Luminescent and magnetic properties of mononuclear Ln(III) complexes using N1-substituted 1,2,3-triazole ligand

Supporting Information

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Table S1 Crystal Data and Structural Refinement for compounds **1-3**.

Compound	**1**	**2**	**3**
Empirical formula	$C_{24}H_{18}DyN_{13}O_9 \cdot 2CH_3CN$	$C_{24}H_{18}TbN_{13}O_9 \cdot 2CH_3CN$	$C_{24}H_{18}EuN_{13}O_9 \cdot 2CH_3CN$
Fw /g·mol^{-1}	875.10	873.55	866.59
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*C2/c*	*C2/c*	*C2/c*
a /Å	19.69338 (9)	19.5199(1)	19.5223(2)
b /Å	11.64098 (5)	11.4695(1)	11.4455(1)
c /Å	16.29945 (9)	16.2186(1)	16.2870(1)
α /°	90	90	90
β /°	111.3480 (6)	111.286(1)	111.382
γ /°	90	90	90
V /Å ^{3}	3480.27 (3)	3383.37(5)	3388.72(6)
Z	4	4	4

Dc /(g/cm^3)	1.670	1.715	1.699
μ /mm^{-1}	12.13	10.943	13.913
Index ranges	-24≤ h ≤24, -14 ≤ k ≤ 14, -20 ≤ l ≤ 20	-24≤ h ≤24, -13 ≤ k ≤ 14, -20 ≤ l ≤ 20	-22≤ h ≤24, -14 ≤ k ≤ 14, -20 ≤ l ≤ 20
θ range/(°)	4.5-73.7	2.9150-73.9820	4.565-74.189
Reflns collected	36711	36703	20050
Independent reflns	3518	3415	3397
Observed reflections	3462	3372	3303
R_{int}	0.027	0.03	0.03
GOF on F^2	1.08	1.052	1.050
R_1, wR_2[I≥2σ(I)]	0.0211, 0.0582	0.0311, 0.0821	0.0319, 0.0809
R_1, wR_2(all data)	0.0213, 0.0584	0.0315, 0.0821	0.0324, 0.0809

Table S2 Geometry analysis for compound **1-3** by using SHAPE 2.1 program.

Point group	Geometry	Polyhedron	**1**	**2**	**3**
D_{10h}	DP-10	Decagon	36.31418	35.98005	36.01793
C_{9v}	EPY-10	Enneagonal pyramid	23.23773	23.01462	23.09622
D_{8h}	OBPY-10	Octagonal bipyramid	16.45394	16.76161	16.78624
D_{5h}	PPR-10	Pentagonal prism	9.34815	8.89390	8.73073
D_{5d}	PAPR-10	Pentagonal antiprism	13.30349	13.05802	12.89469
D_{4h}	JBCCU-10	Bicapped cube (Elongated square bipyramid J15)	12.44866	12.70499	12.75918
D_{4d}	JBCSAPR-10	Bicapped square antiprism (Gyroelongated square bipyramid J17)	4.23444	4.45696	4.62532
C_{2v}	JMBIC-10	Metabidiminished icosahedron (J62)	6.83173	6.68276	6.68330
C_{3v}	JATDI-10	Augmented tridiminished icosahedron (J64)	18.12801	17.76050	17.67328
C_{2v}	JSPC-10	Sphenocorona (J87)	4.19714	4.18951	4.28811
D_2	SDD-10	Staggered dodecahedron (2:6:2) #	4.31009	4.35091	4.29758
C_{2v}	TD-10	Tetradecahedron (2:6:2)	4.31035	4.41930	4.39560
D_{4h}	HD-10	Tetradecahedron (2:6:2)	10.06093	10.33854	10.34790

Table S3 Selected bond distances (Å) and angles (deg) for compound **1**.

