Electronic Supplementary Information

Metal-organic frameworks constructed from flexible ditopic ligands: conformational diversity of an aliphatic ligand

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Table S1 Selected bond distances (Å) and angles (deg) of **1**.

Mn(1)-O(1A)	2.131(2)	Mn(2)-O(2A)	2.068(2)
Mn(1)-O(4A)$^{\#1}$	2.132(2)	Mn(2)-O(3A)$^{\#5}$	2.085(2)
Mn(1)-O(1B)	2.175(2)	Mn(2)-O(1C)	2.137(2)
Mn(1)-O(3B)$^{\#2}$	2.189(2)	Mn(2)-O(2B)	2.212(2)
Mn(1)-O(2B)$^{\#3}$	2.258(2)	Mn(2)-O(3B)$^{\#2}$	2.253(2)
Mn(1)-O(4B)$^{\#4}$	2.261(2)	Mn(2)-O(4B)$^{\#2}$	2.380(2)
O(1A)-Mn(1)-O(4A)$^{\#1}$	175.14(8)	O(2A)-Mn(2)-O(3A)$^{\#5}$	94.56(8)
O(1A)-Mn(1)-O(1B)	90.47(8)	O(2A)-Mn(2)-O(1C)	99.95(9)
O(4A)$^{\#1}$-Mn(1)-O(1B)	90.61(8)	O(3A)$^{\#5}$-Mn(2)-O(1C)	88.85(9)
O(1A)-Mn(1)-O(3B)$^{\#2}$	93.44(8)	O(2A)-Mn(2)-O(2B)	101.47(8)
O(4A)$^{\#1}$-Mn(1)-O(3B)$^{\#2}$	91.29(8)	O(3A)$^{\#5}$-Mn(2)-O(2B)	87.49(8)
O(1B)-Mn(1)-O(3B)$^{\#2}$	90.39(8)	O(1C)-Mn(2)-O(2B)	158.49(8)
O(1A)-Mn(1)-O(2B)$^{\#3}$	84.95(7)	O(2A)-Mn(2)-O(3B)$^{\#2}$	101.63(8)
O(4A)$^{\#1}$-Mn(1)-O(2B)$^{\#3}$	90.20(7)	O(3A)$^{\#5}$-Mn(2)-O(3B)$^{\#2}$	163.74(8)
O(1B)-Mn(1)-O(2B)$^{\#3}$	100.63(8)	O(1C)-Mn(2)-O(3B)$^{\#2}$	89.86(8)
O(3B)$^{\#2}$-Mn(1)-O(2B)$^{\#3}$	168.87(7)	O(2B)-Mn(2)-O(3B)$^{\#2}$	87.79(7)
O(1A)-Mn(1)-O(4B)$^{\#4}$	89.54(7)	O(2A)-Mn(2)-O(4B)$^{\#2}$	157.77(7)
O(4A)$^{\#1}$-Mn(1)-O(4B)$^{\#4}$	89.19(8)	O(3A)$^{\#5}$-Mn(2)-O(4B)$^{\#2}$	107.18(7)
O(1B)-Mn(1)-O(4B)$^{\#4}$	177.62(8)	O(1C)-Mn(2)-O(4B)$^{\#2}$	85.41(8)
O(3B)$^{\#2}$-Mn(1)-O(4B)$^{\#4}$	91.99(7)	O(2B)-Mn(2)-O(4B)$^{\#2}$	75.48(7)
O(2B)$^{\#3}$-Mn(1)-O(4B)$^{\#4}$	77.00(7)	O(3B)$^{\#2}$-Mn(2)-O(4B)$^{\#2}$	56.56(7)

[a] Symmetry transformation used to generate equivalent atoms:

$^{\#1}$ x,-y+3/2,z+1/2 $^{\#2}$ x+1,y,z $^{\#3}$ x,-y+3/2,z-1/2 $^{\#4}$ x+1,-y+3/2,z-1/2 $^{\#5}$ x,y,z+1

Table S2 Selected bond distances (Å) and angles (deg) of **2**.

