Electronic Supplementary Material (ESI) for CrystEngComm.

A seven-coordinated Dy^{III} single ion magnet with C_{2v} symmetry constructed by multidentate Schiff-base ligand

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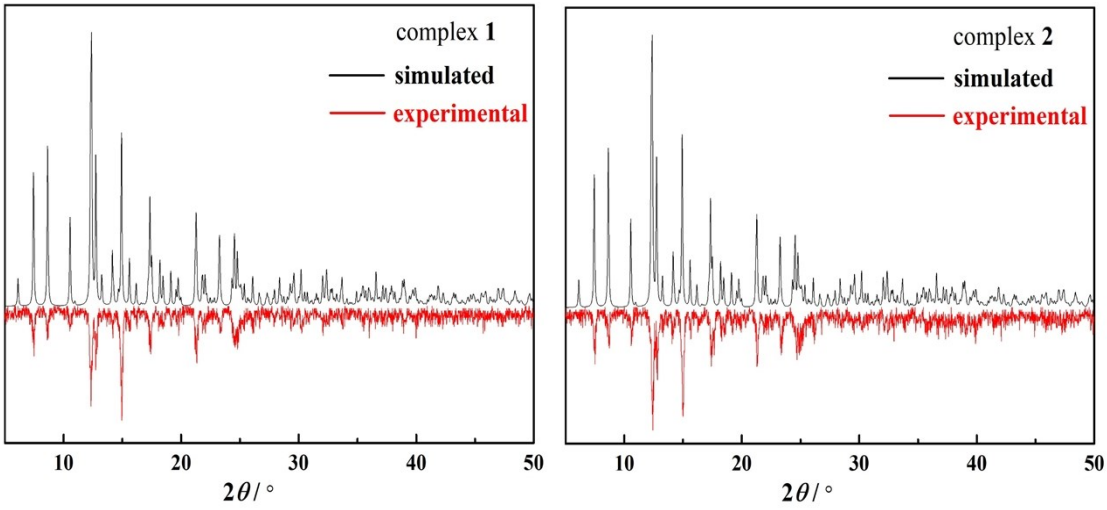

