Supplementary Material (ESI) for *Dalton Transactions*

Supporting Information

A Dodecanuclear Metallamacrocycle Having a Multidentate Bridging Ligand with Two Different Binding Modes

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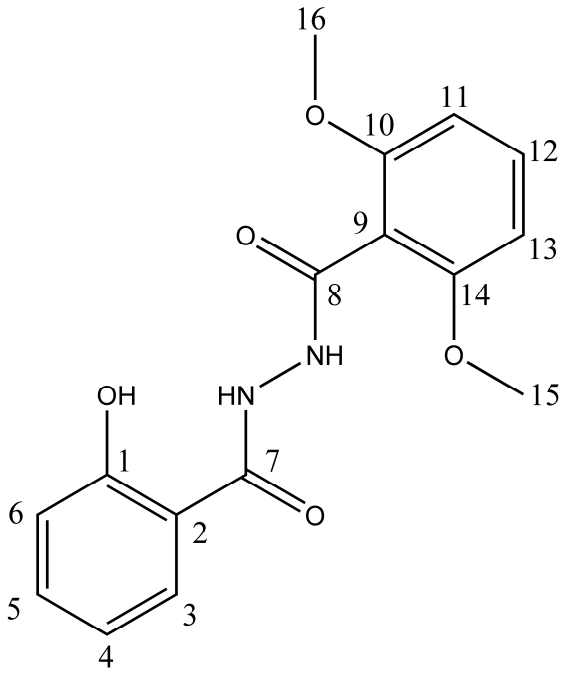

Scheme S1. A numbering scheme of the ligand, H_3dmbshz.

Table S1. Crystal data and structure refinement for complex **1.**

Empirical formula	C230 H294 Mn12 N24 O82	
Formula weight	5366.17	
Temperature	100(2) K	
Wavelength	0.70000 Å	
Crystal system	Rhombohedral	
Space group	R-3	
Unit cell dimensions	a = 29.040(4) Å	α= 90°.
	b = 29.040(4) Å	β= 90°.
	c = 26.733(5) Å	γ = 120°.
Volume	19524(5) $Å^3$	
Z	3	
Density (calculated)	1.369 Mg/m^3	
Absorption coefficient	0.648 mm^{-1}	
F(000)	8394	
Crystal size	0.06 x 0.04 x 0.04 mm^3	
Theta range for data collection	1.09 to 26.57°.	
Index ranges	-37<=h<=23, -37<=k<=37, -34<=l<=29	
Reflections collected	25353	
Independent reflections	9406 [R(int) = 0.0711]	
Completeness to theta = 26.57°	99.0 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9745 and 0.9621	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9406 / 1 / 462	
Goodness-of-fit on F^2	0.890	
Final R indices [I>2sigma(I)]	R1 = 0.0656, wR2 = 0.1896	
R indices (all data)	R1 = 0.1299, wR2 = 0.2123	
Largest diff. peak and hole	0.535 and -0.454 $e.Å^{-3}$	

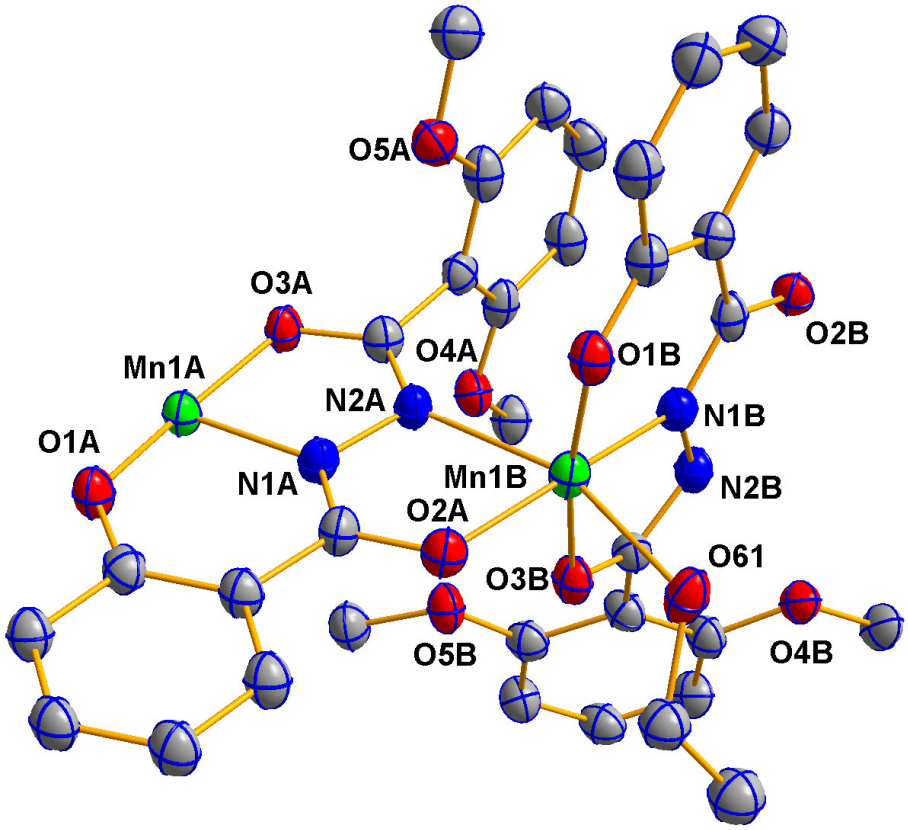

Figure S1. An ORTEP diagram of the asymmetric unit of **1** drawn with 20% probability ellipsoids.