Bond lengths (Å)			
Dy1-O3	2.5037 (17)	Dy1-N2	2.5359 (16)
Dy1-O3	2.5038 (17)	Dy1-N2	2.5358 (16)

Dy1-O1	2.4604 (16)	Dy1-N1	2.6531 (16)
Dy1-O1	2.4604 (16)	Dy1-N1	2.6531 (16)
Dy1-O5	2.4067 (15)	Dy1-N7	2.8802 (18)
Dy1-O5	2.4066 (15)	Dy1-N7	2.8802 (18)
Bond angles (deg)			
O3-Dy1-O3	179.27 (7)	O5-Dy1-O3	127.53 (5)
O3-Dy1-N2	111.15 (5)	O5-Dy1-O3	127.53 (5)
O3-Dy1-N2	68.51 (5)	O5-Dy1-O3	51.79 (5)
O3-Dy1-N2	68.51 (5)	O5-Dy1-O1	119.22 (6)
O3-Dy1-N2	111.15 (5)	O5-Dy1-O1	119.22 (6)
O3-Dy1-N1	110.81 (5)	O5-Dy1-O1	145.90 (6)
O3-Dy1-N1	69.43 (5)	O5-Dy1-O1	145.90 (6)
O3-Dy1-N1	69.43 (5)	O5-Dy1-N2	70.23 (5)
O3-Dy1-N1	110.81 (5)	O5-Dy1-N2	72.65 (5)
O3-Dy1-N7	153.39 (6)	O5-Dy1-N2	72.65 (5)
O3-Dy1-N7	25.92 (5)	O5-Dy1-N2	70.23 (5)
O3-Dy1-N7	153.39 (6)	O5-Dy1-O5	85.87 (8)
O3-Dy1-N7	25.92 (5)	O5-Dy1-N1	75.83 (5)
O1-Dy1-O3	67.96 (6)	O5-Dy1-N1	75.83 (5)
O1-Dy1-O3	112.75 (6)	O5-Dy1-N1	135.13 (5)
O1-Dy1-O3	67.97 (6)	O5-Dy1-N1	135.13 (5)
O1-Dy1-O3	112.75 (6)	O5-Dy1-N7	25.92 (6)
O1-Dy1-O1	51.97 (9)	O5-Dy1-N7	25.92 (6)
O1-Dy1-N2	135.04 (6)	O5-Dy1-N7	106.73 (6)
O1-Dy1-N2	135.03 (6)	O5-Dy1-N7	106.73 (6)
O1-Dy1-N2	94.23 (6)	N1-Dy1-N1	143.06 (7)
O1-Dy1-N2	94.23 (6)	N1-Dy1-N7	125.29 (5)
O1-Dy1-N1	70.08 (6)	N1-Dy1-N7	71.76 (5)
O1-Dy1-N1	76.77 (6)	N1-Dy1-N7	71.76 (5)
O1-Dy1-N1	70.08 (6)	N1-Dy1-N7	125.29 (5)
O1-Dy1-N1	76.77 (6)	N7-Dy1-N7	130.62 (9)
O1-Dy1-N7	133.27 (6)	N7-O3-Dy1	93.94 (12)
O1-Dy1-N7	93.75 (6)	N6-O1-Dy1	95.94 (14)
O1-Dy1-N7	93.75 (6)	N3-N2-Dy1	128.03 (12)
O1-Dy1-N7	133.27 (6)	C6-N2-Dy1	121.91 (13)
N2-Dy1-N2	128.48 (8)	N7-O5-Dy1	98.31 (12)

Table S4 Selected bond distances (Å) and angles (deg) for compound **2**.

