Supplementary Information

Origin of SMM behaviour in asymmetric Er(III) Schiff base complex: A combined experimental and theoretical study

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Experimental:

Unless otherwise mentioned all the reactions were carried out in aerobic conditions. All the chemicals were purchased from commercially available sources and were used without further purification. The synthesis of the Schiff base ligand is reported elsewhere.[1, 2]

Synthesis of **1**:
The ligand HL (0.3 g, 1.3 mmol)) and $Er(NO_3)_3.5H_2O$ (0.2896 g, 0.66mmol) were added to ethanol (60 mL) resulting in an orange solution, which was refluxed for 7-8 hours. Orange/ yellow coloured crystals could originally be obtained at room temperature upon slow evaporation of the solvent. These however were found to be unsuitable for X-ray diffraction. The collected crystalline material was then recrystallized from methanol, upon slow evaporation of solvent, single crystals suitable for X-ray diffraction grown in 3-4 days. IR: (KBr pellet), 3423.54 cm^{-1}(b,(NH)), 2930.17 cm^{-1}(s,(Ar-H)),1642.24 cm^{-1}(s,(C=N)).

Synthesis of **2:**
same procedure was followed as **1** simply by replacing $Er(NO_3)_3.5H_2O$ by $Lu(NO)_3.xH_2O$**.** Suitable crystals for x-ray diffraction were obtained after 2-3 days from methanol at room temperature. IR: (KBr pellet), 3412 cm^{-1}(b,(NH)), 2933.17 cm^{-1}(s,(Ar-H)),1636 cm^{-1}(s,(C=N)).

50% Diluted sample were prepared by reacting ligand HL (0.3 g, 1.3 mmol), $Lu(NO)_3.xH_2O$ (0.1192 g, 0.33 mmol) and $Er(NO_3)_3.5H_2O$ (0.1464g, 0.33 nmol) in ethanol. The resulting mixture was refluxed for 7-8 hrs. Similar procedure was followed for the synthesis of 5% diluted sample with corresponding molar mixture of metal precursor and ligand.

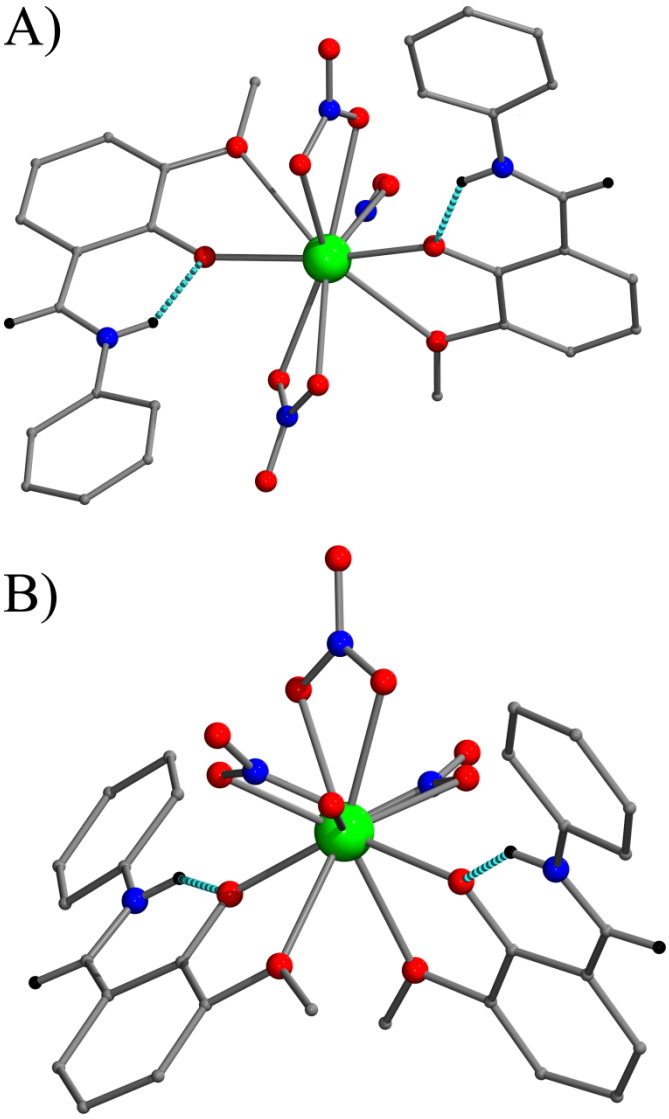

Fig S1. Ball and stick representation of crystal structure of **2**. A) Crystal structure of one of the molecule in the unit cell of **2**, where three nitrates ion arranged in near trigonal planar arrangement, (B) A geometric isomer (second molecule) with distinctly different orientation of nitrates and Schiff base ligands are shown. The sky blue dotted bonds represent the intramolecular hydrogen bonding. Colour code: Green = Lu(III), blue = N, red = O, grey = C.

The crystal structure of **2** is analogous to complex **1**, please refer main article for the detailed structural description.

Table S1. X-ray crystallographic parameters of **1** and **2**

	1	**2**
Formula	$Er_1C_{28}H_{26}N_5O_{13}$	$Lu_1C_{28}H_{26}N_5O_{13}$
Size	0.2 × 0.2 × 0.2	0.2 × 0.2 × 0.2
System	Orthorhombic	Orthorhombic
Space group	*Aba2*	*Aba2*
a [Å]	17.572(5)	17.439(3)
b [Å]	54.043(16)	54.451(11)
c [Å]	9.580(3)	9.5702(19)
α[°]	90	90
β [°]	90	90
γ [°]	90	90
V [Å^3]	9098(5)	9088(3)
Z	12	12
ρ_{calcd}[g/cm^{-3}]	1.769	1.788
$2\Theta_{max}$	58.30	58.24
Radiation	MoK_α	MoK_α
λ [Å]	0.71075	0.71075
T [K]	100	100
Reflns	59128	55796
Ind. Reflns	11965	12162
reflns with >2σ(I)	10593	10958
R1	0.0830	0.0446
wR2	0.1964	0.0807

Table S2. Selected bond lengths and bond angles for **1**.

Selected bond lengths for **1a**.

Er(1)-O(11)	2.2473(6)
Er(1)-O(31)	2.2625(6)
Er(1)-O(62)	2.3881(6)
Er(1)-O(52)	2.4781(5)
Er(1)-O(72)	2.4865(6)
Er(1)-O(51)	2.5430(7)
Er(1)-O(71)	2.5279(5)
Er(1)-O(61)	2.4153(6)
Er(1)-O(12)	2.6852(5)
Er(1)-O(32)	2.8032(5)

Selected bond lengths for **1b**.

Er(2)-O(111)#1	2.2339 (5)
Er(2)-O(111)	2.2339 (5)
Er(2)-O(151)	2.5110 (4)
Er(2)-O(151)#1	2.5110 (4)
Er(2)-O(161)	2.63490 (6)
Er(2)-O(161)#1	2.63490 (6)
Er(2)-O(152)	2.4324 (5)
Er(2)-O(152)#1	2.4324 (5)
Er(2)-O(112)	2.5430 (6)
Er(2)-O(112)#1	2.5430 (6)

Selected Bond angles for **1**

N(151)-Er(2)-N(161)	73.625 (19)
N(151)#1-Er(2)-N(161)	73.625 (19)
N(151)#1-Er(2)-N(151)	147.25 (19)
N(61)-Er(1)-N(51)	110.712 (23)
N(61)-Er(1)-N(71)	114.49 (22)
N(71)-Er(1)-N(51)	138.799 (18)

Table S3. Atoms involved in intermolecular hydrogen bonds for complex **1**

Hydrogen bond donor (D)…acceptor(A)	D… A (Å)
C(17)-H(17)…O(61)_$1	3.359(8)
C(43)-H(43)...O(72A_b)_$2	3.322(7)
C(44)-H(44B)...O(153)_$3	3.200(9)
C(124)-H(12A)...O(53)_$4	3.358(6)
C(44)-H(12B)...O(111)_$5	3.225(7)
C(117)-H(117)...O(161)_$6	3.275(5)

$1 = -X+3/2, Y, Z-1/2; $2 = -X+1/2, Y, Z-1/2; $3 = X, Y, Z+2; $4 = X, Y, Z-2; $5 = -X+1, -Y, Z; $6 = X+1/2, -Y, Z-1/2

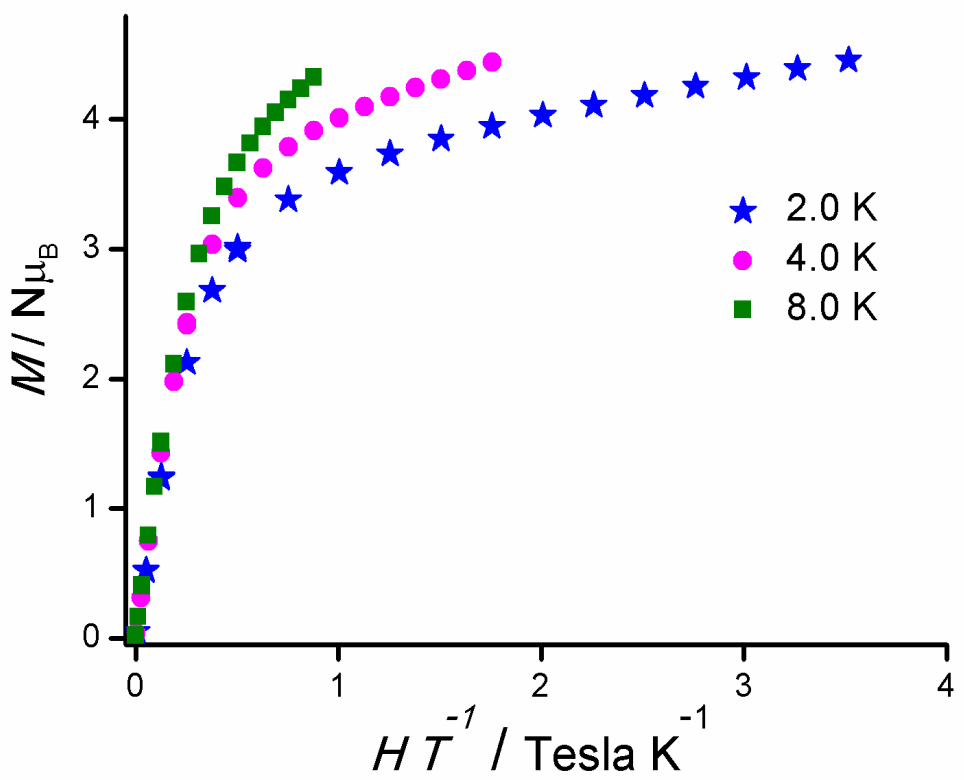

Fig S2. Reduced magnetization data of **1** (100%) measured at the indicated temperatures.

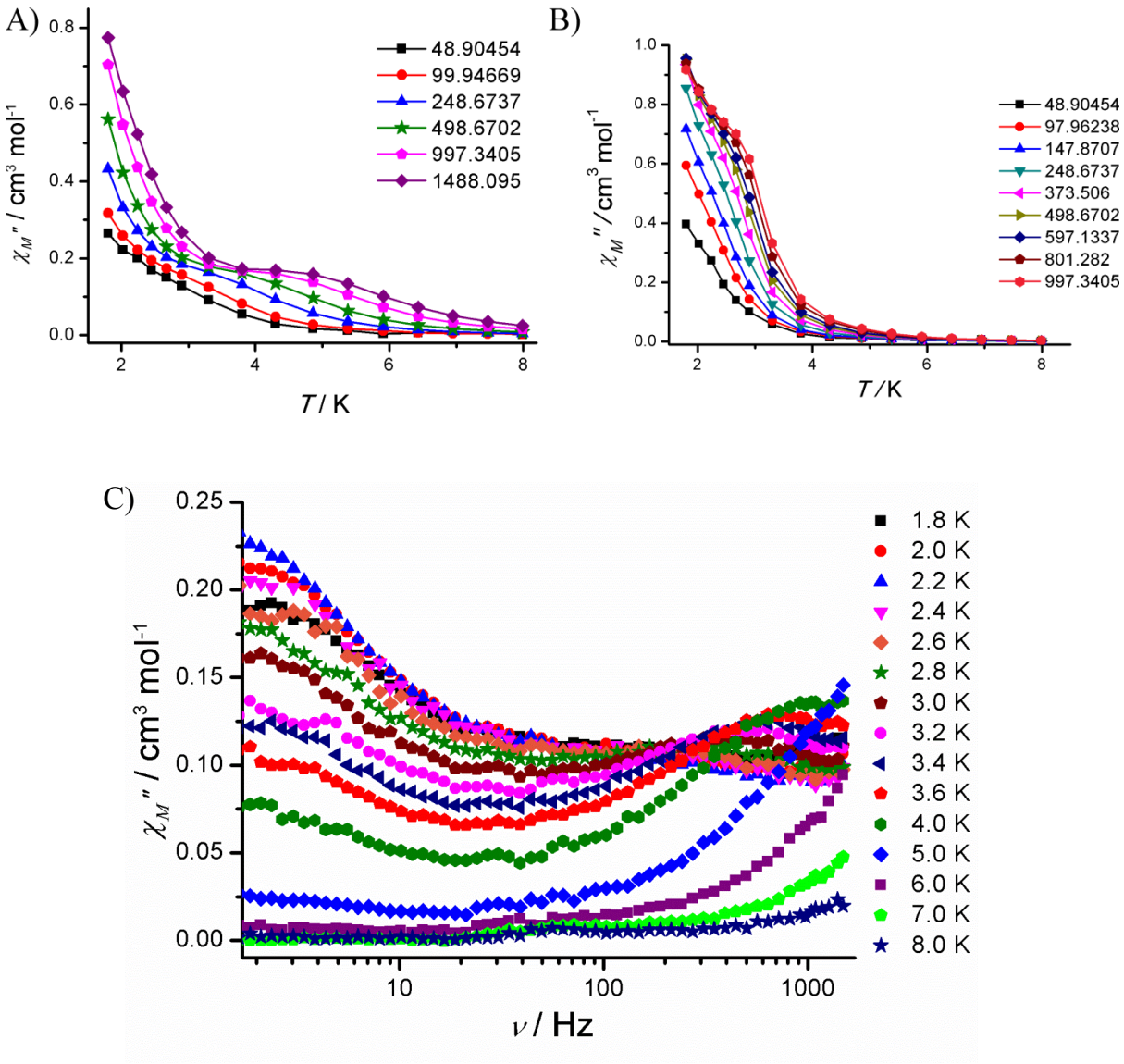

Fig S3. Frequency dependent out-of-phase susceptibility signals observed for **1** (100%) at 0.2 Tesla (A), 0.5 Tesla (C) and for 50 % dilution sample of **1** at 0.2 Tesla (B).

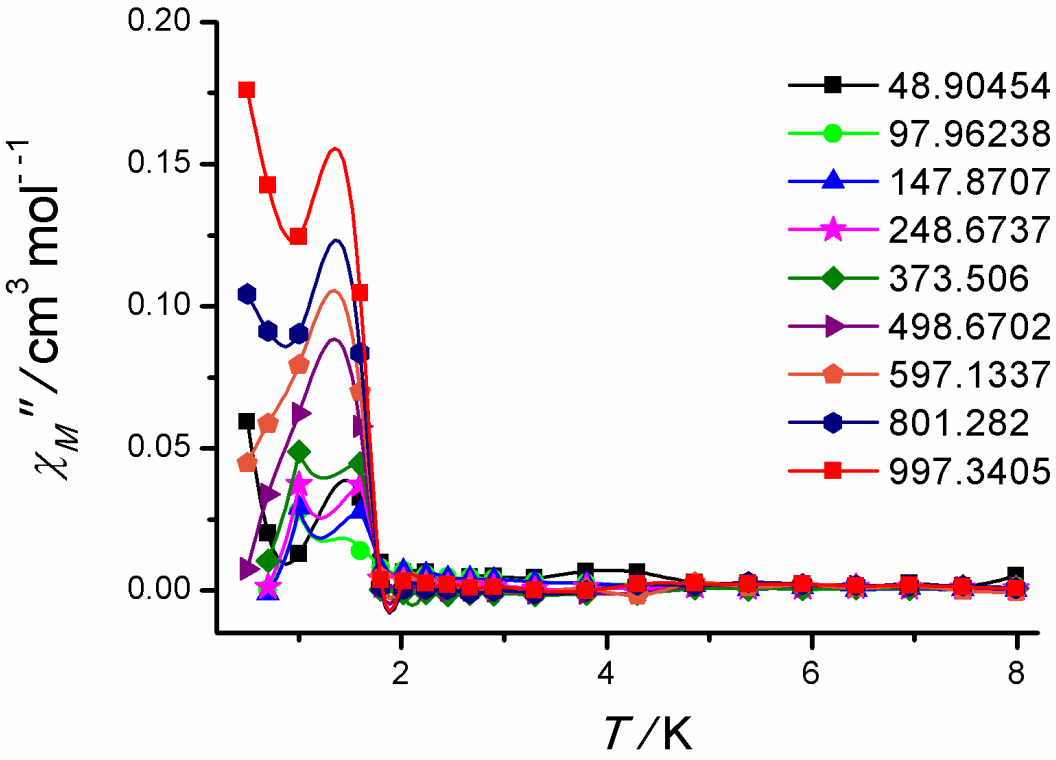

Fig S4. Frequency dependent out-of-phase susceptibility signals observed for **50 %** diluted sample at zero dc field.

