Electronic Supplementary Material for CrystEngComm

<Supplementary Information>

2D Layered Metal-Organic Frameworks Built Using a Hexanuclear Metallamacrocycle and an Octanuclear Metallamacrocycle as Supramolecular Building Blocks

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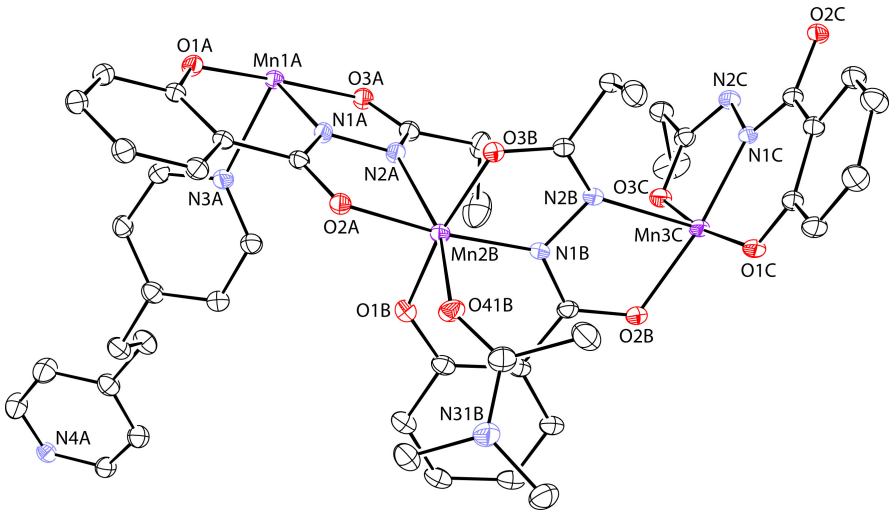

Figure S1. An ORTEP drawing of the asymmetric unit for the network, **2**, with 20% probability ellipsoids.

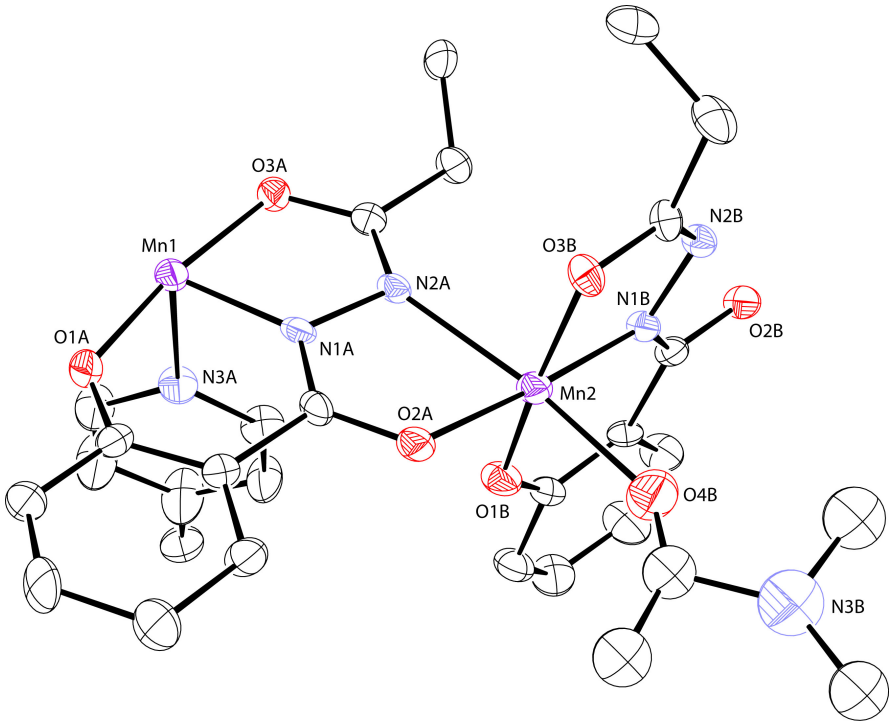

Figure S2. An ORTEP drawing of the asymmetric unit for the network, **3**, with 20% probability ellipsoids.