Co(1)-O(2B)	2.046(3)	Co(2)-O(1B)	2.024(3)
Co(1)-O(3A)$^{\#1}$	2.059(3)	Co(2)-O(2A)$^{\#4}$	2.038(3)
Co(1)-O(1A)	2.070(3)	Co(2)-O(1C)	2.106(3)
Co(1)-O(4A)$^{\#2}$	2.103(3)	Co(2)-O(3B)$^{\#5}$	2.110(3)
Co(1)-O(3B)$^{\#3}$	2.143(3)	Co(2)-O(4A)$^{\#2}$	2.116(3)
Co(1)-O(4B)$^{\#3}$	2.198(3)	Co(2)-O(1A)	2.139(3)
O(2B)-Co(1)-O(3A)$^{\#1}$	169.62(15)	O(1B)-Co(2)-O(2A)$^{\#4}$	175.32(15)
O(2B)-Co(1)-O(1A)	93.69(13)	O(1B)-Co(2)-O(1C)	89.64(14)
O(3A)$^{\#1}$-Co(1)-O(1A)	95.73(13)	O(2A)$^{\#4}$-Co(2)-O(1C)	87.14(14)
O(2B)-Co(1)-O(4A)$^{\#2}$	90.41(13)	O(1B)-Co(2)-O(3B)$^{\#5}$	92.50(13)
O(3A)$^{\#1}$-Co(1)-O(4A)$^{\#2}$	87.08(13)	O(2A)$^{\#4}$-Co(2)-O(3B)$^{\#5}$	90.81(13)
O(1A)-Co(1)-O(4A)$^{\#2}$	79.29(13)	O(1C)-Co(2)-O(3B)$^{\#5}$	88.50(13)
O(2B)-Co(1)-O(3B)$^{\#3}$	93.35(13)	O(1B)-Co(2)-O(4A)$^{\#2}$	88.37(13)
O(3A)$^{\#1}$-Co(1)-O(3B)$^{\#3}$	88.25(13)	O(2A)$^{\#4}$-Co(2)-O(4A)$^{\#2}$	94.76(13)
O(1A)-Co(1)-O(3B)$^{\#3}$	105.91(13)	O(1C)-Co(2)-O(4A)$^{\#2}$	177.55(14)
O(4A)$^{\#2}$-Co(1)-O(3B)$^{\#3}$	173.35(13)	O(3B)$^{\#5}$-Co(2)-O(4A)$^{\#2}$	93.02(13)
O(2B)-Co(1)-O(4B)$^{\#3}$	88.14(13)	O(1B)-Co(2)-O(1A)	87.92(13)
O(3A)$^{\#1}$-Co(1)-O(4B)$^{\#3}$	83.70(13)	O(2A)$^{\#4}$-Co(2)-O(1A)	89.37(13)
O(1A)-Co(1)-O(4B)$^{\#3}$	166.58(14)	O(1C)-Co(2)-O(1A)	101.02(13)
O(4A)$^{\#2}$-Co(1)-O(4B)$^{\#3}$	114.02(13)	O(3B)$^{\#5}$-Co(2)-O(1A)	170.48(13)
O(3B)$^{\#3}$-Co(1)-O(4B)$^{\#3}$	60.69(13)	O(4A)$^{\#2}$-Co(2)-O(1A)	77.49(13)

[a] Symmetry transformation used to generate equivalent atoms:

$^{\#1}$ -x+3/2,-y,z+1/2 $^{\#2}$ y+3/4,-x+3/4,z+3/4 $^{\#3}$ -x+2,-y,-z+1 $^{\#4}$ -y+3/4,x-3/4,z+1/4 $^{\#5}$ y+3/4, -x+5/4,-z+5/4

Table S3 Selected bond distances (Å) and angles (deg) of **3**.

