Supplementary Materials: Synthesis, Crystal Structures, and magnetic Properties of Lanthanide (III) Amino-Phosphonate cages

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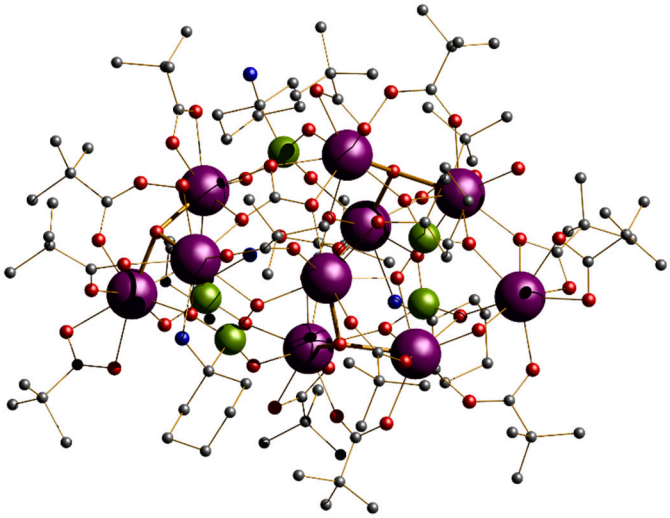

Figure S1. Crystal structure of {$Ln_{10}P_5$} cluster. Scheme: Ln, purple; P, green; O, red; C, grey; N, cyan; (H omitted for clarity).

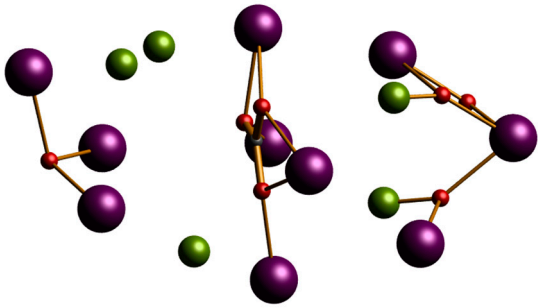

Figure S2. Metal and phosphonate core in {$Gd_{10}P_5$}. Scheme: Ln, purple; P, green; O, red.

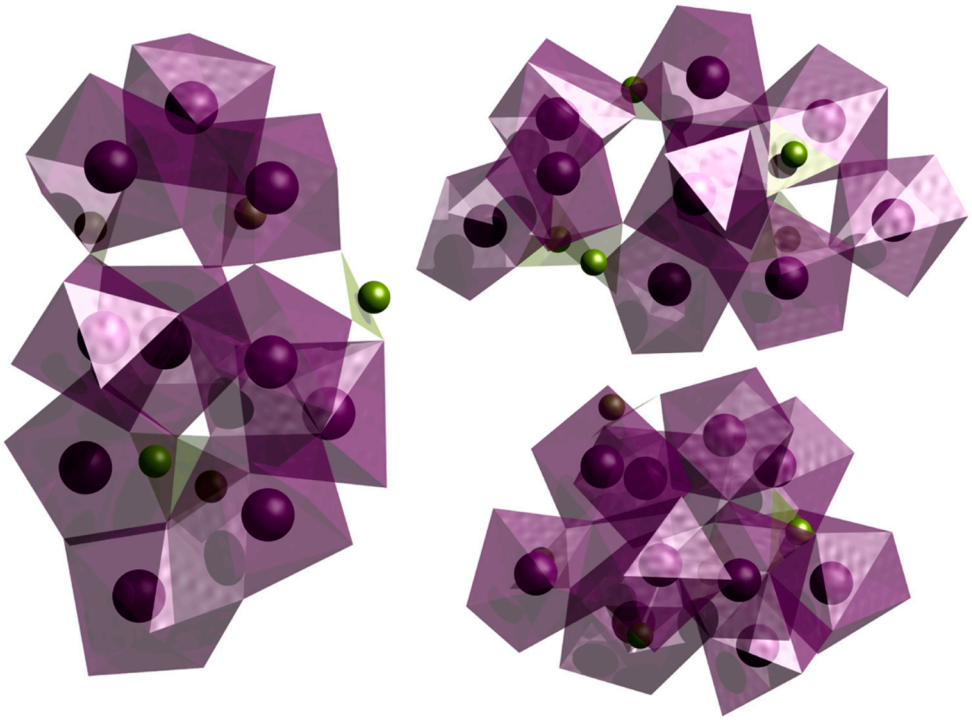

Figure S3. Polyhedral view of {$Ln_{10}P_5$} core.

