

Electronic Supplementary Information

Wheel-type Heterometallic Ferromagnetic Clusters: $[\text{Ni}_{7-x}\text{M}_x(\text{HL})_6(\mu_3\text{-OMe})_4(\mu_3\text{-OH})_2]\text{Cl}_2$ ($\text{M} = \text{Zn}, \text{Co}, \text{Mn}; x = 1, 3$)

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Table S1. Synthetic details and estimated compositions for **1–7**.

Substrates for synthesis of $[\text{Ni}_{7-x}\text{M}_x]$									
x	Amount of Ni^{II}		Amount of Zn^{II}		Amount of Co^{II}		Amount of Mn^{II}		Nominal composition of cluster core
	[mmol]	[mg]	[mmol]	[mg]	[mmol]	[mg]	[mmol]	[mg]	
0	1.17	277	-	-	-	-	-	-	$[\text{Ni}_7]$
1	1.0	237	0.17	23.2	-	-	-	-	$[\text{Ni}_6\text{Zn}]$
1	1.0	237	-	-	0.17	40.4	-	-	$[\text{Ni}_6\text{Co}]$
1	1.0	237	-	-	-	-	0.17	33.6	$[\text{Ni}_6\text{Mn}]$
3	0.67	158	0.5	68.2	-	-	-	-	$[\text{Ni}_4\text{Zn}_3]$
3	0.67	158	-	-	0.5	119.0	-	-	$[\text{Ni}_4\text{Co}_3]$
3	0.67	158	-	-	-	-	0.5	99.0	$[\text{Ni}_4\text{Mn}_3]$

