

Supporting information

Windmill-Shaped Octanuclear $\text{Zn}^{\text{II}}_4/\text{Ln}^{\text{III}}_4$ ($\text{Ln}^{\text{III}} = \text{Dy}, \text{Tb}, \text{Ho}$) Heterometallic Ensembles Supported by a Tetraferrocene Scaffold.

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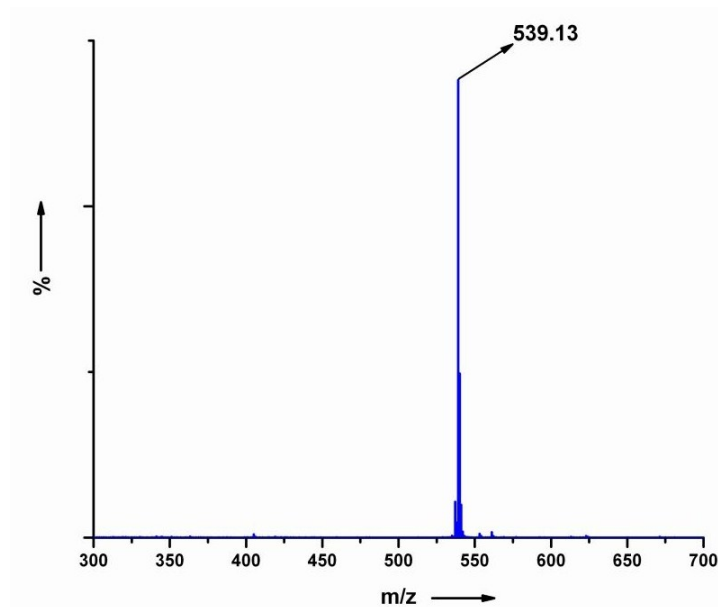


Figure S1. ESI-MS mass spectrum of H₄L (**1**) showing the parent ion at m/z 539.13(H₅L)⁺.