Fig S1 The PXRD pattern of complexes **1** and **2**

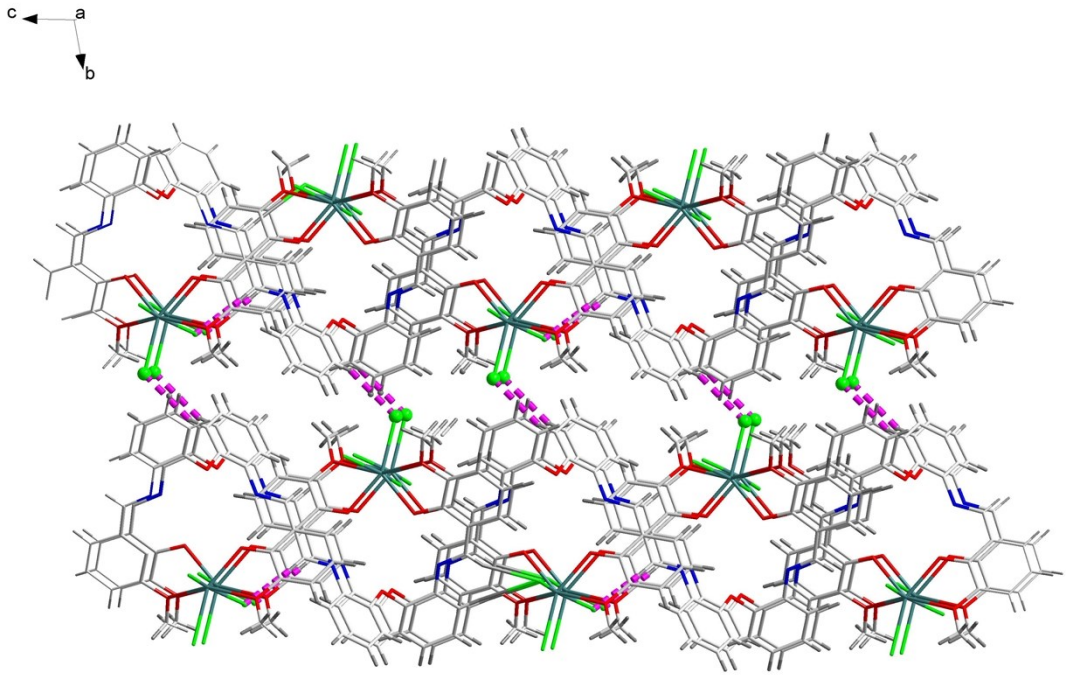

Fig S2 The 3D packing structure of complex **1**

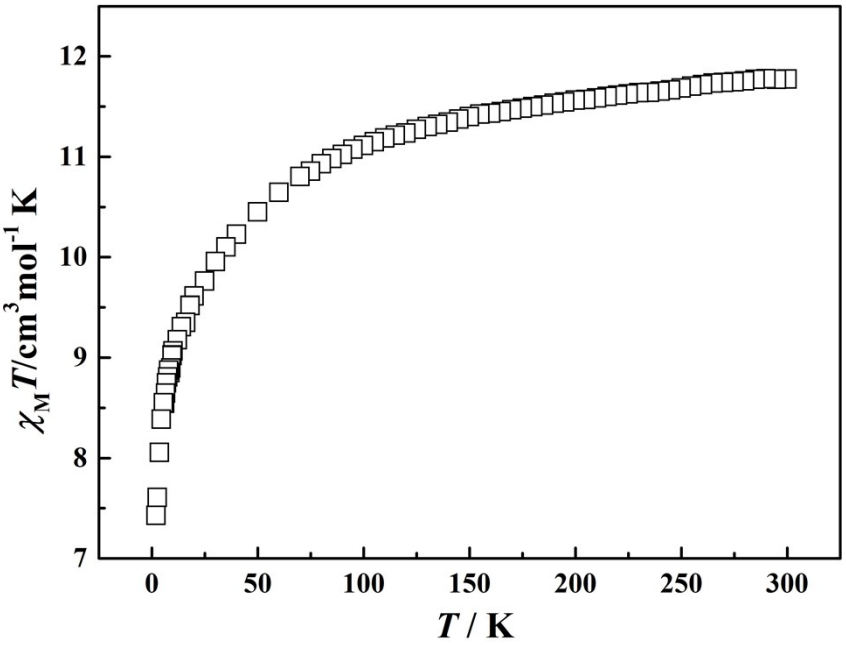

Fig S3 The temperature-dependence of the $\chi_M T$ for complex **2**

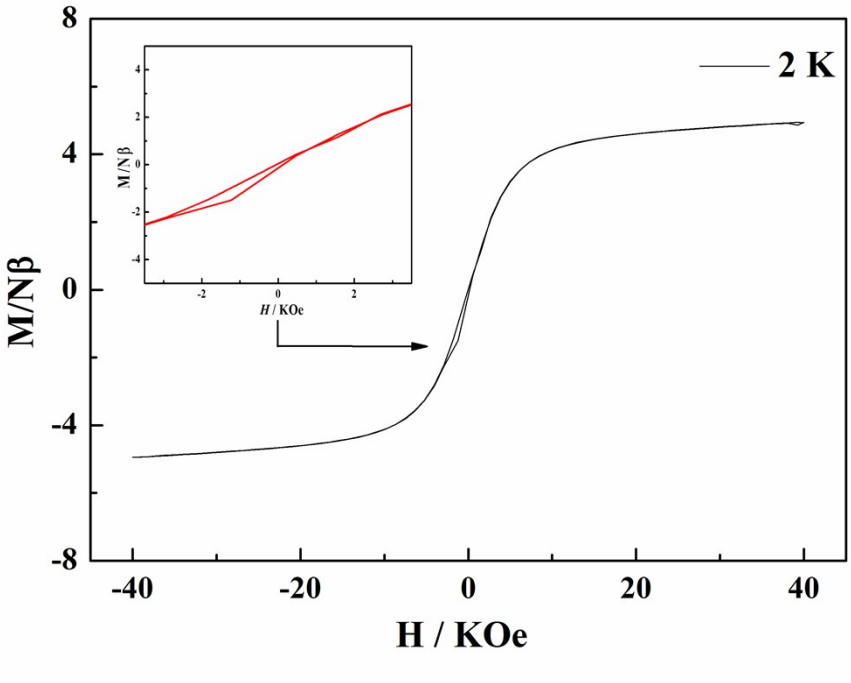

Fig S4 Magnetization curve versus applied field measured at 2 K for complex **1**.

