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Supporting information

One-dimensional lanthanide coordination polymers supported by pentadentate Schiff-base and diphenyl phosphate ligands: single molecule magnet behavior and photoluminescence

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Table S1 Crystallographic data and structure refinement for complexes 1-4.

	1	2	3	4
Formula	$C_{86}H_{88}Cl_2$	$C_{86}H_{88}Cl_2$	$C_{86}H_{88}Cl_2$	$C_{86}H_{88}Cl_2$
Formula	$N_{11}O_{31}P_3Tb_2\\$	$Dy_2N_{11}O_{31}P_3$	$Er_2N_{11}O_{31}P_3$	$N_{11}O_{31}P_3Yb_2$
$M_{\rm r}$ (g mol ⁻¹)	2253.32	2260.48	2270.00	2281.56
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2(1)/n	P2(1)/n	P2(1)/n	P2(1)/n
<i>T</i> (K)	173(2)	173(2)	173(2)	173(2)
<i>a</i> (Å)	13.1608(6)	13.0937(4)	13.0197(5	12.9888(6)
<i>b</i> (Å)	25.5433(13)	25.4261(8) A	25.3950(11)	25.3643(10)
<i>c</i> (Å)	28.7541(12)	28.7090(8)	28.8323(13)	28.8567(13)
α (°)	90	90	90	90
β (°)	99.6190(10)	99.7250(10)	99.940(2)	99.708(2)
γ (°)	90	90	90	90
$V(Å^3)$	9530.4(8)	9420.5(5)	9389.9(7)	9370.8(7)
Ζ	4	4	4	4
$D_{\rm c}~({\rm g~cm^{-3}})$	1.570	1.594	1.606	1.617

$\mu ({\rm mm}^{-1})$	1.664	1.769	1.970	2.179
<i>F</i> (000)	4552	4560	4576	4592
Reflns collected	54480	48351	51031	47242
Unique reflns	16551	17063	16251	17009
$R_{\rm int}$	0.0671	0.0810	0.1163	0.0727
GOF	1.021	1.091	1.171	1.189
$R_1(I > 2\sigma)$	0.0455	0.0576	0.0847	0.0715
w R_2 (all data)	0.1240	0.1790	0.2098	0.2275
Max. diff. peak /	1.064 /	1 0 4 1 / 1 0 1 1	2 017/ 2 009	2 (05/ 2 ((0
hole (e Å ⁻³)	-0.839	1.941/-1.811	2.01//-2.998	2.695/-2.669



Fig. S1 Experimental and simulated PXRD patterns for complexes 1-4.



Fig. S2 IR spectra for complexes 1-4.

	Tb1	Dy1	Er1	Yb1		Tb2	Dy2	Er2	Yb2
OP-8	31.805	32.024	32.671	32.339	EP-9	31.405	31.795	31.975	31.953
HPY-8	20.582	20.634	20.581	20.820	OPY-9	23.086	23.080	23.015	23.103
HBPY- 8	10.654	10.523	10.392	10.634	HBPY- 9	16.847	16.852	17.003	17.133
CU-8	11.056	10.879	10.667	10.965	JTC-9	14.924	15.007	15.014	15.121
SAPR- 8	5.847	5.646	5.328	5.280	JCCU- 9	6.991	6.959	6.979	7.053
TDD-8	4.088	3.999	3.902	3.689	CCU-9	6.120	6.037	6.126	6.163
JGBF- 8	8.102	8.011	7.745	7.833	JCSAP R-9	3.394	3.426	3.269	3.118
JETBP Y-8	21.715	22.043	22.301	22.488	CSAP R-9	2.702	2.704	2.580	2.459
JBTPR -8	4.810	4.867	4.986	4.685	JTCTP R-9	2.586	2.670	2.555	2.379
BTPR- 8	4.070	4.118	4.378	4.087	TCTP R-9	2.700	2.668	2.604	2.465
JSD-8	4.827	4.777	4.651	4.481	JTDIC	11.864	11.892	11.803	12.080

Table S2 Continuous shape measures (CShM) for complexes 1-4.

