Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information

Functionalized phosphonates as building units for multi-dimensional homo- and heterometallic 3d-4f inorganic-organic hybrid-materials and their magnetic characterization.

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Table S1. Crystallographic parameters for compounds **1a** and **1b**, and the ligand **H2H'L**.

	1a	**1b**	**H_2H'L**
Empirical formula	$C_{10}H_{18}CoN_2O_{12.5}P_2$	$C_{10}H_{19.5}N_2NiO_{12.5}P_2$	$C_{10}H_{10}N_2O_6P_2$
Formula weight	487.13	488.42	316.14
Crystal system	monoclinic	monoclinic	Orthorhombic
Space group	$P2_1/n$	$P2_1/n$	$Pbcn$
a/Å	10.9975(11)	10.9582(16)	13.6133(9)
b/Å	10.0662(10)	10.0015(11)	13.0066(8)
c/Å	18.303(2)	18.204(2)	14.3436(9)
α/°	90	90	90
β/°	105.790(3)	105.491(5)	90
γ/°	90	90	90
V/Å^3	1949.8(4)	1922.6(4)	2539.7(3)
Z	4	4	8
$\rho_{calc}g$/cm^3	1.659	1.687	1.654
μ/mm^{-1}	1.108	1.241	0.37
2Θ/°	3.914-55.992	3.934-55.926	4.332-56.038
F(000)	996	1006	1296
Data/restraints/parameters	4698/0/273	4605/0/277	3074/0/185
GOF (F^2)	0.897	0.989	1.059
R_1, wR_2 (I>=2σ (I))	0.0388, 0.0792	0.0449, 0.0902	0.0316, 0.0853
R_1, wR_2 (all data)	0.0771, 0.0867	0.0810, 0.1029	0.0351, 0.0879

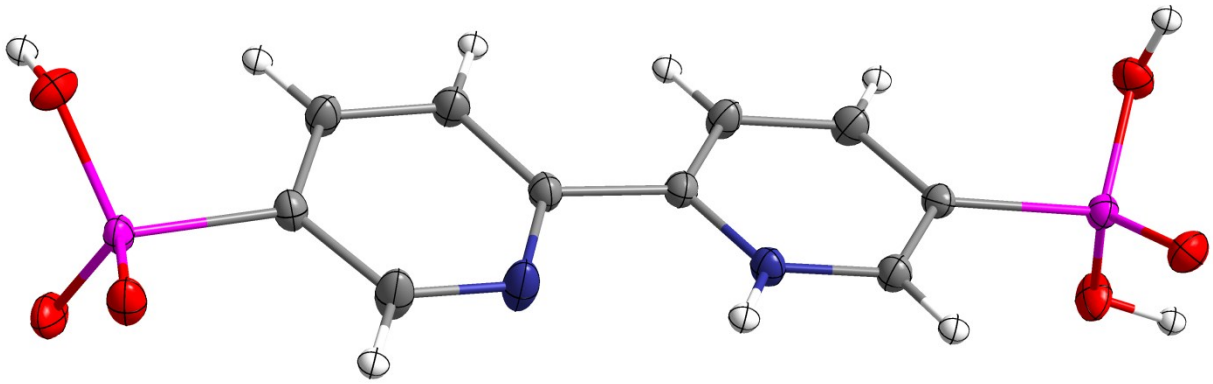

Figure S1. Molecular structure of the ligand **H_3H'L** with thermal ellipsoids. Colour scheme: pink - phosphorus, red - oxygen, dark blue – nitrogen, grey - carbon, white - hydrogen.