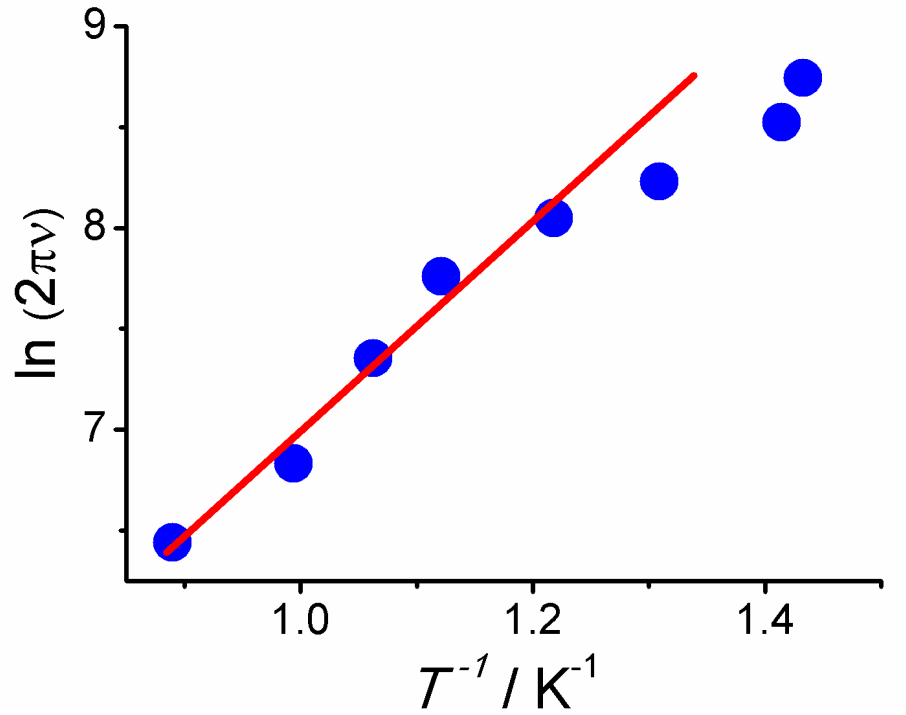

Fig S5. Arrhenius plot derived from the AC relaxation dynamics for complex **1** (100%).

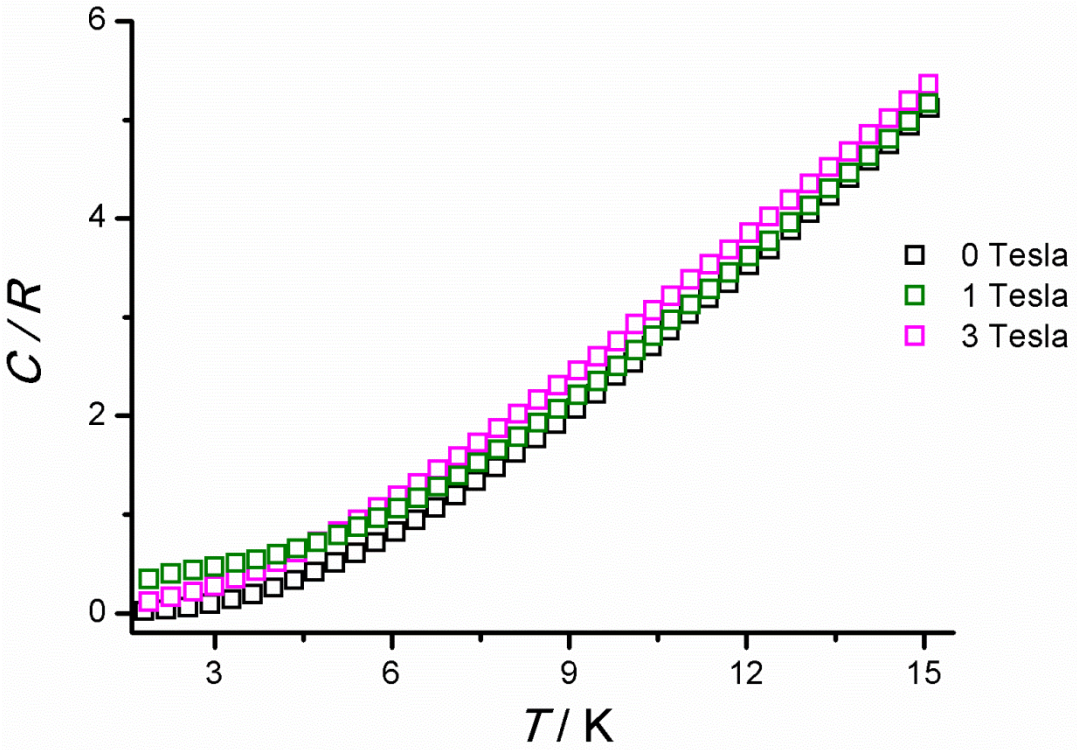

Fig S6. Temperature dependent heat capacity measurement performed on polycrystalline sample of **1** at the indicated external magnetic field.

The above plot shows that there is no magnetic phase transition at low temperature region. Hence, the out-of-phase signal observed for **1** is of purely molecular origin.

Table S4. List of Er(III) based SIM and SMMs reported in literature to date based on Sci-Finder and Cambridge Structure database.

S.No	Complex	Coordination number of Er(III)	Geometry around Erbium(III)	U_{eff}(Bias field)	References
1.	$[Er(pqc)(Hpqc)(NO_3)_2]_n$	8	Distorted Square antiprism	-	[3]
2.	$[Co^{III}_2Er^{III}_4(\mu_3\text{-}OH)_2(hmp)_4(piv)_8(\mu\text{-}N_3)_2(NO_3)_2].2CH_3CN$	8 and 9	Distorted square anti-prism and distorted tricapped trigonal prism	-	[4]
3.	$[Cu_5Er_2(L)_2(\mu_3\text{-}OH)_4(\mu\text{-}OH_2)_2\text{-}(\mu\text{-}OAc)_2(OAc)_2(HOEt)_2](NO_3)_2$	8	Distorted square-antiprismatic	-	[5]
4.	[K(18-crown-6)][Er(COT)2]	16	-	286 K	[6]
5.	$[Er_2(hfac)_6(L^1)_2]$	8	Distorted bicapped square face trigonal prism (Er1)and and a square antiprism(Er2)	-	[7]
6.	$[Er_2H_2OL^1_2(acac)_2]\cdot(C_2H_5)_2O$	7 and 8	Distorted capped trigonalprism and Distorted square antiprismatic geometry	-	[8]
7.	A. $[Er^{III}_2(COT'')_3]$ and B. $K_2(THF)_4[Er^{III}_2(COT)_4]$	16	-	A. 323 K (powder) and 335 K (solution) B. 306K and 170 K, 293K	[9]
8.	A. $Er[N(SiMe_3)_2]_3$ B. $Er(NHPh^iPr_2)_3(THF)_2$	A.3 B. 5	A. Triangle B.Trigonalbipyramidal	A. 122 K B. 25 K (0.04 Tesla)	[10]
9.	$[Er_4(salen)_6].13H_2O$	8 and 7	Distorted dodecahedron and distorted capped trigonal prism	13.5 K (1 Tesla)	[11]
10.	(Cp*)Er(COT)	13	-	197 K and 323 K	[12]
11.	$[Er_4(\mu_3\text{-}OH)_2(mdeaH)_2(piv)_8]$	8 and 7	Between dodecahedral and bicapped trigonal-prismatic (Er1), Distorted Dodecahedral(Er2)	-	[13]
12.	$[Er^{III}_2Mn^{III}_2O_2(ccnm)_6(dcnm)_2(H_2O)_2]\cdot 9H_2O\cdot MeCN$	8	-	-	[13]
13.	A.$[Er(W_5O_{18})_2]^{9-}$ B. $[Er(\beta_2\text{-}SiW_{11}O_{39})_2]^{13-}$	8 8	A.Squareantiprism B.Squareantiprism	A. 55K B. -	[14]
14.	$[Mn^{III}_4Er_4(^nBu\text{-}dea)_4\text{-}(\mu3\text{-}HCOO)_4(\mu\text{-}OMe)_4(\mu\text{-}O_2CEt)_4(O_2CEt)_4(MeOH)_4]$	8	Bicapped trigonal prism	-	[15]
15.	$[Ni_3Er_3(\mu_3\text{-}O)(\mu_3\text{-}OH)_3(L)_3(\mu\text{-}OOCCMe_3)_3]\cdot(ClO_4)\cdot 3CH_2Cl_2\cdot 2CH_3OH\cdot 3H_2O$	8	Distorted trigonal-dodecahedron	-	[16]

16.	$[Er^{III}_4(NO_3)_2(pdmH)_6(pdmH_2)_2](NO_3)_4$	8	Triangular dodecahedron and biaugmented trigonal prismatic	-	[17]
17.	A.$[Zn(\mu\text{-}L)(\mu\text{-}OAc)Er(NO_3)_2]$ B.$[Zn(\mu\text{-}L)(\mu\text{-}NO_3)Er(NO_3)_2]$ C.$[Zn(\mu\text{-}L)(\mu\text{-}9\text{-}An)Er(NO_3)_2]\cdot 2CH_3CN$	9 9 9	-	A.41 K (0.1 T) B.22 K (0.1T) C.-	[18]
18.	$[Er^{III}Zn^{II}_3(L1)\text{-}(OAc)(NO_3)_2(H_2O)_{1.5}(MeOH)_{0.5}]$	9	-	8.1 K	[19]
19.	$[Li(DME)_3][Er^{III}(COT^{\cdot\cdot})_2]$	16	-	187 K	[20]

The Debye function used to fit the Cole-Cole plot of **1**is given below, with the obtained parameters listed in **Table S5**

$$\chi_{AC}(\omega) = \chi_S + \frac{\chi_T - \chi_S}{1 + (i\omega\tau)^{(1-\alpha)}}$$

Table S5. Best fit parameters obtained for Cole-Cole plot for **1**

S.No.	Temperature (K)	χ_S	χ_T	τ	α
1	1.8	0.922321	1.45409	0.0622439	0.167697
2	2.0	0.882094	1.54263	0.0759809	0.241992
3	2.2	0.838938	1.57376	0.0885510	0.280378
4	2.4	0.887778	1.56724	0.0756959	0.296328
5	2.6	0.926243	1.56739	0.0781771	0.294814
6	2.8	0.968856	1.54055	0.0728937	0.282621
7	3.0	1.00876	1.52132	0.0725359	0.281886
8	3.2	1.08203	1.41132	0.0724387	0.262153
9	3.4	1.07472	1.44822	0.0757356	0.254543
10	3.6	1.09606	1.40616	0.0783945	0.218108
11	4.0	1.10822	1.34622	0.0910395	0.248496

Computational Details:

All the ab initio calculations have been performed using MOLCAS 7.8 code. Here we have employed the [ANO-RCC...8s7p5d3f2g1h.] basis set for Er atom, the [.ANO-RCC...3s2p1d.] for N and O atoms, [.ANO-RCC...3s2p.] for C atoms and [.ANO-RCC...2s.] for H atoms. The ground state f-electron configuration for Er(III) is $4f^{11}$ having $^4I_{15/2}$multiplet as a ground state. First, we have generated the guess orbitals from there we have selected seven Er(III) based starting orbitals to perform the CASSCF calculations. CASSCF calculations have been performed where eleven electrons are in the seven active orbitals with an active space of CAS(11,7). Using this active space first we have computed 35 quartets and 112 doublets using the configuration interaction (CI) procedure. After computing all these excited states, we have mixed all these 35 quartets and all 112 doublets using RASSI-SO module to compute the spin-orbit coupled states. After computing these SO states, we have performed the SINGLE_ANISO code to extract the corresponding g-tensors. Here we have computed the g-tensors for the eight low-lying Kramers Doublets. The cholesky decomposition for two electron integrals is employed throughout in the calculations to reduce the disk space. Using SINGLE_ANISO code we have also extracted the crystal field parameters as implemented in MOLCAS 7.8 code.[21]

Table S6. CASSCF+RASSI computed spin-free and spin-orbit state energies for complex **1a**.

Spin-free energies for complex 1a		Spin-Orbit energies for complex 1a	
0	44609.171	0	40908.125
46.088	44609.311	49.608	40941.674
98.38	44754.721	121.537	41047.096
179.217	44757.291	179.432	41095.713
249.44	44863.241	297.778	41404.658
320.175	44867.097	332.841	41426.628
377.006	44953.256	350.242	41502.2
421.9	44978.613	494.373	42069.432
450.386	45031.028	6654.75	42208.707
482.661	45105.323	6692.332	42297.108
498.665	45127.272	6735.842	49495.719
639.1	45285.904	6792.522	49527.856
658.787	45291.442	6822.154	49757.683
18335.418	45519.816	6835.758	49867.419
18340.445	45520.275	6954.751	49979.237
18443.773	45744.238	10716.362	50007.117
18522.993	45744.276	10753.644	50059.887
18524.162	50293.963	10788.785	50087.462
18622.251	50302.162	10818.612	50113.934
18642.41	50321.83	10840.368	50148.37
18735.372	50325.934	10920.145	50206.597
28709.687	50359.163	13443.912	50238.358
28771.134	50370.212	13492.952	50258.101
28831.602	50428.675	13640.421	50335.592
28899.053	50449.237	13663.447	50351.315
28936.701	50462.742	13761.272	50445.351
28960.382	50549.614	19019.333	50596.293
28977.864	50557.328	19116.185	50788.113
29057.835	51454.982	19182.155	50994.966
29191.433	51518.308	19235.089	51204.059
46698.779	51636.919	19290.017	51446.392
46924.19	51918.369	22757.917	51597.923
47032.554	51934.255	22771.079	51794.7
47409.827	60843.481	22795.701	52007.07
47495.016	60879.388	22810.295	52037.455
18192.741	60902.123	22826.568	52058.505
18193.57	60981.756	22854.483	52093.922
18236.242	60987.625	23680.111	52181.521
18238.012	61048.446	23770.323	52217.548
18254.663	61088.919	25196.198	52293.716
18255.138	77248.63	25294.338	52461.655
18259.119	77260.662	25374.604	54766.252
18268.329	77325.755	25441.142	54845.942
18274.479	77389.96	27340.933	56176.476
18305.293	77405.963	27365.561	56315.105
18311.318	77506.187	27434.349	56426.832
24016.108	77517.097	27648.393	56528.13
24020.073	77699.187	27782.274	56663.695
24141.153	77704.987	27834.054	56849.005
24144.935	110426.743	27874.407	57077.501
24196.969	110473.446	27994.845	57319.384
24213.48	110629.553	28020.007	58696.635
24237.206	110869.592	28067.091	58709.959
24296.628	110963.478	31924.73	58757.863
24307.182	111421.736	32078.285	58801.886
27011.482	111441.993	32156.169	58883.417
27011.906		32203.025	59456.498
27156.275		32262.868	61042.514

27160.095	32350.403	61091.658
27221.315	32483.681	61144.066
27243.186	32685.487	61196.398
27268.135	32836.171	61210.999
27321.053	32857.978	61252.418
27325.61	32915.457	61332.393
27405.055	32952.563	61457.983
27406.365	32973.726	61462.944
27535.005	33023.182	67052.566
27536.032	33316.354	67286.65
27758.803	33361.55	67368.516
27758.955	33385.227	67436.224
33150.23	33403.617	67458.616
33163.395	34059.197	67538.433
33193.576	34067.86	76205.755
33249.251	34083.786	76255.806
33483.517	34104.246	76304.265
33537.25	34134.117	83218.412
33542.398	37498.799	83305.817
33564.195	37635.492	83395.838
43906.631	37702.511	83552.159
43920.999	37754.082	87141.589
43928.194	37817.676	87232.424
43953.376	37890.586	87317.607
43997.691	37954.35	87438.542
44040.457	38079.586	87621.571
44089.626	38228.197	116477.207
44159.412	40493.272	116795.807
44170.471	40679.254	117296.551
44210.882	40752.961	120887.256
44215.108	40763.018	121138.588
44362.09	40822.984	121457.238
44362.59	40869.249	121927.083

Table S7. CASSCF+RASSI computed spin-free and spin-orbit state energies for complex **1b**.

