# Supplementary Information

# $Ln^{III}_2Mn^{III}_2$ heterobimetallic "butterfly" complexes displaying antiferromagnetic coupling (Ln = Eu, Gd, Tb, Er)

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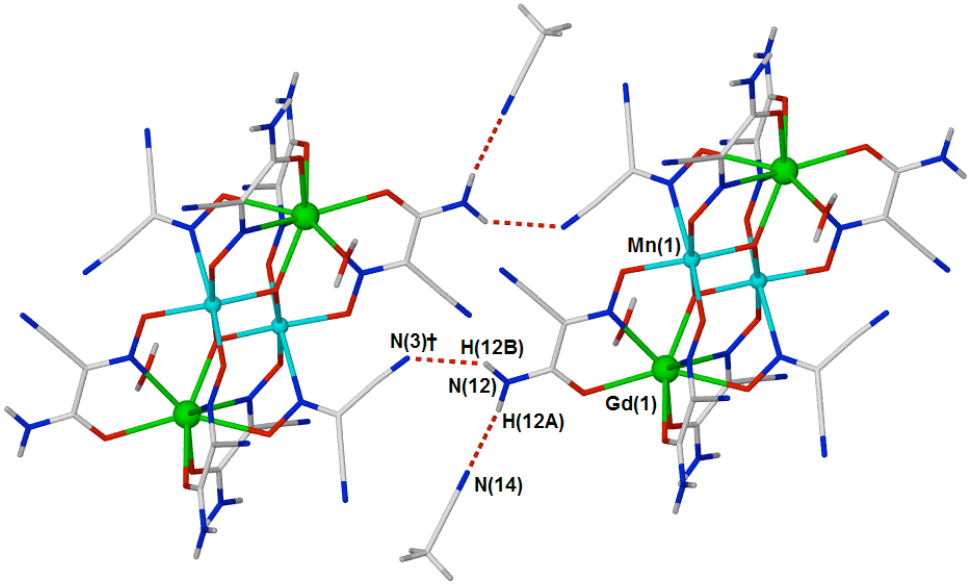


**Fig. S1** Hydrogen bonding within the crystal structure of **1Gd**·3$H_2O$·8MeCN. Complex **1Tb**·3$H_2O$·8MeCN is isostructural. Figures have hydrogen atoms and lattice solvent not participating in hydrogen bonding removed for clarity. Selected bond lengths (Å) and angles (°): N(12)···N(14), 2.962(8); N(12)–H(12A)···N(14), 170; N(12)···N(3)†, 2.943(7); N(12)–H(12B)···N(3)†, 139. Symmetry element used: † = x, 1 + y, z.

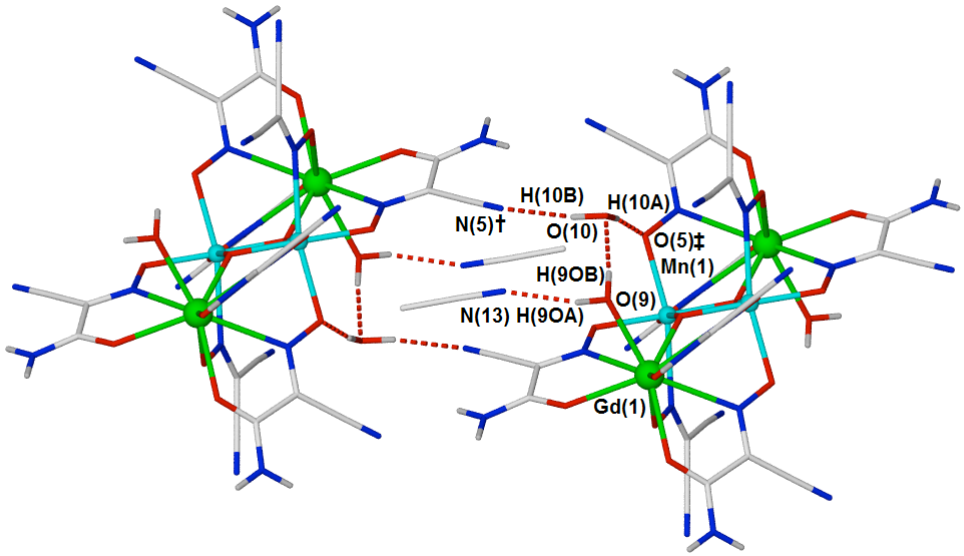


**Fig. S2** Hydrogen bonding within the crystal structure of **1Gd**·3$H_2O$·8MeCN. Complex **1Tb**·3$H_2O$·8MeCN is isostructural. Lattice solvent not participating in hydrogen bonding removed for clarity. Selected bond lengths (Å) and angles (°): O(9)···N(13), 2.808(10); O(9)–H(9OA)···N(13), 147; O(9)···O(10), 2.722(6); O(9)–H(9OB)···O(10), 169; O(10)···N(5)†, 2.911(6); O(10)–H(10B)···N(5)†, 155; O(10)···O(5)‡, 2.866(4); O(10)–H(10A)···O(5)‡, 164. Symmetry elements used: † = 1 − x, −y, 1 − z; ‡ = −x, −y, 1 − z.