Tb(1)-O(2F)$^{\#1}$	2.290(4)	Tb(2)-O(4B)$^{\#2}$	2.445(4)
Tb(1)-O(1B)	2.330(4)	Tb(2)-O(2C)	2.447(4)
Tb(1)-O(3B)$^{\#2}$	2.340(4)	Tb(2)-O(3B)$^{\#2}$	2.607(4)
Tb(1)-O(1G)	2.350(5)	Tb(2)-O(1C)	2.643(4)
Tb(1)-O(2E)$^{\#1}$	2.375(4)	Tb(3)-O(4A)$^{\#4}$	2.282(4)
Tb(1)-O(4D)$^{\#3}$	2.417(4)	Tb(3)-O(1F)	2.328(4)
Tb(1)-O(1A)	2.425(4)	Tb(3)-O(2C)	2.352(4)
Tb(1)-O(2A)	2.508(4)	Tb(3)-O(1E)	2.390(4)
Tb(2)-O(2B)	2.357(4)	Tb(3)-O(2D)	2.443(4)
Tb(2)-O(3A)$^{\#4}$	2.377(4)	Tb(3)-O(4D)$^{\#5}$	2.452(4)
Tb(2)-O(1H)	2.397(5)	Tb(3)-O(3D)$^{\#5}$	2.499(4)
Tb(2)-O(1D)	2.407(3)	Tb(3)-O(1D)	2.514(3)
Tb(2)-O(2A)	2.411(4)	Tb(3)-O(2E)	2.597(4)
O(2F)$^{\#1}$-Tb(1)-O(1B)	100.72(16)	O(3A)$^{\#4}$-Tb(2)-O(3B)$^{\#2}$	145.97(13)
O(2F)$^{\#1}$-Tb(1)-O(3B)$^{\#2}$	81.71(14)	O(1H)-Tb(2)-O(3B)$^{\#2}$	113.33(18)
O(1B)-Tb(1)-O(3B)+	75.11(14)	O(1D)-Tb(2)-O(3B)$^{\#2}$	120.31(12)
O(2F)$^{\#1}$-Tb(1)-O(1G)	90.21(19)	O(2A)-Tb(2)-O(3B)$^{\#2}$	68.13(12)
O(1B)-Tb(1)-O(1G)	143.82(15)	O(4B)$^{\#2}$-Tb(2)-O(3B)$^{\#2}$	51.00(12)
O(3B)$^{\#2}$-Tb(1)-O(1G)	72.50(15)	O(2C)-Tb(2)-O(3B)$^{\#2}$	111.45(13)
O(2F)$^{\#1}$-Tb(1)-O(2E)$^{\#1}$	77.83(15)	O(2B)-Tb(2)-O(1C)	141.83(14)
O(1B)-Tb(1)-O(2E)$^{\#1}$	75.31(13)	O(3A)$^{\#4}$-Tb(2)-O(1C)	138.20(15)
O(3B)$^{\#2}$-Tb(1)-O(2E)$^{\#1}$	139.88(14)	O(1H)-Tb(2)-O(1C)	68.39(17)
O(1G)-Tb(1)-O(2E)$^{\#1}$	140.87(15)	O(1D)-Tb(2)-O(1C)	112.23(13)
O(2F)$^{\#1}$-Tb(1)-O(4D)$^{\#3}$	85.20(14)	O(2A)-Tb(2)-O(1C)	100.25(13)
O(1B)-Tb(1)-O(4D)$^{\#3}$	142.16(13)	O(4B)$^{\#2}$-Tb(2)-O(1C)	69.19(14)
O(3B)$^{\#2}$-Tb(1)-O(4D)$^{\#3}$	142.46(14)	O(2C)-Tb(2)-O(1C)	50.59(12)
O(1G)-Tb(1)-O(4D)$^{\#3}$	72.52(15)	O(3B)$^{\#2}$-Tb(2)-O(1C)	69.63(13)
O(2E)$^{\#1}$-Tb(1)-O(4D)$^{\#3}$	69.47(13)	O(4A)$^{\#4}$-Tb(3)-O(1F)	81.56(15)
O(2F)$^{\#1}$-Tb(1)-O(1A)	155.12(14)	O(4A)$^{\#4}$-Tb(3)-O(2C)	79.47(14)
O(1B)-Tb(1)-O(1A)	83.21(15)	O(1F)-Tb(3)-O(2C)	143.12(14)
O(3B)$^{\#2}$-Tb(1)-O(1A)	122.74(13)	O(4A)$^{\#4}$-Tb(3)-O(1E)	148.35(14)
O(1G)-Tb(1)-O(1A)	101.07(17)	O(1F)-Tb(3)-O(1E)	127.79(14)
O(2E)$^{\#1}$-Tb(1)-O(1A)	79.51(13)	O(2C)-Tb(3)-O(1E)	80.58(13)
O(4D)$^{\#3}$-Tb(1)-O(1A)	77.33(13)	O(4A)$^{\#4}$-Tb(3)-O(2D)	123.86(14)

