0(1)	O8–Mg2–O11	90.1(1)
O1–Mg1–O4	91.2(1)	O8–Mg2–O13	178.0(2)
O1–Mg1–O5	79.9(1)	O8–Mg2–O14	87.4(1)
O1–Mg1–O7	102.1(1)	O9–C12–C11	116.7(4)
O2–C7–C1	116.1(4)	O9–C12–C13	123.5(4)
O2–C7–O1	125.1(4)	O9–C26–H26A	109.5
O2–Mg2–Mg1	112.3(1)	O9–C26–H26B	109.5
O2–Mg2–O11	89.1(1)	O9–C26–H26C	109.5
O2–Mg2–O13	92.7(1)		
O2–Mg2–O14	87.2(1)		
O2–Mg2–O3	177.6(1)		
O2–Mg2–O8	89.1(1)		
O3–C8–C4	116.4(4)		
O3–C8–O4	126.4(4)		
O3–Mg2–Mg1	68.0(1)		
O3–Mg2–O11	90.1(1)		
O3–Mg2–O13	85.0(1)		
O3–Mg2–O14	93.7(1)		
O3–Mg2–O8	93.2(1)		
O4–C8–C4	117.1(4)		
O4–Mg1–C18	91.4(1)		
O4–Mg1–Mg2	72.5(1)		

Symmetry transformations used to generate equivalent atoms:
#1: +x, 1+y, +z; #2: -1+x, +y, +z; #3: 1+x, +y, +z; #4: +x, -1+y, +z; #5: 2-x, 2-y, 2-z; #6: 2-x, 1-y, 1-z

Table S10. Torsion angles for $[Mg_2(2,5\text{-DMT})_2(DMF)_2]$ (**4**).

Atom–Atom–Atom–Atom	Torsion Angle [°]	Atom–Atom–Atom–Atom	Torsion Angle [°]
C10–O6–C5–C4	−173.0(4)	Mg1–O10–C18–C15	178.3(4)
C10–O6–C5–C6	8.1(6)	Mg1–O10–C18–O11	3.3(4)
C12–C11–C13–C12$^{\#3}$	−2.3(8)	Mg1–O11–C18–C15	−178.2(4)
C13–C11–C12–C13$^{\#3}$	2.3(8)	Mg1–O11–C18–O10	−3.2(4)
C13–C11–C12–O9	−175.9(4)	Mg1–O1–C7–C1	4.5(6)
C14–C11–C12–C13$^{\#3}$	−179.2(4)	Mg1–O1–C7–O2	−176.3(3)
C14–C11–C12–O9	2.7(7)	Mg1–O5–C2–C1	41.1(5)
C14–C11–C13–C12$^{\#3}$	179.1(4)	Mg1–O5–C2–C3	−142.1(3)
C15–C16–C17–C15$^{\#1}$	2.5(8)	Mg1–O7–C14–C11	172.9(3)
C15–C16–C17–O12	−175.9(4)	Mg1–O7–C14–O8	−9.6(7)
C16–C15–C18–O10	−144.7(4)	Mg2$^{\#2}$–O2–C7–C1	141.3(3)
C16–C15–C18–O11	30.2(6)	Mg2$^{\#2}$–O2–C7–O1	−38.0(7)
C17$^{\#1}$–C15–C18–O10	30.3(7)	Mg2$^{\#4}$–O3–C8–C4	−141.5(3)
C17$^{\#1}$–C15–C18–O11	−154.8(4)	Mg2$^{\#4}$–O3–C8–O4	34.3(7)
C17–C16–C15–C17$^{\#1}$	−2.5(7)	Mg2–O11–C18–C15	52.6(7)
C17–C16–C15–C18	172.7(4)	Mg2–O11–C18–Mg1	−129.2(5)
C19–O12–C17–C15$^{\#1}$	160.5(6)	Mg2–O11–C18–O10	−132.4(4)
C19–O12–C17–C16	−21.1(8)	Mg2–O13–C20–N1	160.7(3)
C1–C2–C3–C4	1.3(6)	Mg2–O14–C23–N2	151.9(4)
C21–N1–C20–O13	−179.6(5)	Mg2–O8–C14–C11	−163.1(3)
C22–N1–C20–O13	−3.7(7)	Mg2–O8–C14–O7	19.4(8)
C24–N2–C23–O14	179.2(6)	O1–C7–C1–C2	−24.3(6)
C25–N2–C23–O14	−4.4(8)	O1–C7–C1–C6	157.1(4)
C26–O9–C12–C11	177.0(4)	O2–C7–C1–C2	156.5(4)
C26–O9–C12–C13$^{\#3}$	−1.1(7)	O2–C7–C1–C6	−22.1(6)
C2–C1–C6–C5	0.0(6)	O5–C2–C3–C4	−175.5(4)
C2–C3–C4–C5	−0.2(7)	O6–C5–C6–C1	179.9(4)
C2–C3–C4–C8	174.7(4)	O7–C14–C11–C12	−133.8(5)
C3–C4–C5–C6	−0.9(7)	O7–C14–C11–C13	44.8(6)
C3–C4–C5–O6	−179.8(4)	O8–C14–C11–C12	48.5(6)
C3–C4–C8–O3	40.7(6)	O8–C14–C11–C13	−132.9(5)
C3–C4–C8–O4	−135.6(4)		
C4–C5–C6–C1	1.1(7)		
C5–C4–C8–O3	−144.7(4)		
C5–C4–C8–O4	39.1(6)		
C6–C1–C2–C3	−1.2(6)		
C6–C1–C2–O5	175.7(4)		
C7–C1–C2–C3	−179.8(4)		
C7–C1–C2–O5	−2.8(6)		
C7–C1–C6–C5	178.7(4)		
C8–C4–C5–C6	−175.5(4)		
C8–C4–C5–O6	5.7(7)		
C9–O5–C2–C1	−166.1(4)		
C9–O5–C2–C3	10.7(6)		
Mg1$^{\#4}$–O4–C8–C4	160.5(3)		
Mg1$^{\#4}$–O4–C8–O3	−15.3(7)		

Symmetry transformations used to generate equivalent atoms:
#1: 2-x, 2-y, 2-z; #2: 1+x, +y, +z; #3: 2-x, 1-y, 1-z; #4: +x, -1+y, +z