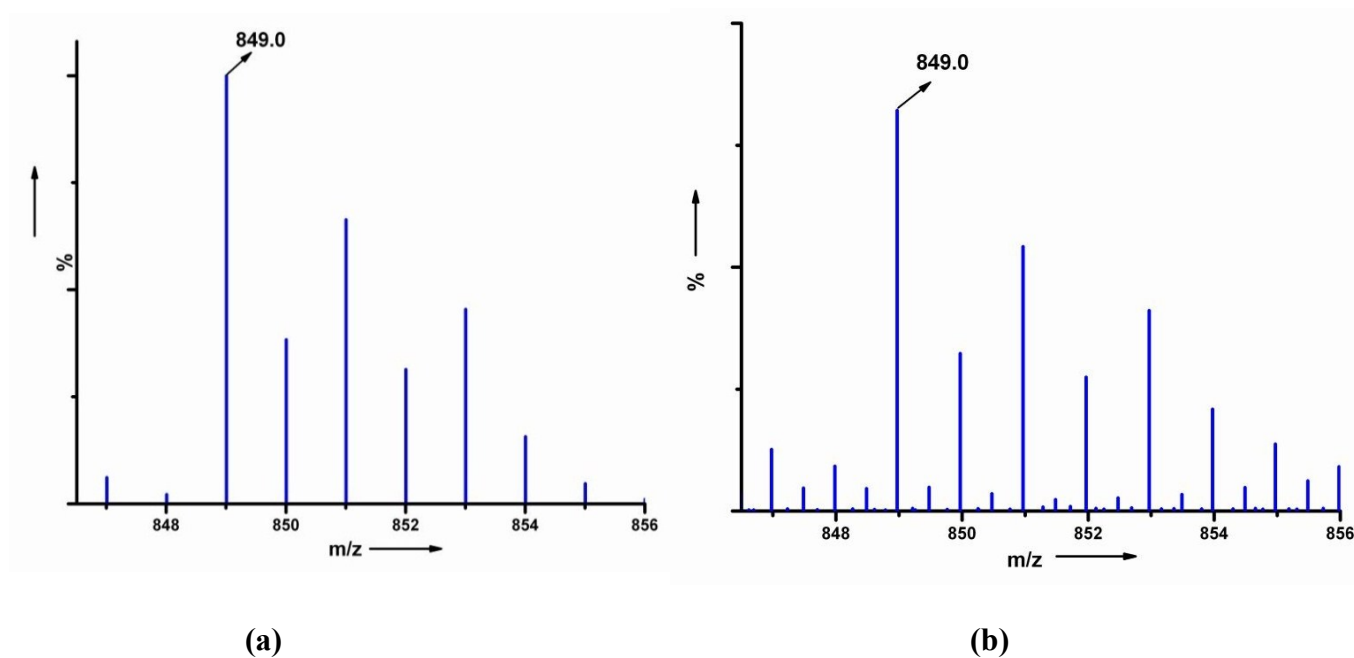


Figure S2. ESI-MS of **3**. (a) Theoretical simulation (b) Experimental spectrum.

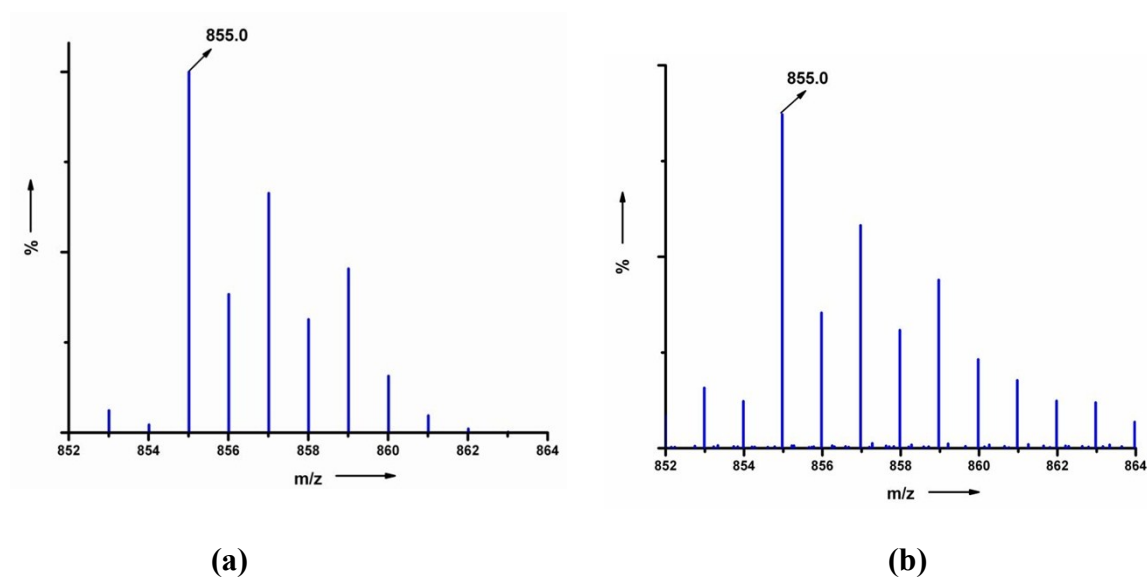


Figure S3. ESI-MS of 4.(a) Theoretical simulation (b) Experimental spectrum.