O(2F)$^{\#1}$-Tb(1)-O(2A)	152.40(14)	O(1F)-Tb(3)-O(2D)	78.27(16)
O(1B)-Tb(1)-O(2A)	75.98(13)	O(2C)-Tb(3)-O(2D)	86.53(14)
O(3B)$^{\#2}$-Tb(1)-O(2A)	70.90(13)	O(1E)-Tb(3)-O(2D)	78.90(14)
O(1G)-Tb(1)-O(2A)	78.55(16)	O(4A)$^{\#4}$-Tb(3)-O(4D)$^{\#5}$	89.82(14)
O(2E)$^{\#1}$-Tb(1)-O(2A)	126.05(13)	O(1F)-Tb(3)-O(4D)$^{\#5}$	78.46(14)
O(4D)$^{\#3}$-Tb(1)-O(2A)	114.49(12)	O(2C)-Tb(3)-O(4D)$^{\#5}$	132.47(12)
O(1A)-Tb(1)-O(2A)	52.46(13)	O(1E)-Tb(3)-O(4D)$^{\#5}$	85.79(13)
O(2B)-Tb(2)-O(3A)$^{\#4}$	79.78(15)	O(2D)-Tb(3)-O(4D)$^{\#5}$	134.94(13)
O(2B)-Tb(2)-O(1H)	138.92(16)	O(4A)$^{\#4}$-Tb(3)-O(3D)$^{\#5}$	75.36(15)
O(3A)$^{\#4}$-Tb(2)-O(1H)	74.39(18)	O(1F)-Tb(3)-O(3D)$^{\#5}$	124.73(15)
O(2B)-Tb(2)-O(1D)	77.73(12)	O(2C)-Tb(3)-O(3D)$^{\#5}$	80.13(13)
O(3A)$^{\#4}$-Tb(2)-O(1D)	72.91(13)	O(1E)-Tb(3)-O(3D)$^{\#5}$	77.21(14)
O(1H)-Tb(2)-O(1D)	122.53(17)	O(2D)-Tb(3)-O(3D)$^{\#5}$	154.20(16)
O(2B)-Tb(2)-O(2A)	75.07(13)	O(4D)$^{\#5}$-Tb(3)-O(3D)$^{\#5}$	52.42(12)
O(3A)$^{\#4}$-Tb(2)-O(2A)	84.84(14)	O(4A)$^{\#4}$-Tb(3)-O(1D)	72.26(13)
O(1H)-Tb(2)-O(2A)	71.33(16)	O(1F)-Tb(3)-O(1D)	77.27(13)
O(1D)-Tb(2)-O(2A)	147.42(13)	O(2C)-Tb(3)-O(1D)	66.94(12)
O(2B)-Tb(2)-O(4B)$^{\#2}$	79.80(15)	O(1E)-Tb(3)-O(1D)	120.98(13)
O(3A)$^{\#4}$-Tb(2)-O(4B)$^{\#2}$	143.34(14)	O(2D)-Tb(3)-O(1D)	52.40(12)
O(1H)-Tb(2)-O(4B)$^{\#2}$	137.54(17)	O(4D)$^{\#5}$-Tb(3)-O(1D)	151.61(13)
O(1D)-Tb(2)-O(4B)$^{\#2}$	73.19(13)	O(3D)$^{\#5}$-Tb(3)-O(1D)	137.06(12)
O(2A)-Tb(2)-O(4B)$^{\#2}$	118.43(12)	O(4A)$^{\#4}$-Tb(3)-O(2E)	149.58(13)
O(2B)-Tb(2)-O(2C)	141.97(13)	O(1F)-Tb(3)-O(2E)	76.53(13)
O(3A)$^{\#4}$-Tb(2)-O(2C)	102.58(14)	O(2C)-Tb(3)-O(2E)	130.08(13)
O(1H)-Tb(2)-O(2C)	75.68(15)	O(1E)-Tb(3)-O(2E)	51.82(12)
O(1D)-Tb(2)-O(2C)	67.21(12)	O(2D)-Tb(3)-O(2E)	71.91(12)
O(2A)-Tb(2)-O(2C)	142.77(13)	O(4D)$^{\#5}$-Tb(3)-O(2E)	65.41(12)
O(4B)$^{\#2}$-Tb(2)-O(2C)	76.47(13)	O(3D)$^{\#5}$-Tb(3)-O(2E)	100.19(13)
O(2B)-Tb(2)-O(3B)$^{\#2}$	73.70(13)	O(1D)-Tb(3)-O(2E)	121.89(12)

[a] Symmetry transformation used to generate equivalent atoms:

$^{\#1}$ x+1/2,-y+3/2,z-1/2 $^{\#2}$ -x+3/2,y-1/2,-z+3/2 $^{\#3}$ x+1,y,z $^{\#4}$ -x+2,-y+2,-z+2 $^{\#5}$ x+1/2,-y+3/2,z+1/2

