

Supporting Information

[(Cu-Radical)₂-Ln]: Structure and Magnetic Properties of a Hetero-tri-spin Chain of Rings (Ln = Y^{III}, Gd^{III}, Tb^{III}, Dy^{III})

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CONTENT

- Figure S1. Crystal structure of complex **1**.
- Figure S2. Crystal structure of complex **2**.
- Figure S3. Crystal structure of complex **4**.
- Figure S4. Crystal packing of complex **1**.
- Figure S5. Crystal packing of complex **2**.
- Figure S6. Crystal packing of complex **3**.
- Figure S7. Crystal packing of complex **4**.
- Table S1 Crystallographic data for complexes **1-4**.
- Table S2 SHAPE analysis for complexes **1-4**.
- Scheme S1. Spin polarization mechanism for the magnetic coupling mediated by NIT3Py ligand.
- Figure S8. *M* versus *H* curves for complex **3**.
- Figure S9. *M* versus *H* curves for complex **4**.
- Figure S10. Temperature dependence of the out-of-phase components of ac susceptibility for **4** in zero dc field and an applied DC field of 1 kOe, 2 kOe and 3 kOe.

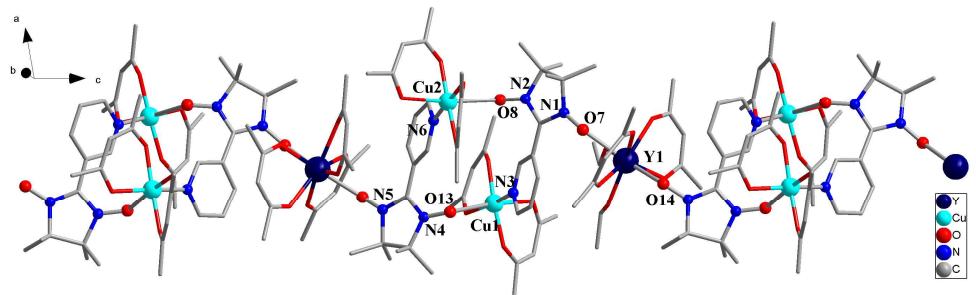


Figure S1. Crystal structure of complex 1. (All hydrogen and fluorine atoms are omitted for clarity).

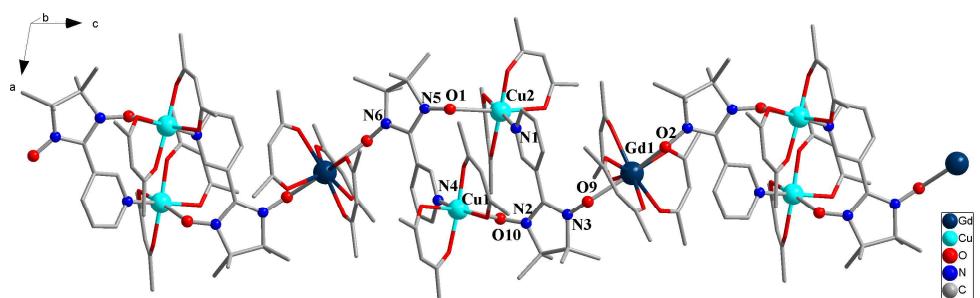


Figure S2. Crystal structure of complex 2. (All hydrogen and fluorine atoms are omitted for clarity).

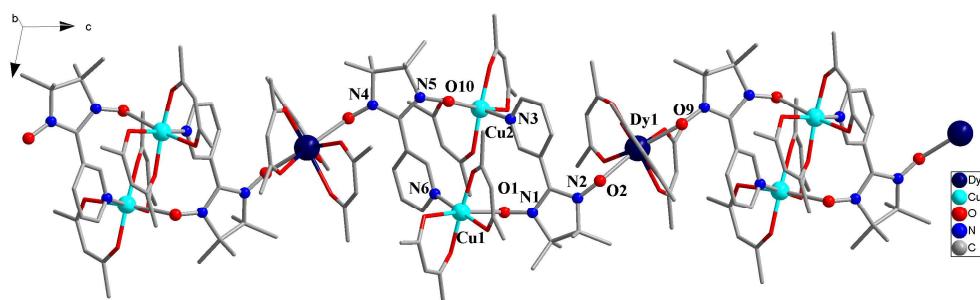


Figure S3. Crystal structure of complex 4. (All hydrogen and fluorine atoms are omitted for clarity).

