Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic supplementary information

Fluoride-bridged $\{Ln_2Cr_2\}$ polynuclear complexes from semi-labile *mer*-$[CrF_3(py)_3]$ and $[Ln(hfac)_3(H_2O)_2]$

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1 Crystallographic data

Table S1. Single-crystal data and structure refinement details. Note that **1Ln** (Ln = Y (powder), Tb, Ho, Er) are isomorphous to **1Dy**, see Fig. S1a below.

	1Y	**1Gd**	**1Dy**	**2Tb**	**3Dy**
Formula	$C_{50}H_{28}Cr_2F_{40}N_4O_{14}Y_2$	$C_{50}H_{28}Cr_2F_{40}Gd_2N_4O_{14}$	$C_{50}H_{28}Cr_2Dy_2F_{40}N_4O_{14}$	$C_{60}H_{36}Cr_2F_{42}N_6O_{12}Tb_2$	$C_{35}H_{21}CrDyF_{26}N_3O_9{\cdot}0.82(CH_2Cl_2)$
M_r	1950.58	2087.26	2097.76	2252.79	1406.11
Crystal size/mm	0.20 × 0.08 × 0.03	0.18 × 0.09 × 0.07	0.12 × 0.07 × 0.06	0.37 × 0.13 × 0.13	0.23 × 0.12 × 0.09
Shape	Plate	Prism	Prism	Rod	Prism
Colour	Pink	Pink	Pink	pink	Pink
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
T/K	122	122	122	122	122
a/Å	12.181(2)	12.158(3)	11.115(4)	12.5395(9)	12.404(3)
b/Å	12.530(3)	12.5405(14)	12.695(3)	13.2423(10)	20.093(3)
c/Å	12.550(2)	12.5573(10)	12.939(3)	15.094(2)	20.130(2)
α/°	65.253(11)	65.482(10)	95.30(2)	97.193(16)	88.972(9)
β/°	78.007(12)	78.496(14)	99.06(3)	110.446(8)	85.810(11)
γ/°	77.683(13)	77.792(12)	101.86(2)	116.354(7)	83.452(11)
V/Å^3	1684.4(6)	1689.1(5)	1749.7(7)	1983.6(3)	4970.7(14)
Z	1	1	1	1	4
ρ/g cm^{-3}	1.923	2.052	1.991	1.886	1.879
μ(Mo Kα)/mm^{-1}	2.19	2.42	2.58	2.19	1.95
$2\theta_{max}$/°	28.1	40.0	27.7	40.0	27.7
F(000)	954	1004	1008	1090	2731
Reflections collected	63568	90679	63297	130374	184854
Unique reflections	8156	20879	8083	24542	22902
R_{int}	0.060	0.094	0.097	0.056	0.105
Refl. Observed [$I > 2\sigma(I)$]	6691	16431	6597	20391	16551
Parameters/restraints	508/1	508/1	508/1	559/0	1417/4
GOF on F^2	1.07	1.09	1.06	1.06	1.14
$R[F^2 > 2\sigma(F^2)]$	0.043	0.042	0.046	0.030	0.052
wR_2 (all data)	0.096	0.103	0.108	0.071	0.120
Largest residuals/e Å^{-3}	1.24/–0.90	1.52/–1.59	1.79/–1.49	2.13/–0.90	1.39/–0.94

2 Powder diffractograms

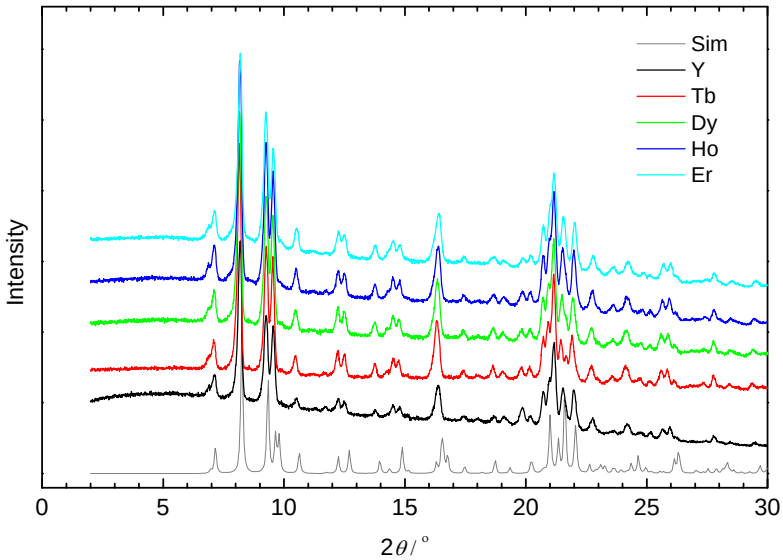


Fig. S1a. Powder diffractograms of the **1Ln** series. The grey diffractogram is calculated from the crystal structure of **1Dy**.