TT-8	11.861	11.677	11.495	11.768	HH-9	6.705	6.629	6.664	6.918
ETBP Y-8	18.230	18.557	18.981	19.248	MFF-9	2.491	2.411	2.403	2.374
OP-8=Oct	agon, HPY	-8=Heptago	nal pyrami	d, HBPY-	8=Hexagonal	bipyrami	d, CU-8=Cu	ube, SAPI	R-8=Square
antiprism,	TDD-8=T	riangular o	dodecahedro	on, JGBF-	-8=Johnson	gyrobifast	igium J26,	JETBPY	-8=Johnson
elongated	triangular b	pipyramid J	14, JBTPR-	8=Biaugm	ented trigona	l prism J5	0, BTPR-8=	Biaugment	ted trigonal
prism, JS	D-8=Snub	diphenoid	J84, TT-8	3=Triakis	tetrahedron,	ETBPY-8	=Elongated	trigonal	bipyramid;
EP-9=Enn	eagon, OPY	-9=Octagoi	nal pyramid	, HBPY-9=	=Heptagonal	bipyramid,	HBPY-9=H	Ieptagonal	bipyramid,
JCCU-9=0	Capped cub	e J8, CCU-	-9=Spherica	l-relaxed	capped cube,	JCSAPR-	9=Capped s	square anti	iprism J10,
CSAPR-9	=Spherical	capped squa	are antipris	m, JTCTP	R-9=Tricappo	ed trigonal	prism J51,	TCTPR-9	9=Spherical
tricapped t	trigonal pris	m, JTDIC-9	=Tridiminis	shed icosah	edron J63, Hl	H-9=Hula-	hoop, MFF-9	=Muffin.	

 $\textbf{Table S3} \ \text{Lanthanide complexes with DAPBH or /and DPP derivatives as ligands and}$

Complexes	Nuclearity	Dimensionality	Coordination mode	Ref.
[Yb ₂ (DAPBH) ₂ (DPP) ₃ (CH ₃ OH)](NO ₃)(ClO ₄) ₂ ·3CH ₃ OH	2	1D	HN YD NH O O O	This work
Eu(DAPBH)2(NO3)3·2H2O	1	0D	HN N EU N NH	1
[Dy(H2DABPH)2](NO3)3· 2.5H2O	1	0D		
[Dy(H2DABPH)(HDABPH)] (NO3)2·EtOH·4H2O	1	0D		
[Dy ₂ (DAPBH ₂) ₂ (µ ₂ -TCNQ) ₂ (TCNQ) ₂ (EtOH) ₂ (TCNQ) ₂ · 2EtOH·2CH ₂ Cl ₂	2	0D		2,3,4
[Dy(DAPBH)NO ₃ (H ₂ O) ₂]· (NO ₃) ₂	1	0D		

their nuclearity and dimensionality.

[Tb ₂ (DAPBH ₂) ₂ (µ ₂ -TCNQ) ₂ (TCNQ) ₂ (EtOH) ₂ (TCNQ) ₂ · 4EtOH	2	0D		3
[Ln2(DAPBH2)2(µ2-TCNQ)2 (TCNQ)2(MeOH)2(TCNQ)2·2M eOH (Ln=Gd,Tb,Dy)	2	0D		3,5
[Ln(DAPBH ₂)(CH ₃ OH) (H ₂ O) ₃]Cl ₃ ·2CH ₃ OH (Ln=Tb and Dy)	1	0D		
La(DAPBH)(NO ₃) ₃	1	0D		
Trinitrato-(2,6-diacetylpyridine -bis(benzoic- acid- hydrazone))lanthanum(iii)	1	0D		4,6
Yb(DAPBH)(NO3)3(H2O)2	1	0D	HN YD N HH	7
[Ln(H2dapsc)(H2O)4](NO3)3 (Ln=Dy, Ho, Er, and Tb)	1	0D		8
[Dy(H4daps)(H2O)3(NO3)] (NO3)2 [.] (H2O)	1	0D		
[Dy(H3daps)(H2O)2(NO3)] (NO3)·(MeOH)	1	0D		9,10
[Dy(H4daps)(H2O)3(NO3)] (NO3)2 [.] (H2O)	1	0D		
(Et ₃ NH)[(H ₂ L)LnCl ₂] (Ln = Tb, Dy)	1	0D		11
{[Ln(DAPMBH)(N ₃)C ₂ H ₅ OH] \cdot C ₂ H ₅ OH} _n (Ln = Dy, Er, and Gd)	1	1D		12