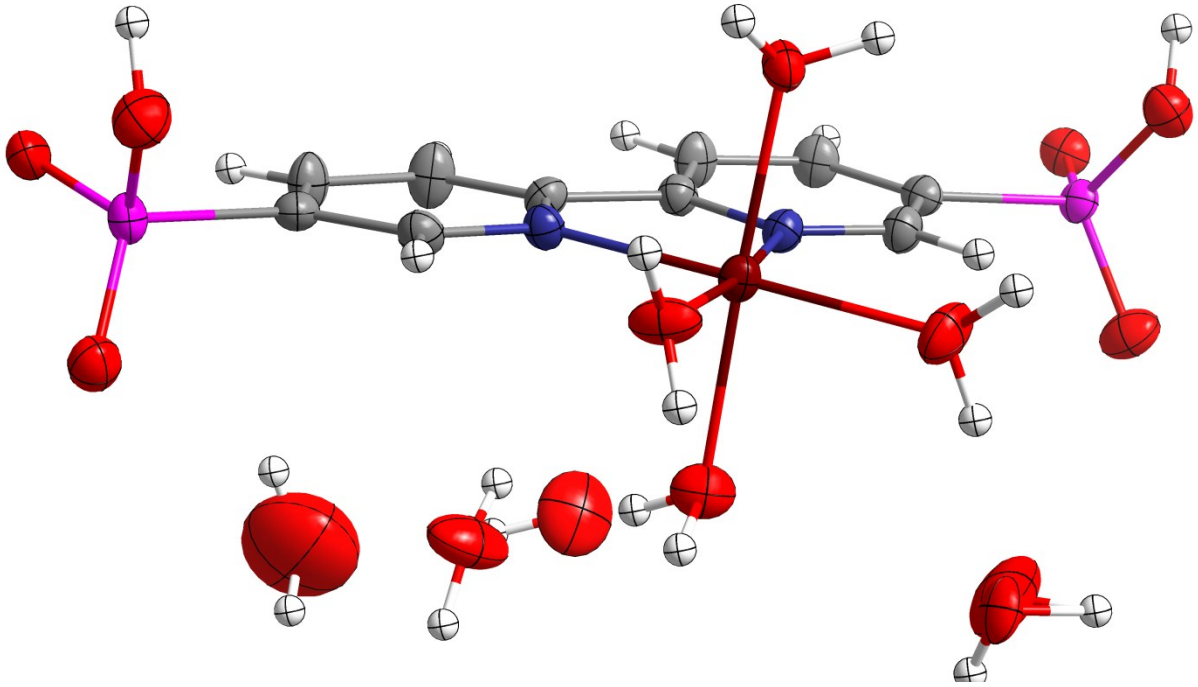

Figure S2. Molecular structure of compound **1a** with thermal ellipsoids. Colour scheme: dark red - cobalt, pink - phosphorus, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