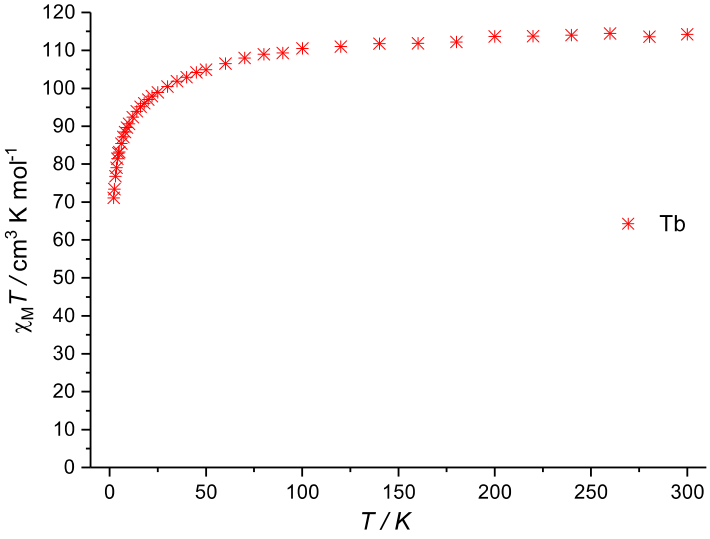

Figure S4. Variation of $\chi_M T$ vs. T for **2** at 1kOe from 2–300K.

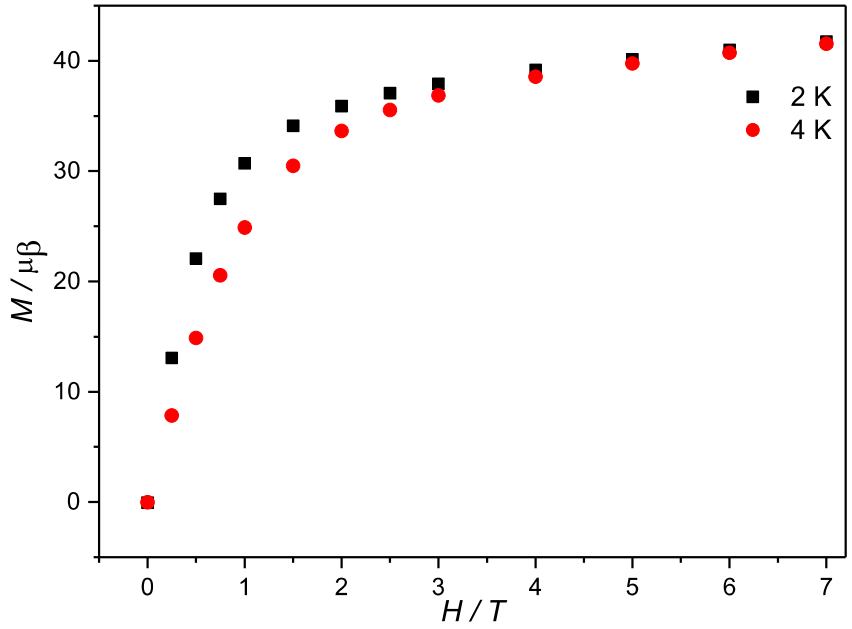

Figure S5. M_β vs. H for **2** at different temperatures (2 - 9 K) in the field range comprising 0 to 7 T.