Spin-free energies for complex 1b		Spin-Orbit energies for complex 1b	
0	44691.496	0	40923.102
0.861	44692.264	105.966	40955.47
121.386	44747.816	160.877	41038.96
200.312	44754.986	204.318	41119.528
236.758	44813.545	328.69	41414.484
365.435	44847.096	354.605	41443.537
384.84	44878.738	375.444	41485.508
428.767	44959.063	499.004	42090.129
438.772	44967.164	6683.48	42217.565
482.455	45089.724	6731.161	42292.344
491.587	45096.264	6767.871	49512.242
624.299	45260.843	6812.616	49541.511
644.3	45262.494	6842.821	49776.232
18337.122	45458.896	6869.635	49869.669
18362.445	45458.923	6952.271	49967.259
18479.836	45635.025	10751.958	50066.072
18480.923	45635.08	10779.479	50080.714
18518.637	50277.591	10813.503	50134.056
18616.666	50283.943	10839.031	50160.219
18649.208	50314.667	10870.255	50168.801
18670.664	50323.722	10924.425	50196.577
28728.987	50325.991	13460.376	50248.332
28783.925	50345.572	13523.023	50285.451
28824.243	50361.652	13664.458	50323.854
28863.275	50438.227	13690.506	50356.72
28893.791	50454.1	13777.183	50457.447
28959.929	50512.476	19050.223	50606.936
28980.559	50520.782	19153.278	50781.022
29057.041	51447.898	19204.016	50964.441
29113.77	51545.084	19239.578	51131.129
46821.89	51603.253	19292.556	51491.453
46837.167	51865.689	22785.559	51606.289
47007.669	51889.55	22792.692	51776.495
47339.706	60822.711	22814.949	52019.254
47444.089	60855.548	22827.548	52033.527
18202.096	60884.074	22838.389	52077.192
18202.359	60944.896	22861.55	52103.444
18210.786	60952.878	23701.702	52147.504
18218.303	61032.132	23780.77	52211.624
18240.398	61043.284	25232.529	52317.9
18258.825	77239.948	25298.592	52406.077
18263.27	77242.043	25409.034	54771.431
18265.918	77321.346	25440.699	54842.552
18268.611	77346.458	27368.598	56280.164
18286.768	77383.995	27387.537	56344.22
18290.405	77457.09	27447.144	56430.823
24032.163	77459.048	27668.624	56527.886
24035.193	77644.531	27783.199	56664.222
24126.837	77647.375	27852.046	56842.076
24128.212	110453.797	27888.904	57045.325
24195.493	110481.902	28020.588	57247.822
24210.22	110603.282	28033.569	58706.468
24244.802	110828.802	28084.319	58730.844
24259.484	110848.325	32051.013	58739.471
24273.101	111326.697	32066.01	58808.225
27096.164	111334.390	32139.708	58870.333
27105.646		32197.172	59459.094
27109.92		32290.963	61070.297

27129.172	32402.286	61118.766
27178.036	32511.8	61177.996
27220.902	32599.943	61196.132
27228.471	32868.107	61209.349
27307.715	32886.283	61235.023
27314.634	32933.19	61313.483
27420.304	32963.664	61433.5
27423.226	32970.82	61442.331
27543.097	33018.408	67072.674
27543.232	33333.878	67287.007
27655.387	33369.339	67377.269
27655.445	33400.295	67420.438
33153.199	33411.62	67453.255
33170.852	34073.835	67521.96
33208.362	34080.819	76210.832
33238.635	34087.334	76248.267
33463.003	34120.984	76295.568
33496.071	34136.671	83231.294
33513.261	37594.04	83293.048
33526.177	37631.828	83384.193
43961.374	37688.672	83520.074
43963.267	37765.783	87159.464
43979.039	37837.76	87236.353
43979.056	37899.645	87303.908
44024.689	38000.928	87412.114
44029.841	38112.008	87585.505
44048.863	38142.939	116511.085
44092.182	40510.747	116757.753
44092.516	40699.239	117228.127
44205.253	40765.299	120929.403
44206.739	40796.118	121137.489
44331.207	40826.768	121390.757
44331.417	40875.196	121847.817

Table S8. SINGLE_ANISO computed g-tensors and relative energies of eight low lying Kramers of complex **1a** along with the deviation from the principal magnetization axes of first KD.

KDs Energy(cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ
0	1.03429	2.77774	13.99637	0
49.6	0.01569	3.22007	11.29990	86.8
121.5	0.12834	2.77998	11.24686	8.884
179.4	2.97204	5.36462	8.66974	56.050
297.7	0.47838	4.90701	10.05109	60.771
332.8	0.084751	1.53586	14.26651	150.875
350.2	1.44322	3.95959	10.24188	136.796
494.3	0.43262	0.53955	15.96924	108.300

Table S9. SINGLE_ANISO computed g-tensors and relative energies of eight low lying Kramers doublets of complex **1b** along with the deviation from the principal magnetization axes of first KD.

KDs Energy(cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ
0	0.04317	0.07420	15.78162	0
105.9	1.31487	5.09789	12.34400	90.015
160.8	0.08586	2.76276	10.69054	10.629
204.3	5.13221	4.30873	2.901179	2.254
328.69	0.25778	0.40376	14.27241	140.888
354.6	1.28919	1.65590	10.88598	57.401
375.4	0.07487	0.07758	16.88782	15.645
499.0	0.21768	0.43583	15.59827	71.883

Table S10. SINGLE_ANISO computed crystal field parameters for complex **1a** and **1b**. The majorcomponents in the Table are in the bold font. The crystal field Hamiltonian parameter:

$$\hat{H}_{CF} = \sum \sum_{k=-q}^{q} B_q^k \hat{O}_q^k$$

Where B_q^k the crystal is field parameter and O_q^k is the extended Stevens operator.
Quantization axis is chosen to be the main magnetic axes of the ground Kramer Doublet.

k	q	B_q^k	B_q^k
		Complex **1a**	Complex **1b**
2	-2	-0.128 x 10^{-2}	0.904 x 10^{-1}
	-1	0.229 x 10^{-2}	-0.200
	0	**-0.562**	**-0.614**
	1	**-0.236 x 10^{1}**	-0.336 x 10^{1}
	2	**0.146 x 10^{1}**	0.139 x 10^{1}
4	-4	-0.371 x 10^{-4}	0.265 x 10^{-2}
	-3	0.110 x 10^{-3}	**0.107 x 10^{-1}**
	-2	0.344 x 10^{-4}	0.795 x 10^{-3}
	-1	-0.575 x 10^{-4}	0.203 x 10^{-2}
	0	0.129 x 10^{-2}	0.177 x 10^{-2}
	1	0.415 x 10^{-2}	-0.594 x 10^{-2}
	2	0.227 x 10^{-2}	**-0.137 x 10^{-1}**
	3	**0.217 x 10^{-1}**	0.482 x 10^{-2}
	4	-0.701 x 10^{-2}	**0.126 x 10^{-1}**
6	-6	-0.924 x 10^{-8}	-0.406 x 10^{-4}
	-5	-0.717 x 10^{-6}	-0.205 x 10^{-3}
	-4	0.398 x 10^{-6}	0.923 x 10^{-5}
	-3	-0.673 x 10^{-6}	-0.101 x 10^{-3}
	-2	0.731 x 10^{-6}	0.285 x 10^{-4}
	-1	-0.115 x 10^{-5}	-0.374 x 10^{-5}
	0	0.421 x 10^{-4}	0.326 x 10^{-4}
	1	**-0.114 x 10^{-2}**	-0.693 x 10^{-3}
	2	0.281 x 10^{-3}	0.601 x 10^{-3}
	3	-0.336 x 10^{-3}	-0.429 x 10^{-3}
	4	-0.649 x 10^{-4}	0.182 x 10^{-3}
	5	-0.681 x 10^{-4}	**-0.186 x 10^{-2}**
	6	-0.440 x 10^{-4}	0.941 x 10^{-4}

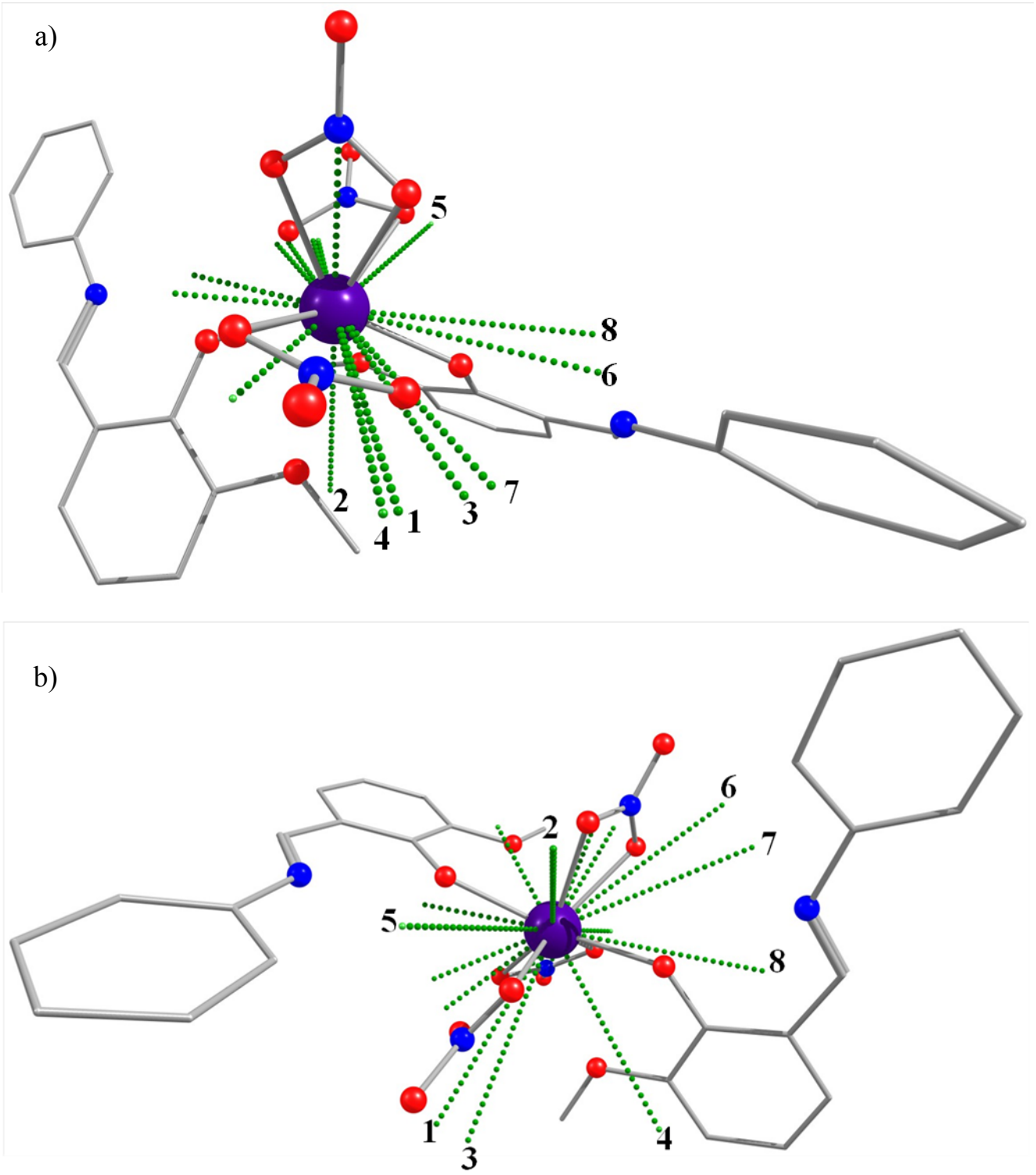

Figure S7.SINGLE_ANISO computed orientation of principal magnetization axes g_{zz} for all the eight low-lying Kramers Doublets. The light dotted green line indicates the orientation of principal magnetization axes (g_{zz}) of each Kramers doublet. a) for complex **1b**; b) for complex **1a**.

Table S11. SINGLE_ANISO computed g-tensors and relative energies of eight low lying Kramers of model **1a-A**.

KDs Energy(cm^{-1})	g_{xx}	g_{yy}	g_{zz}
0	0.9235	1.0238	16.3037
77.575	3.4005	4.1848	10.6449
112.946	0.4689	1.8275	13.2483
130.163	1.3880	2.7744	11.1946
236.803	0.3345	0.5378	14.9379
410.896	10.3245	6.2687	0.5426
439.633	8.0858	4.8037	0.8282
489.614	0.2347	1.6161	14.5559

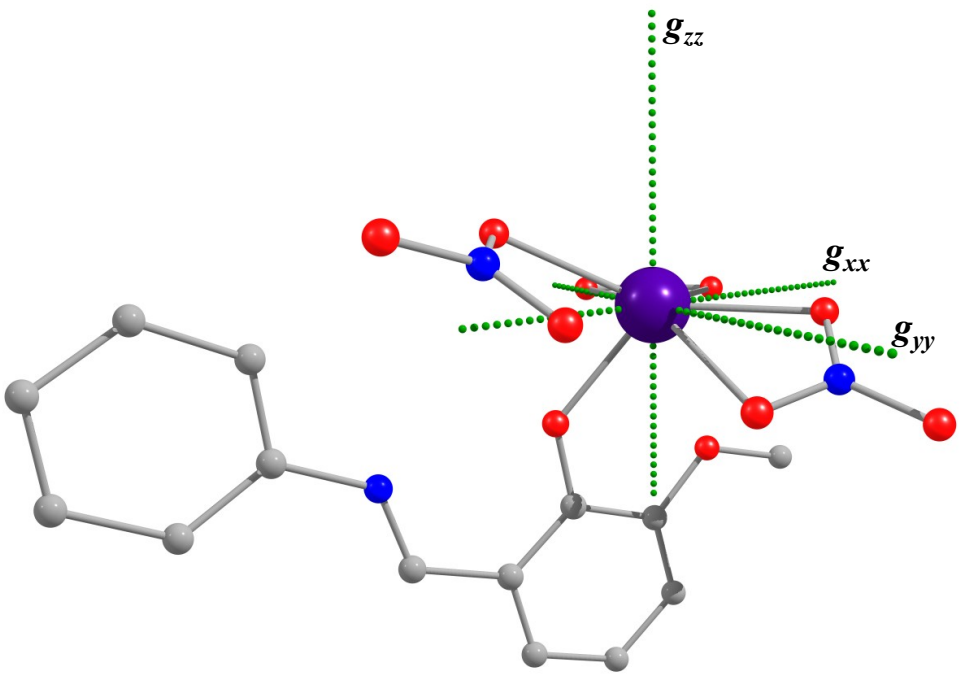

Figure S8.SINGLE_ANISO computed g-tensor orientation of ground state KD for complex **1a-A**. The light dotted green line indicates the orientation of principal magnetization axes. Color code: violet, Er; red, O; blue; N; grey, C; hydrogens are omitted for clarity

Table S12. SINGLE_ANISO computed g-tensors and relative energies of eight low lying Kramers of model **1a-B**.