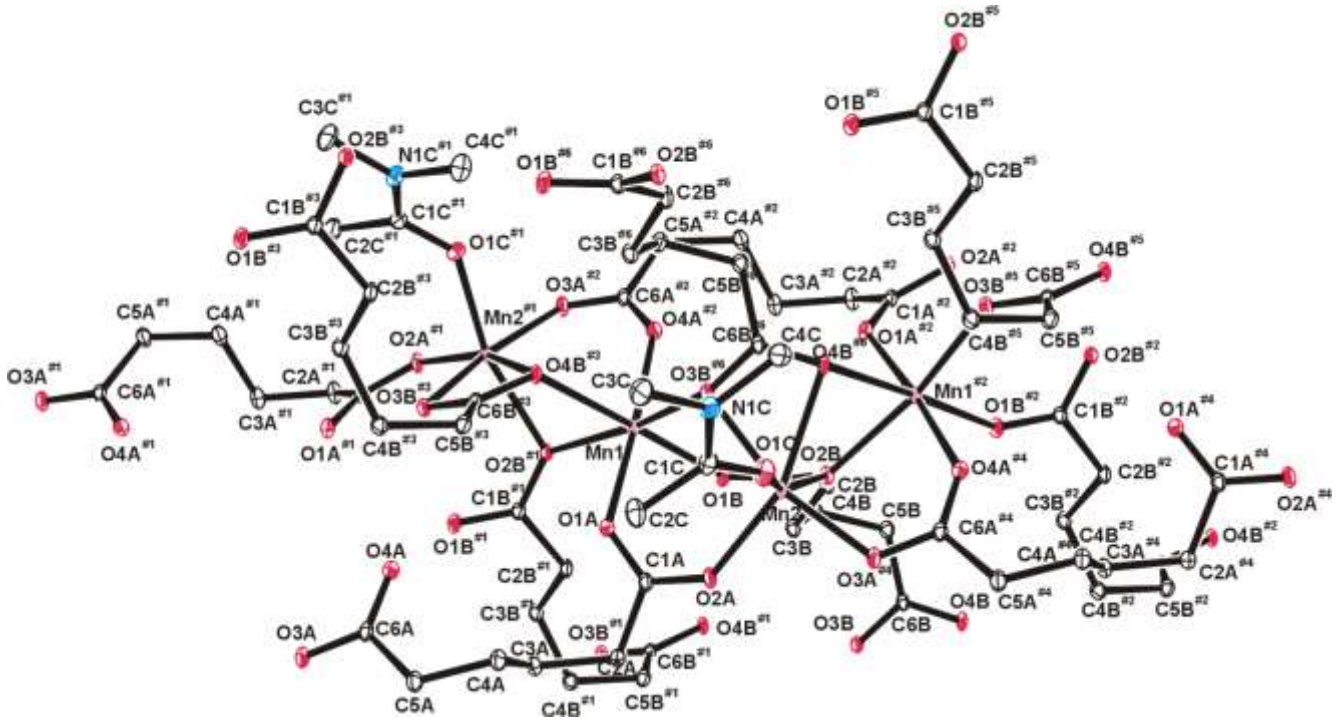

Fig. S1 An ORTEP drawing of **1** with atomic numbering scheme (thermal ellipsoids at 30% probability). Symmetry operation: #1 x,-y+3/2,z-1/2 #2 x,-y+3/2,z+1/2 #3 x+1,-y+3/2,z-1/2 #4 1+x,y,z #5 x+1,-y+3/2,z+1/2 #6 x+1,y,z.