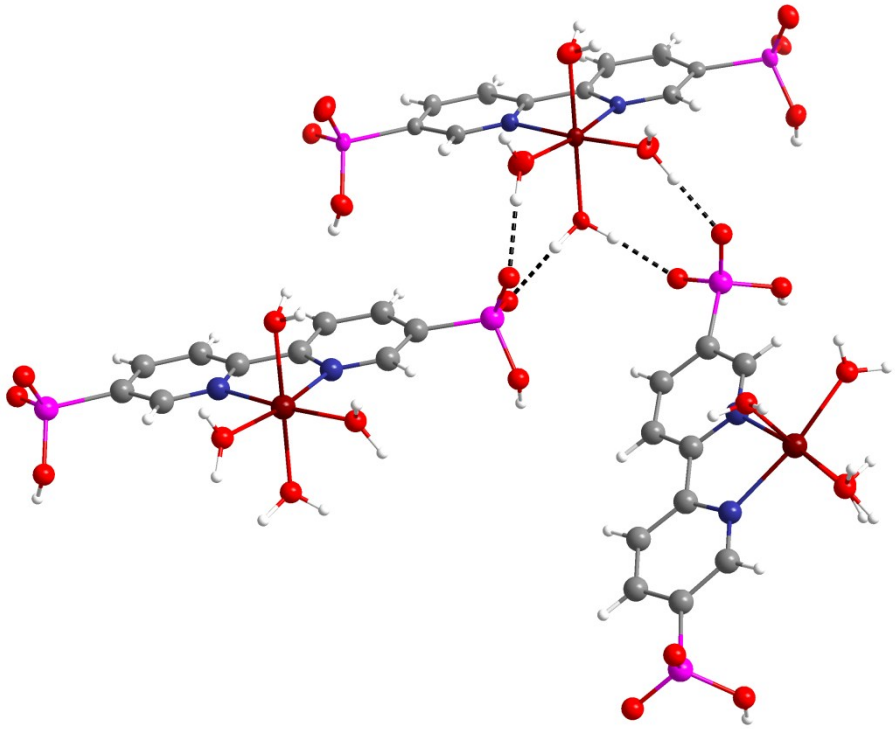

Figure S3. Intermolecular connections in compound **1a** mediated by hydrogen bonds between crystal water molecules and phosphonate groups.

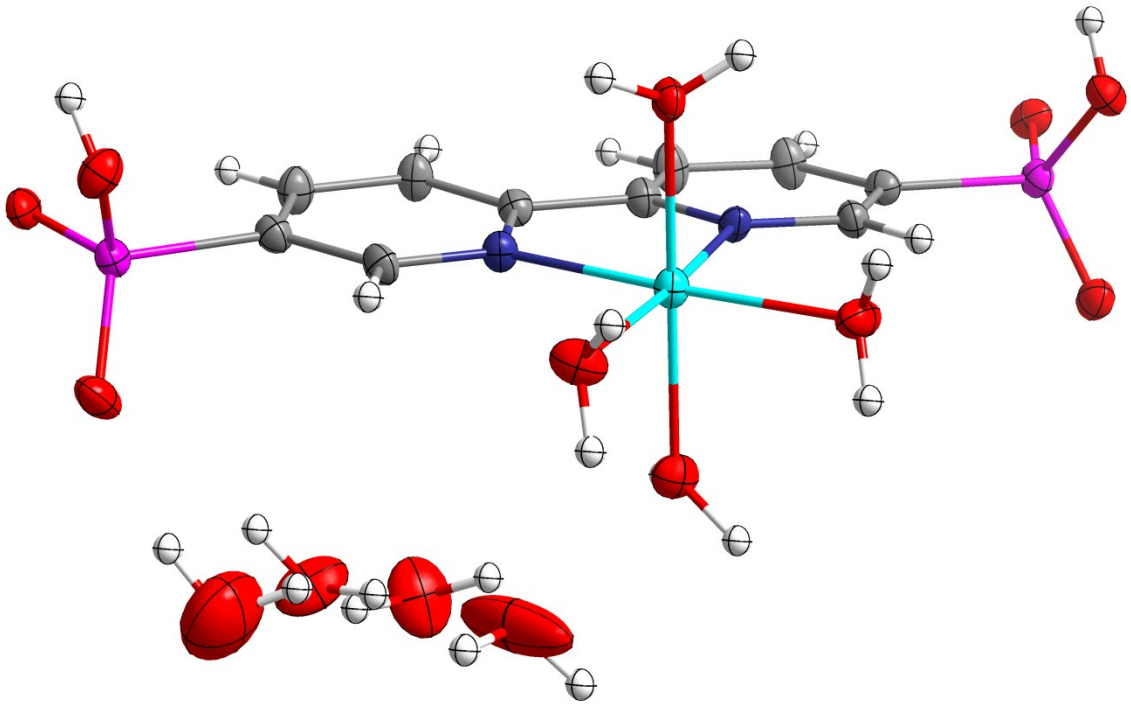

Figure S4. Molecular structure of compound **1b** with thermal ellipsoids. Colour scheme: light blue - nickel, pink - phosphorus, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