KDs Energy(cm^{-1})	g_{xx}	g_{yy}	g_{zz}
0	0.04015	0.07977	17.8067
131.5	2.0577	2.5199	14.2072
209.6	0.6597	5.0387	10.6518
267.0	6.9034	6.3991	1.5351
313.1	2.4528	3.8497	12.6382
618.1	0.4091	2.6550	13.5780
653.1	0.2933	0.7966	10.6891
683.84	0.28273	2.6835	14.7009

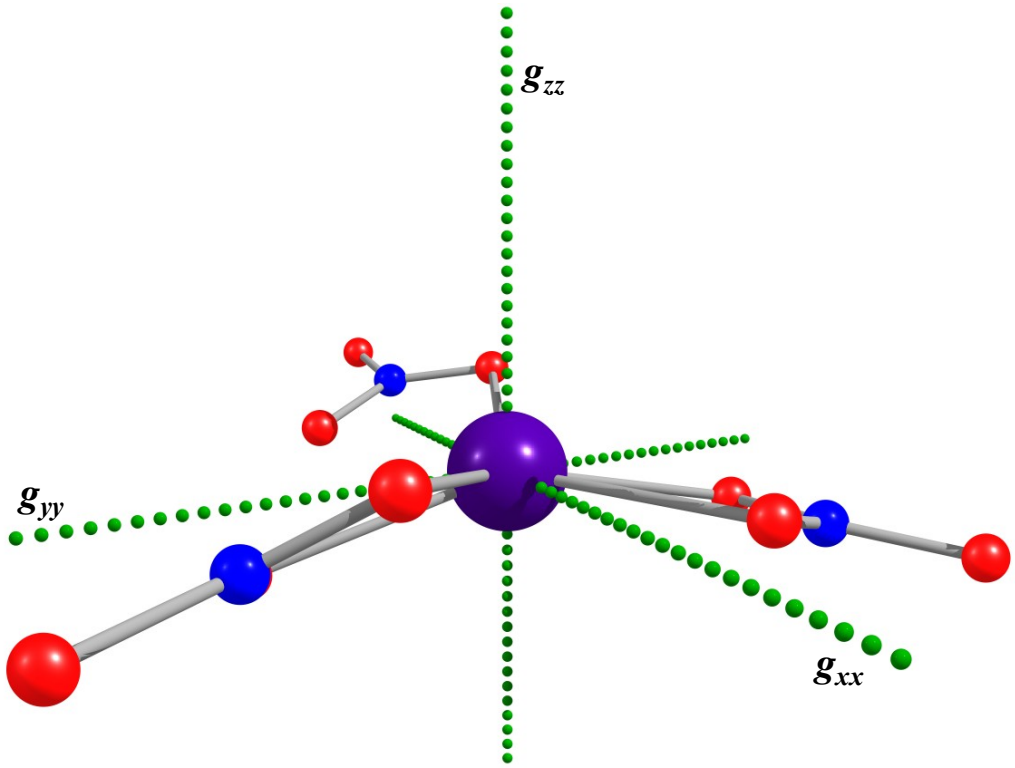

Figure S9.SINGLE_ANISO computed g-tensor orientation of ground state KD for complex **1a-B**. The light dotted green line indicates the orientation of principal magnetization axes. Color code: violet, Er; red, O; blue; N; grey, C; hydrogens are omitted for clarity

Table S13. Composition of wavefunctions for complex **1a** as derived from CASSCF/RASSI/single_aniso calculations.

| JM >	w.f.1		w.f.2		w.f.3		w.f.4	
-15/2	0.557800	-0.001894	0.000000	0.000000	-0.044797	0.000251	-0.010367	0.000058
-13/2	0.727077	-0.001425	-0.000752	0.000002	-0.010503	-0.000156	0.091203	-0.000437
-11/2	-0.380762	-0.000227	-0.001242	-0.000001	0.078269	-0.000403	0.181791	-0.000453
-9/2	0.048000	0.000450	0.001667	-0.000008	-0.104926	0.000730	-0.194641	0.000874
-7/2	0.071421	-0.000411	0.001494	-0.000015	0.157283	-0.000184	-0.023591	0.000406
-5/2	0.082182	0.000157	-0.002795	-0.000006	0.363409	-0.001806	0.270759	-0.001174
-3/2	0.008922	0.000007	-0.015228	0.000046	0.244288	-0.001388	0.584715	-0.001793
-1/2	-0.021835	0.000045	-0.016464	-0.000020	-0.339201	0.000212	0.392530	-0.000040
1/2	-0.016464	0.000076	0.021835	-0.000029	-0.392524	0.002158	-0.339197	0.001687
3/2	0.015229	-0.000005	0.008922	-0.000037	0.584716	-0.001480	-0.244292	-0.000020
5/2	-0.002795	0.000015	-0.082181	0.000436	-0.270761	0.000342	0.363413	-0.000229
7/2	-0.001494	-0.000010	0.071422	0.000168	-0.023593	-0.000274	-0.157281	0.000696
9/2	0.001667	0.000002	-0.047998	0.000613	0.194643	-0.000216	-0.104929	-0.000143
11/2	0.001242	-0.000005	-0.380759	0.001520	0.181791	-0.000564	-0.078270	0.000035
13/2	-0.000752	0.000001	-0.727078	0.001043	-0.091204	0.000074	-0.010502	0.000215
15/2	0.000000	0.000000	0.557803	0.000000	-0.010367	0.000000	0.044798	0.000000
| JM >	w.f.5		w.f.6		w.f.7		w.f.8	
-15/2	-0.014488	0.000129	0.031839	-0.000284	-0.009864	0.000107	0.058821	-0.000636
-13/2	-0.336684	0.001363	0.171319	0.000258	0.058868	-0.000419	0.089932	-0.000743
-11/2	-0.598373	0.000877	0.259042	0.001419	0.132411	-0.000435	0.071327	-0.000758
-9/2	0.506222	-0.000397	-0.192371	-0.001653	-0.119840	0.000138	0.007556	-0.000450
-7/2	-0.023330	0.000403	-0.161961	0.001216	0.199201	-0.001539	-0.512563	0.003508
-5/2	0.014380	0.001372	-0.200863	0.000934	-0.030622	-0.000820	-0.529901	0.003254
-3/2	0.071238	-0.000337	-0.009600	-0.000360	-0.354915	0.001053	-0.096426	-0.000072
-1/2	0.145160	-0.001429	0.209918	-0.001862	-0.454237	0.002087	0.148606	-0.002168
1/2	-0.209926	0.000007	0.145167	0.000137	-0.148620	-0.000561	-0.454233	0.002827
3/2	-0.009596	0.000445	-0.071238	0.000297	-0.096419	0.001115	0.354906	-0.002787
5/2	0.200863	-0.000854	0.014367	-0.001500	0.529906	-0.002479	-0.030612	0.001151
7/2	-0.161966	0.000226	0.023332	0.000196	-0.512571	0.002037	-0.199206	0.000616
9/2	0.192348	-0.003365	0.506206	-0.004110	-0.007561	-0.000368	-0.119834	0.001158
11/2	0.259019	-0.003725	0.598357	-0.004451	0.071331	-0.000014	-0.132408	0.000998
13/2	-0.171309	0.001783	-0.336683	0.001634	-0.089935	0.000230	0.058869	-0.000218
15/2	0.031841	0.000000	0.014488	0.000000	0.058824	0.000000	0.009864	0.000000
| JM >	w.f.9		w.f.10		w.f.11		w.f.12	
-15/2	0.007172	-0.000084	-0.264845	0.003116	0.055226	-0.000181	0.156974	-0.000514
-13/2	0.005033	-0.000084	-0.025565	0.001004	-0.000616	0.000136	-0.019703	-0.000017
-11/2	0.032664	-0.000194	-0.572300	0.006543	0.063696	-0.000348	0.184167	-0.000838
-9/2	0.013921	-0.000335	-0.657267	0.007567	0.160756	0.000342	0.273065	-0.000274
-7/2	0.073131	-0.000188	-0.320162	0.003157	-0.419401	0.000183	-0.499668	0.000258
-5/2	-0.030089	-0.000114	-0.003990	-0.000490	0.195576	0.000276	0.124755	-0.000011
-3/2	-0.096071	0.000090	0.067224	-0.001257	0.269750	-0.000445	0.110522	-0.000538
-1/2	-0.026590	-0.000241	-0.212092	0.002038	-0.150699	0.000088	-0.496454	0.000826
1/2	-0.212101	0.000457	0.026585	-0.000554	0.496454	-0.000801	-0.150698	0.000405
3/2	-0.067234	-0.000466	-0.096066	0.001040	0.110524	0.000175	-0.269750	0.000439
5/2	-0.003984	0.000537	0.030085	-0.000468	-0.124755	0.000397	0.195575	-0.000917
7/2	0.320177	-0.000609	0.073128	-0.000672	-0.499666	0.001379	0.419399	-0.001191
9/2	-0.657311	0.000165	-0.013924	-0.000172	-0.273064	0.000620	0.160754	-0.000869
11/2	0.572337	-0.000189	0.032664	-0.000190	0.184169	0.000235	-0.063697	-0.000139
13/2	-0.025575	-0.000703	-0.005033	-0.000025	0.019703	-0.000081	-0.000616	-0.000134
15/2	0.264864	0.000000	0.007172	0.000000	0.156975	0.000000	-0.055226	0.000000
| JM >	w.f.13		w.f.14		w.f.15		w.f.16	

-15/2	0.026411	0.000006	0.761161	0.000187	0.001124	0.000002	0.063248	0.000135
-13/2	-0.022063	-0.000033	-0.551672	-0.000785	-0.004007	0.000012	-0.052459	-0.000051
-11/2	-0.006002	0.000052	0.015569	0.000910	-0.011641	0.000019	0.032265	-0.000206
-9/2	-0.023876	-0.000053	-0.317647	-0.000585	-0.017293	0.000070	-0.081734	0.000438
-7/2	0.026641	0.000072	0.052301	0.000541	-0.014439	0.000201	-0.321444	-0.001062
-5/2	-0.020750	-0.000012	-0.079046	-0.000416	0.002255	0.000277	0.635717	0.001406
-3/2	-0.001888	0.000064	0.051748	-0.000074	0.051733	0.000466	-0.594637	-0.001243
-1/2	0.020815	0.000113	-0.010919	0.000004	0.095369	0.000306	0.334707	0.000544
1/2	0.010919	0.000006	0.020815	-0.000108	0.334707	0.000169	-0.095370	0.000103
3/2	0.051748	0.000087	0.001888	0.000065	0.594638	0.000023	0.051734	-0.000355
5/2	0.079046	-0.000396	-0.020750	0.000007	0.635718	-0.000053	-0.002256	0.000272
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9/2	0.317647	-0.000507	-0.023876	0.000047	-0.081733	-0.000611	0.017292	0.000107
11/2	0.015569	-0.000906	0.006002	0.000053	-0.032264	-0.000275	-0.011641	-0.000044
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2^, conventional R-factors R are based

on F, with F set to zero for negative F^2^. The threshold expression of F^2^ >2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Structure refinement and structure solution was found using a twinned reflection data.

Due to twinning reflection several restrains and constraints such as DFIX, DANG, FLAT, SIMU, DELU, ISOR etc. were used for better convergence
of the structure.

Hydrogen atoms were added based on the geometric position in the respective atoms.

All the non-hydrogen atoms were refined anisotropically except the disordered atoms.

The largest Q-peak with intensity 4.0 is very close to the Er(III) which is unreliable, hence these Q-peaks were not treated further.
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O11 O 0.6276(4) 0.16500(12) 0.2137(7) 0.0175(13) Uani 1 1 d U A .
O12 O 0.6022(4) 0.19877(13) 0.4003(8) 0.0247(15) Uani 1 1 d U A .
O31 O 0.3849(4) 0.16865(12) 0.1873(8) 0.0224(14) Uani 1 1 d U A .
O32 O 0.3967(4) 0.13389(13) 0.3763(8) 0.0230(14) Uani 1 1 d U . .
O51 O 0.5417(6) 0.12224(17) 0.2829(8) 0.063(3) Uani 1 1 d DU A .
O52 O 0.5045(4) 0.13691(13) 0.0834(9) 0.055(3) Uani 1 1 d DU A .
O53 O 0.5367(8) 0.09826(13) 0.1014(10) 0.072(3) Uani 1 1 d DU A .
N11 N 0.7234(5) 0.13881(14) 0.0654(9) 0.0179(16) Uani 1 1 d U . .
H11A H 0.6773 0.1440 0.0861 0.021 Uiso 1 1 calcR . .
N31 N 0.3011(5) 0.19383(15) 0.0133(9) 0.0230(18) Uani 1 1 d U A .
H31A H 0.3452 0.1885 0.0449 0.028 Uiso 1 1 calcR . .
N61 N 0.5011(3) 0.16521(13) 0.5635(6) 0.050(3) Uiso 1 1 d DU . .
O61 O 0.5456(5) 0.15138(16) 0.4974(9) 0.049(2) Uiso 1 1 d DU A .
O62 O 0.4550(5) 0.17869(16) 0.4989(9) 0.051(2) Uiso 1 1 d DU A .
O63 O 0.5027(6) 0.1656(3) 0.6943(6) 0.094(5) Uiso 1 1 d DU A .
N71 N 0.4859(6) 0.21309(16) 0.1507(10) 0.044(5) Uiso 0.60(2) 1 d PDU A 1
O71 O 0.5132(7) 0.1952(2) 0.0846(13) 0.032(4) Uiso 0.60(2) 1 d PDU A 1
O72 O 0.4628(10) 0.2101(3) 0.2734(11) 0.054(4) Uiso 0.60(2) 1 d PDU A 1
O73 O 0.4816(12) 0.2339(2) 0.0941(16) 0.068(6) Uiso 0.60(2) 1 d PDU A 1
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O71A O 0.5063(12) 0.2111(4) 0.136(2) 0.059(8) Uiso 0.40(2) 1 d PDU A 2
N71A N 0.4618(9) 0.2210(3) 0.2222(15) 0.058(7) Uiso 0.40(2) 1 d PDU A 2
O72A O 0.4423(15) 0.2095(4) 0.330(2) 0.059(7) Uiso 0.40(2) 1 d PDU A 2
O73A O 0.4368(16) 0.2424(3) 0.200(3) 0.075(10) Uiso 0.40(2) 1 d PDU A 2
N51 N 0.5276(3) 0.11913(11) 0.1559(7) 0.056(3) Uani 1 1 d DU . .
C11 C 0.7637(3) 0.16776(10) 0.2409(7) 0.0195(19) Uani 1 1 d GU . .
C12 C 0.8252(2) 0.17852(11) 0.3091(7) 0.0199(19) Uani 1 1 d GU . .
H12A H 0.8756 0.1736 0.2861 0.024 Uiso 1 1 calcR . .
C13 C 0.8129(3) 0.19642(11) 0.4108(7) 0.021(2) Uani 1 1 d GU . .
H13A H 0.8549 0.2038 0.4574 0.025 Uiso 1 1 calcR . .
C14 C 0.7391(3) 0.20356(10) 0.4444(7) 0.0188(19) Uani 1 1 d GU A .
H14A H 0.7308 0.2158 0.5139 0.023 Uiso 1 1 calcR . .
C15 C 0.6777(2) 0.19279(11) 0.3762(7) 0.0179(18) Uani 1 1 d GU . .
C16 C 0.6899(3) 0.17489(10) 0.2745(7) 0.0153(16) Uani 1 1 d GU A .
C17 C 0.7787(6) 0.14950(18) 0.1348(10) 0.0183(19) Uani 1 1 d U . .
H17A H 0.8298 0.1451 0.1147 0.022 Uiso 1 1 calcR . .
C18 C 0.7272(4) 0.12030(12) -0.0373(8) 0.0227(19) Uani 1 1 d GU . .
C19 C 0.6599(3) 0.11291(15) -0.1008(9) 0.047(3) Uani 1 1 d GU . .
H19A H 0.6130 0.1203 -0.0743 0.056 Uiso 1 1 calcR . .
C20 C 0.6610(3) 0.09470(15) -0.2033(9) 0.045(3) Uani 1 1 d GU . .
H20A H 0.6150 0.0896 -0.2467 0.054 Uiso 1 1 calcR . .
C21 C 0.7296(4) 0.08388(13) -0.2422(8) 0.036(3) Uani 1 1 d GU . .
H21A H 0.7304 0.0714 -0.3122 0.043 Uiso 1 1 calcR . .
C22 C 0.7970(3) 0.09127(13) -0.1786(8) 0.037(3) Uani 1 1 d GU . .
H22A H 0.8438 0.0839 -0.2052 0.044 Uiso 1 1 calcR . .
C23 C 0.7958(3) 0.10948(13) -0.0762(8) 0.026(2) Uani 1 1 d GU . .
H23A H 0.8419 0.1145 -0.0327 0.031 Uiso 1 1 calcR . .
C24 C 0.5860(6) 0.21801(19) 0.5008(12) 0.026(2) Uani 1 1 d U . .
H24A H 0.5987 0.2121 0.5947 0.039 Uiso 1 1 calc R A .
H24B H 0.5318 0.2222 0.4969 0.039 Uiso 1 1 calcR . .
H24C H 0.6164 0.2327 0.4790 0.039 Uiso 1 1 calcR . .
C31 C 0.2493(4) 0.16627(11) 0.1855(7) 0.026(2) Uani 1 1 d GU A .
C32 C 0.1830(3) 0.15596(13) 0.2392(8) 0.026(2) Uani 1 1 d GU . .
H32A H 0.1349 0.1613 0.2056 0.032 Uiso 1 1 calcR . .
C33 C 0.1872(3) 0.13788(12) 0.3421(8) 0.028(2) Uani 1 1 d GU . .
H33A H 0.1419 0.1308 0.3788 0.034 Uiso 1 1 calcR . .
C34 C 0.2577(4) 0.13011(11) 0.3913(7) 0.024(2) Uani 1 1 d GU . .
H34A H 0.2606 0.1177 0.4616 0.028 Uiso 1 1 calcR . .
C35 C 0.3240(3) 0.14042(11) 0.3375(7) 0.0159(17) Uani 1 1 d GU A .
C36 C 0.3198(3) 0.15850(11) 0.2346(7) 0.0175(18) Uani 1 1 d GU . .
C37 C 0.2415(5) 0.18454(16) 0.0728(10) 0.0167(17) Uani 1 1 d U . .
H37A H 0.1923 0.1896 0.0435 0.020 Uiso 1 1 calc R A .
C38 C 0.3045(4) 0.21126(12) -0.0951(7) 0.026(2) Uani 1 1 d GU . .