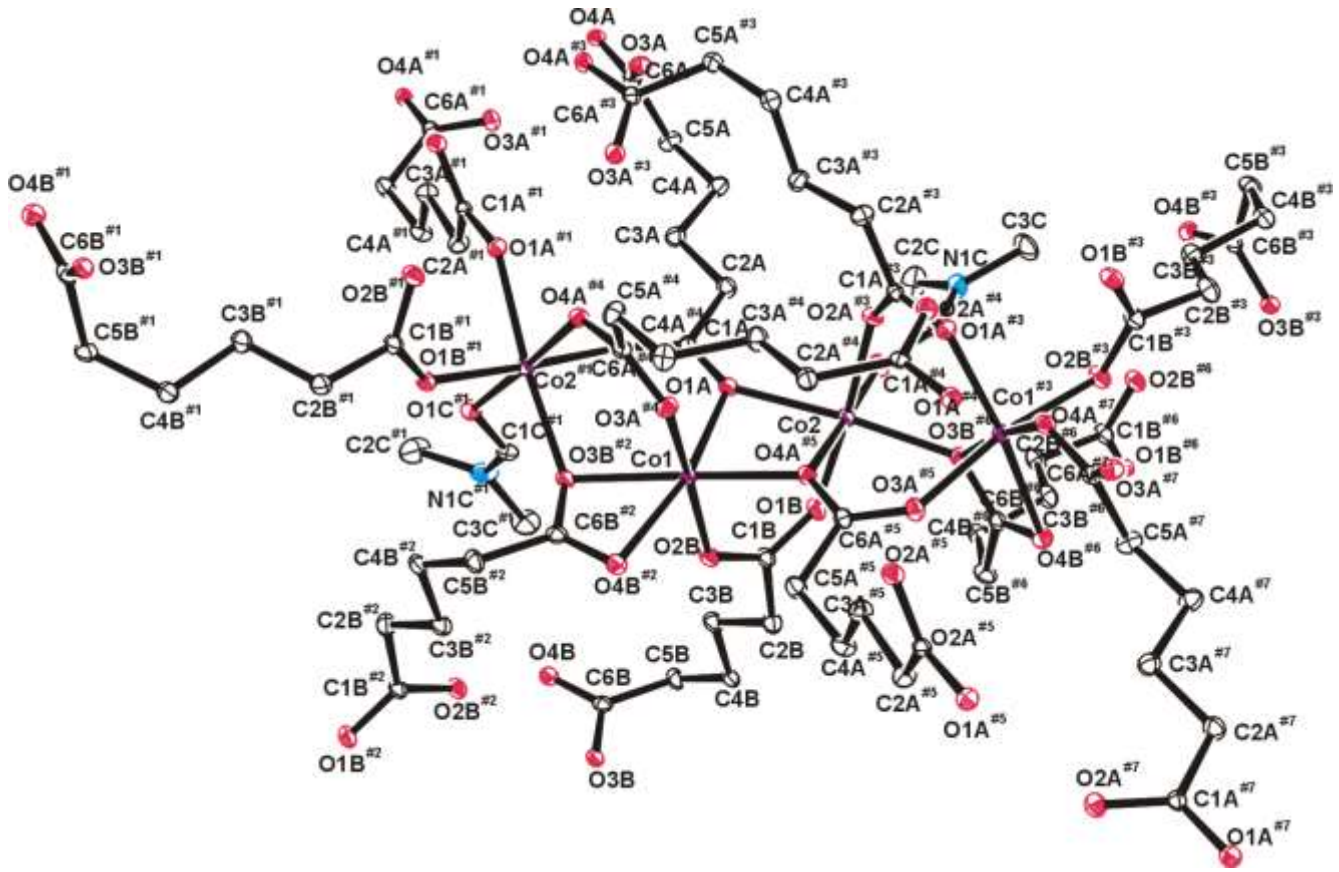

Fig. S2 An ORTEP drawing of **2** with atomic numbering scheme (thermal ellipsoids at 30% probability). Symmetry operation: #1 y+3/4,-x+3/4,z-1/4 #2 -x+2,-y,-z+1 #3 -y+3/4,x-3/4,z+1/4 #4 -x+3/2,-y,z+1/2 #5 y+3/4,-x+3/4,z+3/4 #6 y+3/4,-x+5/4,z+5/4 #7 x, y,z+1.