Bond lengths (Å)			
Tb1-O1	2.474 (2)	Tb1-N4	2.550 (2)
Tb1-O1	2.474 (2)	Tb1-N4	2.550 (2)
Tb1-O3	2.504 (2)	Tb1-N7	2.890 (2)
Tb1-O3	2.504 (2)	Tb1-N7	2.890 (2)
Tb1-O4	2.4237 (19)	Tb1-N5	2.635 (2)
Tb1-O4	2.4237 (19)	Tb1-N5	2.635 (2)
Bond angles (deg)			
O1-Tb1-O1	51.92 (10)	O1-Tb1-N4	136.00 (7)
O1-Tb1-O3	112.28 (6)	O1-Tb1-N4	95.61 (7)
O1-Tb1-O3	67.07 (6)	O1-Tb1-N4	95.61 (7)
O1-Tb1-O3	67.07 (6)	O1-Tb1-N7	93.02 (7)
O1-Tb1-O3	112.28 (6)	O1-Tb1-N7	133.43 (7)
O1-Tb1-N4	136.00 (7)	O1-Tb1-N7	133.43 (7)
O1-Tb1-N7	93.02 (7)	O1-Tb1-N5	70.71 (7)
O1-Tb1-N5	70.71 (7)	O1-Tb1-N5	77.21 (7)
O1-Tb1-N5	77.21 (7)	O3-Tb1-N7	26.04 (6)

O3-Tb1-O3	179.33 (8)	O3-Tb1-N7	154.60 (6)
O3-Tb1-N4	68.71 (7)	O3-Tb1-N7	154.60 (6)
O3-Tb1-N4	68.71 (7)	O3-Tb1-N7	26.04 (6)
O3-Tb1-N4	111.62 (7)	O3-Tb1-N5	69.87 (7)
O3-Tb1-N4	111.62 (7)	O3-Tb1-N5	109.92 (7)
O3-Tb1-N5	69.87 (7)	O4-Tb1-O3	128.70 (6)
O3-Tb1-N5	109.92 (7)	O4-Tb1-O3	51.92 (6)
O4-Tb1-O1	118.41 (7)	O4-Tb1-O3	128.70 (6)
O4-Tb1-O1	145.99 (7)	O4-Tb1-O3	51.92 (6)
O4-Tb1-O1	145.99 (7)	O4-Tb1-O4	86.96 (9)
O4-Tb1-O1	118.41 (7)	O4-Tb1-N4	71.58 (7)
O4-Tb1-N4	69.92 (7)	O4-Tb1-N7	107.56 (7)
O4-Tb1-N4	71.57 (7)	O4-Tb1-N5	134.31 (7)
O4-Tb1-N4	69.91 (7)	O4-Tb1-N5	134.31 (7)
O4-Tb1-N7	25.99 (6)	O4-Tb1-N5	75.33 (7)
O4-Tb1-N7	25.99 (6)	O4-Tb1-N5	75.33 (7)
O4-Tb1-N7	107.56 (6)	N4-Tb1-N4	125.94 (10)
N4-Tb1-N7	91.75 (7)	N4-Tb1-N5	62.83 (7)
N4-Tb1-N7	66.13 (6)	N4-Tb1-N5	137.35 (7)
N4-Tb1-N7	66.13 (6)	N7-Tb1-N7	131.40 (9)
N4-Tb1-N7	91.75 (7)	N5-Tb1-N7	72.27 (6)
N4-Tb1-N5	62.83 (7)	N5-Tb1-N7	72.27 (6)
N4-Tb1-N5	137.35 (7)	N5-Tb1-N7	123.86 (6)
N5-Tb1-N7	123.86 (6)	C7-N4-Tb1	121.28 (17)
N5-Tb1-N5	144.27 (10)	O3-N7-Tb1	59.80 (13)
N6-O1-Tb1	96.10 (16)	O5-N7-Tb1	173.82 (18)
N7-O3-Tb1	94.16 (15)	O4-N7-Tb1	56.18 (12)
N7-O4-Tb1	97.83 (14)	C12-N5-Tb1	121.84 (18)
O1-N6-Tb1	57.94 (16)	O1-N6-Tb1	57.94 (16)
N3-N4-Tb1	128.65 (16)	C8-N5-Tb1	121.05 (17)

Table S5 Selected bond distances (Å) and angles (deg) for compound **3**.