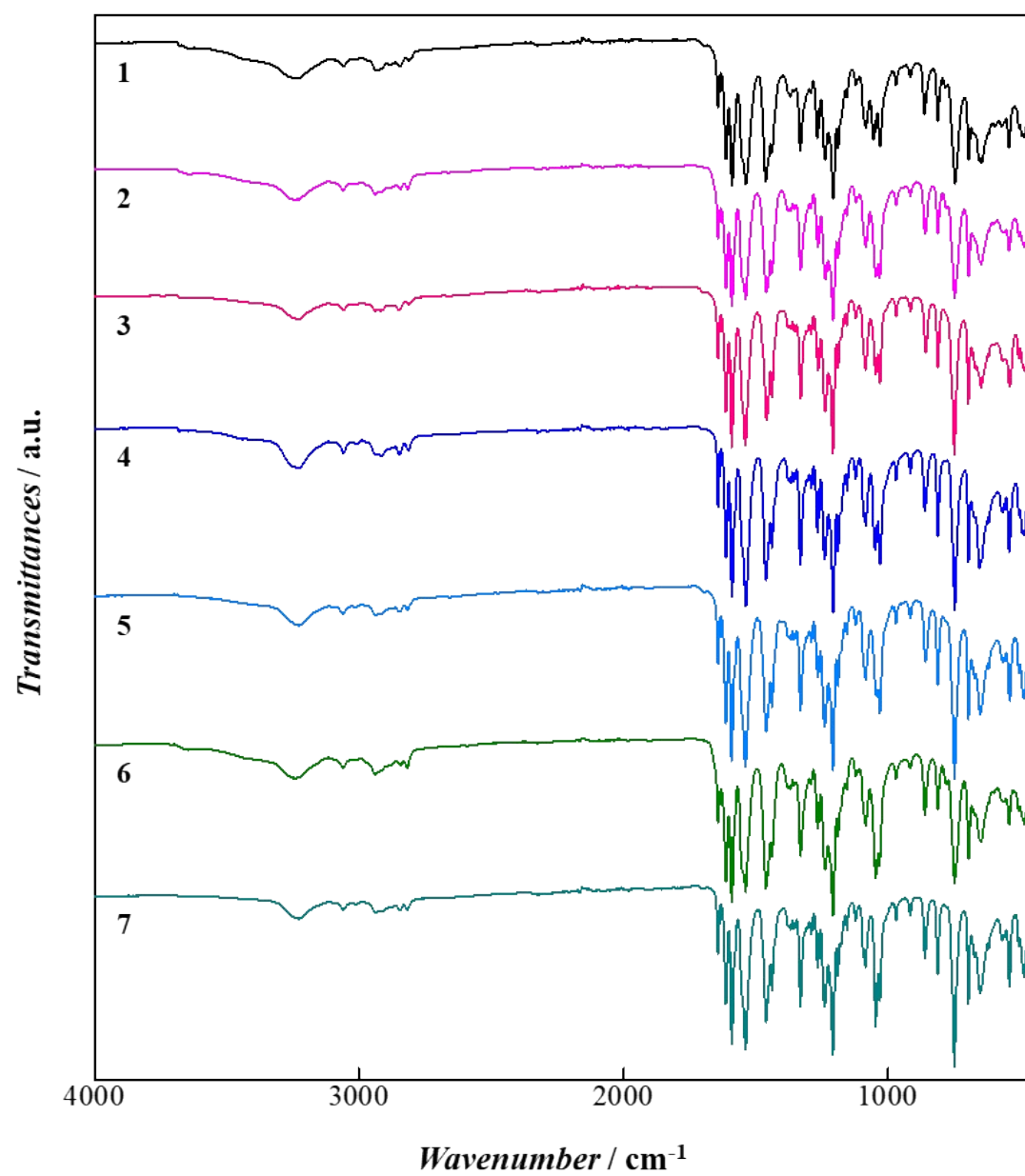


Figure S1. FT-IR spectra for 1–7.

