

Supplementary Information

Synthetic ability of dinuclear mesocates containing 1,3-bis(diazinecarboxamide)benzene bridging ligands to form complexes of increased nuclearity. Crystal Structures, magnetic properties and theoretical studies.

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Bond Lengths / Å		Bond Angles / °	
Ni1-N1	2.118(2)	N1-Ni1-N3	78.06(9)
Ni1-N3	2.083(2)	N1- Ni1- N1'	91.44(9)
O1-C5	1.268(3)	<i>cis</i> -N1-Ni-N3'	91.99(9)
N1-C1	1.332(4)	<i>cis</i> -N3-Ni1-N3'	98.91(7)
N1-C4	1.342(4)	<i>trans</i> -N1-Ni1-N3'	169.03(9)
N3-C5	1.303(4)	C1-N1-Ni1	129.1(2)
N3-C6	1.426(3)	C1-N1-C4	117.4(2)
N2-C1	1.326(4)	C4-N1-Ni1	113.26(17)
N2-C2	1.329(5)	C5-N3-N1	117.67(17)
C2-C3	1.382(5)	C5-N3-C6	117.8(2)
C3-C4	1.390(4)	C6-N3-Ni1	124.48(17)
C4-C5	1.509(4)	C1-N2-C2	115.6(3)
C6-C7	1.392(3)	N2-C1-N1	126.2(3)
C6-C8	1.388(4)	N2-C2-C3	123.5(3)
C8-C9	1.386(3)	C2-C3-C4	116.5(3)
		N1-C4-C3	120.7(3)
		N1-C4-C5	116.8(2)
		C3-C4-C5	122.5(3)
		O1-C5-N3	128.7(2)
		O1-C5-C4	117.3(2)
		N3-C4-C4	114.0(2)
		C7-C6-N3	119.4(2)
		C8-C6-N3	120.7(2)
		C8-C6-C7	119.9(3)
		C6-C7-C6	120.2(3)
		C9-C8-C6	119.4(3)
		C8-C9-C8	121.2(4)
		N2-C1-N1	126.2(3)

Table S1.- Selected bond distances (Å) and angles (°) for complex **1**.

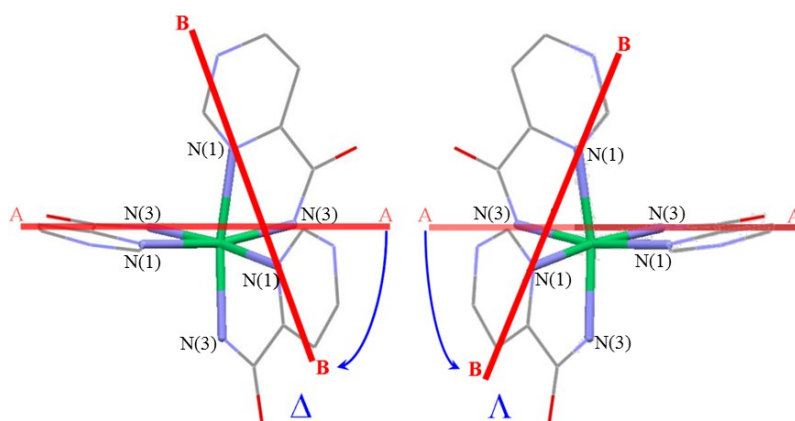


Figure S1: Coordination sphere of Ni²⁺ centres in the [Ni₂(bpcb)₃]²⁻ unit showing opposite Λ and Δ conformations according to the skew line convention