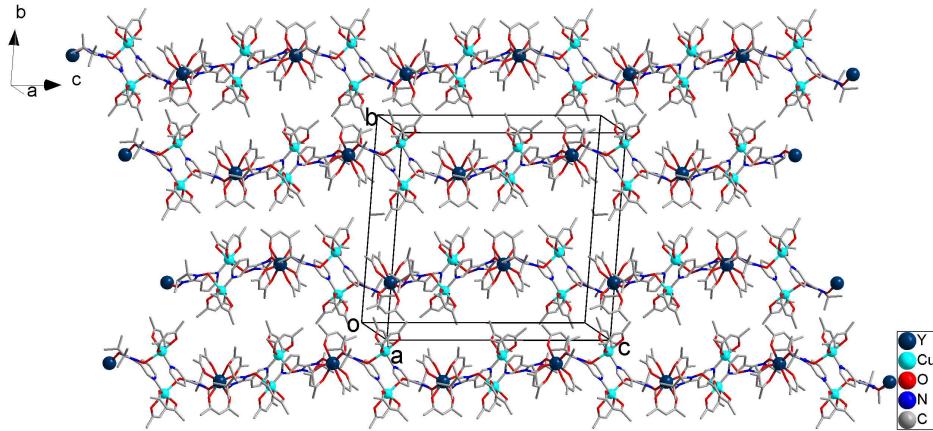


Figure S4. Crystal packing of complex 1. (All hydrogen and fluorine atoms are omitted for clarity).

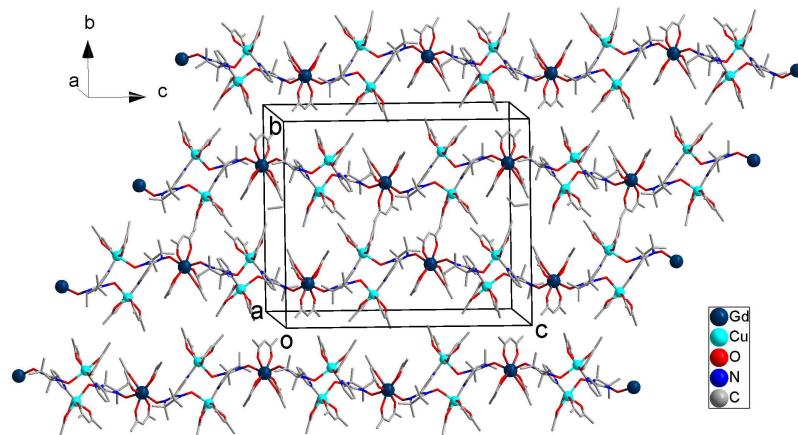


Figure S5. Crystal packing of complex 2. (All hydrogen and fluorine atoms are omitted for clarity).

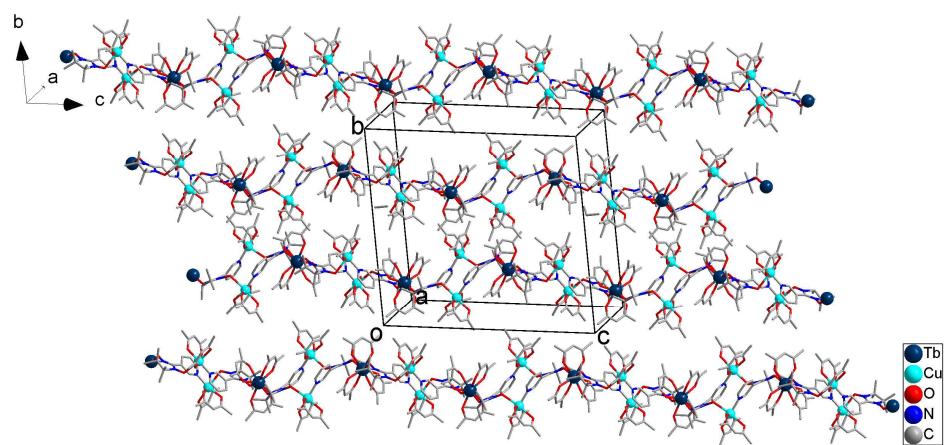


Figure S6. Crystal packing of complex 3. (All hydrogen and fluorine atoms are omitted for clarity).