C39 C 0.3750(3) 0.21541(13) -0.1567(8) 0.027(2) Uani 1 1 d GU A .
H39A H 0.4185 0.2067 -0.1246 0.033 Uiso 1 1 calcR . .
C40 C 0.3817(3) 0.23231(14) -0.2654(8) 0.036(3) Uani 1 1 d GU A .
H40A H 0.4299 0.2351 -0.3075 0.043 Uiso 1 1 calcR . .
C41 C 0.3180(4) 0.24506(13) -0.3125(8) 0.037(3) Uani 1 1 d GU A .
H41A H 0.3226 0.2566 -0.3868 0.044 Uiso 1 1 calcR . .
C42 C 0.2475(4) 0.24091(14) -0.2509(8) 0.037(3) Uani 1 1 d GU A .
H42A H 0.2040 0.2496 -0.2831 0.044 Uiso 1 1 calcR . .
C43 C 0.2408(3) 0.22401(14) -0.1422(8) 0.030(2) Uani 1 1 d GU A .
H43A H 0.1926 0.2212 -0.1001 0.036 Uiso 1 1 calcR . .
C44 C 0.4050(7) 0.1134(2) 0.4674(13) 0.033(2) Uani 1 1 d U . .
H44A H 0.3762 0.1164 0.5533 0.050 Uiso 1 1 calcR . .
H44B H 0.4589 0.1111 0.4901 0.050 Uiso 1 1 calcR . .
H44C H 0.3855 0.0984 0.4216 0.050 Uiso 1 1 calcR . .
O112 O 0.5266(4) 0.02644(13) -1.7382(9) 0.0231(14) Uani 1 1 d U . .
C111 C 0.7204(3) 0.00519(10) -1.7677(7) 0.0166(18) Uani 1 1 d GU . .
C112 C 0.7483(3) 0.01856(11) -1.8806(7) 0.0184(19) Uani 1 1 d GU . .
H11B H 0.7994 0.0163 -1.9103 0.022 Uiso 1 1 calcR . .
C113 C 0.7016(3) 0.03527(11) -1.9499(6) 0.023(2) Uani 1 1 d GU . .
H11C H 0.7207 0.0444 -2.0270 0.027 Uiso 1 1 calcR . .
C114 C 0.6268(3) 0.03861(11) -1.9063(7) 0.025(2) Uani 1 1 d GU . .
H11D H 0.5948 0.0500 -1.9537 0.030 Uiso 1 1 calcR . .
C115 C 0.5988(3) 0.02525(11) -1.7935(7) 0.0149(17) Uani 1 1 d GU . .
C116 C 0.6456(3) 0.00853(10) -1.7242(6) 0.0158(16) Uani 1 1 d GU . .
C124 C 0.4721(7) 0.0417(2) -1.8153(13) 0.031(2) Uani 1 1 d U . .
H12B H 0.4913 0.0587 -1.8216 0.047 Uiso 1 1 calcR . .
H12C H 0.4231 0.0416 -1.7665 0.047 Uiso 1 1 calcR . .
H12D H 0.4654 0.0349 -1.9094 0.047 Uiso 1 1 calcR . .
C117 C 0.7689(5) -0.01272(15) -1.7070(9) 0.0139(16) Uani 1 1 d U . .
H11E H 0.8206 -0.0135 -1.7358 0.017 Uiso 1 1 calcR . .
C118 C 0.7831(3) -0.04863(9) -1.5502(7) 0.0172(18) Uani 1 1 d G . .
C119 C 0.7484(3) -0.06005(11) -1.4368(7) 0.022(2) Uani 1 1 d G . .
H11F H 0.7007 -0.0542 -1.4037 0.026 Uiso 1 1 calcR . .
C120 C 0.7836(4) -0.08001(10) -1.3718(6) 0.020(2) Uani 1 1 d G . .
H12E H 0.7599 -0.0878 -1.2943 0.024 Uiso 1 1 calcR . .
C121 C 0.8533(4) -0.08855(10) -1.4202(7) 0.023(2) Uani 1 1 d G . .
H12F H 0.8773 -0.1022 -1.3758 0.028 Uiso 1 1 calcR . .
C122 C 0.8880(3) -0.07713(12) -1.5336(8) 0.027(2) Uani 1 1 d G . .
H12G H 0.9357 -0.0830 -1.5667 0.033 Uiso 1 1 calcR . .
C123 C 0.8529(3) -0.05717(11) -1.5986(7) 0.0204(19) Uani 1 1 d G . .
H12H H 0.8766 -0.0494 -1.6761 0.024 Uiso 1 1 calcR . .
N111 N 0.7443(5) -0.02844(15) -1.6112(9) 0.0201(16) Uani 1 1 d U . .
H11G H 0.6975 -0.0260 -1.5816 0.024 Uiso 1 1 calcR . .

N151 N 0.5051(3) 0.05041(8) -1.4405(6) 0.035(2) Uani 1 1 d DU . .
O111 O 0.6171(3) -0.00392(10) -1.6123(7) 0.0099(11) Uani 1 1 d U . .
O151 O 0.4457(3) 0.04274(10) -1.4987(8) 0.0244(16) Uani 1 1 d DU . .
O152 O 0.5630(3) 0.03690(11) -1.4358(9) 0.0276(16) Uani 1 1 d DU . .
O153 O 0.5065(5) 0.07154(12) -1.3868(12) 0.065(4) Uani 1 1 d DU . .
O161 O 0.4472(2) 0.00846(14) -1.3039(3) 0.0361(18) Uani 1 1 d DU . .
N161 N 0.5000 0.0000 -1.2324(3) 0.022(2) Uani 1 2 d SDU . .
O163 O 0.5000 0.0000 -1.1029(3) 0.044(3) Uani 1 2 d SDU . .

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O11 0.0170(16) 0.0179(16) 0.0175(16) -0.0002(10) 0.0008(10) 0.0002(10)
O12 0.0245(17) 0.0244(17) 0.0251(17) -0.0005(10) 0.0006(10) -0.0002(10)
O31 0.0217(17) 0.0226(17) 0.0227(17) 0.0012(10) -0.0003(10) -0.0006(10)
O32 0.0230(17) 0.0228(17) 0.0232(17) 0.0008(10) 0.0000(10) 0.0004(10)
O51 0.059(6) 0.059(6) 0.072(6) -0.013(6) 0.001(6) 0.006(5)
O52 0.018(4) 0.035(5) 0.111(7) -0.028(5) -0.003(4) 0.004(3)
O53 0.073(8) 0.052(7) 0.090(9) -0.018(6) 0.013(7) -0.005(6)
N11 0.0178(18) 0.0178(18) 0.0180(18) -0.0001(10) 0.0005(10) 0.0001(10)
N31 0.0229(19) 0.0230(19) 0.0229(19) 0.0001(10) -0.0009(10) 0.0004(10)
N51 0.039(5) 0.047(5) 0.081(6) -0.026(5) -0.001(5) -0.013(5)
C11 0.020(2) 0.019(2) 0.019(2) -0.0003(10) -0.0003(10) 0.0004(10)
C12 0.020(2) 0.020(2) 0.020(2) -0.0002(10) -0.0001(10) -0.0003(10)
C13 0.021(2) 0.020(2) 0.021(2) -0.0002(10) -0.0002(10) -0.0006(10)
C14 0.019(2) 0.019(2) 0.019(2) -0.0005(10) 0.0003(10) 0.0002(10)
C15 0.018(2) 0.018(2) 0.018(2) 0.0002(10) 0.0003(10) -0.0001(10)
C16 0.0155(18) 0.0150(18) 0.0154(18) 0.0001(10) -0.0001(10) -0.0009(10)
C17 0.018(2) 0.018(2) 0.018(2) 0.0004(10) -0.0001(10) -0.0001(10)
C18 0.023(2) 0.023(2) 0.023(2) -0.0002(10) 0.0003(10) 0.0001(10)
C19 0.047(3) 0.047(3) 0.047(3) -0.0004(10) 0.0001(10) 0.0000(10)
C20 0.045(3) 0.045(3) 0.045(3) -0.0006(10) 0.0002(10) -0.0004(10)
C21 0.036(3) 0.035(3) 0.035(3) -0.0002(10) 0.0003(10) -0.0005(10)
C22 0.037(3) 0.037(3) 0.037(3) 0.0000(10) 0.0005(10) 0.0001(10)
C23 0.026(2) 0.026(2) 0.026(2) 0.0000(10) 0.0006(10) 0.0000(10)
C24 0.026(2) 0.026(2) 0.026(2) -0.0002(10) 0.0003(10) -0.0001(10)

C31 0.026(2) 0.025(2) 0.026(2) -0.0001(10) -0.0003(10) 0.0000(10)
C32 0.026(2) 0.027(2) 0.027(2) -0.0003(10) -0.0001(10) 0.0002(10)
C33 0.028(2) 0.028(2) 0.028(2) 0.0001(10) 0.0008(10) -0.0006(10)
C34 0.024(2) 0.023(2) 0.024(2) 0.0003(10) -0.0001(10) 0.0001(10)
C35 0.0160(19) 0.0155(19) 0.0163(19) -0.0009(10) 0.0002(10) -0.0001(10)
C36 0.017(2) 0.017(2) 0.018(2) -0.0003(10) 0.0001(10) -0.0003(10)
C37 0.0168(19) 0.0167(19) 0.0165(19) -0.0002(10) -0.0004(10) -0.0003(10)
C38 0.026(2) 0.026(2) 0.026(2) -0.0002(10) -0.0005(10) 0.0001(10)
C39 0.028(2) 0.027(2) 0.027(2) -0.0004(10) 0.0000(10) -0.0002(10)
C40 0.037(3) 0.036(3) 0.036(3) 0.0001(10) -0.0003(10) 0.0001(10)
C41 0.038(3) 0.037(3) 0.037(3) 0.0001(10) -0.0005(10) 0.0004(10)
C42 0.037(3) 0.037(3) 0.036(3) 0.0000(10) -0.0004(10) 0.0008(10)
C43 0.030(3) 0.030(3) 0.029(3) -0.0002(10) -0.0001(10) 0.0004(10)
C44 0.033(3) 0.033(3) 0.033(3) 0.0002(10) 0.0002(10) 0.0002(10)
O112 0.0228(16) 0.0231(16) 0.0234(16) 0.0002(10) 0.0002(10) -0.0007(10)
C111 0.017(2) 0.016(2) 0.016(2) 0.0000(10) 0.0001(10) -0.0006(10)
C112 0.018(2) 0.019(2) 0.018(2) -0.0003(10) 0.0003(10) -0.0001(10)
C113 0.023(2) 0.022(2) 0.023(2) 0.0003(10) 0.0003(10) -0.0007(10)
C114 0.025(2) 0.024(2) 0.025(2) 0.0000(10) -0.0003(10) -0.0002(10)
C115 0.0151(19) 0.0144(19) 0.0152(19) 0.0003(10) -0.0003(10) -0.0001(10)
C116 0.0159(17) 0.0159(18) 0.0156(18) 0.0003(10) -0.0003(10) -0.0005(10)
C124 0.031(3) 0.031(3) 0.031(3) 0.0005(10) -0.0003(10) 0.0002(10)
C117 0.0141(18) 0.0133(18) 0.0142(18) -0.0003(10) 0.0003(10) -0.0001(10)
C118 0.017(4) 0.010(4) 0.025(5) -0.001(3) -0.006(4) 0.010(3)
C119 0.022(5) 0.021(4) 0.022(5) -0.007(4) 0.001(4) 0.005(4)
C120 0.040(6) 0.004(4) 0.017(5) -0.004(3) -0.003(4) -0.003(4)
C121 0.029(5) 0.019(5) 0.022(5) -0.001(4) -0.010(4) 0.000(4)
C122 0.020(5) 0.027(5) 0.035(6) -0.005(5) -0.008(5) 0.004(4)
C123 0.019(5) 0.025(5) 0.017(4) -0.011(4) -0.002(4) 0.001(4)
N111 0.0201(18) 0.0200(18) 0.0200(18) -0.0008(10) -0.0001(10) 0.0001(10)
N151 0.039(5) 0.020(4) 0.047(5) -0.004(4) -0.021(4) 0.000(3)
O111 0.0106(14) 0.0084(14) 0.0107(14) 0.0000(9) 0.0004(10) 0.0004(9)
O151 0.028(4) 0.004(2) 0.041(4) -0.004(3) -0.018(3) 0.003(2)
O152 0.029(4) 0.017(3) 0.036(4) 0.009(3) -0.011(3) 0.001(3)
O153 0.077(9) 0.024(5) 0.092(9) -0.025(5) -0.046(6) 0.015(4)
O161 0.030(4) 0.030(4) 0.049(5) -0.005(4) 0.005(4) 0.000(3)
N161 0.016(5) 0.013(4) 0.038(6) 0.000 0.000 0.004(4)
O163 0.059(9) 0.042(7) 0.029(6) 0.000 0.000 -0.007(6)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken

into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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C18 N11 H11A 115.3 . . ?

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O51 Er1 O31 C36 60.1(7) . . . . ?
O72A Er1 O31 C36 -102.2(8) . . . . ?
O12 Er1 O31 C36 -108.6(7) . . . . ?
O71A Er1 O31 C36 -152.0(8) . . . . ?
N71 Er1 O31 C36 -146.0(7) . . . . ?
O11 Er1 O32 C35 -151.2(5) . . . . ?
O31 Er1 O32 C35 -14.0(5) . . . . ?
O71 Er1 O32 C35 -26.9(7) . . . . ?
O62 Er1 O32 C35 89.0(5) . . . . ?
O72 Er1 O32 C35 36.3(7) . . . . ?
O61 Er1 O32 C35 147.0(6) . . . . ?
O52 Er1 O32 C35 -92.4(5) . . . . ?
O51 Er1 O32 C35 -143.9(6) . . . . ?
O72A Er1 O32 C35 44.8(8) . . . . ?
O12 Er1 O32 C35 116.5(5) . . . . ?
O71A Er1 O32 C35 5.0(9) . . . . ?
N71 Er1 O32 C35 10.0(7) . . . . ?
O11 Er1 O32 C44 34.9(9) . . . . ?
O31 Er1 O32 C44 172.2(9) . . . . ?
O71 Er1 O32 C44 159.3(8) . . . . ?