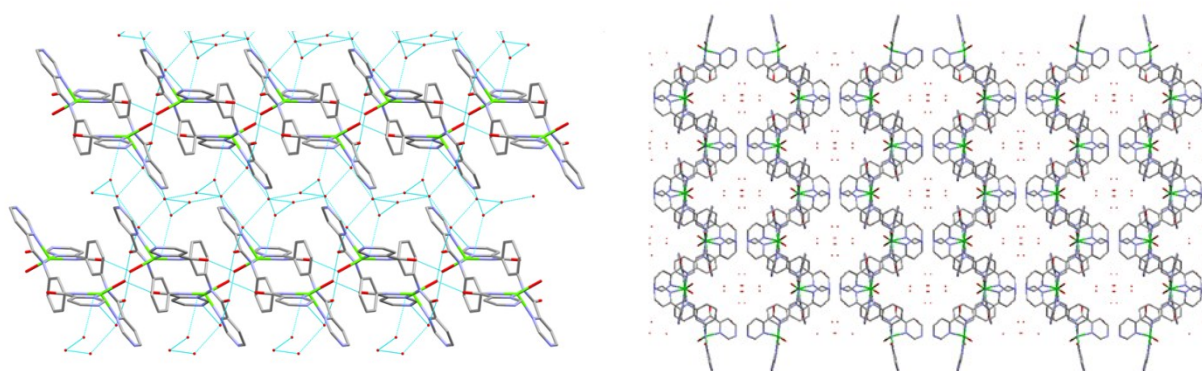


Figure S2: View along plan *ac* (left) and along plan *ab* (right) of **3**

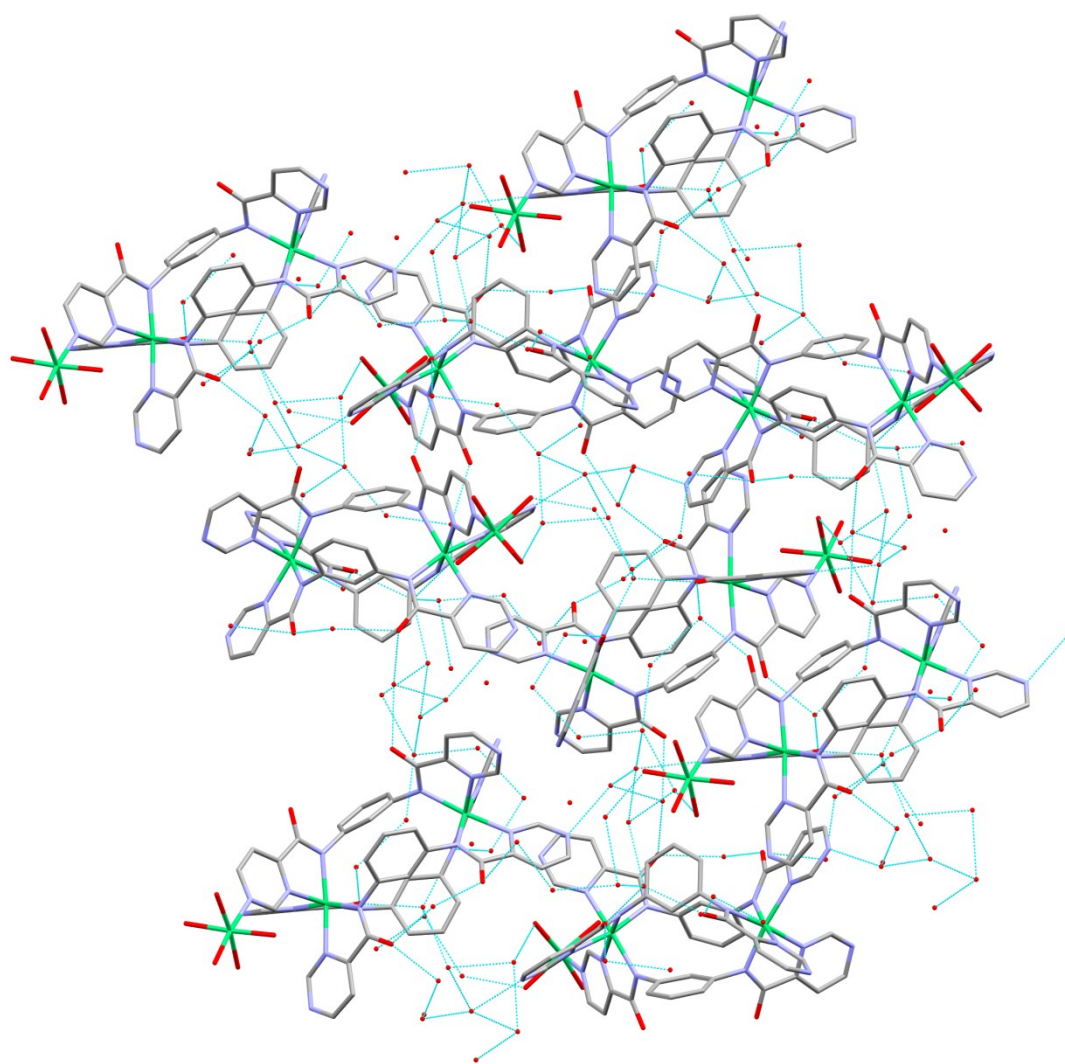


Figure S3: Perspective view of the three-dimensional array of **5** along the [100] direction. Hydrogen atoms have been omitted for the sake of clarity.