(C ₂₃ H ₂₃ N ₇ O ₂)Ln(NO ₃) ₃ . CH ₃ OH (Ln=Dy, Tb, Gd, Eu)	1	0D		13
(C ₂₃ H ₂₃ N ₇ O ₂)Er(NO ₃) ₃ ·2H ₂ O	1	0D		15
[Yb2(DAPBH)2(DPP)3(CH3OH)](NO3)(ClO4)2·3CH3OH	2	1D	Vb-0 ^P O-Yb	This work
[ErNa(valdien)Cl((PhO)2PO2)]n	2	1D	Er-O ^P O-Na	14
[Er(valdien)((PhO)2PO2)]n	1	1D		14
[LnNa(valdien)((PhO) ₂ PO ₂)Cl] _n (Ln=Dy, Gd, Tb and Ho)	2	1D		15
[Ln(valdien)((PhO)2PO2)]n (Ln=Dy and Ho)	1	1D		15
[Dy2(HL)2((PhO)2PO2)4]· 2CH3OH	2	0D	Dy-O ^P O-Dy	16
DyTx(P1)2	1	0D	O O Dy	17
$ \{ Nd[(2,6-Me_2C_6H_3O)_2PO_2]_3[(2, 6-Me_2C_6H_3-O)_2PO_2H]_3 \} $	1	0D	C O O Nd	18

			Nd OF OH	
			Nd OP Nd	
{Nd2[(2,6-Me2C6H3O)2PO2]6[(2 ,6-Me2C6H3-O)2PO2H]}	2	0D		
			Nd P OH	
${Nd_2[(2,4-Cl_2-6-MeC_6H_3O)_2PO_2]_6(H_2O)_2(OCMe_2)_2}$	2	0D		
[Ln(C ₂₄ H ₃₄ O ₄ P)Cl(CH ₄ O)4] · 2CH ₃ OH (Ln=Nd and Lu)	1	0D		10.20
[Ln(C24H34O4P)3(CH3OH)5]· CH3OH (Ln=La and Ce)	1	0D		19,20
[Nd2(C24H34O4P)4(OH)(H2O)4]· 2C6H14·2 (heptane)	2	0D		21



Fig. S3 The π - π interactions in 4.



Fig. S4 Intermolecular N/O-H···O hydrogen bonds in **4**. The pyridine and benzene rings were omitted for clarity.

Fig. S5 Intermolecular C-H···O hydrogen bonds in 4.

Table S4 Intermolecular N/O-H···O and C-H···O hydrogen bonds in 4 [Å and °].

D-H···A	d(D-H)	$d(H^{\dots}A)$	$d(D^{\dots}A)$	<(DHA)
N(4)-H(4) ···O(7)	0.88	2.22	2.896(13)	133
N(6)-H(6)····O(27)	0.88	2.19	2.956(14)	145
N(9)-H(9)···O(26)	0.88	2	2.792(13)	149
N(11)-H(11)····O(5)	0.88	2.36	3.240(13)	174
O(24)-H(24B)····O(25)	0.85	2.16	2.861(14)	140
O(25)-H(25A)····O(4A)	0.85	2.16	2.97(3)	160
O(25)-H(25A)····O(4Z)	0.85	2.12	2.96(4)	170
O(26)-H(26B)····O(6)	0.85	1.92	2.764(17)	172
O(27)-H(27B)····O(1B)	0.84	2.59	3.28(3)	140

O(27)-H(27B)····O(2B)	0.84	2.02	2.81(3)	154	
O(27)-H(27B)····O(1Y)	0.84	2.37	3.16(4)	155	
O(27)-H(27B)····O(3Y)	0.84	1.93	2.68(5)	147	
C(9)-H(9A)…O(1Z)	0.95	2.32	3.15(5)	146	
C(32)-H(32A)····O(6)	0.95	2.25	3.156(19)	159	
C(40)-H(40A)····O(3A)	0.95	2.43	3.26(3)	146	
C(40)-H(40A)····O(3Z)	0.95	2.38	3.24(3)	151	
C(49)-H(49A)…O(7)	0.95	2.52	3.391(18)	154	
C(50)-H(50A)····O(5)	0.98	2.57	3.421(18)	145	
C(56)-H(56A)····O(2Y)	0.95	2.56	3.39(4)	146	
C(59)-H(59A)····O(27)	0.98	2.42	3.227(17)	140	
C(59)-H(59A)····O(3Y)	0.98	2.55	3.45(5)	152	
C(63)-H(63A)····O(2A)	0.95	2.59	3.52(3)	166	
C(63)-H(63A)····O(3A)	0.95	2.54	3.19(3)	126	
C(63)-H(63A)····O(2Z)	0.95	2.49	3.37(4)	154	
C(63)-H(63A)····O(3Z)	0.95	2.55	3.28(3)	134	
C(68)-H(68A)····O(25)	0.95	2.48	3.42(2)	170	
C(71)-H(71A)····O(2A)	0.95	2.5	3.41(3)	160	
C(71)-H(71A)····O(2Z)	0.95	2.33	3.25(4)	163	
C(73)-H(73A)····O(7)	0.98	2.33	3.312(18)	175	
C(82)-H(82A)····O(5)	0.98	2.55	3.293(15)	132	