Bond lengths (Å)			
Eu1-O4	2.498 (2)	Eu1-N4	2.572 (2)
Eu1-O4	2.498 (2)	Eu1-N4	2.572 (2)
Eu1-O1	2.4510 (18)	Eu1-N5	2.658 (2)
Eu1-O1	2.4510 (17)	Eu1-N5	2.658 (2)
Eu1-O3	2.523 (2)	Eu1-N6	2.909 (2)
Eu1-O3	2.523 (2)	Eu1-N6	2.909 (2)
Bond angles (deg)			
O4-Eu1-O4	51.42 (9)	O4-Eu1-O3	112.18 (6)
O4-Eu1-O3	67.29 (6)	O4-Eu1-N4	96.08 (6)
O4-Eu1-O3	67.29 (6)	O4-Eu1-N4	135.92 (6)
O4-Eu1-O3	112.18 (6)	O4-Eu1-N4	135.92 (6)
O4-Eu1-N4	96.08 (6)	O4-Eu1-N5	77.48 (6)
O4-Eu1-N5	70.80 (6)	O4-Eu1-N6	133.31 (6)
O4-Eu1-N5	70.80 (6)	O1-Eu1-O4	118.24 (6)
O4-Eu1-N5	77.48 (6)	O1-Eu1-O4	146.21 (6)
O4-Eu1-N6	92.97 (6)	O1-Eu1-O4	118.24 (6)
O4-Eu1-N6	92.97 (6)	O1-Eu1-O4	146.20 (6)
O4-Eu1-N6	133.32 (6)	O1-Eu1-O1	87.27 (8)
O1-Eu1-O3	51.52 (6)	O1-Eu1-N4	70.16 (6)
O1-Eu1-O3	128.98 (6)	O1-Eu1-N4	70.17 (6)
O1-Eu1-O3	128.98 (6)	O1-Eu1-N5	75.52 (6)
O1-Eu1-O3	51.52 (6)	O1-Eu1-N5	133.50 (6)

O1-Eu1-N4	71.17 (6)	O1-Eu1-N5	133.50 (6)
O1-Eu1-N4	71.17 (6)	O1-Eu1-N5	75.52 (6)
O1-Eu1-N6	107.89 (6)	O3-Eu1-N4	111.49 (7)
O1-Eu1-N6	25.86 (6)	O3-Eu1-N4	68.78 (6)
O1-Eu1-N6	107.89 (6)	O3-Eu1-N4	111.49 (6)
O1-Eu1-N6	25.86 (6)	O3-Eu1-N4	68.78 (6)
O3-Eu1-O3	179.46 (7)	O3-Eu1-N5	70.35 (6)
O3-Eu1-N5	109.48 (7)	O3-Eu1-N6	25.76 (6)
O3-Eu1-N5	70.35 (7)	N4-Eu1-N4	125.56 (9)
O3-Eu1-N5	109.47 (6)	N4-Eu1-N5	62.39 (6)
O3-Eu1-N6	25.76 (6)	N4-Eu1-N5	137.77 (6)
O3-Eu1-N6	154.75 (6)	N4-Eu1-N5	62.39 (6)
O3-Eu1-N6	154.75 (6)	N4-Eu1-N5	137.77 (6)
N4-Eu1-N6	65.94 (6)	N4-Eu1-N6	91.90 (6)
N4-Eu1-N6	65.94 (6)	N5-Eu1-N5	144.75 (9)
N4-Eu1-N6	91.90 (6)	N5-Eu1-N6	72.71 (6)
N5-Eu1-N6	123.04 (6)	N6-O3-Eu1	94.37 (14)
N5-Eu1-N6	72.71 (6)	N3-N4-Eu1	128.80 (15)
N5-Eu1-N6	123.04 (6)	C7-N4-Eu1	121.56 (16)
N6-Eu1-N6	131.66 (9)	C12-N5-Eu1	121.54 (18)
N7-O4-Eu1	96.45 (15)	C8-N5-Eu1	121.20 (16)
N6-O1-Eu1	97.47 (13)	O1-N6-Eu1	56.67 (11)
O3-N6-Eu1	59.87 (13)	O4-N7-Eu1	57.84 (15)
O2-N6-Eu1	173.09 (17)	O4-N7-Eu1	57.84 (15)