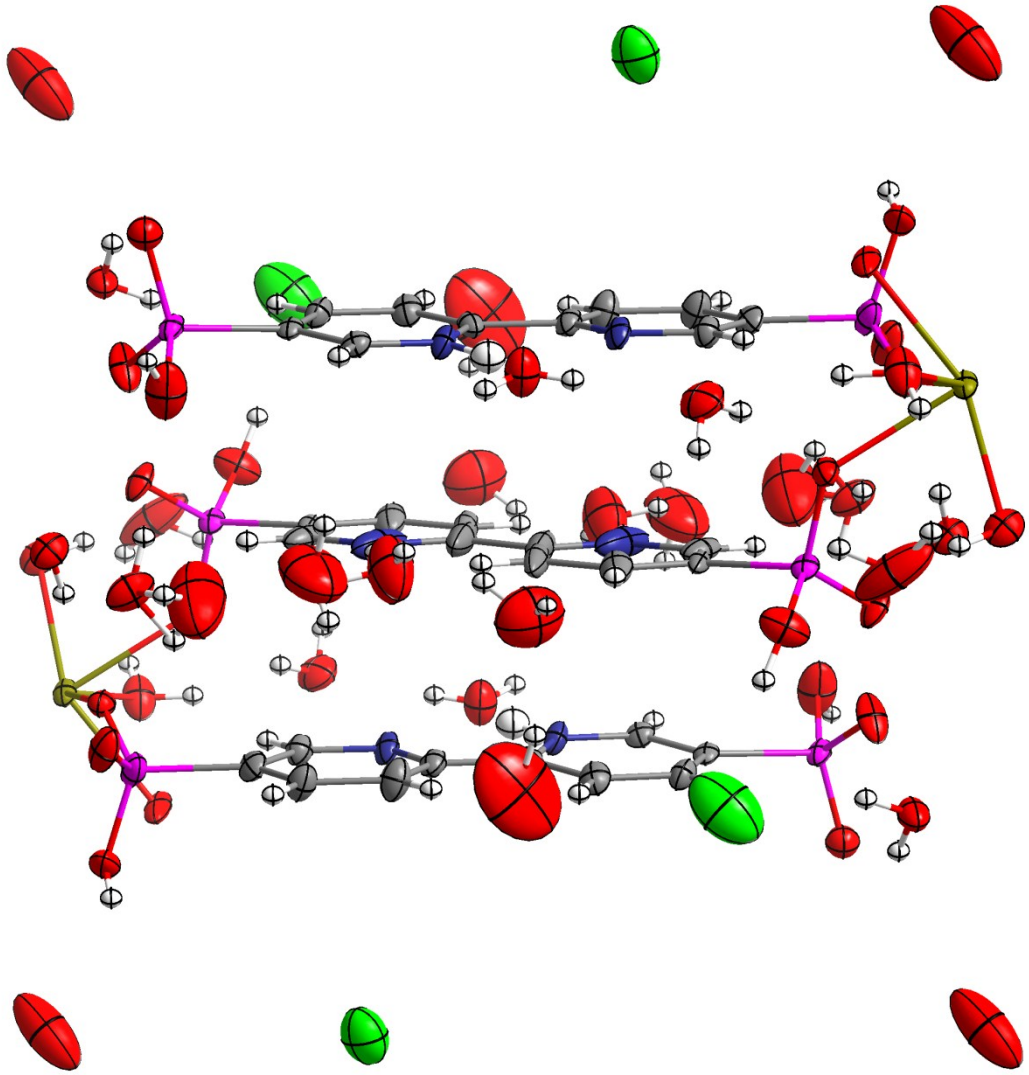

Figure S5. Molecular structure of compound **2** with thermal ellipsoids. Colour scheme: brown - gadolinium, light green – chlorine, pink - phosphorus, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