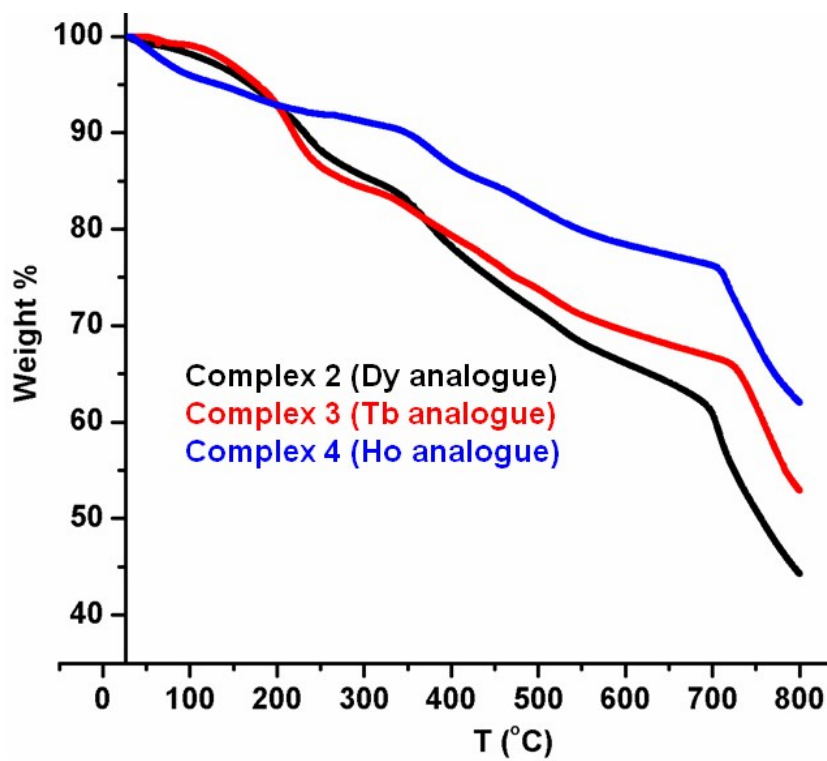


Figure S4. TGA plots of the complexes 2, 3 and 4.

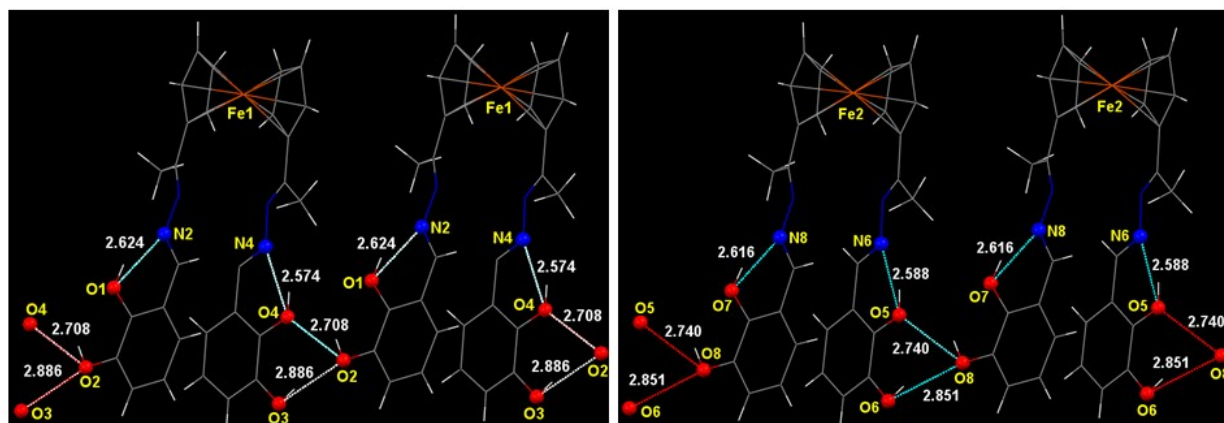


Figure S5. Intra- and inter-molecular H-bonding interactions in the solid state packing of the ligand H₄L (**1**). The H-bond donors and acceptors are highlighted with *ball-and-stick* representation.

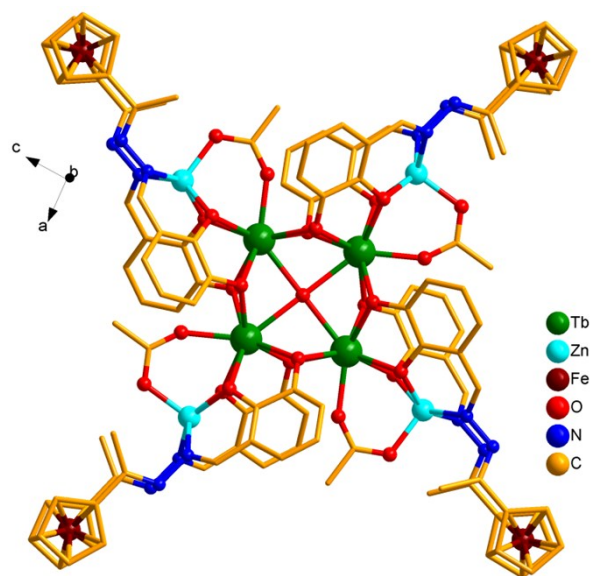


Figure S6. Molecular structure of **3**. Hydrogen atoms and solvent molecules are omitted for clarity.