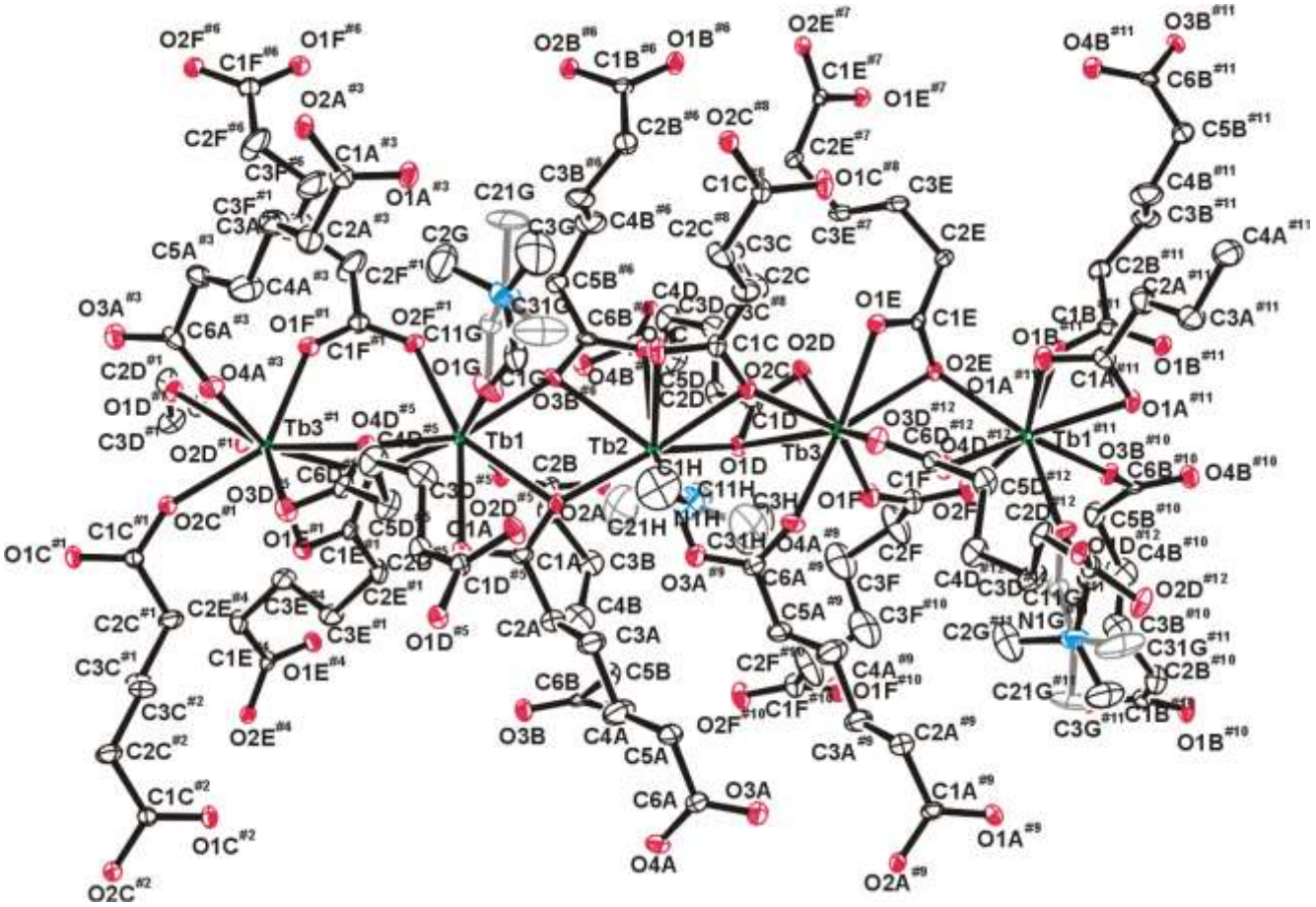

Fig. S3 An ORTEP drawing of **3** with atomic numbering scheme (thermal ellipsoids at 30% probability). DMF coordinating to Tb 1 is disordered. Symmetry operation: #1 x+1/2,-y+3/2,z-1/2 #2 -x+2/5,y+1/2,-z+3/2 #3 -x+5/2,y-1/2,-z+3/2 #4 -x+3/2,y+1/2,-z+3/2 #5 x+1,y,z #6 -x+3/2,y-1/2,-z+3/2 #7 -x+1,-y+1,-z+2 #8 -x+2,-y+1,-z+2 #9 -x+2,-y+2,-z+2 #10 -x+1,-y+2,-z+2 #11 x-1/2,-y+3/2,z+1/2 #12 x+1/2,-y+3/2,z+1/2.

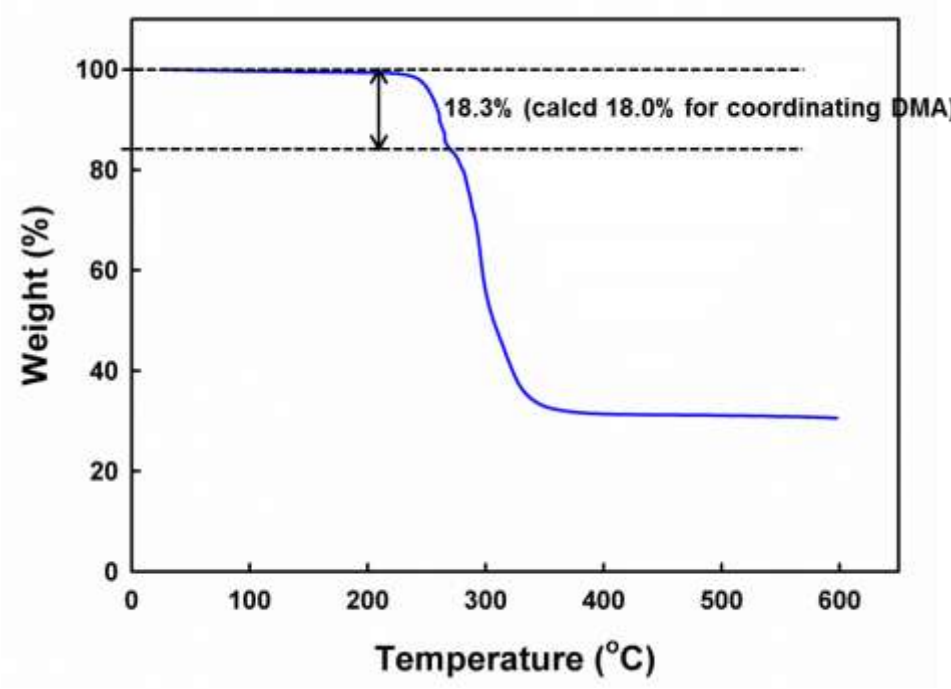

Fig. S4 TGA trace for **1**.