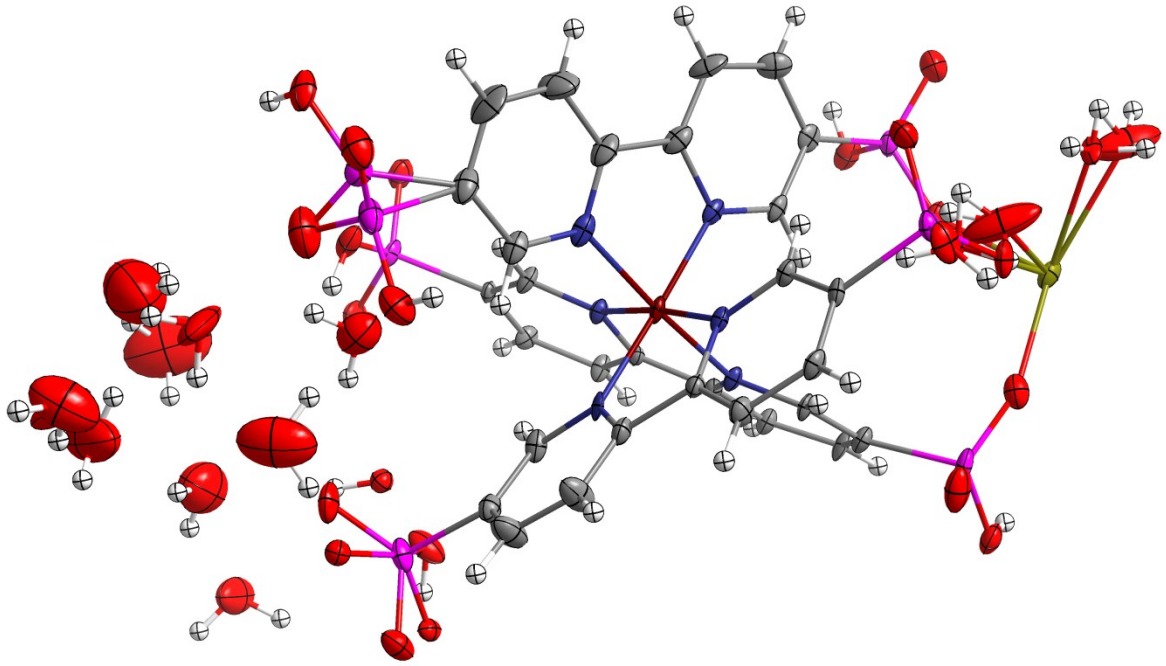

Figure S6. Molecular structure of compound **3a** with thermal ellipsoids. Colour scheme: brown - gadolinium, dark red - cobalt, pink - phosphorus, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