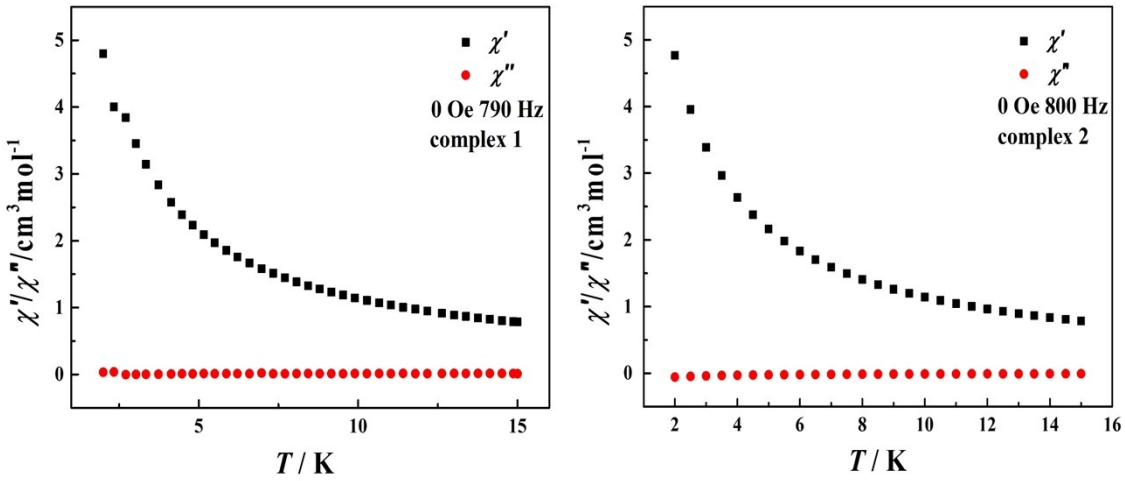

Fig S5 Temperature dependence of the χ' and χ'' ac magnetic susceptibility for **1** and **2** under zero dc field.

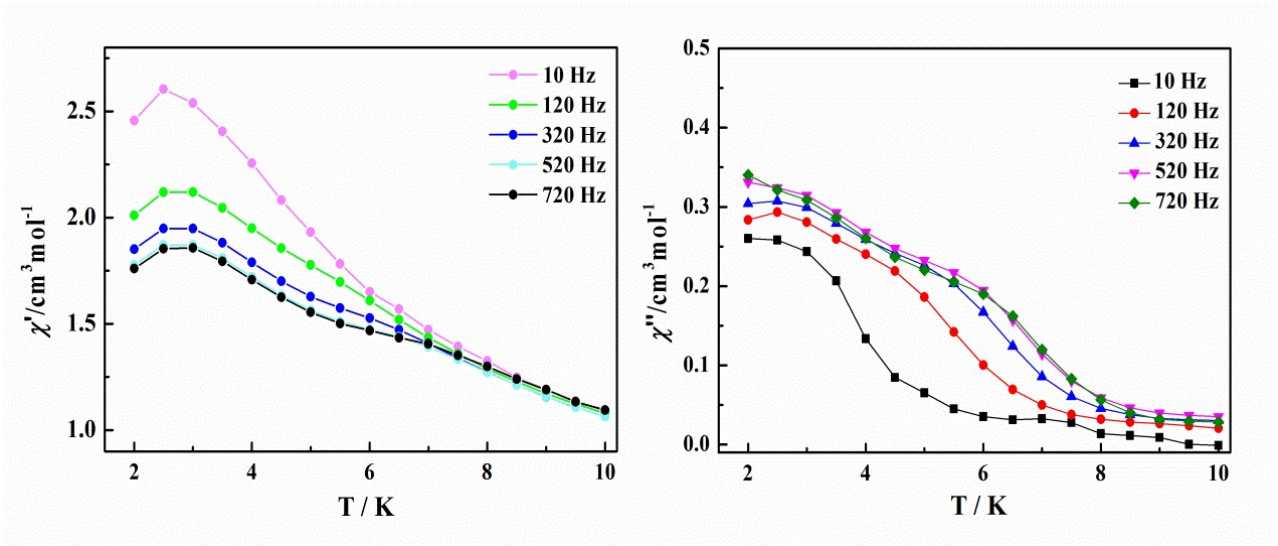

Fig S6 Temperature dependence of the χ' and χ'' ac magnetic susceptibility for **1** under 1500 Oe dc field.