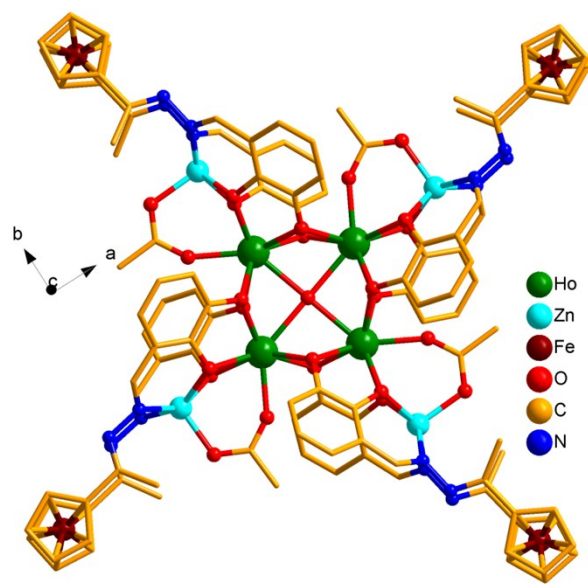
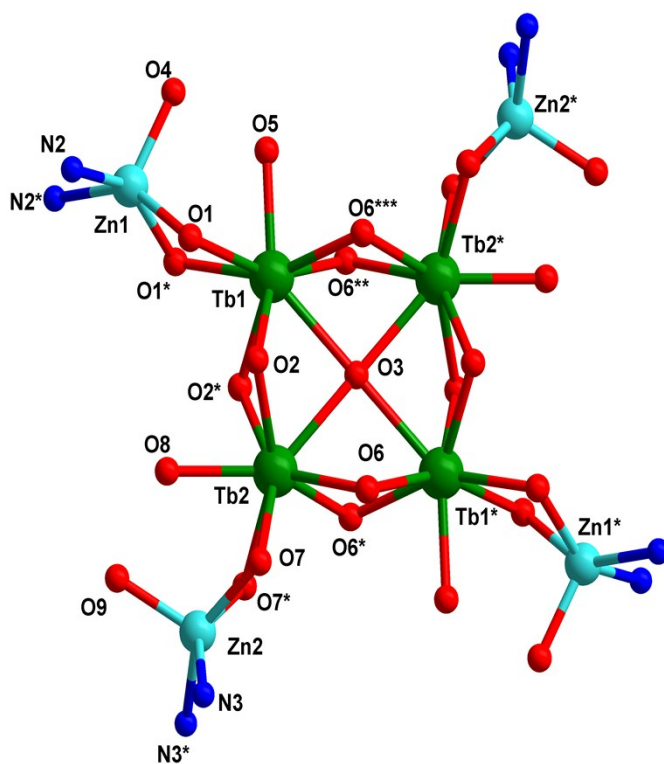


Figure S7. Molecular structure of **4**. Hydrogen atoms and solvent molecules are omitted for clarity.

Table S1.