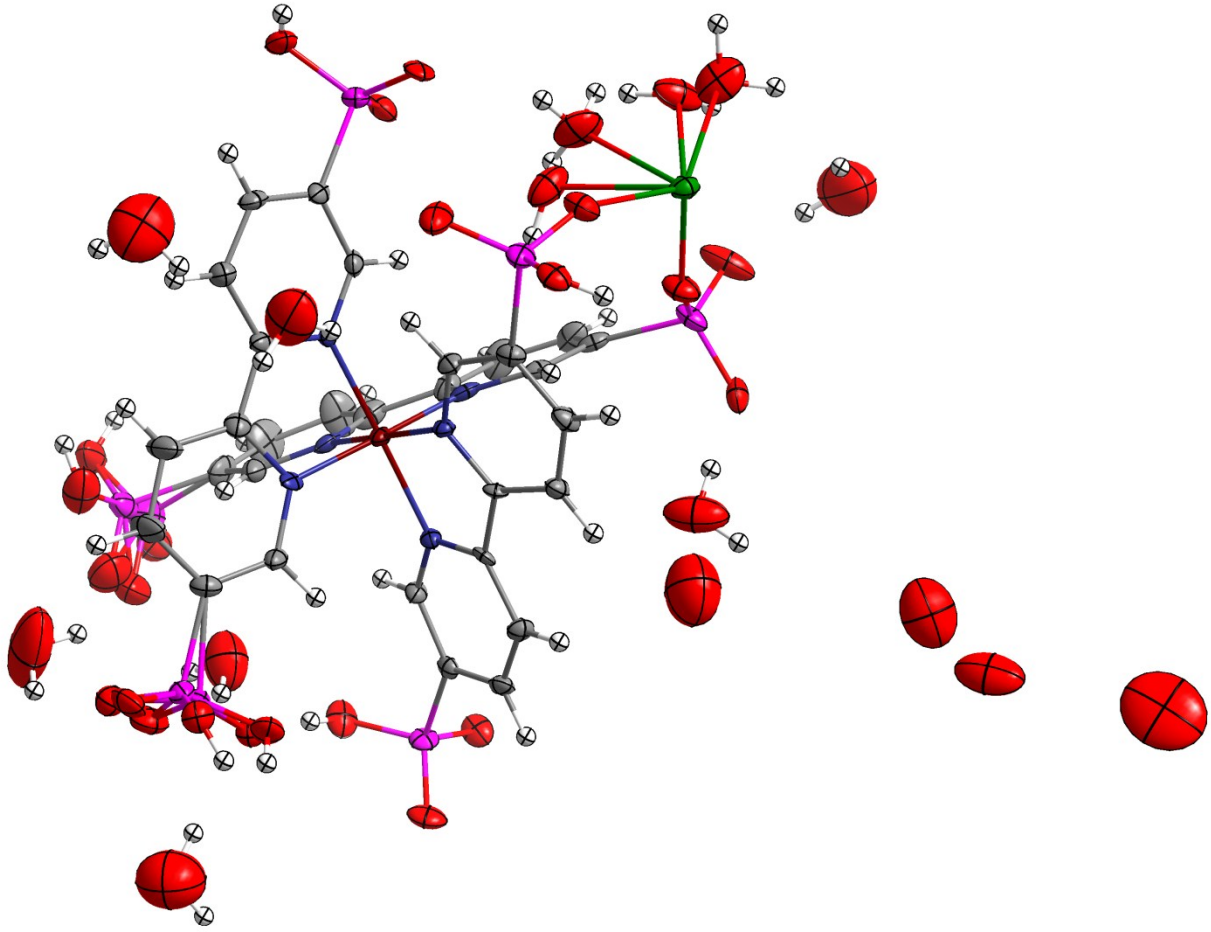

Figure S7. Molecular structure of compound **3b** with thermal ellipsoids. Colour scheme: green - dysprosium, dark red - cobalt, pink - phosphorus, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

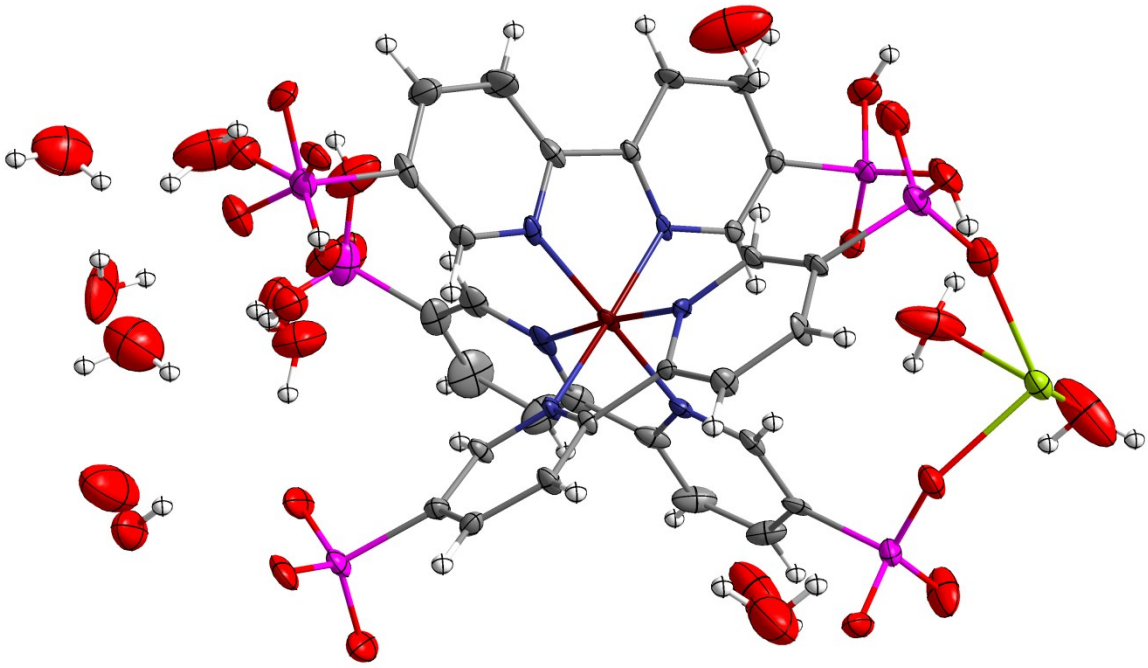

Figure S8. Molecular structure of compound **3c** with thermal ellipsoids. Colour scheme: yellow - terbium, dark red - cobalt, pink - phosphorus, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