O62 Er1 O32 C44 -84.8(8) . . . . ?
O72 Er1 O32 C44 -137.5(9) . . . . ?
O61 Er1 O32 C44 -26.8(8) . . . . ?
O52 Er1 O32 C44 93.8(8) . . . . ?
O51 Er1 O32 C44 42.3(8) . . . . ?
O72A Er1 O32 C44 -129.0(10) . . . . ?
O12 Er1 O32 C44 -57.3(9) . . . . ?
O71A Er1 O32 C44 -168.8(10) . . . . ?
N71 Er1 O32 C44 -163.8(8) . . . . ?
O11 Er1 O51 N51 -86.6(5) . . . . ?
O31 Er1 O51 N51 54.7(5) . . . . ?
O71 Er1 O51 N51 -29.7(7) . . . . ?
O62 Er1 O51 N51 149.4(5) . . . . ?
O72 Er1 O51 N51 102(8) . . . . ?
O61 Er1 O51 N51 179.6(6) . . . . ?
O52 Er1 O51 N51 -0.3(3) . . . . ?
O72A Er1 O51 N51 129(2) . . . . ?
O12 Er1 O51 N51 -133.6(4) . . . . ?
O71A Er1 O51 N51 -39.8(13) . . . . ?
N71 Er1 O51 N51 -28.9(10) . . . . ?
O11 Er1 O52 N51 78.6(4) . . . . ?
O31 Er1 O52 N51 -125.0(5) . . . . ?
O71 Er1 O52 N51 157.3(5) . . . . ?
O62 Er1 O52 N51 -59.9(6) . . . . ?
O72 Er1 O52 N51 -175.9(6) . . . . ?
O61 Er1 O52 N51 0.2(5) . . . . ?
O51 Er1 O52 N51 0.3(3) . . . . ?
O72A Er1 O52 N51 -159.4(8) . . . . ?
O12 Er1 O52 N51 85.4(5) . . . . ?
O71A Er1 O52 N51 160.3(6) . . . . ?
N71 Er1 O52 N51 168.1(4) . . . . ?
O11 Er1 N61 O61 -40.7(5) . . . . ?
O31 Er1 N61 O61 135.0(5) . . . . ?
O71 Er1 N61 O61 -130.7(7) . . . . ?
O62 Er1 N61 O61 174.9(6) . . . . ?
O72 Er1 N61 O61 -153.1(7) . . . . ?
O52 Er1 N61 O61 45.8(6) . . . . ?
O51 Er1 N61 O61 29.6(5) . . . . ?
O72A Er1 N61 O61 -160.7(8) . . . . ?
O12 Er1 N61 O61 -90.3(5) . . . . ?
O71A Er1 N61 O61 -135.3(7) . . . . ?
N71 Er1 N61 O61 -143.7(5) . . . . ?
O11 Er1 N61 O63 60(4) . . . . ?

O31 Er1 N61 O63 -124(4) . . . . ?
O71 Er1 N61 O63 -30(4) . . . . ?
O62 Er1 N61 O63 -84(4) . . . . ?
O72 Er1 N61 O63 -52(4) . . . . ?
O61 Er1 N61 O63 101(4) . . . . ?
O52 Er1 N61 O63 147(4) . . . . ?
O51 Er1 N61 O63 131(4) . . . . ?
O72A Er1 N61 O63 -60(4) . . . . ?
O12 Er1 N61 O63 11(4) . . . . ?
O71A Er1 N61 O63 -34(4) . . . . ?
N71 Er1 N61 O63 -43(4) . . . . ?
O11 Er1 N61 O62 144.3(5) . . . . ?
O31 Er1 N61 O62 -40.0(5) . . . . ?
O71 Er1 N61 O62 54.4(7) . . . . ?
O72 Er1 N61 O62 32.0(7) . . . . ?
O61 Er1 N61 O62 -174.9(6) . . . . ?
O52 Er1 N61 O62 -129.1(6) . . . . ?
O51 Er1 N61 O62 -145.3(6) . . . . ?
O72A Er1 N61 O62 24.4(8) . . . . ?
O12 Er1 N61 O62 94.8(5) . . . . ?
O71A Er1 N61 O62 49.8(7) . . . . ?
N71 Er1 N61 O62 41.3(6) . . . . ?
O63 N61 O61 Er1 -175.0(6) . . . . ?
O62 N61 O61 Er1 5.0(6) . . . . ?
O11 Er1 O61 N61 141.0(5) . . . . ?
O31 Er1 O61 N61 -57.0(6) . . . . ?
O71 Er1 O61 N61 92.4(8) . . . . ?
O62 Er1 O61 N61 -2.8(3) . . . . ?
O72 Er1 O61 N61 30.3(7) . . . . ?
O52 Er1 O61 N61 -146.3(4) . . . . ?
O51 Er1 O61 N61 -146.4(6) . . . . ?
O72A Er1 O61 N61 19.7(8) . . . . ?
O12 Er1 O61 N61 78.5(5) . . . . ?
O71A Er1 O61 N61 63.7(8) . . . . ?
N71 Er1 O61 N61 51.2(7) . . . . ?
O61 N61 O62 Er1 -5.1(6) . . . . ?
O63 N61 O62 Er1 175.0(6) . . . . ?
O11 Er1 O62 N61 -44.5(6) . . . . ?
O31 Er1 O62 N61 143.1(5) . . . . ?
O71 Er1 O62 N61 -144.3(5) . . . . ?
O72 Er1 O62 N61 -145.7(7) . . . . ?
O61 Er1 O62 N61 2.8(3) . . . . ?
O52 Er1 O62 N61 81.9(7) . . . . ?

O51 Er1 O62 N61 36.6(6) . . . . ?
O72A Er1 O62 N61 -150.7(10) . . . . ?
O12 Er1 O62 N61 -74.7(5) . . . . ?
O71A Er1 O62 N61 -138.4(7) . . . . ?
N71 Er1 O62 N61 -144.1(5) . . . . ?
O11 Er1 N71 O72 -131.3(9) . . . . ?
O31 Er1 N71 O72 83.9(9) . . . . ?
O71 Er1 N71 O72 176.3(9) . . . . ?
O62 Er1 N71 O72 -3.4(9) . . . . ?
O61 Er1 N71 O72 -44.5(9) . . . . ?
O52 Er1 N71 O72 152.1(9) . . . . ?
O51 Er1 N71 O72 175.0(11) . . . . ?
O72A Er1 N71 O72 4.8(16) . . . . ?
O12 Er1 N71 O72 -71.1(9) . . . . ?
O71A Er1 N71 O72 -142(4) . . . . ?
O11 Er1 N71 O73 -19(9) . . . . ?
O31 Er1 N71 O73 -164(9) . . . . ?
O71 Er1 N71 O73 -72(10) . . . . ?
O62 Er1 N71 O73 109(9) . . . . ?
O72 Er1 N71 O73 112(9) . . . . ?
O61 Er1 N71 O73 68(9) . . . . ?
O52 Er1 N71 O73 -96(9) . . . . ?
O51 Er1 N71 O73 -73(9) . . . . ?
O72A Er1 N71 O73 117(10) . . . . ?
O12 Er1 N71 O73 41(9) . . . . ?
O71A Er1 N71 O73 -30(10) . . . . ?
O11 Er1 N71 O71 52.4(7) . . . . ?
O31 Er1 N71 O71 -92.4(7) . . . . ?
O62 Er1 N71 O71 -179.7(7) . . . . ?
O72 Er1 N71 O71 -176.3(9) . . . . ?
O61 Er1 N71 O71 139.2(7) . . . . ?
O52 Er1 N71 O71 -24.2(7) . . . . ?
O51 Er1 N71 O71 -1.3(10) . . . . ?
O72A Er1 N71 O71 -171.5(13) . . . . ?
O12 Er1 N71 O71 112.6(7) . . . . ?
O71A Er1 N71 O71 42(4) . . . . ?
O72 N71 O71 Er1 -3.7(9) . . . . ?
O73 N71 O71 Er1 176.3(9) . . . . ?
O11 Er1 O71 N71 -125.7(7) . . . . ?
O31 Er1 O71 N71 80.0(7) . . . . ?
O62 Er1 O71 N71 0.4(8) . . . . ?
O72 Er1 O71 N71 2.1(5) . . . . ?
O61 Er1 O71 N71 -75.6(9) . . . . ?

O52 Er1 O71 N71 156.6(7) . . . . ?
O51 Er1 O71 N71 179.3(6) . . . . ?
O72A Er1 O71 N71 6.1(10) . . . . ?
O12 Er1 O71 N71 -62.5(6) . . . . ?
O71A Er1 O71 N71 -15.3(16) . . . . ?
O73 N71 O72 Er1 -176.4(9) . . . . ?
O71 N71 O72 Er1 3.7(9) . . . . ?
O11 Er1 O72 N71 53.3(9) . . . . ?
O31 Er1 O72 N71 -87.5(8) . . . . ?
O71 Er1 O72 N71 -2.1(5) . . . . ?
O62 Er1 O72 N71 176.4(9) . . . . ?
O61 Er1 O72 N71 148.5(6) . . . . ?
O52 Er1 O72 N71 -35.5(11) . . . . ?
O51 Er1 O72 N71 -136(7) . . . . ?
O72A Er1 O72 N71 -167(4) . . . . ?
O12 Er1 O72 N71 99.1(8) . . . . ?
O71A Er1 O72 N71 9.2(11) . . . . ?
O11 Er1 O71A N71A -143.8(11) . . . . ?
O31 Er1 O71A N71A 69.9(10) . . . . ?
O71 Er1 O71A N71A 150(2) . . . . ?
O62 Er1 O71A N71A -16.9(12) . . . . ?
O72 Er1 O71A N71A -4.6(12) . . . . ?
O61 Er1 O71A N71A -66.3(13) . . . . ?
O52 Er1 O71A N71A 141.5(10) . . . . ?
O51 Er1 O71A N71A 172.1(8) . . . . ?
O72A Er1 O71A N71A -3.4(7) . . . . ?
O12 Er1 O71A N71A -81.0(10) . . . . ?
N71 Er1 O71A N71A 26(4) . . . . ?
Er1 O71A N71A O72A 6.0(13) . . . . ?
Er1 O71A N71A O73A -174.0(13) . . . . ?
O71A N71A O72A Er1 -6.4(14) . . . . ?
O73A N71A O72A Er1 173.7(14) . . . . ?
O11 Er1 O72A N71A 51.5(14) . . . . ?
O31 Er1 O72A N71A -89.2(12) . . . . ?
O71 Er1 O72A N71A -6.9(11) . . . . ?
O62 Er1 O72A N71A 167.5(16) . . . . ?
O72 Er1 O72A N71A 6(3) . . . . ?
O61 Er1 O72A N71A 145.6(11) . . . . ?
O52 Er1 O72A N71A -53.7(16) . . . . ?
O51 Er1 O72A N71A -168.6(14) . . . . ?
O12 Er1 O72A N71A 86.2(12) . . . . ?
O71A Er1 O72A N71A 3.4(8) . . . . ?
N71 Er1 O72A N71A -2.7(8) . . . . ?

Er1 O52 N51 O53 179.6(6) . . . . ?
Er1 O52 N51 O51 -0.6(6) . . . . ?
Er1 O51 N51 O52 0.6(6) . . . . ?
Er1 O51 N51 O53 -179.7(6) . . . . ?
O11 Er1 N51 O52 -94.2(5) . . . . ?
O31 Er1 N51 O52 52.3(5) . . . . ?
O71 Er1 N51 O52 -23.3(6) . . . . ?
O62 Er1 N51 O52 141.8(5) . . . . ?
O72 Er1 N51 O52 7.5(10) . . . . ?
O61 Er1 N51 O52 -179.8(5) . . . . ?
O51 Er1 N51 O52 -179.4(6) . . . . ?
O72A Er1 N51 O52 43.9(12) . . . . ?
O12 Er1 N51 O52 -119.4(5) . . . . ?
O71A Er1 N51 O52 -24.1(8) . . . . ?
N71 Er1 N51 O52 -15.2(5) . . . . ?
O11 Er1 N51 O53 -106(20) . . . . ?
O31 Er1 N51 O53 41(20) . . . . ?
O71 Er1 N51 O53 -35(20) . . . . ?
O62 Er1 N51 O53 130(20) . . . . ?
O72 Er1 N51 O53 -4(20) . . . . ?
O61 Er1 N51 O53 168(20) . . . . ?
O52 Er1 N51 O53 -12(20) . . . . ?
O51 Er1 N51 O53 169(20) . . . . ?
O72A Er1 N51 O53 32(20) . . . . ?
O12 Er1 N51 O53 -131(20) . . . . ?
O71A Er1 N51 O53 -36(20) . . . . ?
N71 Er1 N51 O53 -27(20) . . . . ?
O11 Er1 N51 O51 85.2(5) . . . . ?
O31 Er1 N51 O51 -128.2(5) . . . . ?
O71 Er1 N51 O51 156.2(6) . . . . ?
O62 Er1 N51 O51 -38.7(6) . . . . ?
O72 Er1 N51 O51 -173.0(10) . . . . ?
O61 Er1 N51 O51 -0.4(5) . . . . ?
O52 Er1 N51 O51 179.4(6) . . . . ?
O72A Er1 N51 O51 -136.6(13) . . . . ?
O12 Er1 N51 O51 60.0(6) . . . . ?
O71A Er1 N51 O51 155.4(8) . . . . ?
N71 Er1 N51 O51 164.3(6) . . . . ?
C16 C11 C12 C13 0.0 . . . . ?
C17 C11 C12 C13 179.2(7) . . . . ?
C11 C12 C13 C14 0.0 . . . . ?
C12 C13 C14 C15 0.0 . . . . ?
C24 O12 C15 C16 -177.5(6) . . . . ?

Er1 O12 C15 C16 10.6(6) . . . . ?
C24 O12 C15 C14 1.7(10) . . . . ?
Er1 O12 C15 C14 -170.2(3) . . . . ?
C13 C14 C15 O12 -179.1(7) . . . . ?
C13 C14 C15 C16 0.0 . . . . ?
Er1 O11 C16 C15 -12.2(8) . . . . ?
Er1 O11 C16 C11 167.0(4) . . . . ?
O12 C15 C16 O11 -1.6(6) . . . . ?
C14 C15 C16 O11 179.2(6) . . . . ?
O12 C15 C16 C11 179.2(6) . . . . ?
C14 C15 C16 C11 0.0 . . . . ?
C12 C11 C16 O11 -179.2(6) . . . . ?
C17 C11 C16 O11 1.6(8) . . . . ?
C12 C11 C16 C15 0.0 . . . . ?
C17 C11 C16 C15 -179.2(7) . . . . ?
C18 N11 C17 C11 -177.9(8) . . . . ?
C12 C11 C17 N11 -179.2(7) . . . . ?
C16 C11 C17 N11 0.0(11) . . . . ?
C17 N11 C18 C19 -176.7(8) . . . . ?
C17 N11 C18 C23 3.1(12) . . . . ?
C23 C18 C19 C20 0.0 . . . . ?
N11 C18 C19 C20 179.8(7) . . . . ?
C18 C19 C20 C21 0.0 . . . . ?
C19 C20 C21 C22 0.0 . . . . ?
C20 C21 C22 C23 0.0 . . . . ?
C21 C22 C23 C18 0.0 . . . . ?
C19 C18 C23 C22 0.0 . . . . ?
N11 C18 C23 C22 -179.8(8) . . . . ?
C36 C31 C32 C33 0.0 . . . . ?
C37 C31 C32 C33 177.5(7) . . . . ?
C31 C32 C33 C34 0.0 . . . . ?
C32 C33 C34 C35 0.0 . . . . ?
C44 O32 C35 C34 6.8(10) . . . . ?
Er1 O32 C35 C34 -167.9(3) . . . . ?
C44 O32 C35 C36 -172.0(7) . . . . ?
Er1 O32 C35 C36 13.2(6) . . . . ?
C33 C34 C35 O32 -178.8(7) . . . . ?
C33 C34 C35 C36 0.0 . . . . ?
Er1 O31 C36 C35 -14.5(9) . . . . ?
Er1 O31 C36 C31 163.6(4) . . . . ?
O32 C35 C36 O31 -2.9(7) . . . . ?
C34 C35 C36 O31 178.2(7) . . . . ?
O32 C35 C36 C31 178.9(6) . . . . ?