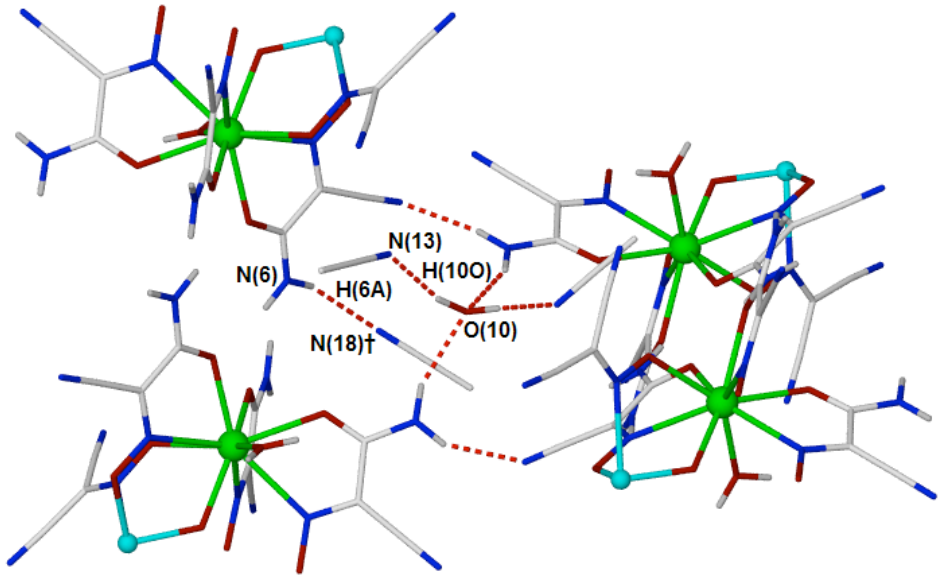


**Fig. S3** Hydrogen bonding within the crystal structure of **1Er**·$H_2O$·11MeCN. Lattice solvent not participating in hydrogen bonding removed for clarity. Selected bond lengths (Å) and angles (°): O(10)···N(13), 2.859(8); O(10)–H(10O)···N(13), 164(6); N(6)···N(18)†, 3.119(10); N(6)–H(6A)···N(18)†, 157. Symmetry element used: † = −x, 2 − y, −z.

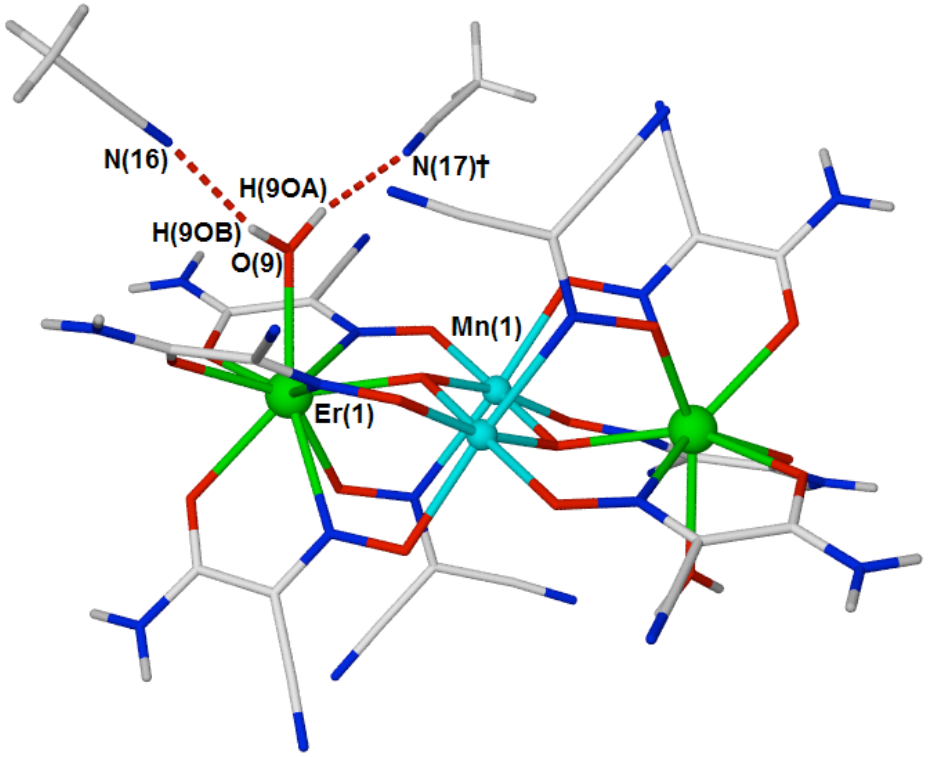


**Fig. S4** Hydrogen bonding within the crystal structure of **1Er**·$H_2O$·11MeCN. Selected bond lengths (Å) and angles (°): O(9)···N(16), 2.886(6); O(9)–H(9OA)···N(16), 159; O(9)···N(17)†, 2.787(7); O(9)–H(9OB)···N(17)†, 165. Symmetry element used: † = $^1/_2$ − x, $^3/_2$ − y, −z.

**Table S1.** Results of bond valence sum calculations of complexes **1Gd** – **1Er**.[1]

| Complex | $Mn^{II}$ | $Mn^{III}$ |
|---|---|---|
| **1Gd** | 3.426 | 3.147 |
| **1Tb** | 3.433 | 3.168 |
| **1Er** | 3.416 | 3.208 |

## References

1. C. Hormillosa, S. Healy, T. Stephen, Bond Valence Calculator V.200, McMaster University, **1993**.