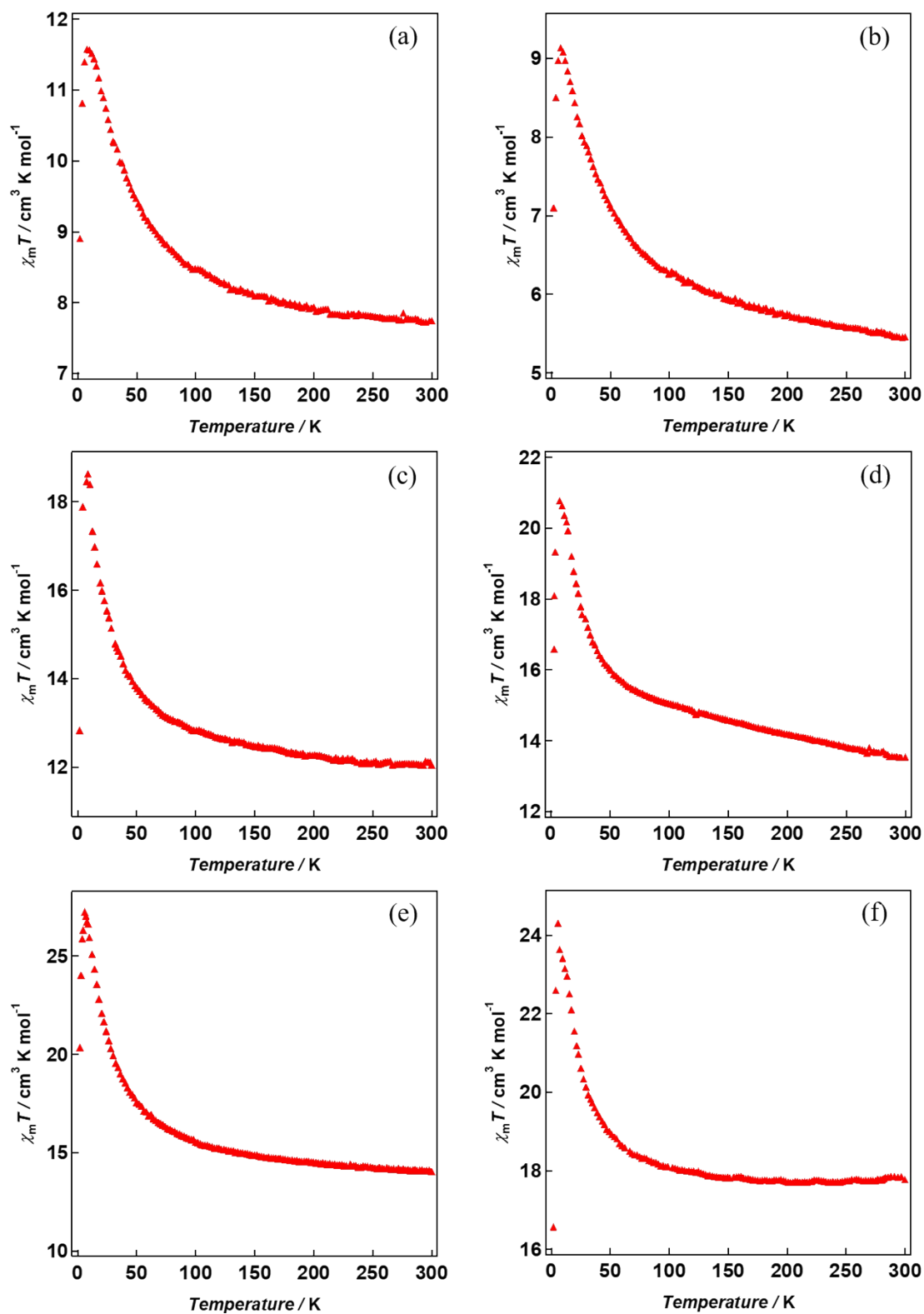


Figure S2. Magnetic behaviors for (a) 2, (b) 3, (c) 4, (d) 5, (e) 6, (f) 7.

Table S2. Crystallographic data for **2** after PLATON SQUEEZE treatment.¹ An additional methanol molecule was added to the final formula.

Compound	2·3CH₃OH
formula	C ₁₀₉ H ₁₂₈ Ni ₆ ZnN ₁₂ O ₂₇ Cl ₂
formula weight	2526.76
crystal system	cubic
space group	<i>Pa</i> ³
<i>a</i> / Å	22.6686(17)
<i>b</i> / Å	22.6686(17)
<i>c</i> / Å	22.6686(17)
<i>α</i> / °	90
<i>β</i> / °	90
<i>γ</i> / °	90
<i>V</i> / Å ³	11648.6(15)
<i>Z</i>	4
<i>T</i> / K	123
<i>R</i> 1	0.0710
w <i>R</i> 2	0.2507
G.O.F.	1.041
CCDC	1853458

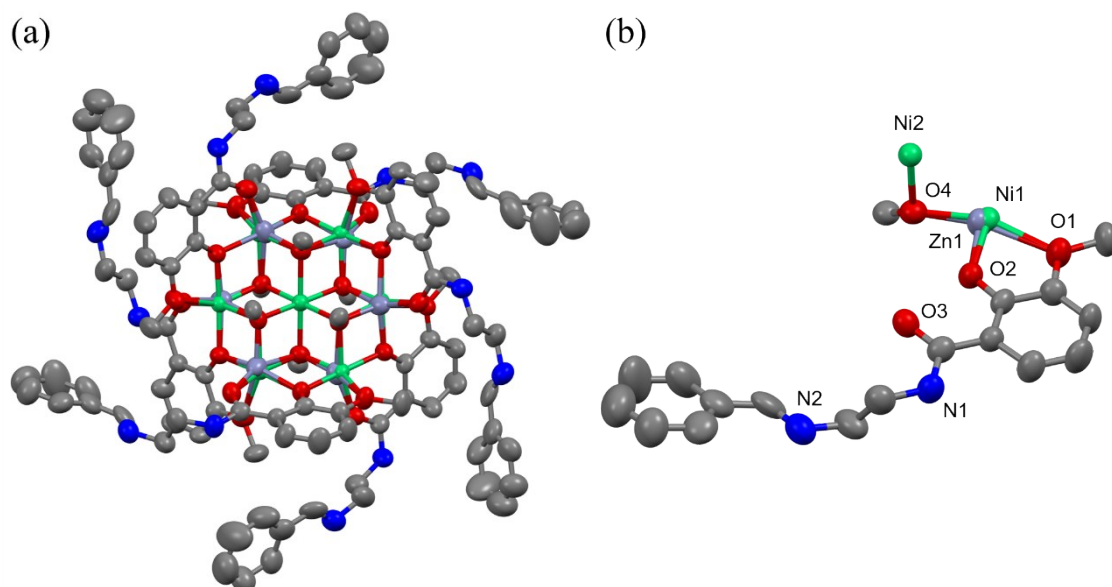


Figure S3. (a) Crystal structure and (b) an asymmetric unit of Ni₆Zn (**2·3CH₃OH**) at 123 K. Ni1 and Zn1 atoms are existed in 0.83333:0.16667 disorder occupancy ratio. All disordered atoms, hydrogen atoms, counter anions, and solvent molecules are omitted for clarity.