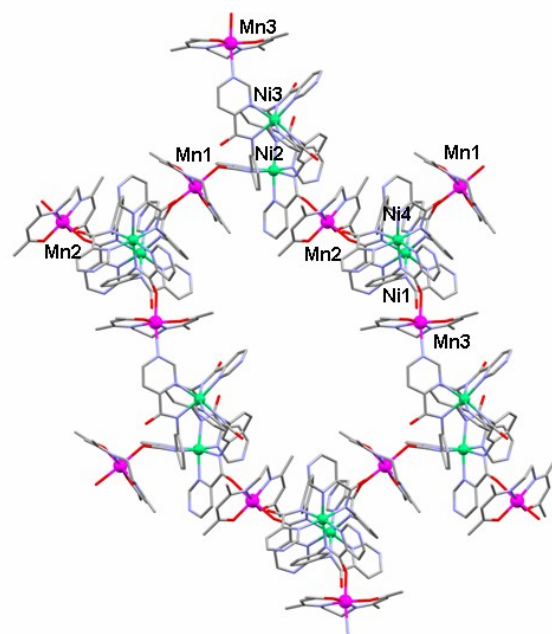


Figure S4: Representation of the hexagon formed by the Ni²⁺ dimers and Mn³⁺ units in 7.

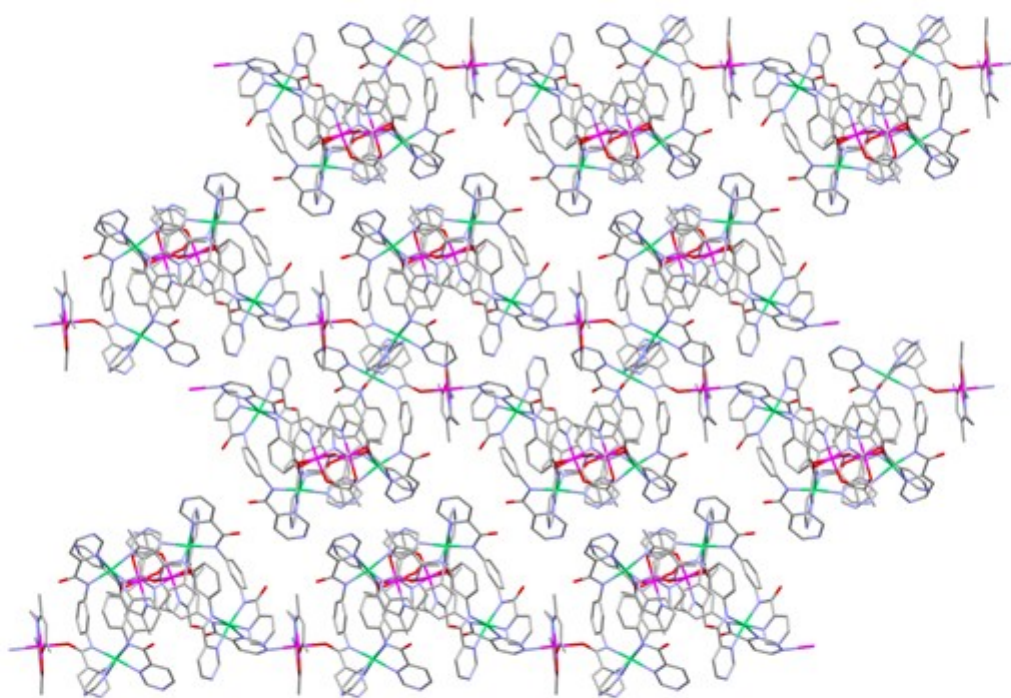


Figure S5: Stacking of 7

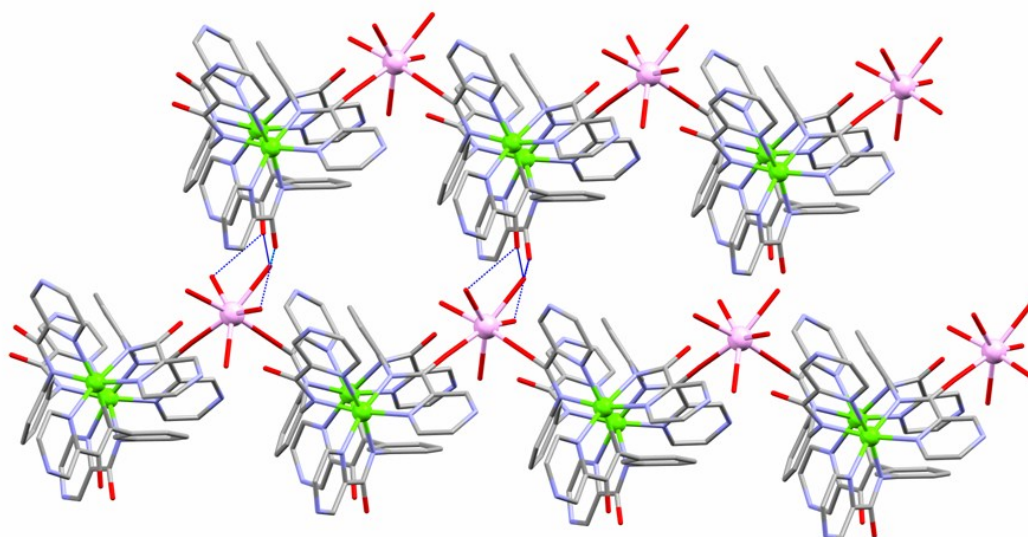


Figure S6: 2D system for compound **8**