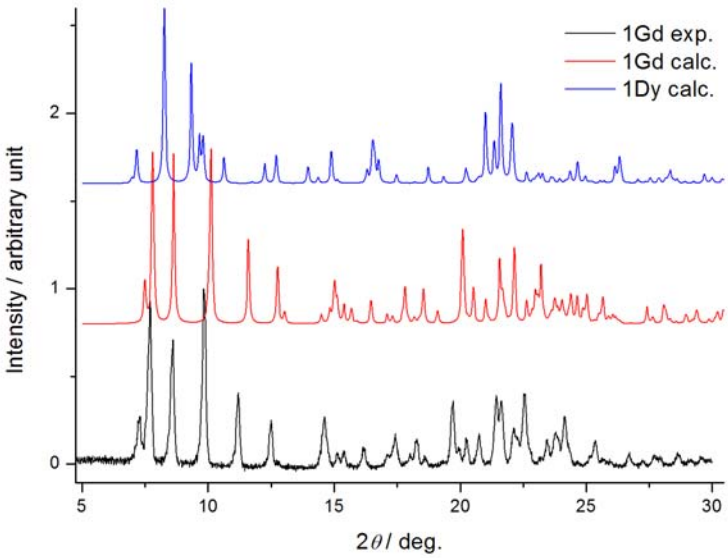


Fig. S1b. Powder diffractogram of **1Gd**. The different nature of **1Gd** as compared to **1Dy** (**1Ln**) illustrated by experimental and calculated powder diffractograms.

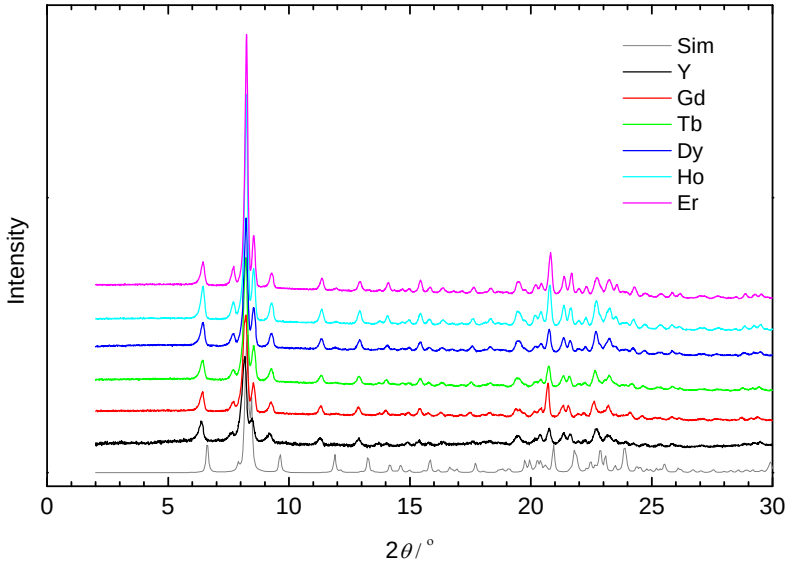
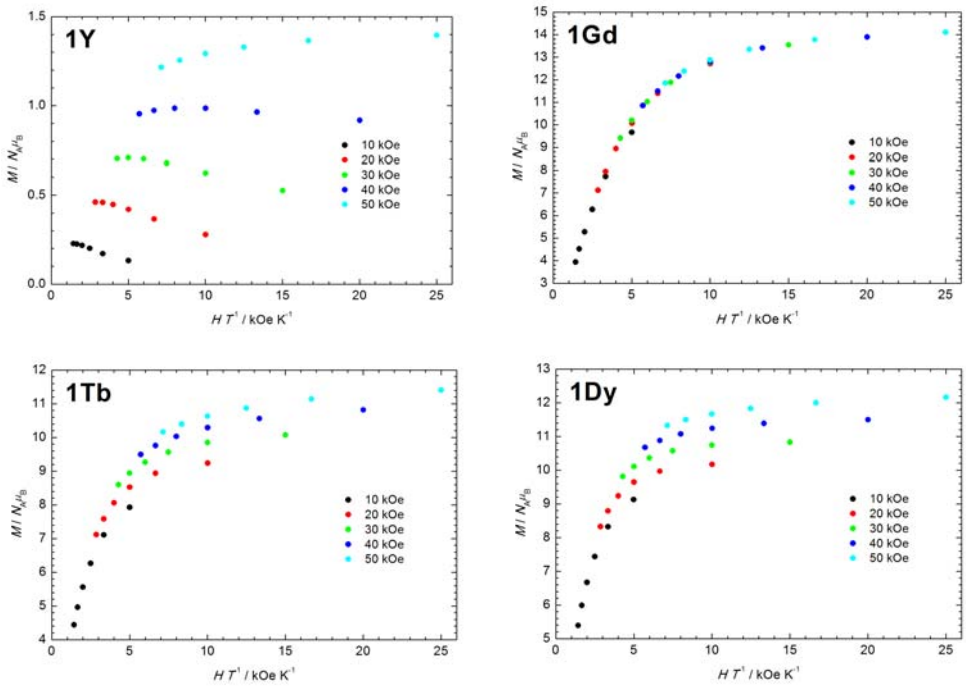


Fig. S2. Powder diffractograms of the **2Ln** series. The grey diffractogram is calculated from the crystal structure of **2Dy**.