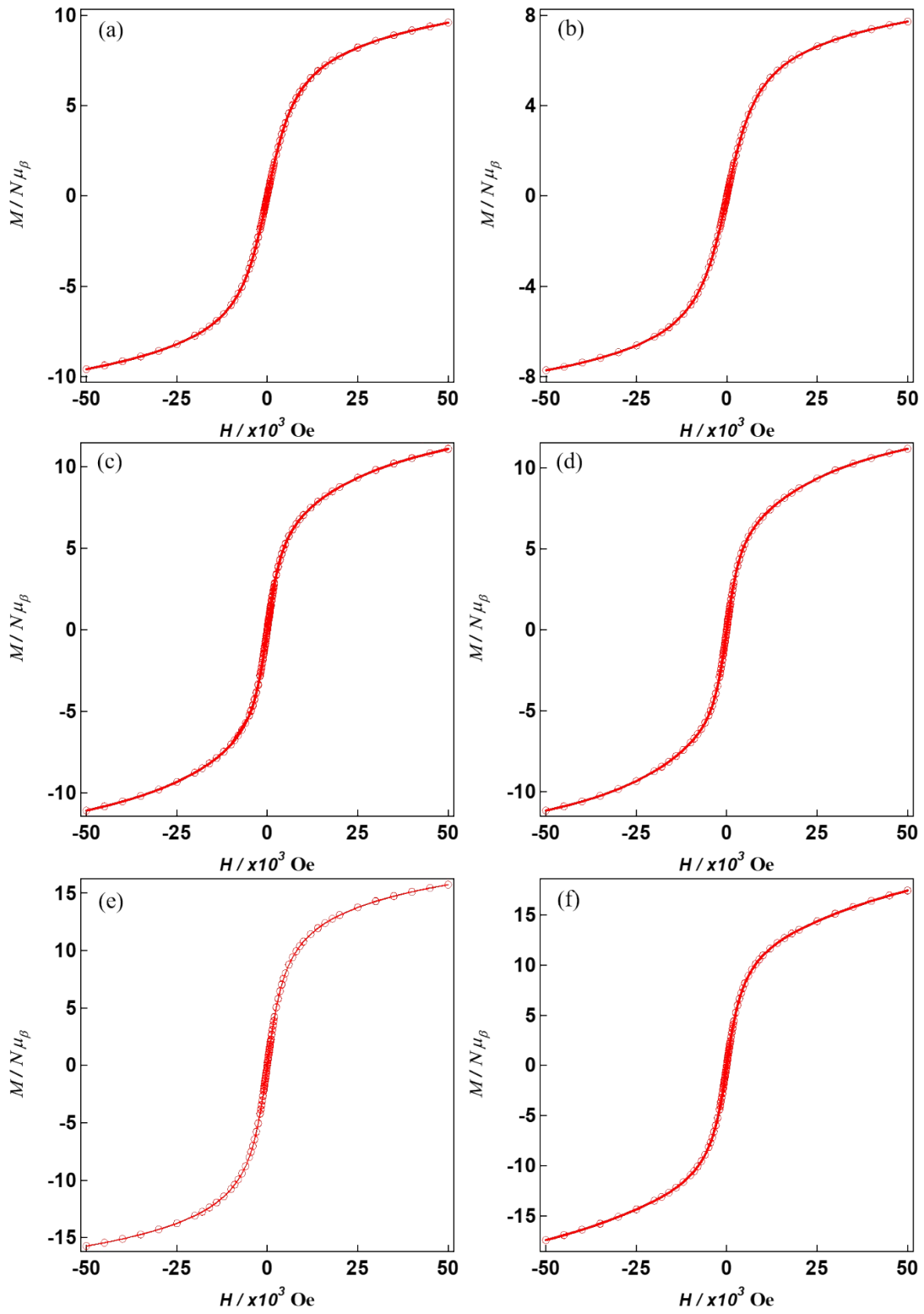


Figure S4. Magnetizations for (a) 2, (b) 3, (c) 4, (d) 5, (e) 6, (f) 7.