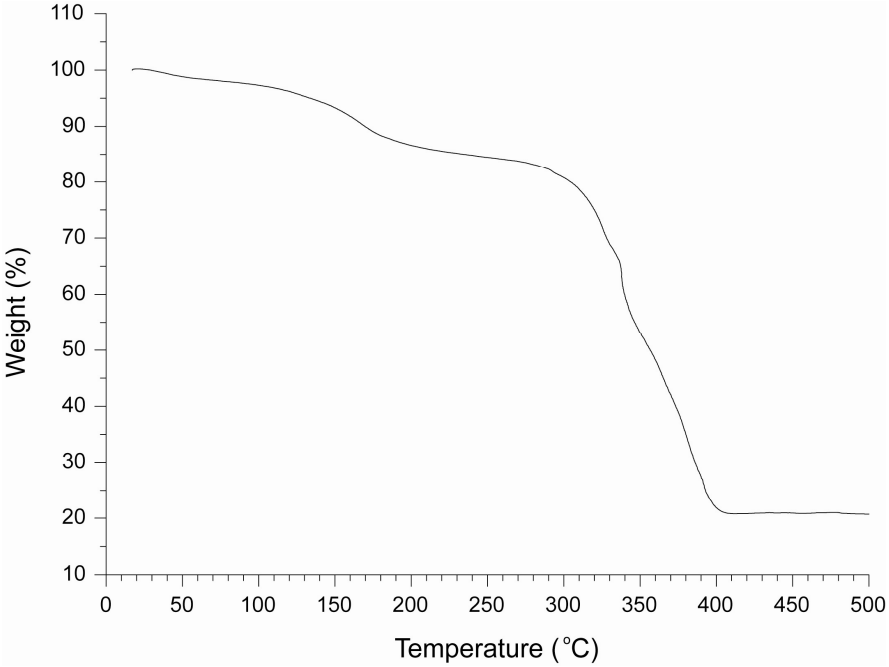

Figure S3. TGA data of for network **2**.

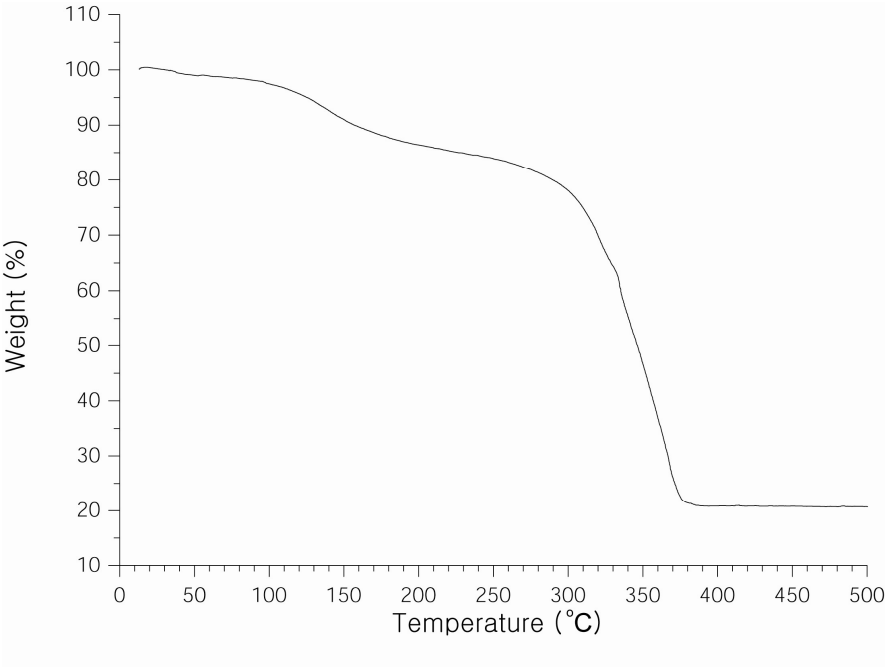

Figure S4. TGA data for network **3**.