Table S6 Hydrogen bonds donor/acceptor scheme (Å, °) for compounds **1-3**.

Compound	D-H···A	H···A (Å)	D···A (Å)	D-H···A (°)
1	C(1)-H(1)···O(1)	2.51	3.115 (3)	123
	C(2)-H(2)···O(4)	2.55	3.183 (3)	125
	C(6)-H(6)···O(4)	2.57	3.337 (3)	140
2	C(11)-H(11)···O(3)	2.56	3.186 (4)	125
	C(12)-H(12)···O(4)	2.52	3.138 (3)	124
	C(6)-H(6)···O(4)	2.58	3.347 (4)	140
3	C(11)-H(11)···O(3)	2.56	3.194 (5)	125
	C(12)-H(12)···O(4)	2.54	3.163 (5)	125

Table S7 π···π interactions of compounds **1-3**.

Compound	π···π	Centroid-to-centroid Distance/ Å
1	C_2N_3···C_5N_1	3.6544 (13)
2	C_2N_3···C_5N_1	3.5888 (2)
3	C_2N_3···C_5N_1	3.5963 (2)

Table S8 Lifetime and fluorescence quantum yield of Dy^{3+} complexes containing triazole-based ligands.

Complex	Dy^{3+} lifetime, μs	fluorescence quantum yield, %	Lambda ex, nm	Ref.
$Dy(C_2H_6O_2)(H_2O)_2(NO_3)_3$·2bpt·$2H_2O$	2.2	4.15	375	1

Table S9 Lifetime and fluorescence quantum yield of Tb^{3+} complexes containing triazole-based ligands.

Complex	Tb^{3+} lifetime, μs	Fluorescence quantum yield, %	Lambda ex, nm	Ref.
$Tb(C_2H_6O_2)(H_2O)_2(NO_3)_3{\cdot}2bpt{\cdot}2H_2O$	755	7.77	375	1
$[Tb_2(TDA)_2(H_2O)_3]{\cdot}5H_2O$	800.5 and 349.4		270	2
$[Tb(TDA)(H_2O)_3]{\cdot}H2O$	475		350	3
$[Tb(TDA)]_n$	366		350	3
$[Tb(TDA)(D_2O)_3]{\cdot}D_2O$	529		350	3

Table S10 Lifetime and fluorescence quantum yield of Eu^{3+} complexes containing triazole-based ligands.

Complex	Eu^{3+} lifetime, μs	fluorescence quantum yield, %	Lambda ex, nm	Ref.
$Eu(C_2H_6O_2)(H_2O)_2(NO_3)_3{\cdot}2bpt{\cdot}2H_2O$	283	10.17	375	1
$[Eu_2(TDA)_2(H_2O)_3]{\cdot}5H_2O$	308.5 and 169.2		396	2
$[Eu(TDA)(H_2O)_3]{\cdot}H_2O$	292		394	3
Eu(TDA)	388		394	3
$[Eu(TDA)(D_2O)_3]{\cdot}D_2O$	712		394	3
$(NMe_2H_2)[Eu(TAD)(HCOO)]$	645		254	4
$[Eu(H_2L)_{1.5}(H_2O)_2]{\cdot}1.75H_2O$	320	2.08	390	5