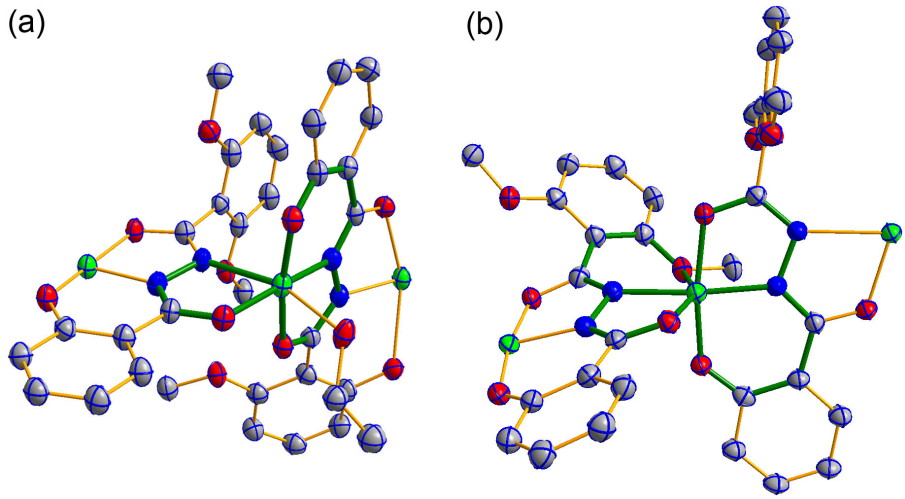

Figure S2. The two different types of chelation modes observed around the metal centers. (a) A bidentate–tridentate chelation mode leads to a Λ/Δ–type chiral configuration. (b) A tridentate–tridentate chelation mode leads to a *C*/*A*–type chiral configuration.

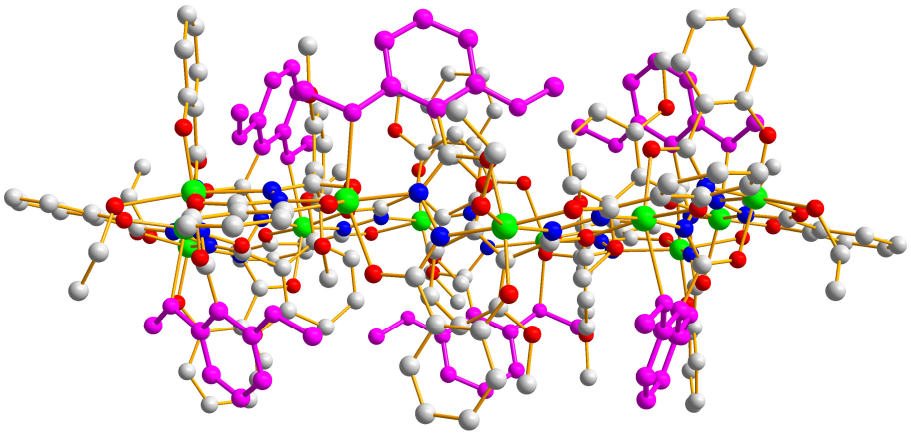

Figure S3. A ball-and-stick side view of 1. Six 2,6-dimethoxyphenyl groups involved in the ligation to the ring metal centers are arranged vertically up and down relative to the metalladiazamacrocyclic ring plane.

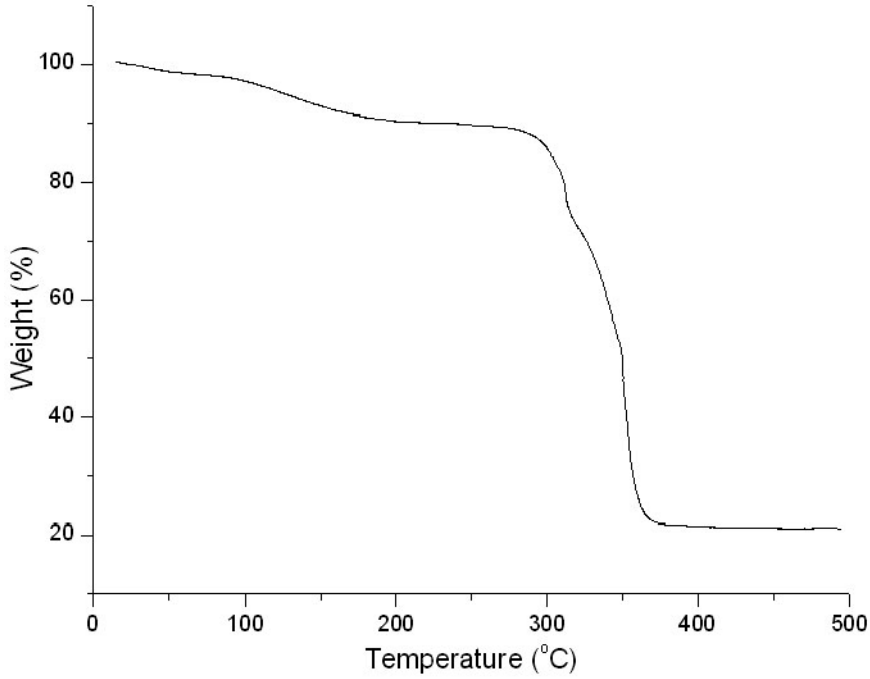

Figure S4. TGA of the dodecanuclear metalladiazamacrocycle, **1**.