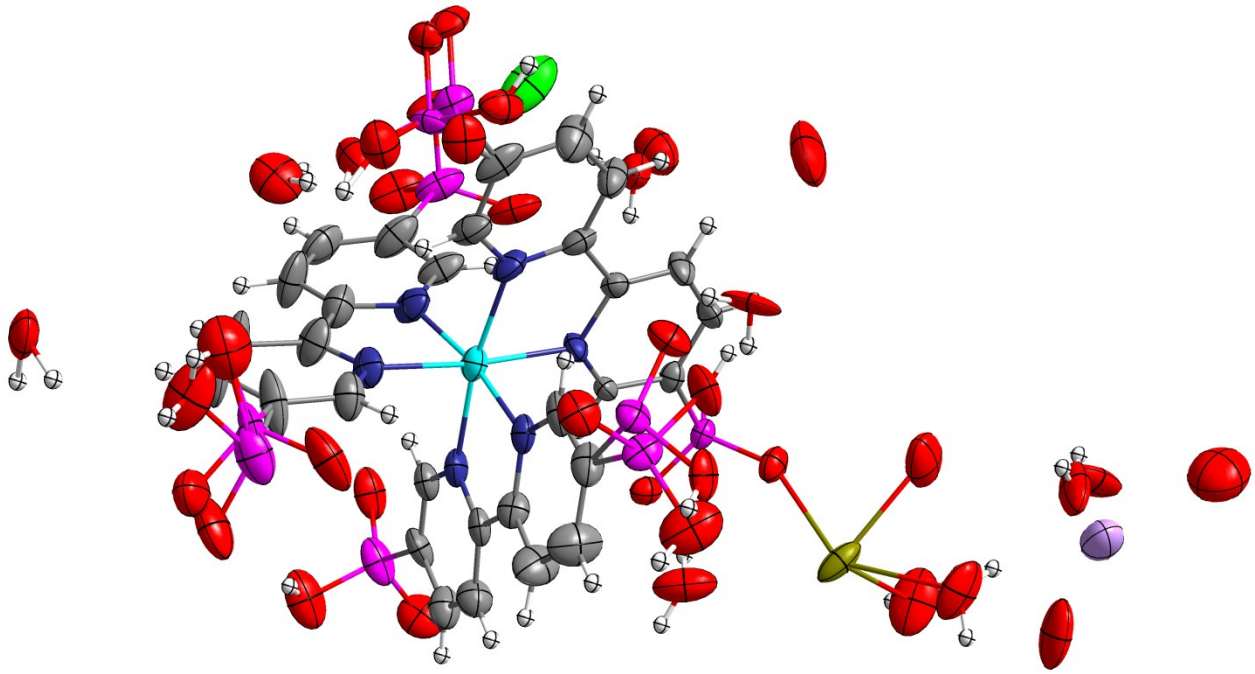

Figure S9. Molecular structure of compound **4** with thermal ellipsoids. Colour scheme: brown - gadolinium, light blue - nickel, light green - chlorine, pink - phosphorus, purple - sodium, red - oxygen, dark blue - nitrogen, grey - carbon, white - hydrogen.