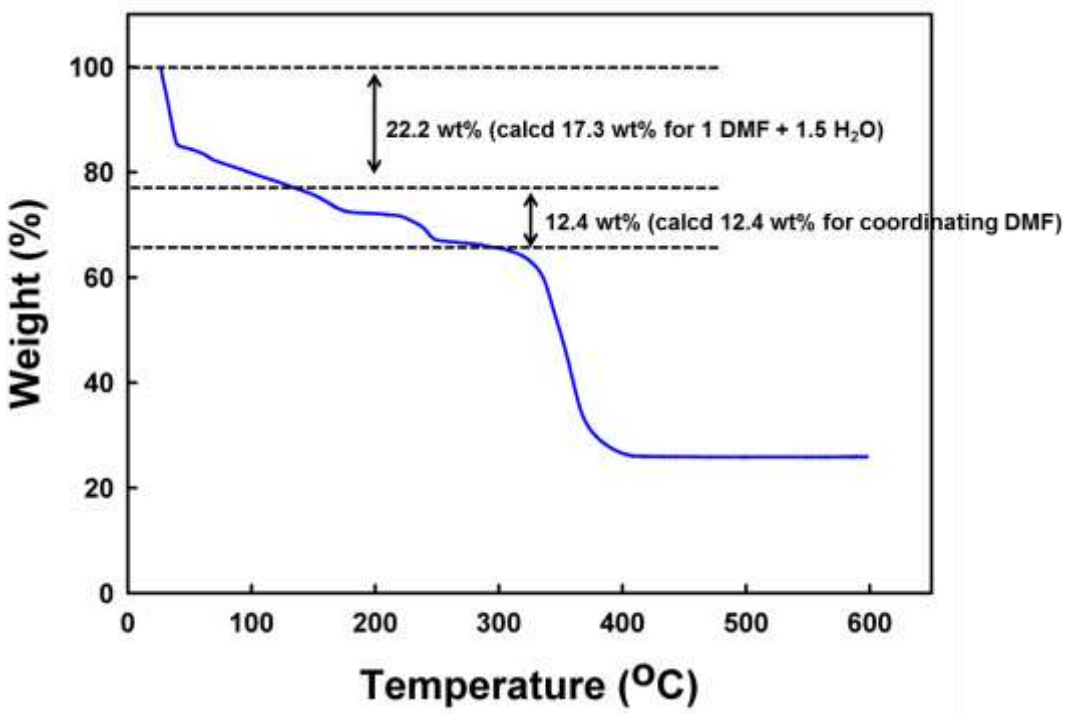

Fig. S5 TGA trace for **2**.

5

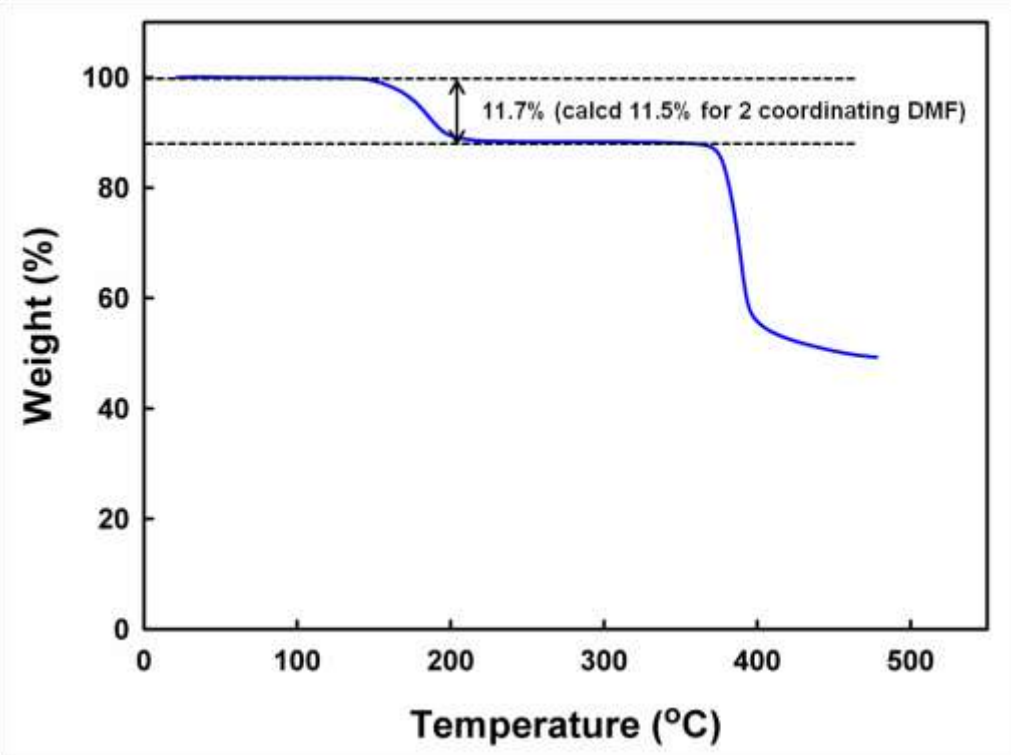

Fig. S6 TGA trace for **3**.