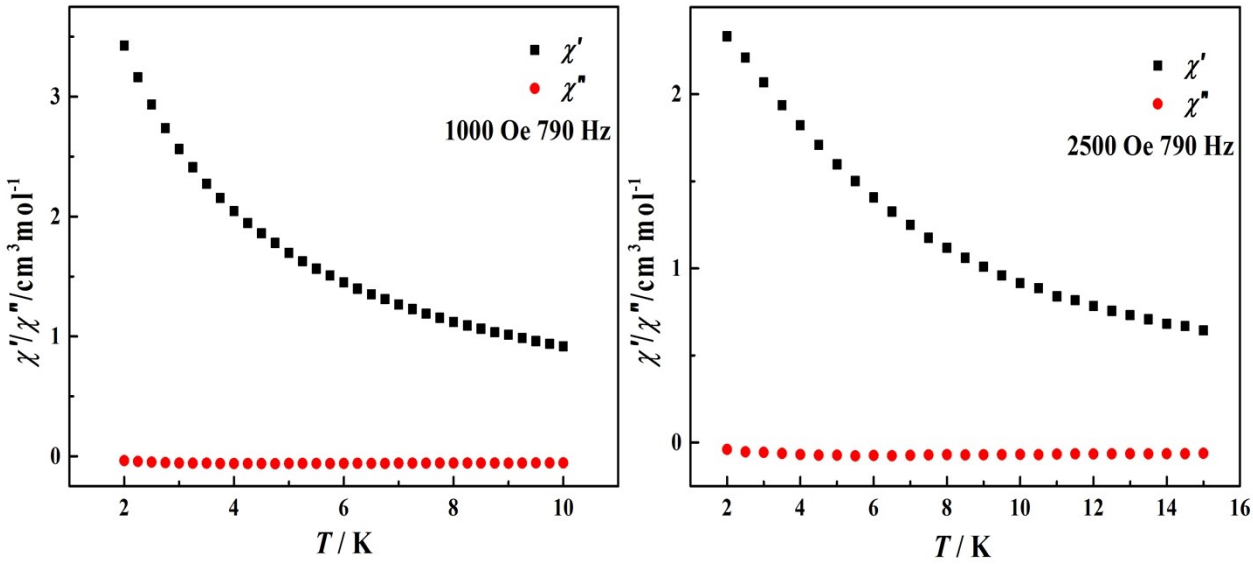

Fig S7 Temperature dependence of the χ' and χ'' ac magnetic susceptibility for **2** under 1000 Oe and 2500 Oe dc field.

Table S1 Selected bond lengths [Å] and-angles [°] for complex **1**

Bond Lengths			
Dy1-O2	2.272(3)	Dy1-O3	2.526(3)
Dy1-O4	2.317(3)	Dy1-O5	2.497(3)
Dy1-Cl6	2.665(1)	Dy1-Cl7	2.621(1)
Dy1 Cl8	2.639(1)	N9-C15	1.306(5)
O2-C4	1.302(5)	O4-C22	1.305(5)
O11-C8	1.395(5)	O11-C40	1.396(5)
O3-C68	1.389(5)	O3-C49	1.425(5)
O5-C36	1.390(5)	O5-C65	1.435(5)
N10-C13	1.421(5)	N10-C25	1.300(5)
N9-C2	1.427(5)		
Bond angles			
Cl7-Dy1-Cl8	87.52(4)	Cl7-Dy1-Cl6	90.15(4)
Cl8-Dy1-Cl6	159.31(4)	O4-Dy1-O3	140.47(10)
O2-Dy1-Cl7	150.11(8)	O4-Dy1-O5	64.87(10)
O2-Dy1-Cl8	89.23(8)	O4-Dy1-Cl6	115.40(8)
O2-Dy1-O4	80.19(10)	O3-Dy1-Cl7	84.72(7)
O2-Dy1-O3	65.50(10)	O3-Dy1-Cl8	79.05(7)
O2-Dy1-O5	128.77(11)	O3-Dy1-Cl6	80.27(7)
O2-Dy1-Cl6	82.61(8)	O5-Dy1-Cl7	77.79(8)
O4-Dy1-Cl7	128.51(8)	O5-Dy1-Cl8	119.10(8)
O4-Dy1-Cl8	81.58(8)	O5-Dy1-O3	153.73(10)
O5-Dy1-Cl6	80.33(8)		