Core view of 2

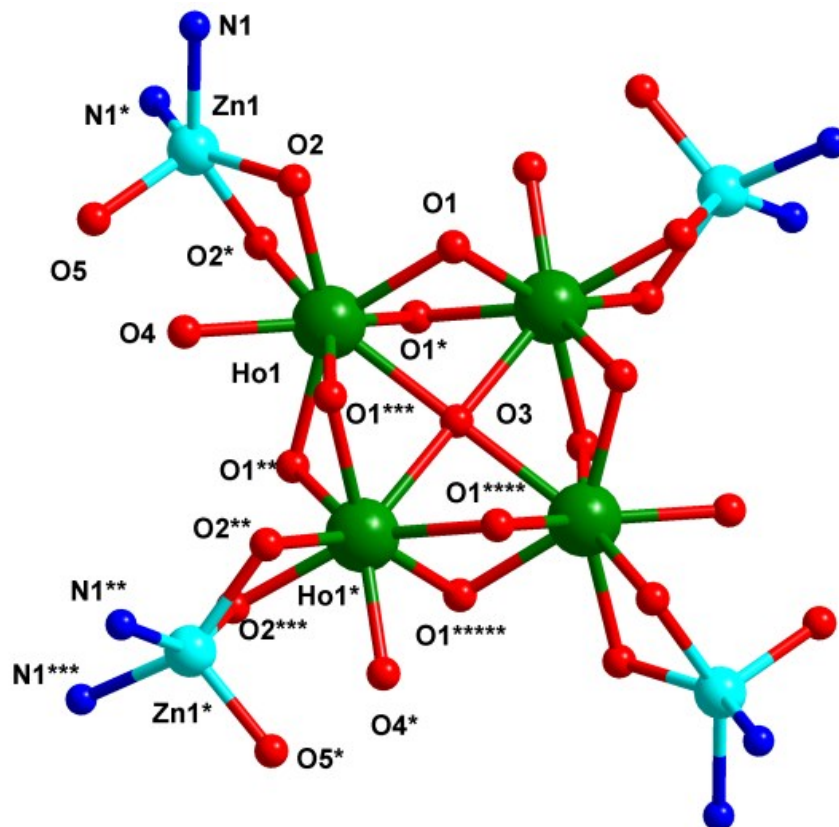


Bond lengths around Zn ^{II} (Å)	Bond angles around Zn ^{II} (°)	Bond lengths around Tb ^{III} (Å)	Bond angles around Tb ^{III} (°)
Zn(1)-O(4), 1.964(5)	Zn(1)-O(1)-Tb(1), 101.2(2)	Tb(1)-O(5), 2.298(5)	Tb(2)-O(3)-Tb(1), 89.61(2)
Zn(1)-O(1)*, 2.066(4)	Zn(2)-O(7)-Tb(2), 100.3(2)	Tb(1)-O(1)*, 2.338(4)	Tb(2)*-O(3)-Tb(1), 90.39(2)
Zn(1)-O(1), 2.066(4)		Tb(1)-O(1), 2.338(4)	Tb(2)-O(3)-Tb(1)*, 90.38 (2)
Zn(1)-N(2), 2.113(5)		Tb(1)-O(2)*, 2.359(5)	Tb(2)*-O(3)-Tb(1)*,
Zn(1)-N(2)*, 2.113(5)		Tb(1)-O(2), 2.359(5)	89.62(2)
Zn(2)-O(9), 1.955(5)		Tb(1)-O(6), 2.365(4)	Tb(1)-O(6)-Tb(2), 96.2(2)
Zn(2)-O(7)*, 2.061(4)		Tb(1)-O(6), 2.365(4)	Tb(1)-O(2)-Tb(2)*, 97.30(2)
Zn(2)-O(7), 2.061(4)		Tb(1)-O(3), 2.5192(5)	
Zn(2)-N(3), 2.101(5)		Tb(1)-Zn(1), 3.4081(10)	

Zn(2)-N(3)*, 2.101(5)		Tb(1)-Tb(2), 3.5302(7) Tb(1)-Tb(2), 3.5542(7) Tb(2)-O(8), 2.300(5) Tb(2)-O(7), 2.352(4) Tb(2)-O(7)*, 2.352(4) Tb(2)-O(2)*, 2.376(5) Tb(2)-O(2)*, 2.376(4) Tb(2)-O(6)*, 2.376(5) Tb(2)-O(6), 2.376(5) Tb(2)-O(3), 2.4902(5) Tb(2)-Zn(2), 3.3928(10) Tb(2)-Tb(1)*, 3.5541(7)	
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Table S2.

Core view of 3



Bond lengths around Zn ^{II} (Å)	Bond angles around Zn ^{II} (°)	Bond lengths around Ho ^{III} (Å)	Bond angles around Ho ^{III} (°)
Zn(1)-O(9), 1.978(8)	Zn(1)-O(7)-Ho(1), 101.0(3)	Ho(1)-O(8), 2.250(8)	Ho(2)-O(3)-Ho(1), 89.99(8)
Zn(1)-O(7), 2.070(6)	Zn(2)-O(1)-Ho(2), 101.9(3)	Ho(1)-O(7)*, 2.311(6)	Ho(2)*-O(3)-Ho(1), 90.02(8)
Zn(1)-O(7)*, 2.070(6)		Ho(1)-O(7) , 2.311(6)	Ho(2)-O(3)-Ho(1), 90.01(8)
Zn(1)-N(3), 2.107(9)		Ho(1)-O(4)*, 2.334(6)	Ho(2)*-O(3)-Ho(1)*, 89.98(8)
		Ho(1)-O(4), 2.334(6)	
		Ho(1)-O(2)**, 2.344(7)	
		Ho(1)-O(2)*, 2.344(7)	
		Ho(1)-O(3)*, 2.451(6)	