C34 C35 C36 C31 0.0 . . . . ?
C32 C31 C36 O31 -178.1(7) . . . . ?
C37 C31 C36 O31 4.5(8) . . . . ?
C32 C31 C36 C35 0.0 . . . . ?
C37 C31 C36 C35 -177.4(7) . . . . ?
C38 N31 C37 C31 179.8(8) . . . . ?
C32 C31 C37 N31 -176.3(7) . . . . ?
C36 C31 C37 N31 1.2(11) . . . . ?
C37 N31 C38 C39 -169.9(8) . . . . ?
C37 N31 C38 C43 9.6(13) . . . . ?
C43 C38 C39 C40 0.0 . . . . ?
N31 C38 C39 C40 179.5(7) . . . . ?
C38 C39 C40 C41 0.0 . . . . ?
C39 C40 C41 C42 0.0 . . . . ?
C40 C41 C42 C43 0.0 . . . . ?
C41 C42 C43 C38 0.0 . . . . ?
C39 C38 C43 C42 0.0 . . . . ?
N31 C38 C43 C42 -179.4(8) . . . . ?
O111 Er2 O112 C115 -2.1(5) . . . . ?
O111 Er2 O112 C115 -155.0(6) 4_655 . . . ?
O161 Er2 O112 C115 129.0(5) . . . . ?
O161 Er2 O112 C115 49.9(7) 4_655 . . . ?
O152 Er2 O112 C115 81.4(5) . . . . ?
O152 Er2 O112 C115 -106.3(5) 4_655 . . . ?
O151 Er2 O112 C115 136.2(6) . . . . ?
O151 Er2 O112 C115 -38.4(6) 4_655 . . . ?
O112 Er2 O112 C115 -87.9(6) 4_655 . . . ?
N161 Er2 O112 C115 92.1(6) . . . . ?
N151 Er2 O112 C115 -63.0(6) 4_655 . . . ?
O111 Er2 O112 C124 173.6(8) . . . . ?
O111 Er2 O112 C124 20.6(8) 4_655 . . . ?
O161 Er2 O112 C124 -55.3(8) . . . . ?
O161 Er2 O112 C124 -134.4(7) 4_655 . . . ?
O152 Er2 O112 C124 -102.9(8) . . . . ?
O152 Er2 O112 C124 69.4(9) 4_655 . . . ?
O151 Er2 O112 C124 -48.1(7) . . . . ?
O151 Er2 O112 C124 137.2(7) 4_655 . . . ?
O112 Er2 O112 C124 87.8(8) 4_655 . . . ?
N161 Er2 O112 C124 -92.2(8) . . . . ?
N151 Er2 O112 C124 112.7(7) 4_655 . . . ?
C116 C111 C112 C113 0.0 . . . . ?
C117 C111 C112 C113 176.0(7) . . . . ?
C111 C112 C113 C114 0.0 . . . . ?

C112 C113 C114 C115 0.0 . . . . ?
C124 O112 C115 C116 -173.7(7) . . . . ?
Er2 O112 C115 C116 2.5(6) . . . . ?
C124 O112 C115 C114 6.2(10) . . . . ?
Er2 O112 C115 C114 -177.6(3) . . . . ?
C113 C114 C115 O112 -179.9(7) . . . . ?
C113 C114 C115 C116 0.0 . . . . ?
O112 C115 C116 O111 -1.4(7) . . . . ?
C114 C115 C116 O111 178.7(6) . . . . ?
O112 C115 C116 C111 179.9(6) . . . . ?
C114 C115 C116 C111 0.0 . . . . ?
C112 C111 C116 O111 -178.7(6) . . . . ?
C117 C111 C116 O111 5.6(7) . . . . ?
C112 C111 C116 C115 0.0 . . . . ?
C117 C111 C116 C115 -175.8(7) . . . . ?
C112 C111 C117 N111 -171.3(7) . . . . ?
C116 C111 C117 N111 4.5(11) . . . . ?
C123 C118 C119 C120 0.0 . . . . ?
N111 C118 C119 C120 -180.0(6) . . . . ?
C118 C119 C120 C121 0.0 . . . . ?
C119 C120 C121 C122 0.0 . . . . ?
C120 C121 C122 C123 0.0 . . . . ?
C121 C122 C123 C118 0.0 . . . . ?
C119 C118 C123 C122 0.0 . . . . ?
N111 C118 C123 C122 180.0(7) . . . . ?
C111 C117 N111 C118 173.7(7) . . . . ?
C119 C118 N111 C117 170.7(7) . . . . ?
C123 C118 N111 C117 -9.3(12) . . . . ?
O111 Er2 N151 O153 -114.6(18) . . . . ?
O111 Er2 N151 O153 108.3(17) 4_655 . . . ?
O161 Er2 N151 O153 22.2(17) . . . . ?
O161 Er2 N151 O153 -27.9(17) 4_655 . . . ?
O152 Er2 N151 O153 -81.2(18) . . . . ?
O152 Er2 N151 O153 32.8(17) 4_655 . . . ?
O151 Er2 N151 O153 107.5(16) . . . . ?
O151 Er2 N151 O153 -53.7(18) 4_655 . . . ?
O112 Er2 N151 O153 -174.1(18) . . . . ?
O112 Er2 N151 O153 160.8(18) 4_655 . . . ?
N161 Er2 N151 O153 -4.1(17) . . . . ?
N151 Er2 N151 O153 -4.1(17) 4_655 . . . ?
O111 Er2 N151 O151 137.9(4) . . . . ?
O111 Er2 N151 O151 0.8(4) 4_655 . . . ?
O161 Er2 N151 O151 -85.3(4) . . . . ?

O161 Er2 N151 O151 -135.4(4) 4_655 . . . ?
O152 Er2 N151 O151 171.3(5) . . . . ?
O152 Er2 N151 O151 -74.7(5) 4_655 . . . ?
O151 Er2 N151 O151 -161.3(5) 4_655 . . . ?
O112 Er2 N151 O151 78.4(4) . . . . ?
O112 Er2 N151 O151 53.3(5) 4_655 . . . ?
N161 Er2 N151 O151 -111.7(4) . . . . ?
N151 Er2 N151 O151 -111.7(4) 4_655 . . . ?
O111 Er2 N151 O152 -33.4(4) . . . . ?
O111 Er2 N151 O152 -170.5(4) 4_655 . . . ?
O161 Er2 N151 O152 103.4(4) . . . . ?
O161 Er2 N151 O152 53.3(4) 4_655 . . . ?
O152 Er2 N151 O152 114.0(6) 4_655 . . . ?
O151 Er2 N151 O152 -171.3(5) . . . . ?
O151 Er2 N151 O152 27.5(5) 4_655 . . . ?
O112 Er2 N151 O152 -92.9(4) . . . . ?
O112 Er2 N151 O152 -118.0(5) 4_655 . . . ?
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Crystallographic information file of 2

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2^ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All non-hydrogen atoms exept the solvent molecules refined anisotropically and the hydrogen atoms refined as riding model.

For better convergence of disordered solvent molecules,restraints and constraints
such as DFIX, DANG SIMU, DELU, ISOR etc.were used.

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C118 C 0.7844(3) 0.04896(8) 0.2637(5) 0.0210(10) Uani 1 1 d . . .
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H11F H 0.7010 0.0549 0.1181 0.030 Uiso 1 1 calc R . .
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H12B H 0.7622 0.0876 0.0070 0.036 Uiso 1 1 calc R . .
C121 C 0.8560(3) 0.08811(10) 0.1344(6) 0.0325(13) Uani 1 1 d . . .
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C122 C 0.8891(3) 0.07697(9) 0.2492(7) 0.0302(11) Uani 1 1 d . . .
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C124 C 0.4726(3) -0.04142(12) 0.5303(7) 0.0407(15) Uani 1 1 d . . .
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H12G H 0.4529 -0.0542 0.4679 0.061 Uiso 1 1 calc R . .
H12H H 0.4299 -0.0314 0.5651 0.061 Uiso 1 1 calc R . .
N111 N 0.7446(2) 0.02873(7) 0.3244(4) 0.0210(8) Uani 1 1 d . . .
H11G H 0.6978 0.0261 0.2934 0.025 Uiso 1 1 calc R . .
O111 O 0.61696(17) 0.00425(6) 0.3288(4) 0.0188(7) Uani 1 1 d . . .
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Lu1 Lu 0.493726(11) 0.169951(7) 0.45026(13) 0.03597(8) Uani 1 1 d . A .
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C13 C 0.8146(3) 0.13729(10) 0.3755(7) 0.0344(14) Uani 1 1 d . . .
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C14 C 0.7430(3) 0.12935(9) 0.3261(6) 0.0310(12) Uani 1 1 d . . .
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C16 C 0.6781(3) 0.15817(9) 0.4779(5) 0.0225(11) Uani 1 1 d . . .
C17 C 0.7570(3) 0.18321(9) 0.6382(7) 0.0316(13) Uani 1 1 d . . .
H17A H 0.8066 0.1879 0.6695 0.038 Uiso 1 1 calc R A .
C18 C 0.6950(4) 0.21050(9) 0.8097(6) 0.0310(12) Uani 1 1 d . . .
C19 C 0.6243(4) 0.21447(10) 0.8712(6) 0.0347(13) Uani 1 1 d . A .
H19A H 0.5804 0.2057 0.8398 0.042 Uiso 1 1 calc R . .
C20 C 0.6183(4) 0.23139(10) 0.9794(7) 0.0474(17) Uani 1 1 d . . .
H20A H 0.5698 0.2342 1.0221 0.057 Uiso 1 1 calc R A .
C21 C 0.6809(5) 0.24405(11) 1.0252(7) 0.054(2) Uani 1 1 d . A .
H21A H 0.6759 0.2557 1.0984 0.065 Uiso 1 1 calc R . .
C22 C 0.7515(5) 0.23988(11) 0.9650(7) 0.0536(19) Uani 1 1 d . . .
H22A H 0.7952 0.2485 0.9985 0.064 Uiso 1 1 calc R A .
C23 C 0.7598(4) 0.22302(10) 0.8549(6) 0.0417(16) Uani 1 1 d . A .
H23A H 0.8083 0.2203 0.8125 0.050 Uiso 1 1 calc R . .
C24 C 0.5947(4) 0.11235(10) 0.2457(7) 0.0426(14) Uani 1 1 d . A .
H24A H 0.5402 0.1099 0.2250 0.064 Uiso 1 1 calc R . .
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O11 O 0.61491(18) 0.16809(7) 0.5235(4) 0.0293(8) Uani 1 1 d . A .
O12 O 0.6037(2) 0.13330(7) 0.3362(5) 0.0357(9) Uani 1 1 d . . .
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H11A H 0.6531 0.1885 0.6644 0.033 Uiso 1 1 calc R . .
C31 C 0.2343(2) 0.16812(8) 0.4753(5) 0.0192(10) Uani 1 1 d . A .
C32 C 0.1723(3) 0.17891(9) 0.4044(6) 0.0268(11) Uani 1 1 d . . .
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C36 C 0.3107(2) 0.17544(7) 0.4444(6) 0.0169(8) Uani 1 1 d . . .
C37 C 0.2201(3) 0.14954(9) 0.5774(6) 0.0214(10) Uani 1 1 d . . .
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C38 C 0.2679(3) 0.11973(8) 0.7510(6) 0.0305(12) Uani 1 1 d . . .
C39 C 0.3349(4) 0.11196(13) 0.8091(8) 0.057(2) Uani 1 1 d . A .
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C40 C 0.3328(5) 0.09358(13) 0.9111(9) 0.068(2) Uani 1 1 d . . .
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C41 C 0.2637(5) 0.08382(10) 0.9503(8) 0.0531(19) Uani 1 1 d . A .
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C42 C 0.1979(5) 0.09192(13) 0.8912(7) 0.0535(19) Uani 1 1 d . . .
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O62 O 0.5329(7) 0.1746(2) 0.2044(13) 0.025(3) Uani 0.391(13) 1 d PDU A 1
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N61A N 0.5015(4) 0.16802(17) 0.1595(9) 0.048(3) Uani 0.609(13) 1 d PDU A 2
O61A O 0.4534(4) 0.15438(15) 0.2233(8) 0.040(2) Uani 0.609(13) 1 d PDU A 2
O62A O 0.5474(4) 0.17990(17) 0.2355(8) 0.039(2) Uani 0.609(13) 1 d PDU A 2
O63A O 0.5021(4) 0.1693(3) 0.0309(6) 0.075(4) Uani 0.609(13) 1 d PDU A 2
N51 N 0.5344(3) 0.22202(14) 0.5010(8) 0.049(3) Uani 0.542(9) 1 d PDU A 1
O51 O 0.4889(5) 0.21099(18) 0.5822(10) 0.047(3) Uani 0.542(9) 1 d PDU A 1
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O52A O 0.5293(7) 0.2102(2) 0.4635(11) 0.069(4) Uani 0.458(9) 1 d PDU A 2
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O73 O 0.4619(5) 0.09857(13) 0.6146(10) 0.046(3) Uani 0.467(6) 1 d PDU A 3
O72 O 0.4578(4) 0.12331(13) 0.4364(8) 0.037(2) Uani 0.467(6) 1 d PDU A 3
N71A N 0.4982(2) 0.14236(17) 0.6838(10) 0.047(3) Uani 0.533(6) 1 d PDU A 4
O73A O 0.5073(4) 0.12817(15) 0.7865(9) 0.053(3) Uani 0.533(6) 1 d PDU A 4
O71A O 0.4968(4) 0.16488(12) 0.7071(10) 0.041(3) Uani 0.533(6) 1 d PDU A 4
O72A O 0.4909(6) 0.13386(17) 0.5633(9) 0.046(3) Uani 0.533(6) 1 d PDU A 4

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O161 0.0291(19) 0.032(2) 0.055(3) -0.011(2) 0.022(2) -0.0037(16)
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O152 0.085(6) 0.101(6) 0.018(3) 0.000 0.000 0.035(5)
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C112 0.025(3) 0.024(2) 0.030(3) -0.005(2) -0.013(2) 0.005(2)
C113 0.043(3) 0.022(2) 0.023(3) 0.002(2) -0.011(2) 0.009(2)
C114 0.039(3) 0.023(2) 0.026(3) 0.007(2) 0.001(2) 0.010(2)
C115 0.025(2) 0.024(2) 0.023(2) 0.003(2) 0.001(2) 0.003(2)
C116 0.019(2) 0.022(2) 0.016(2) -0.0019(19) 0.000(2) 0.0071(18)
C117 0.0138(19) 0.021(2) 0.027(3) -0.006(2) -0.0055(18) 0.0036(17)
C118 0.026(2) 0.0158(19) 0.021(3) -0.0072(19) 0.002(2) -0.0021(17)
C119 0.031(3) 0.022(2) 0.023(2) -0.008(2) 0.001(2) -0.002(2)
C120 0.040(3) 0.025(2) 0.024(3) -0.006(2) 0.001(2) 0.003(2)
C121 0.042(3) 0.024(2) 0.031(3) -0.004(2) 0.015(3) -0.002(2)

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O111 0.0132(15) 0.0247(17) 0.0186(16) 0.0066(13) -0.0030(13) -0.0023(13)
O112 0.0195(15) 0.037(2) 0.0333(19) 0.017(2) -0.0026(19) -0.0034(14)
Lu1 0.01448(10) 0.0680(2) 0.02541(12) -0.00163(15) 0.00075(17) -
0.00533(10)
C11 0.016(2) 0.019(2) 0.041(3) 0.009(2) -0.001(2) -0.0019(19)
C12 0.014(2) 0.032(3) 0.052(4) 0.015(3) 0.002(2) 0.0009(19)
C13 0.026(3) 0.025(3) 0.052(4) 0.009(3) 0.015(3) 0.008(2)
C14 0.036(3) 0.019(2) 0.038(3) 0.004(2) 0.008(3) 0.007(2)
C15 0.022(2) 0.025(2) 0.027(3) 0.006(2) 0.004(2) 0.000(2)
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C17 0.028(3) 0.026(3) 0.041(3) 0.011(2) -0.010(3) -0.008(2)
C18 0.050(3) 0.018(2) 0.025(3) 0.006(2) -0.010(3) -0.006(2)
C19 0.049(3) 0.022(2) 0.033(3) 0.002(2) -0.006(3) 0.001(2)
C20 0.092(5) 0.019(3) 0.031(3) 0.001(2) -0.002(3) 0.006(3)
C21 0.114(7) 0.025(3) 0.023(3) -0.004(2) -0.004(4) -0.019(4)
C22 0.095(5) 0.039(3) 0.026(3) 0.005(3) -0.023(4) -0.042(4)
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C31 0.019(2) 0.022(2) 0.017(3) 0.0005(19) 0.0001(18) 0.0039(17)
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C33 0.025(3) 0.030(3) 0.033(3) 0.005(2) -0.007(2) 0.008(2)
C34 0.034(3) 0.026(2) 0.027(3) 0.003(2) -0.002(2) 0.007(2)
C35 0.024(2) 0.018(2) 0.021(2) -0.0043(19) 0.003(2) 0.0006(19)
C36 0.0201(18) 0.0141(19) 0.0166(19) -0.0050(19) 0.001(2) 0.0020(15)
C37 0.016(2) 0.023(2) 0.025(2) -0.003(2) 0.006(2) 0.0010(18)
C38 0.044(3) 0.019(2) 0.029(3) 0.001(2) 0.008(3) 0.005(2)
C39 0.041(4) 0.055(4) 0.075(5) 0.033(4) 0.015(4) 0.019(3)
C40 0.084(6) 0.050(4) 0.070(6) 0.031(4) 0.008(4) 0.027(4)
C41 0.099(5) 0.020(3) 0.040(3) 0.011(3) 0.033(5) 0.010(3)
C42 0.077(5) 0.043(4) 0.039(4) 0.006(3) 0.023(4) -0.004(4)
C43 0.052(4) 0.031(3) 0.039(3) 0.004(3) 0.015(3) -0.003(3)
C44 0.042(3) 0.027(2) 0.037(3) 0.005(2) 0.003(3) -0.011(2)
O31 0.0155(15) 0.0263(17) 0.0222(17) 0.0048(15) -0.0011(13) 0.0036(13)
O32 0.0273(19) 0.0261(17) 0.037(2) 0.0088(17) 0.0068(17) -0.0045(15)
N31 0.025(2) 0.028(2) 0.024(2) 0.0015(19) 0.0109(19) -0.0009(18)
N61 0.020(3) 0.020(3) 0.021(3) 0.0003(10) -0.0002(10) -0.0003(10)