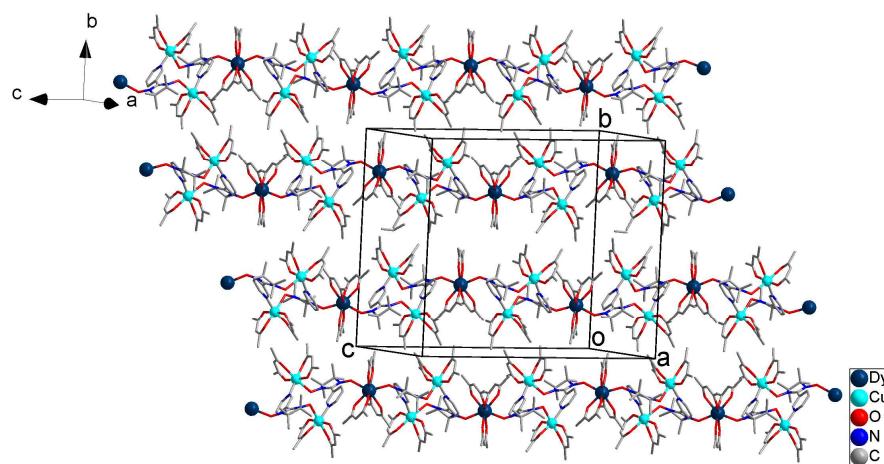


Figure S7. Crystal packing of complex 4. (All hydrogen and fluorine atoms are omitted for clarity).

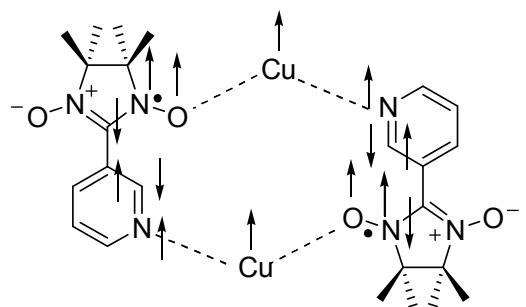
Table S1 Crystallographic data for complexes **1-4**.

Complex	1 Y	2 Gd	3 Tb	4 Dy
Empirical formula	$C_{65}H_{53}Cu_2F_{42}N_6O_{18}Ln$			
Mr	2220.14	2288.48	2290.16	2293.73
T, (K)	113(2)	113(2)	113(2)	113(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a /Å	12.320(3)	12.319(3)	12.342(3)	12.302(3)
b /Å	24.477(5)	24.455(5)	24.479(5)	24.362(5)
c /Å	28.744(6)	28.738(6)	28.691(6)	28.685(6)
β /°	101.86(3)	102.03(3)	101.99(3)	101.92(3)
V/Å³	8483(3)	8468(3)	8479(3)	8412(3)
Z	4	4	4	4
D_{calcd} /g cm⁻³	1.738	1.795	1.794	1.811
μ /mm⁻¹	1.335	1.432	1.482	1.541
θ /°	1.67-25.01	1.45-25.01	1.10-27.96	1.45-25.01
F(000)	4415	4515	4519	4523
Reflections collected	46804	45817	66971	51750
Unique reflns R_{int}	14225/ 0.1340	14911/0.0401	20067/0.0577	14833/0.0458
GOF (F^2)	1.013	1.018	1.080	1.056
R₁, wR₂ ($I > 2\sigma(I)$)	0.1001, 0.2119	0.0470, 0.1316	0.0564, 0.1520	0.0442, 0.1279
R₁, wR₂ (all data)	0.1558, 0.2473	0.0578, 0.1442	0.0719, 0.1669	0.0550, 0.1417

$$R_1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|. \quad wR_2 = [\sum w(|F_o|^2 - |F_c|^2)^2/\sum w(|F_o|^2)^2]^{1/2}.$$

Table S2 SHAPE analysis for complexes **1-4**.

complex	SAPR-8	TDD-8	BTPR-8
1 Y	1.780	0.357	1.910
2 Gd	1.810	0.406	1.932
3 Tb	1.766	0.413	1.935
4 Dy	1.778	0.388	1.908



Scheme S1. Spin polarization mechanism for the magnetic coupling mediated by NIT-3Py ligand.