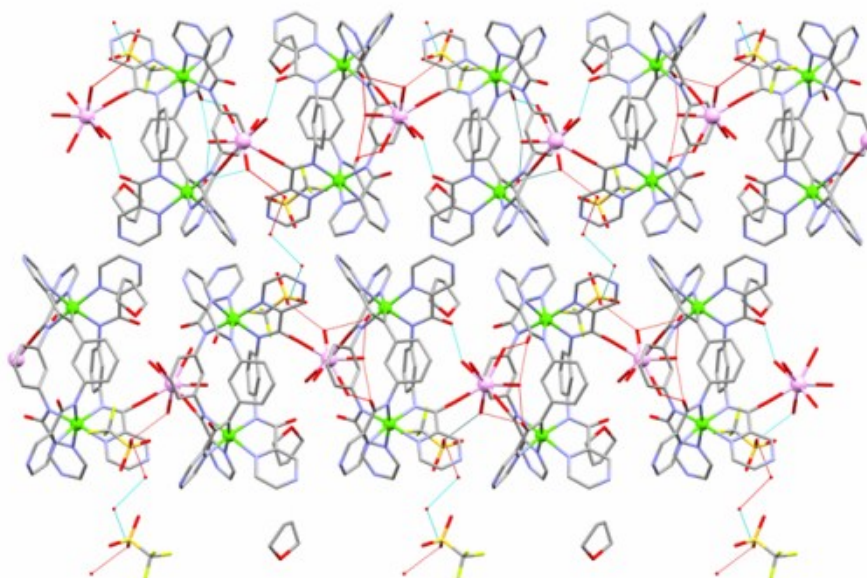


Figure S7: view of the interactions between solvent molecules in **8**

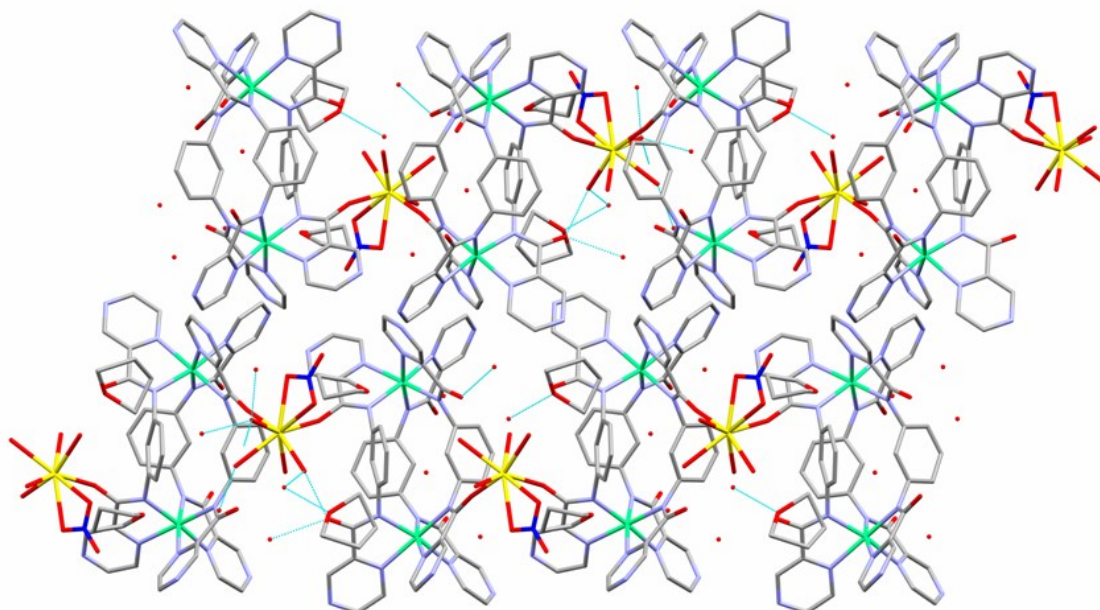


Figure S8: Hydrogen bond for compounds **9** and **10**

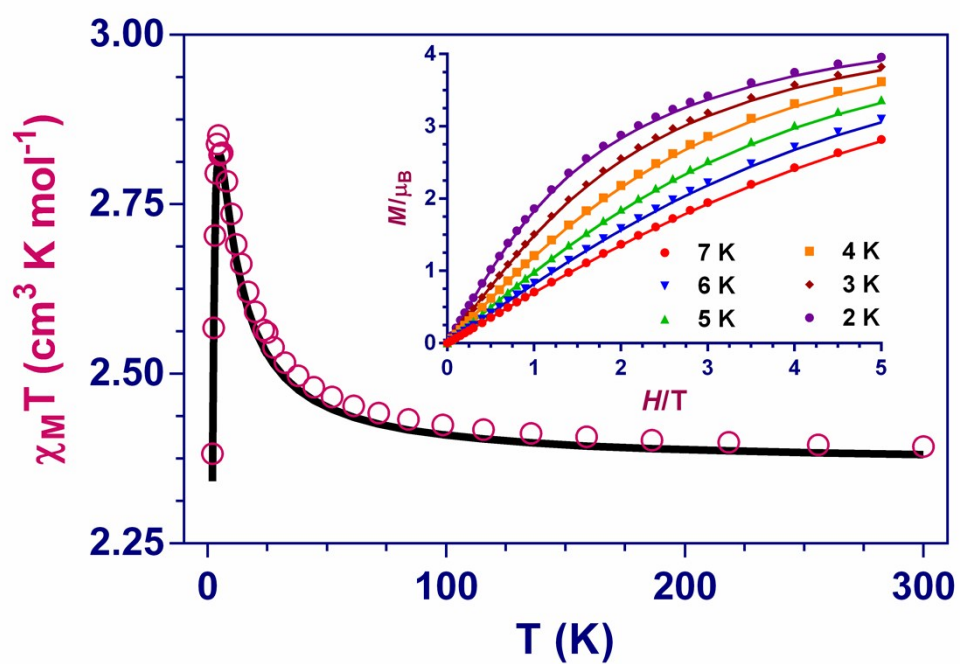


Figure S9.- Temperature dependence of $\chi_M T$ for **2** Inset: Field dependence of the magnetisation. Solid lines represent the best fit results with zJ' fixed at zero.

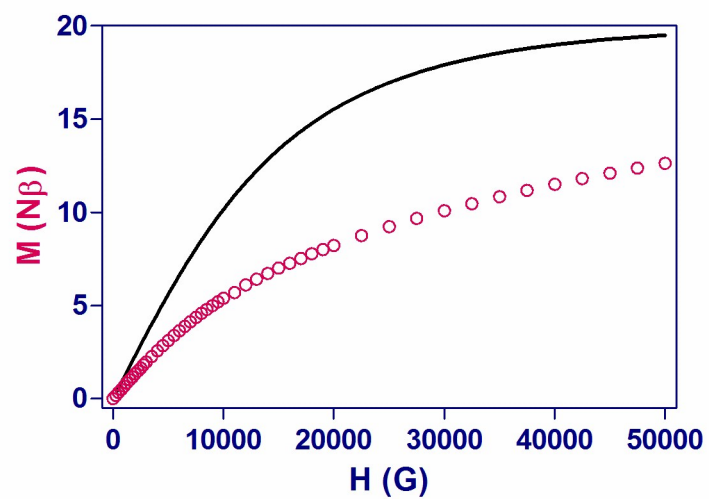


Figure S10.- Field dependence of magnetisation for 7. The solid line corresponds to the Brillouin function with g values for Mn^{3+} and Ni^{2+} equal to 2.