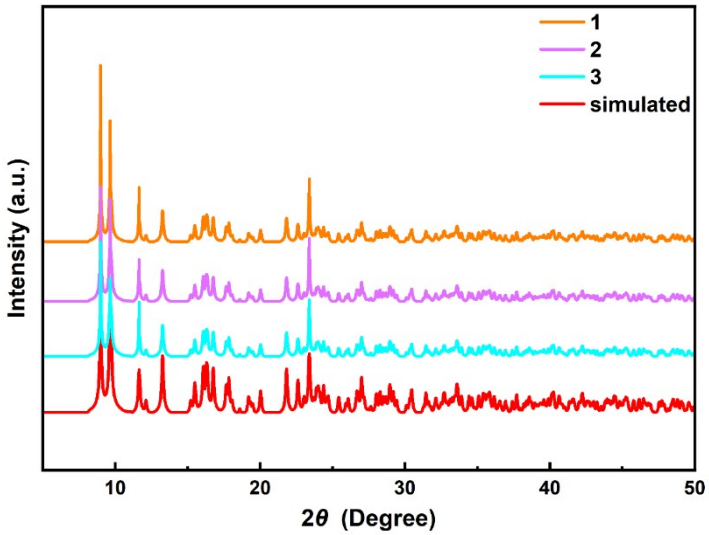

Figure S1. X-ray powder diffraction: measured for compounds **1-3** in comparison with that simulated from the single-crystal structures of compound **1**.

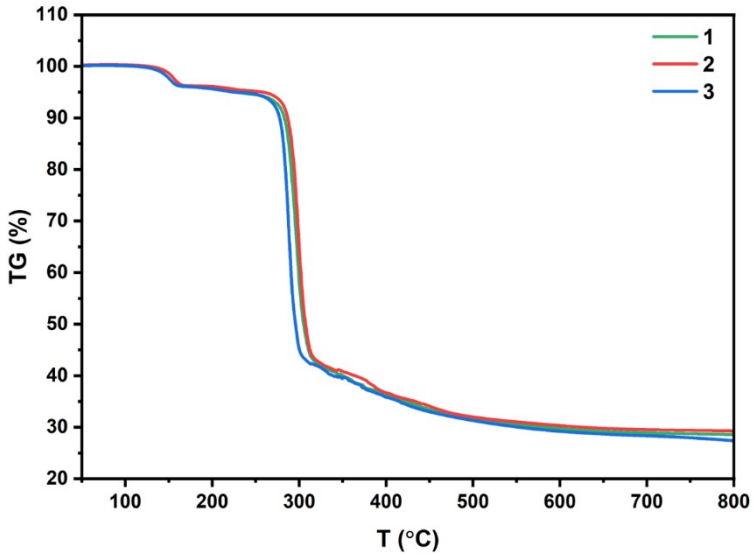

Figure S2. Thermogravimetric curves for **1-3**.

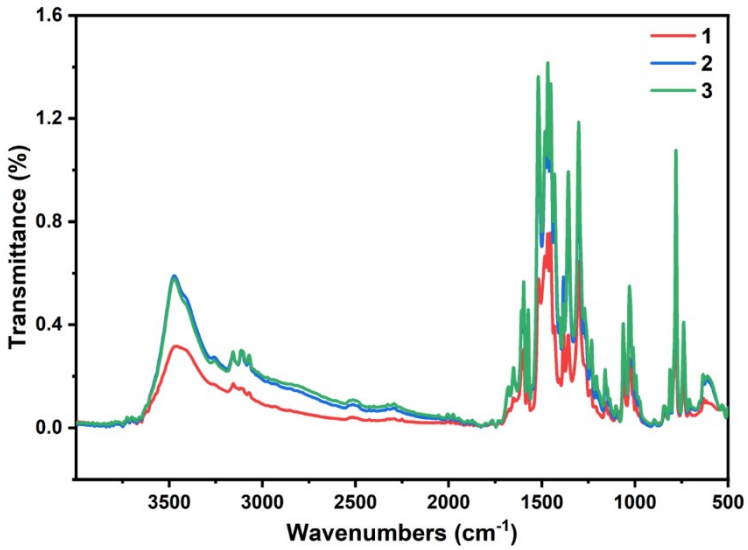

Figure S3. Infrared spectrum for **1-3**.