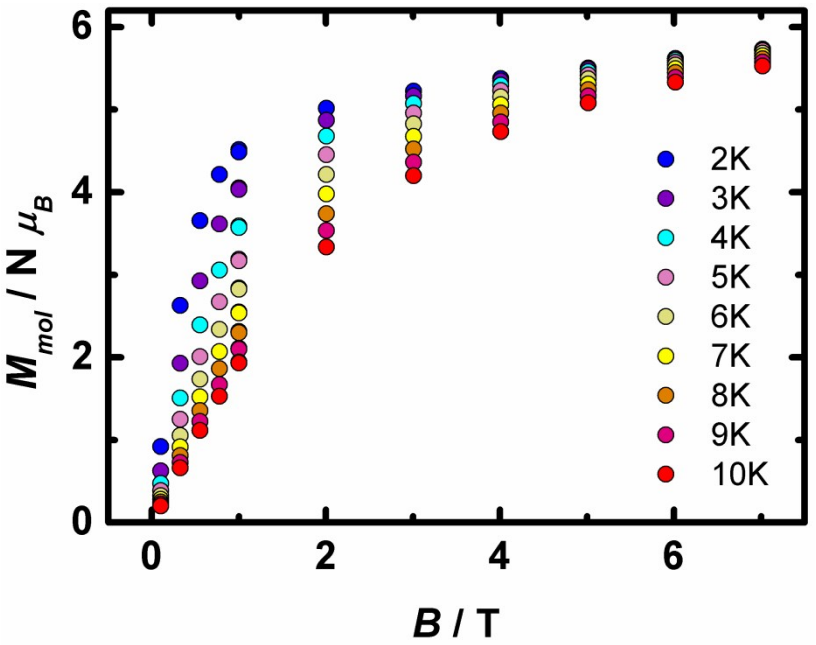

Figure S10. Magnetisation of **3b** in a temperature range between 2 K and 10 K an applied magnetic field of up to 70 kOe. At low fields, a strong increase in the magnetization *M* is observed, which slowly reaches for a value near its saturation at high magnetic fields. The highest obtained values for the magnetization at 2 K and 10 K are 5.73 $N\mu_B$ and 5.53 $N\mu_B$.

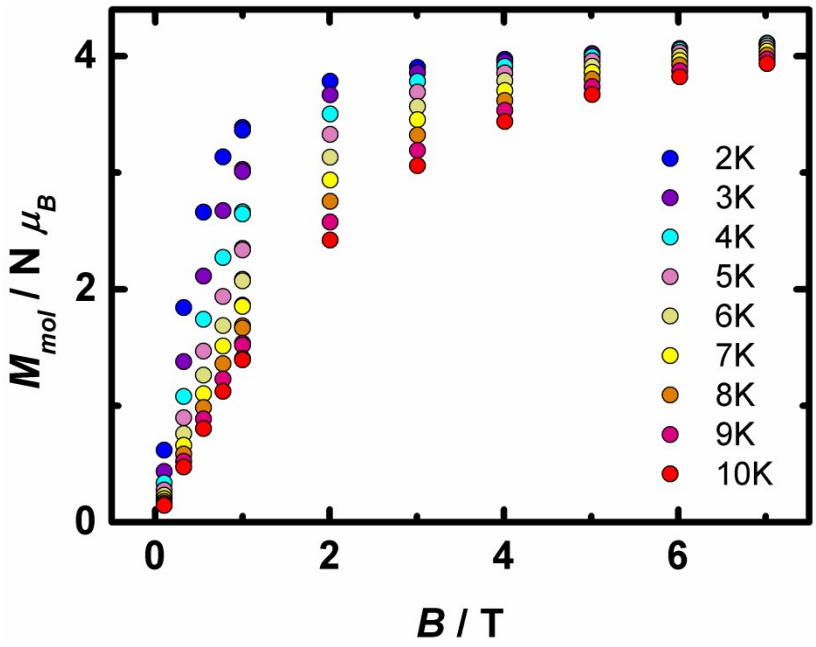

Figure S11. Magnetisation of **3c** in a temperature range between 2 K and 10 K an applied magnetic field of up to 70 kOe. At low fields, a strong increase in the magnetization *M* is observed, which slowly reaches for a value near its saturation at high magnetic fields. The highest obtained values for the magnetization at 2 K and 10 K are 4.10 $N\mu_B$ and 3.94 $N\mu_B$.