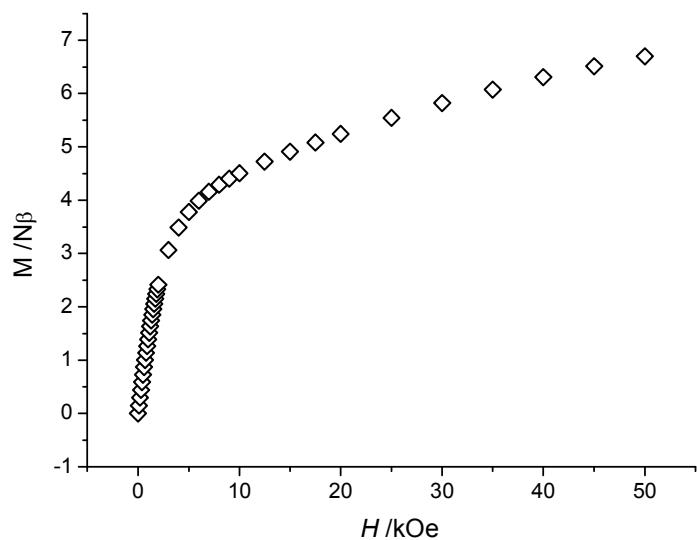


Figure S8. M versus H curves for complex 3.

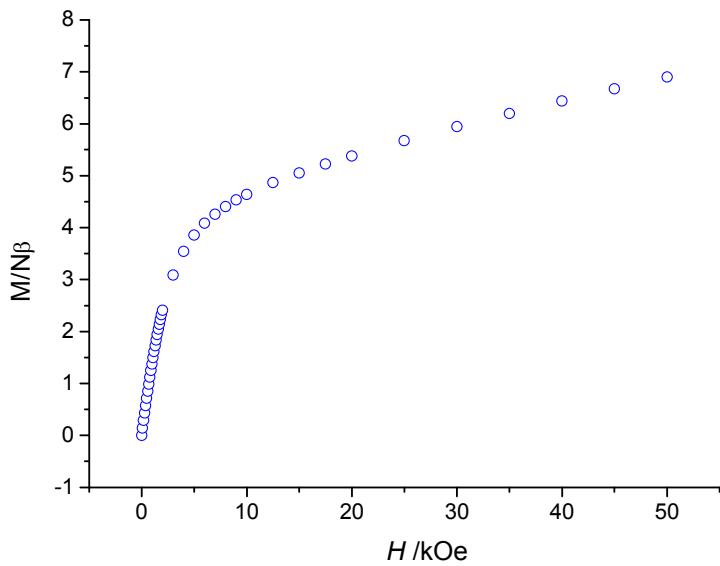


Figure S9. M versus H curves for complex **4**.

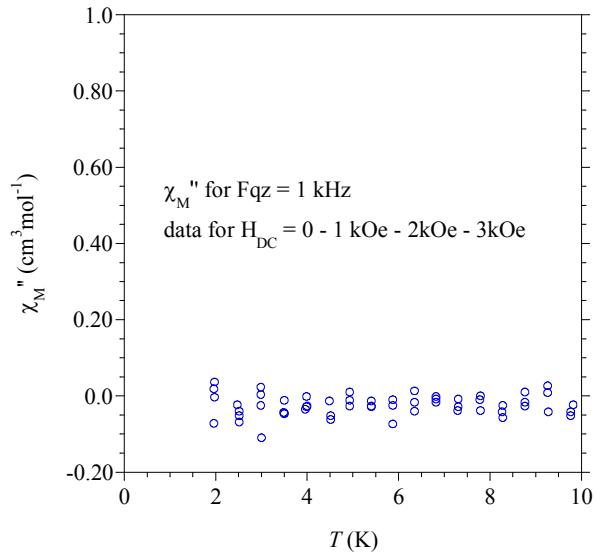


Figure S10. Temperature dependence of the out-of-phase components of ac susceptibility for **4** in zero dc field and an applied DC field of 1 kOe, 2 kOe and 3 kOe.