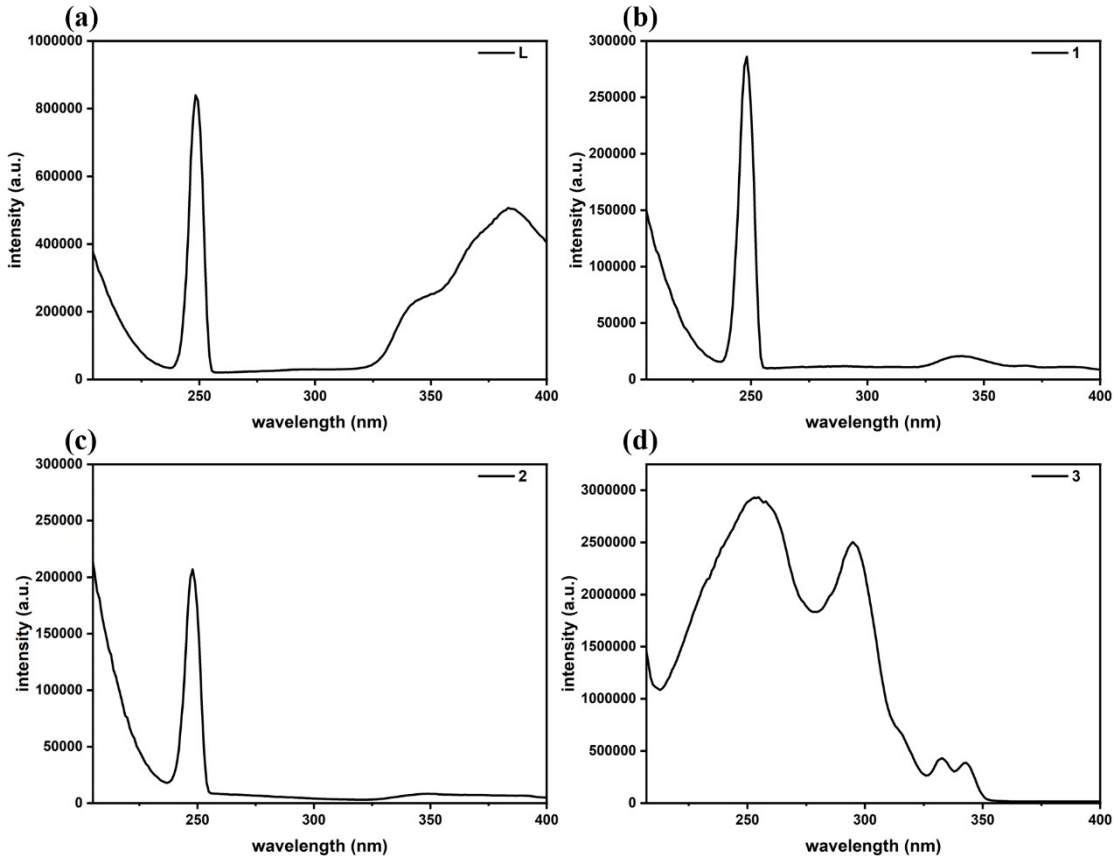

Figure S4. Excitation spectra of free ligand L (a) and the complexes **1**−**3** (b-c).