Zn(1)-N(3), 2.107(9)		Ho(2)-O(5), 2.244(7)	Ho(1)-O(3)-Ho(1)*, 180.0
Zn(2)-O(6)*, 1.951(8)		Ho(2)-O(1)*, 2.314(6)	Ho(2)-O(2)-Ho(1)*, 95.7(3)
Zn(2)-O(1), 2.041(6)		Ho(2)-O(2)*, 2.331(7)	Ho(1)-O(4)-Ho(2)*, 95.7(3)
Zn(2)-O(1), 2.041(6)		Ho(2)-O(4)*, 2.340(6)	Ho(2)-Ho(1)-Ho(2)*, 89.99(2)
Zn(2)-N(2), 2.107(9)		Ho(2)-O(4)*, 2.340(6)	
Zn(2)-N(2), 2.107(9)		Ho(2)-O(3), 2.4505(6)	
Ho(1)-Zn(1), 3.384(4)		Ho(1)-Ho(2), 3.465(8)	
Ho(2)-Zn(2), 3.386(4)		Ho(1)-Ho(2)*, 3.466(8)	

Table S3. Results of Continuous Shape Measures (SHAPE) ⁶⁴⁻⁶⁶ calculation

SAPR-8 5 D4d Square antiprism
TDD-8 6 D2d Triangular dodecahedron
JBTPR-8 9 C2v Biaugmented trigonal prism J50
BTPR-8 10 C2v Biaugmented trigonal prism
JSD-8 11 D2d Snub diphendoid J84

[ML8]	SAPR-8	TDD-8	JBTPR-8	BTPR-8	JSD-8
Dy1	4.367	2.759	2.660	2.117	4.881
Dy2	4.363	2.760	2.581	2.072	4.795
Tb1	4.481	2.849	2.742	2.270	4.921
Tb2	4.453	2.824	2.789	2.202	5.003
Ho	4.217	2.722	2.625	2.024	4.855

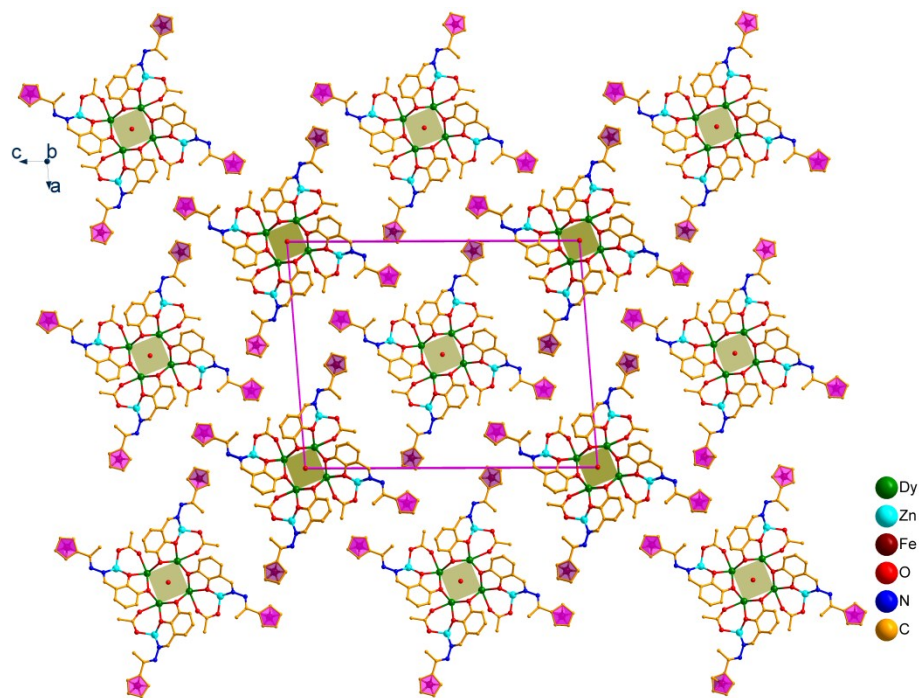


Figure S8. Packing diagram of **2**.