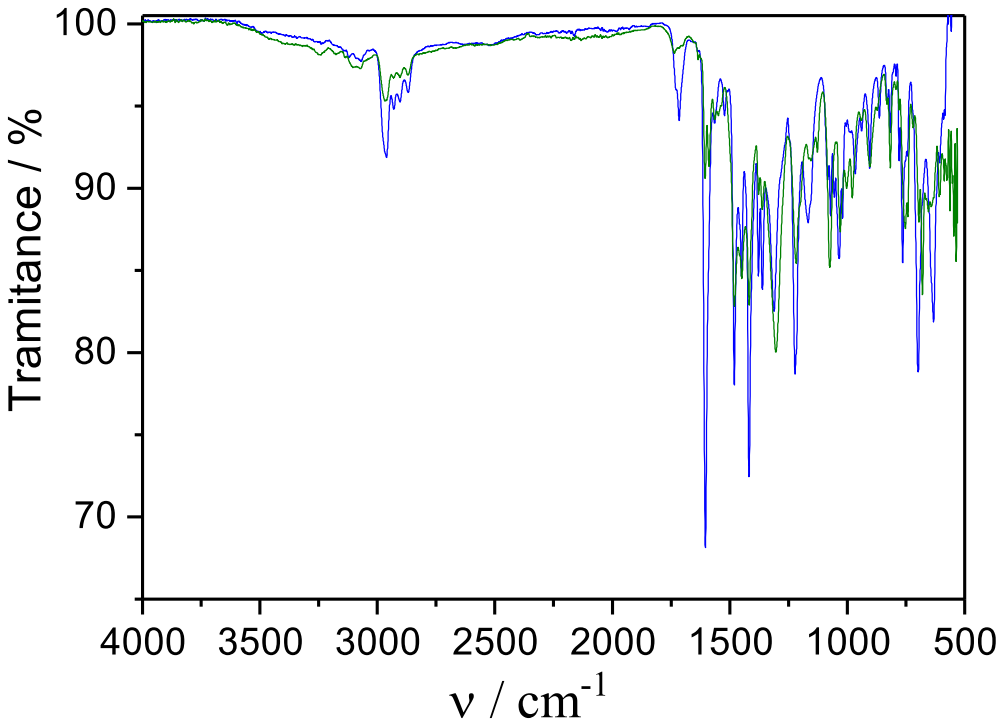

Figure S6. IR spectra for compound **1** (blue trace) and compound **2** (green trace).

Table S1. CShM values for the Gd metal ion centres of **1**.

	Gd2	**Gd3**	**Gd5**	**Gd6**	**Gd8**	**Gd9**	**Gd10**
Geometry	CShM	CShM	CShM	CShM	CShM	CShM	CShM
OP	33.529	32.553	31.632	33.218	30.427	33.651	30.994
HPY	22.259	20.819	23.397	24.964	23.499	24.130	21.996
HBPY	15.799	15.476	15.706	13.774	14.629	16.812	12.928
CU	12.089	13.012	11.651	13.128	8.751	11.807	12.384
SAPR	4.206	4.385	3.434	4.930	3.026	3.767	4.352
TDD	1.750	2.422	0.804	2.505	0.715	3.236	2.316
JGBF	13.932	12.207	11.087	9.514	14.730	13.388	10.812
JETBPY	27.592	26.730	28.154	27.349	29.007	26.910	26.232
JBTPR	3.201	2.798	2.653	3.766	3.289	3.497	3.236
BTPR	2.194	2.121	2.272	3.602	2.828	2.452	3.103
JSD	4.062	4.305	2.307	3.258	2.877	5.641	2.729
TT	12.825	13.504	12.250	13.682	9.374	12.472	12.897
ETBPY	23.150	22.254	24.514	23.444	24.812	21.610	23.757

	Gd1	**Gd4**	**Gd7**
Geometry	CShM	CShM	CShM
EP	33.259	34.429	33.716
OPY	21.105	22.688	22.847
HBPY	19.332	17.111	17.164
JTC	16.037	14.826	14.456
JCCU	11.929	8.821	8.634
CCU	11.113	7.755	7.273
JCSAPR	4.345	2.505	3.302
CSAPR	3.689	1.554	2.227
JTCTPR	5.334	3.737	2.658
TCTPR	3.891	2.307	2.467
JTDIC	12.786	11.591	13.393
HH	10.461	10.028	9.100
MFF	2.776	1.238	1.569

Table S2. Selected bond distances (**Å**) and angles (°) of compounds **1** and **2**.

Bond distances (Å) and angles (◦)	**1**	**2**
Ln1…Ln2	3.8642(6)	3.86034(6)
Ln2…Ln3	3.8104(6)	3.81040(5)
Ln1…Ln3	3.8151(8)	3.81543(7)
Ln4…Ln5	109.1(2)	3.86034(6)
Ln5…Ln6	108.8(3)	3.81040(5)
Ln6…Ln4	108.9(2)	3.81543(7)
Ln7…Ln8	109.1(2)	3.86034(6)
Ln8…Ln9	108.8(3)	3.81040(5)
Ln9…Ln7	108.9(2)	3.81543(7)
Ln1…O1…Ln2/°	109.1(2)	108.9690(1)
Ln2…O1…Ln3/°	108.8(3)	108.3313(5)
Ln1…O1…Ln3/°	108.9(2)	108.8080(1)
Ln4…O1…Ln5/°	109.1(2)	108.9690(1)
Ln5…O1…Ln6/°	108.8(3)	108.3313(5)
Ln6…O1…Ln4/°	108.9(2)	108.8080(1)
Ln7…O1…Ln8/°	109.1(2)	108.9690(1)
Ln8…O1…Ln9/°	108.8(3)	108.3313(5)
Ln9…O1…Ln7/°	108.9(2)	108.8080(1)