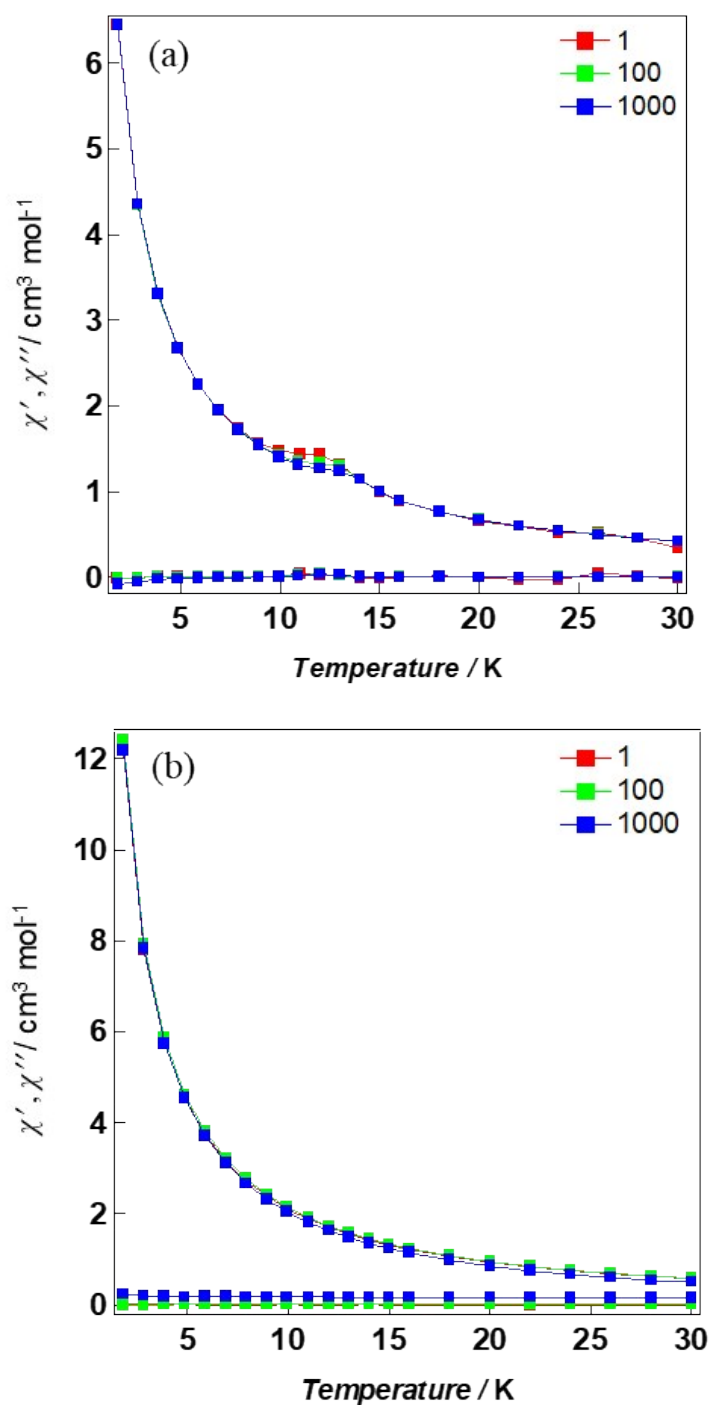


Figure S5. Temperature dependence of alternate current (ac) magnetic susceptibilities measured at $H_{\text{ac}} = 3$ Oe for (a) Ni_7 ; **1**, (b) Ni_4Mn_3 ; **7**.

Reference in ESI

(1) A. L. Spek, *J. Appl. Cryst.*, 2003, **36**, 7–13.