Table S2 Selected bond lengths [Å] and-angles [°] for complex **2**

Bond Lengths			
Tb1-O2	2.288(2)	Tb1-O3	2.555(3)
Tb1-O4	2.316(2)	Tb1-O5	2.517(3)
Tb1-Cl6	2.6468(13)	Tb1-Cl7	2.6269(11)
Tb1-Cl8	2.6678(12)	O3-C1	1.378(5)
O5-C24	1.444(5)	O3-C28	1.424(5)
O4-C22	1.300(4)	O2-C6	1.302(4)
N9-C7	1.304(5)	O11-C9	1.385(5)
N9-C8	1.421(5)	O11-C14	1.388(5)
N10-C15	1.424(5)	O5-C23	1.377(5)
N10-C20	1.301(5)		
Bond angles			
Cl6-Tb1-Cl8	160.38(4)	O2-Tb1-O4	80.94(9)
Cl7-Tb1-Cl8	90.57(4)	O5-Tb1-Cl8	80.66(8)
Cl7-Tb1-Cl6	88.00(5)	O5-Tb1-Cl6	118.04(8)
O3-Tb1-Cl8	80.73(7)	O5-Tb1-Cl7	77.83(7)
O3-Tb1-Cl6	79.65(7)	O5-Tb1-O3	154.08(9)
O3-Tb1-Cl7	84.48(7)	O4-Tb1-Cl8	114.33(8)
O2-Tb1-Cl8	82.60(8)	O4-Tb1-Cl6	81.30(8)
O2-Tb1-Cl6	88.64(8)	O4-Tb1-Cl7	128.67(7)
O2-Tb1-Cl7	149.15(7)	O4-Tb1-O3	140.84(9)
O2-Tb1-O3	64.75(9)	O4-Tb1-O5	64.22(9)
O2-Tb1-O5	129.91(10)		

Table S3 Ln^{III} ion geometry analysis by SHAPE software for two complexes.

Complexes	C_{2v}-CTPR	C_{3v}-COC	D_{5h}-JPBPY
1	1.180	2.912	4.681
2	1.304	3.124	4.410

Table S4 Energy levels and eigenstates for **1** obtained from fitting the $\chi_M T$-T and M-H data.

Energy / cm^{-1}	**Eigenstate**
0	51.7%|±7/2 > +15.0%|± 5/2> +11.7%|± 9/2>+5.5%|± 11/2>+…
61	43.2%|± 5/2> +23.3%|± 9/2 > +16.9%|± 7/2>9.1%|±3/2>+…
64	85.9%|± 13/2> +7.5%|± 11/2 > +4.7%|± 3/2>+…
84	45.2%|± 13/2> +18.5%|± 1/2 > +14.9%|± 7/2> +8.9%|±9/2>+…
89	45.5%|± 9/2> +39.4%|± 1/2 > +1.4%|± 13/2>+12.8%|± 3/2> +…
141	64.5%|± 11/2> +11.1%|± 3/2 > +6.9%|± 3/2> +…
165	30.2%|± 1/2> +17.9%|± 11/2 > +17.4%|± 3/2> +14.4%|± 7/2>+…
179	96.3%|± 13/2 > +2.3%|± 5/2> +…

TableS5 Crystal field parameters from PHI program fitting for complex **1**.

	B_0^2	B_2^2	B_0^4	B_2^4	B_4^4	B_0^6	B_2^6	B_4^6	B_6^6	Residual
1	-36.47	-181.43	11.39	11.93	-43.15	-38.92	-138.38	-153.40	100.17	0.033

TableS6 Fitted parameters α with Debye model under 2.0 K-6.0 K for complex **1**.

Temperature/K	α_1	α_2
2.0	0.50	0.80
2.4	0.45	0.79
2.8	0.41	0.77
3.2	0.35	0.76
3.6	0.29	0.74
4.0	0.25	0.72
4.4	0.23	0.71
4.8	0.23	0.70
5.2	0.22	0.69
5.6	0.11	0.68
6.0	0.02	0.68

Table S7 Examples of seven-coordinate Dy^{III} SIMs with low C_{nv} symmetry.

Formula	Symmetry	U_{eff}	Ref.
$[(LOEt)Dy((R,R)\text{-Salphen})]_2 \cdot 3H_2O$	C_{2v}	24.6 K(2 KOe)	22a
$[DyH_4L/\ (SCN)_2](SCN)_2$	C_{2v}	34.5 K(200 Oe)	22b
$Dy(Hthd)_3(MeOH) \cdot 2,5\text{-Py}$	C_{2v}	26.6 K(1 KOe)	14a
$Dy((R,R)\text{-5-Cl-Salcy})) \cdot CH_3OH \cdot 1/8H_2O$	C_{2v}	13.2 K(2 KOe)	22a
$[(LOEt)Dy(TPP)] \cdot 0.25H_2O$	C_{3v}	8.5 K(2 KOe)	22c
$[(LOEt)Dy(L)] \cdot 0.25H_2O$	C_{3v}	41.6 K(2 KOe)	22d
$Dy(Hthd)_3(Tppo)$	C_{3v}	35.9 K(1 KOe)	14a
$Dy(Hthd)_3(PyNO)$	C_{3v}	42.7 K(1 KOe)	14a
$Dy(Hthd)_3(4\text{-PyNO})$	C_{3v}	55.8 K(1 KOe)	14a