	Table S5 Static magnetic data for 1-4.								
	Ground	Expected χT at	Measured χT	Saturation	Measured				
Compounds	state of	300K	at 300K	magnetization	magnetization				
Compounds	state of	300K		magnetization	at 2K and 7T				
	Ln(III)	(cm ³ Kmol ⁻¹)	(cm ³ Kmol ⁻¹)	(Νβ)	(Νβ)				
1-Tb ₂	${}^{7}F_{6}$	23.64	24.02	18	10.73				
2-Dy ₂	⁶ H _{15/2}	28.34	28.42	20	11.06				
3-E r ₂	${}^{4}I_{15/2}$	22.96	22.85	18	10.37				
4-Yb ₂	${}^{2}F_{7/2}$	5.14	5.36	8	4.11				

Fig. S6 *M* vs. *H* plots for **1** (a), **2** (b), **3** (c) and **4** (d).

Fig. S7 *M* vs. *HT*⁻¹ plots for **1** (a), **2** (b), **3** (c) and **4** (d).

Fig. S8 Field dependence of the magnetization at 2 K for 1 (a), 2 (b), 3 (c) and 4 (d).

Fig. S9 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 3 K for 3.

Fig. S10 Frequency dependence of in-phase (a) and out-of-phase (b) ac susceptibility data under different dc fields at 2 K for 4.

<i>T /</i> K	$\chi_S/$ cm ⁻³ ·mol ⁻¹	$\Delta \chi_l / cm^{-3} \cdot mol^{-1}$	$ au_l/{ m s}$	α_{l}	$\Delta \chi_2 / cm^{-3} \cdot mol^{-1}$	$ au_2$ / s	α_2	R
2	1 12E±00	2 54E±00	1.58E-	2.45	0.99E 01	4.45	2.19	2 07E 02
2	1.13E+00	5.34E+00	04	E-01	9.00E-01	E-01	E-01	5.9/E-02
2.2	1 225+00	2 11E⊥00	1.05E-	2.99	7 17E 01	2.03	1.11E	1 87E 02
2.5	1.22E+00	5.11E+00	04	E-01	/.1/E - 01	E-01	-01	4.0/E-02
26	1.6 2 E±00	2 46E±00	9.88E-	3.06	4.54E.01	1.25	1.81	4 21E 02
2.0	1.02E+00	∠.40£700	05	E-01	4.34E-01	E-01	E-08	4.31E-02

Table S6 Cole-Cole parameters of 3 under 2500 Oe dc field

2.9	1.60E+00	2.31E+00	7.27E-	3.53	3.60E-01	1.58	2.45	3.30E-02
			05	E-01		E-01	E-08	

 $\chi_{\rm S}$ / cm⁻³mol⁻¹ T/K $\chi_{\rm T}$ / cm⁻³mol⁻¹ R τ / s α 2 9.38E-02 7.64E-03 8.79E-02 1.45E+00 4.81E-04 2.2 8.89E-02 1.34E+00 3.72E-04 9.08E-02 1.08E-02 2.4 1.20E-01 1.24E+00 2.95E-04 5.63E-02 1.11E-02 2.6 1.16E-01 1.15E+00 2.29E-04 4.99E-02 1.00E-02 2.8 1.02E-01 1.08E+00 1.78E-04 6.14E-02 8.30E-03 3 1.48E-01 1.01E+00 1.50E-04 2.09E-02 9.85E-03 3.2 1.87E-01 9.49E-01 1.28E-04 9.75E-16 4.51E-03 3.4 2.39E-01 9.07E-01 1.13E-04 1.22E-15 1.03E-02

Table S7 Cole-Cole parameters of 4 under 2000 Oe dc field

Fig. S11 Excitation spectra for DAPBH (a) and DPP (b) ligands.

Fig. S12 Lifetime decay curves for 1 (a), 2 (b) and 4 (c). The red lines are the best fit to the double (a and b) or single (c) exponential functions.

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