3 Magnetic data



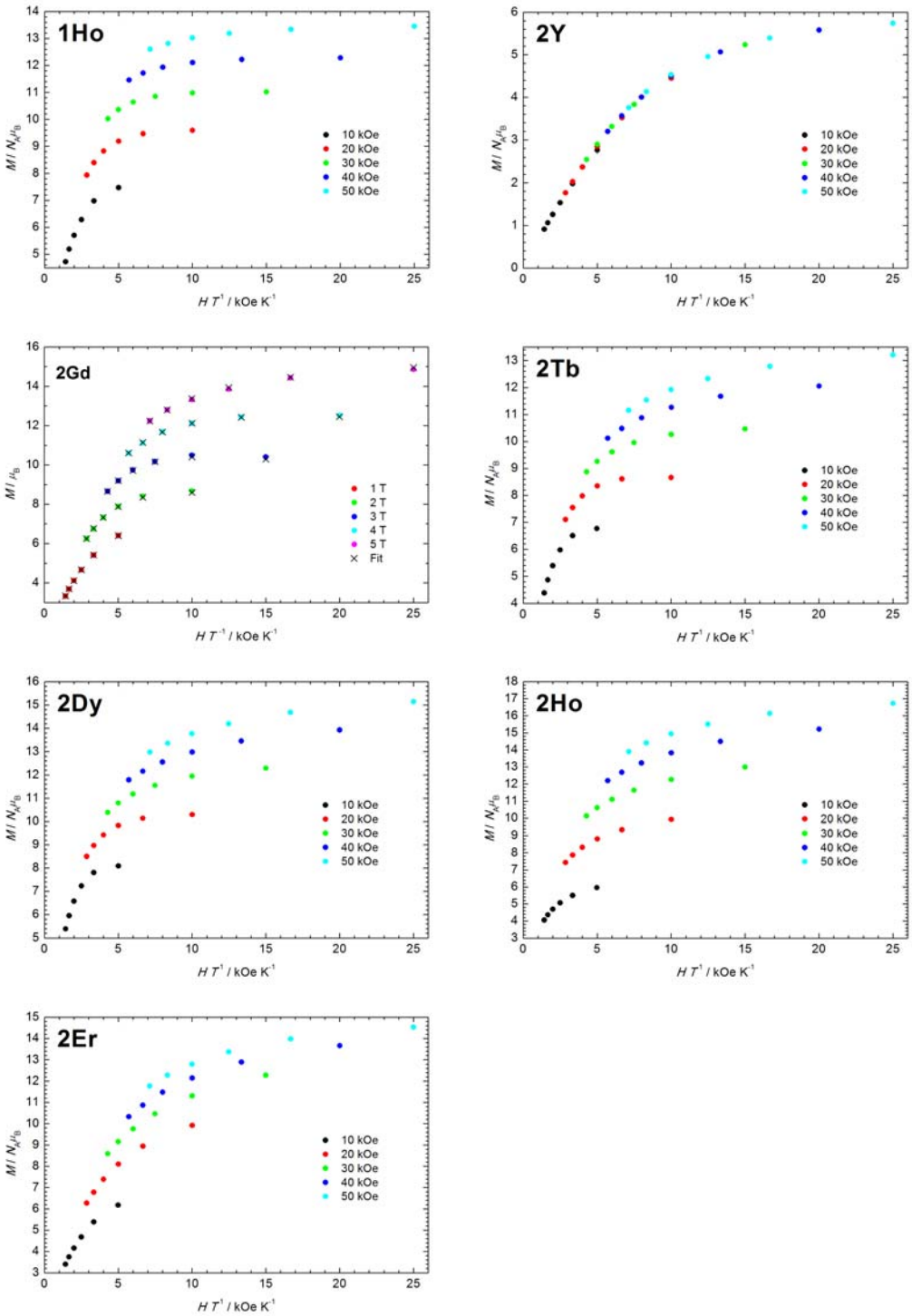


Fig. S5. Magnetization data.