Table S1. Crystal data and structure refinement for **2**.

Empirical formula	$Mn_6C_{104}H_{120}N_{21}O_{24}$	
Formula weight	1188.92	
Temperature	100(2) K	
Wavelength	0.80000 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 16.675(3) Å	α = 90°.
	b = 28.710(6) Å	β = 100.23(3)°.
	c = 23.663(5) Å	γ = 90°.
Volume	11148(4) $Å^3$	
Z	4	
Density (calculated)	1.417 Mg/m^3	
Absorption coefficient	0.739 mm^{-1}	
F(000)	4932	
Crystal size	0.33 x 0.30 x 0.20 mm^3	
Theta range for data collection	1.88 to 30.40°.	
Index ranges	-21<=h<=21, -36<=k<=36, -29<=l<=29	
Reflections collected	39781	
Independent reflections	11692 [R(int) = 0.0598]	
Completeness to theta = 30.40°	99.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8664 and 0.7926	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11692 / 0 / 718	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0646, wR2 = 0.1823	
R indices (all data)	R1 = 0.0675, wR2 = 0.1849	
Largest diff. peak and hole	1.381 and -0.840 e.$Å^{-3}$	

Table S2. Crystal data and structure refinement for **3**.

Empirical formula	$Mn_8C_{165}H_{233.25}N_{35.25}O_{39.25}$	
Formula weight	3778.14	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	*P*4/*ncc*	
Unit cell dimensions	a = 26.988(3) Å	α = 90°.
	b = 26.988(3) Å	β = 90°.
	c = 29.158(5) Å	γ = 90°.
Volume	21238(5) $Å^3$	
Z	4	
Density (calculated)	1.182 Mg/m^3	
Absorption coefficient	0.531 mm^{-1}	
F(000)	7936	
Crystal size	0.48 x 0.48 x 0.30 mm^3	
Theta range for data collection	1.51 to 22.00°.	
Index ranges	-27<=h<=24, -28<=k<=12, -30<=l<=30	
Reflections collected	42577	
Independent reflections	6531 [R(int) = 0.0990]	
Completeness to theta = 22.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8571 and 0.7848	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6531 / 7 / 401	
Goodness-of-fit on F^2	0.883	
Final R indices [I>2sigma(I)]	R1 = 0.0837, wR2 = 0.2243	
R indices (all data)	R1 = 0.1522, wR2 = 0.2523	
Largest diff. peak and hole	0.616 and -0.261 $e.Å^{-3}$	

Table S3. Close contact interactions [Å and °] for **2**.

CH ··· O interactions				
D-H ··· A	d(D-H)	d(H ··· A)	d(D ··· A)	<(DHA)
C(12A)-H(12A) ··· O(1A)[a]	0.95	2.55	3.394(6)	148
C(6C)-H(6C) ··· O(1C)[b]	0.95	2.57	3.468(7)	158
CH ··· π interactions				
D-H ··· A	d(D-H)	d(H ··· A)	d(D ··· A)	<(DHA)
C(13B) -H(13A) ··· C(3C)[b]	0.98	3.12	3.558(6)	109
C(13B) -H(13B) ··· C(4C)[b]	0.98	3.05	3.589(7)	116

Symmetry transformations used to generate equivalent atoms: [a] 1/2-x, -1/2-y, 1-z, [b] 1/2-x, 1/2-y, 1-z

Table S4. Close contact interactions [Å] for **3**.

π···π stacking interactions	
Displacement of the ligated dma molecule from the best plane of the benzene group of the ligand	
O4B[a]	3.65(1)
N3B[a]	3.67(1)
C11B[a]	3.54(2)
C12B[a]	3.50(2)
C13B[a]	3.65(1)
C14B[a]	3.75(2)

Symmetry transformation used to generate equivalent atoms: [a] 2-x, 1-y, -z