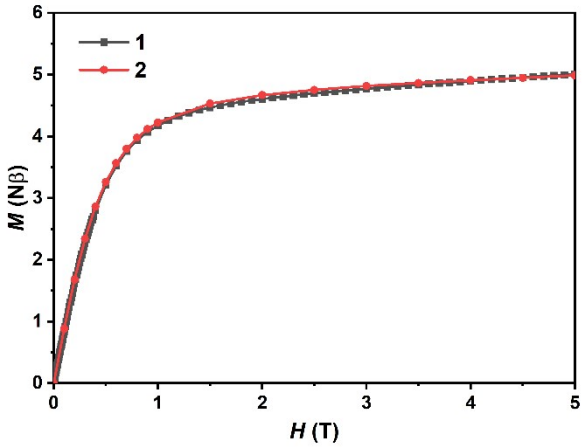

Figure S5 Field dependence of the magnetisation at 2 K for **1** and **2**

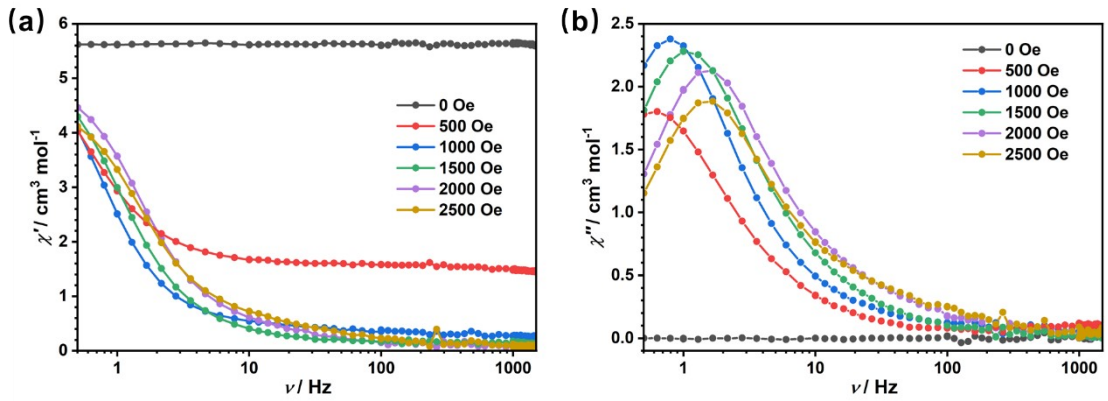

Figure S6 Frequency dependence of the in-phase (χ') (left) and out-of-phase (χ'') (right) ac susceptibility components under the indicated dc fields at 2.0 K for **1**.

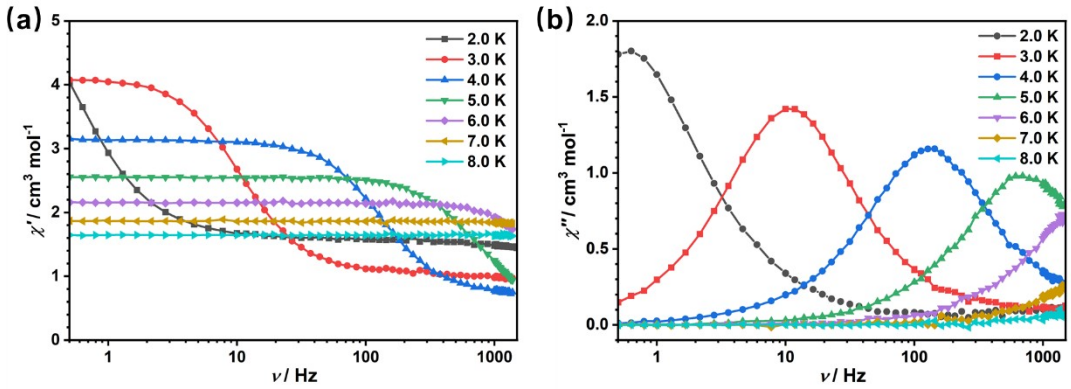

Figure S7 Frequency dependence of the in-phase (χ') (left) and out-of-phase (χ'') (right) ac susceptibility components at different temperatures under 500 Oe dc field for **1**.

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