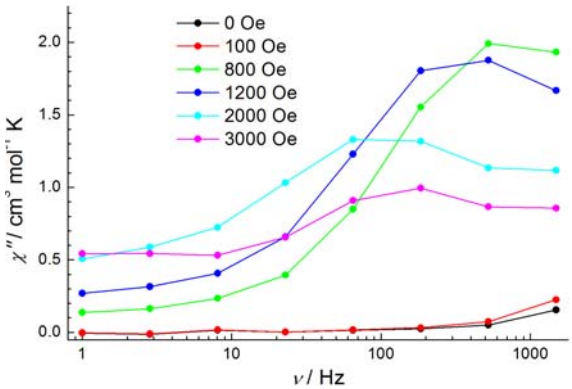


Fig. S6. Field dependence of the out-of-phase component of the ac susceptibility of **1Dy** at T = 1.8 K

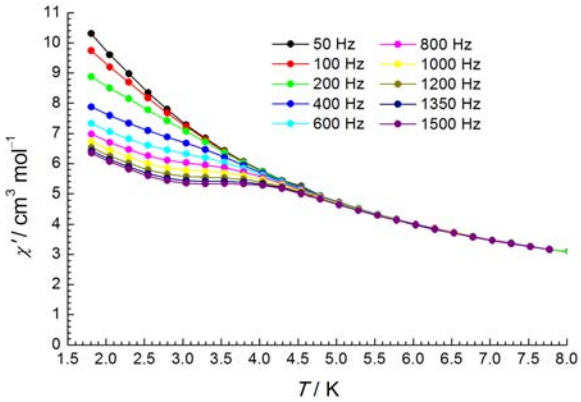


Fig. S7. In-phase component of the ac susceptibility of **1Dy** obtained with H_{dc} = 1200 Oe.

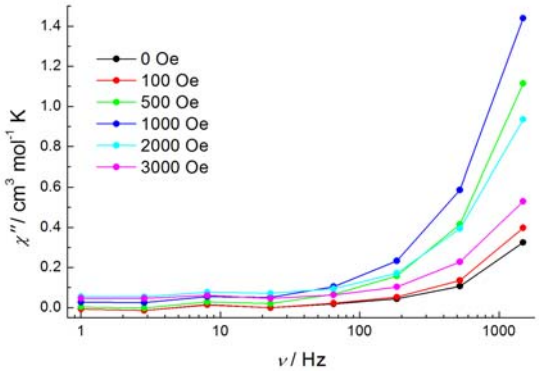


Fig. S8. Field dependence of the out-of-phase component of the ac susceptibility of **2Dy** at T = 1.8 K

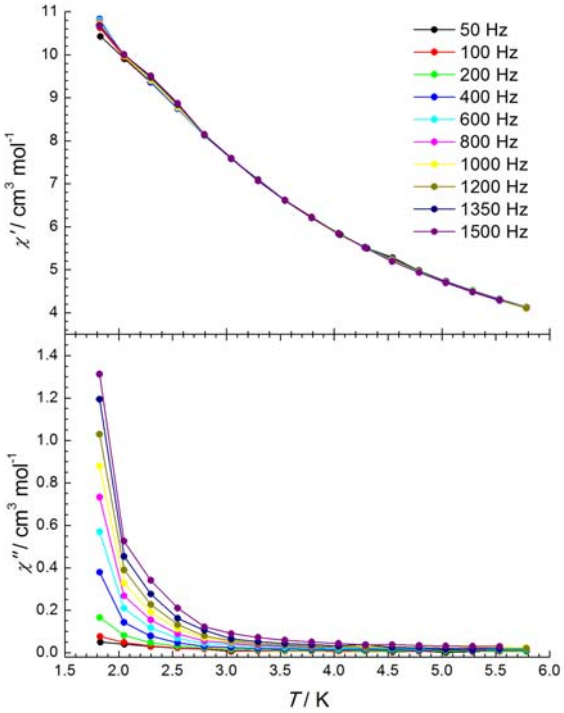


Fig. S9. Out-of-phase (top) and in-phase (bottom) component of the ac susceptibility of **2Dy** obtained with H_{dc} = 1200 Oe.

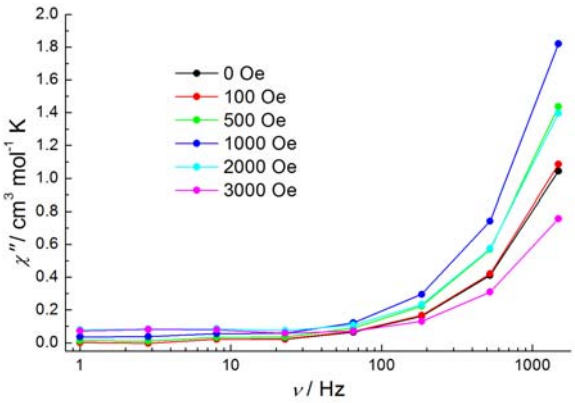


Fig. S10. Field dependence of the out-of-phase component of the ac susceptibility of **2Tb** at T = 1.8 K