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O62 0.024(3) 0.025(3) 0.025(3) -0.0008(10) 0.0003(10) -0.0001(10)
O63 0.026(3) 0.026(3) 0.026(3) -0.0009(10) 0.0005(10) -0.0008(10)
N61A 0.026(4) 0.083(7) 0.035(4) 0.001(5) 0.008(3) 0.020(4)
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O51 0.038(5) 0.039(5) 0.066(6) -0.008(5) -0.014(4) 0.006(4)
O52 0.033(4) 0.046(5) 0.070(6) -0.019(5) -0.012(4) -0.006(4)
O53 0.076(7) 0.031(4) 0.093(8) -0.023(5) -0.023(6) -0.006(4)
N51A 0.064(7) 0.044(6) 0.078(8) -0.047(6) -0.038(6) 0.027(6)
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O52A 0.098(9) 0.028(5) 0.081(8) -0.032(6) -0.047(8) 0.021(6)
N71 0.025(4) 0.032(4) 0.054(5) 0.006(4) 0.004(4) 0.010(4)
O71 0.023(5) 0.041(5) 0.056(7) 0.018(6) -0.018(5) -0.001(4)
O73 0.041(5) 0.029(4) 0.069(7) 0.031(4) 0.014(5) 0.005(4)
O72 0.047(4) 0.032(4) 0.033(4) 0.002(4) 0.014(4) 0.003(3)
N71A 0.029(5) 0.061(5) 0.051(6) 0.011(5) 0.012(5) -0.003(5)
O73A 0.030(4) 0.063(5) 0.065(6) 0.030(5) -0.007(4) 0.005(4)
O71A 0.021(4) 0.044(4) 0.057(7) 0.003(4) 0.014(4) 0.002(4)
O72A 0.035(5) 0.039(5) 0.065(6) 0.010(5) -0.001(5) 0.002(4)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C40 C41 H41A 119.8 . . ?

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N161 Lu2 O112 C115 107.5(4) . . . . ?
O111 Lu2 O112 C124 22.0(5) 4_655 . . . ?
O111 Lu2 O112 C124 175.1(5) . . . . ?
O171 Lu2 O112 C124 -101.9(5) 4_655 . . . ?
O171 Lu2 O112 C124 69.7(5) . . . . ?
O151 Lu2 O112 C124 -53.7(5) 4_655 . . . ?
O151 Lu2 O112 C124 -132.8(4) . . . . ?
O112 Lu2 O112 C124 90.1(5) 4_655 . . . ?
O161 Lu2 O112 C124 138.2(5) 4_655 . . . ?
O161 Lu2 O112 C124 -47.6(5) . . . . ?
N151 Lu2 O112 C124 -89.9(5) . . . . ?
N161 Lu2 O112 C124 -74.9(5) . . . . ?
C17 C11 C12 C13 176.7(5) . . . . ?
C16 C11 C12 C13 -0.5(8) . . . . ?
C11 C12 C13 C14 -0.7(8) . . . . ?
C12 C13 C14 C15 1.1(8) . . . . ?
C13 C14 C15 O12 -179.7(5) . . . . ?
C13 C14 C15 C16 -0.4(8) . . . . ?
O12 C15 C16 O11 -1.6(7) . . . . ?
C14 C15 C16 O11 179.1(5) . . . . ?
O12 C15 C16 C11 178.6(4) . . . . ?
C14 C15 C16 C11 -0.7(7) . . . . ?
C12 C11 C16 O11 -178.6(5) . . . . ?
C17 C11 C16 O11 4.2(7) . . . . ?
C12 C11 C16 C15 1.2(7) . . . . ?
C17 C11 C16 C15 -176.0(5) . . . . ?
C12 C11 C17 N11 -176.8(5) . . . . ?
C16 C11 C17 N11 0.4(8) . . . . ?
C23 C18 C19 C20 0.3(8) . . . . ?
N11 C18 C19 C20 -179.3(5) . . . . ?
C18 C19 C20 C21 0.1(9) . . . . ?
C19 C20 C21 C22 -0.8(9) . . . . ?
C20 C21 C22 C23 1.2(10) . . . . ?
C19 C18 C23 C22 0.0(8) . . . . ?

N11 C18 C23 C22 179.6(5) . . . . ?
C21 C22 C23 C18 -0.8(9) . . . . ?
C15 C16 O11 Lu1 -17.1(7) . . . . ?
C11 C16 O11 Lu1 162.7(4) . . . . ?
O31 Lu1 O11 C16 132.3(4) . . . . ?
O72A Lu1 O11 C16 84.9(5) . . . . ?
O61 Lu1 O11 C16 9.4(6) . . . . ?
O51A Lu1 O11 C16 -179(96) . . . . ?
O52A Lu1 O11 C16 -121.3(5) . . . . ?
O62A Lu1 O11 C16 -47.1(5) . . . . ?
O61A Lu1 O11 C16 -7.0(6) . . . . ?
O62 Lu1 O11 C16 -39.1(5) . . . . ?
O71A Lu1 O11 C16 140.9(5) . . . . ?
O52 Lu1 O11 C16 -102.4(5) . . . . ?
O71 Lu1 O11 C16 100.6(5) . . . . ?
C14 C15 O12 C24 7.1(8) . . . . ?
C16 C15 O12 C24 -172.2(5) . . . . ?
C11 C17 N11 C18 178.7(5) . . . . ?
C19 C18 N11 C17 -167.7(5) . . . . ?
C23 C18 N11 C17 12.7(8) . . . . ?
C36 C31 C32 C33 0.0(7) . . . . ?
C37 C31 C32 C33 -179.3(5) . . . . ?
C31 C32 C33 C34 -0.2(8) . . . . ?
C32 C33 C34 C35 -0.2(8) . . . . ?
C33 C34 C35 O32 179.3(5) . . . . ?
C33 C34 C35 C36 0.7(8) . . . . ?
C34 C35 C36 O31 179.3(5) . . . . ?
O32 C35 C36 O31 0.5(6) . . . . ?
C34 C35 C36 C31 -0.8(7) . . . . ?
O32 C35 C36 C31 -179.6(4) . . . . ?
C32 C31 C36 O31 -179.6(4) . . . . ?
C37 C31 C36 O31 -0.4(7) . . . . ?
C32 C31 C36 C35 0.5(7) . . . . ?
C37 C31 C36 C35 179.7(4) . . . . ?
C32 C31 C37 N31 179.7(5) . . . . ?
C36 C31 C37 N31 0.5(7) . . . . ?
C43 C38 C39 C40 0.1(11) . . . . ?
N31 C38 C39 C40 -180.0(6) . . . . ?
C38 C39 C40 C41 0.0(12) . . . . ?
C39 C40 C41 C42 -0.2(11) . . . . ?
C40 C41 C42 C43 0.2(11) . . . . ?
C39 C38 C43 C42 0.0(9) . . . . ?
N31 C38 C43 C42 180.0(5) . . . . ?

C41 C42 C43 C38 -0.1(10) . . . . ?
C35 C36 O31 Lu1 -11.4(6) . . . . ?
C31 C36 O31 Lu1 168.8(3) . . . . ?
O11 Lu1 O31 C36 157.6(3) . . . . ?
O72A Lu1 O31 C36 -154.3(4) . . . . ?
O61 Lu1 O31 C36 -68.7(5) . . . . ?
O51A Lu1 O31 C36 109.1(5) . . . . ?
O52A Lu1 O31 C36 61.4(5) . . . . ?
O62A Lu1 O31 C36 -23.2(5) . . . . ?
O61A Lu1 O31 C36 -55.9(4) . . . . ?
O62 Lu1 O31 C36 -32.4(5) . . . . ?
O71A Lu1 O31 C36 149.3(4) . . . . ?
O52 Lu1 O31 C36 47.2(5) . . . . ?
O71 Lu1 O31 C36 -170.8(4) . . . . ?
C34 C35 O32 C44 2.6(7) . . . . ?
C36 C35 O32 C44 -178.7(4) . . . . ?
C34 C35 O32 Lu1 -171.1(4) . . . . ?
C36 C35 O32 Lu1 7.6(5) . . . . ?
O11 Lu1 O32 C35 -160.1(3) . . . . ?
O31 Lu1 O32 C35 -9.2(3) . . . . ?
O72A Lu1 O32 C35 12.8(5) . . . . ?
O61 Lu1 O32 C35 75.2(4) . . . . ?
O51A Lu1 O32 C35 -84.9(4) . . . . ?
O52A Lu1 O32 C35 -137.5(4) . . . . ?
O62A Lu1 O32 C35 143.6(4) . . . . ?
O61A Lu1 O32 C35 86.3(4) . . . . ?
O62 Lu1 O32 C35 132.1(4) . . . . ?
O71A Lu1 O32 C35 -59.7(4) . . . . ?
O52 Lu1 O32 C35 -157.6(4) . . . . ?
O71 Lu1 O32 C35 -11.6(5) . . . . ?
O11 Lu1 O32 C44 27.2(5) . . . . ?
O31 Lu1 O32 C44 178.1(4) . . . . ?
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O61 Lu1 O32 C44 -97.5(5) . . . . ?
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O62 Lu1 O32 C44 -40.6(4) . . . . ?
O71A Lu1 O32 C44 127.5(4) . . . . ?
O52 Lu1 O32 C44 29.7(4) . . . . ?
O71 Lu1 O32 C44 175.7(4) . . . . ?
C31 C37 N31 C38 -179.7(5) . . . . ?

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O31 Lu1 N61 O63 -75(6) . . . . ?
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O61A Lu1 N61 O63 -64(6) . . . . ?
O62 Lu1 N61 O63 145(6) . . . . ?
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O52 Lu1 N61 O63 159(6) . . . . ?
O71 Lu1 N61 O63 4(6) . . . . ?
O11 Lu1 N61 O61 126.3(6) . . . . ?
O31 Lu1 N61 O61 -36.7(6) . . . . ?
O72A Lu1 N61 O61 42.3(6) . . . . ?
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O71A Lu1 N61 O61 43.5(8) . . . . ?
O52 Lu1 N61 O61 -161.9(6) . . . . ?
O71 Lu1 N61 O61 42.9(6) . . . . ?
O11 Lu1 N61 O62 -57.1(6) . . . . ?
O31 Lu1 N61 O62 139.9(6) . . . . ?
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O61 Lu1 N61 O62 176.6(6) . . . . ?
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O52A Lu1 N61 O62 24.4(7) . . . . ?
O62A Lu1 N61 O62 -2.2(10) . . . . ?
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O71A Lu1 N61 O62 -139.9(10) . . . . ?
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O71 Lu1 N61 O62 -140.5(7) . . . . ?
O63 N61 O61 Lu1 176.5(6) . . . . ?
O62 N61 O61 Lu1 -3.5(6) . . . . ?
O11 Lu1 O61 N61 -64.9(6) . . . . ?
O31 Lu1 O61 N61 143.3(6) . . . . ?
O72A Lu1 O61 N61 -138.8(6) . . . . ?
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O71 Lu1 O61 N61 -143.2(5) . . . . ?
O63 N61 O62 Lu1 -176.9(5) . . . . ?
O61 N61 O62 Lu1 3.1(5) . . . . ?
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O52 Lu1 O62 N61 -163.9(7) . . . . ?
O71 Lu1 O62 N61 56.5(9) . . . . ?
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O71 Lu1 N61A O63A 159(6) . . . . ?
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O31 Lu1 N61A O62A 150.0(4) . . . . ?
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O61 Lu1 N61A O62A -162.4(7) . . . . ?
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O62 Lu1 N61A O62A -5.4(17) . . . . ?
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O53 N51 O52 Lu1 175.2(5) . . . . ?
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O52A Lu1 N71A O71A 19.5(5) . . . . ?
O62A Lu1 N71A O71A 125.6(6) . . . . ?
O61A Lu1 N71A O71A -160.4(4) . . . . ?
O62 Lu1 N71A O71A 146.5(6) . . . . ?
O52 Lu1 N71A O71A 37.4(4) . . . . ?
O71 Lu1 N71A O71A -170.5(17) . . . . ?
O11 Lu1 N71A O72A -104.3(5) . . . . ?
O31 Lu1 N71A O72A 87.2(5) . . . . ?
O61 Lu1 N71A O72A 14.4(5) . . . . ?
O51A Lu1 N71A O72A 169.7(5) . . . . ?
O52A Lu1 N71A O72A -166.9(6) . . . . ?
O62A Lu1 N71A O72A -60.9(6) . . . . ?
O61A Lu1 N71A O72A 13.2(5) . . . . ?
O62 Lu1 N71A O72A -40.0(6) . . . . ?
O71A Lu1 N71A O72A 173.5(4) . . . . ?
O52 Lu1 N71A O72A -149.1(6) . . . . ?
O71 Lu1 N71A O72A 3.0(19) . . . . ?

O11 Lu1 N71A O73A -45(5) . . . . ?
O31 Lu1 N71A O73A 146(5) . . . . ?
O72A Lu1 N71A O73A 59(5) . . . . ?
O61 Lu1 N71A O73A 74(5) . . . . ?
O51A Lu1 N71A O73A -131(5) . . . . ?
O52A Lu1 N71A O73A -108(5) . . . . ?
O62A Lu1 N71A O73A -2(5) . . . . ?
O61A Lu1 N71A O73A 72(5) . . . . ?
O62 Lu1 N71A O73A 19(5) . . . . ?
O71A Lu1 N71A O73A -127(5) . . . . ?
O52 Lu1 N71A O73A -90(5) . . . . ?
O71 Lu1 N71A O73A 62(5) . . . . ?
O72A N71A O71A Lu1 -6.3(4) . . . . ?
O73A N71A O71A Lu1 173.7(4) . . . . ?
O11 Lu1 O71A N71A -88.2(3) . . . . ?
O31 Lu1 O71A N71A 87.0(3) . . . . ?
O72A Lu1 O71A N71A 3.6(2) . . . . ?
O61 Lu1 O71A N71A 28.3(6) . . . . ?
O51A Lu1 O71A N71A 174.5(6) . . . . ?
O52A Lu1 O71A N71A -162.9(4) . . . . ?
O62A Lu1 O71A N71A -106.3(7) . . . . ?
O61A Lu1 O71A N71A 32.5(6) . . . . ?
O62 Lu1 O71A N71A -88.1(10) . . . . ?
O52 Lu1 O71A N71A -151.1(3) . . . . ?
O71 Lu1 O71A N71A 3.0(5) . . . . ?
O71A N71A O72A Lu1 7.0(4) . . . . ?
O73A N71A O72A Lu1 -173.0(4) . . . . ?
O11 Lu1 O72A N71A 69.0(4) . . . . ?
O31 Lu1 O72A N71A -86.3(4) . . . . ?
O61 Lu1 O72A N71A -166.4(5) . . . . ?
O51A Lu1 O72A N71A -9.4(5) . . . . ?
O52A Lu1 O72A N71A 20.3(9) . . . . ?
O62A Lu1 O72A N71A 143.6(4) . . . . ?
O61A Lu1 O72A N71A -169.0(4) . . . . ?
O62 Lu1 O72A N71A 155.3(4) . . . . ?
O71A Lu1 O72A N71A -3.6(2) . . . . ?
O52 Lu1 O72A N71A 54.4(8) . . . . ?
O71 Lu1 O72A N71A -2.1(13) . . . . ?

_diffrn_measured_fraction_theta_max 0.997
_diffrn_reflns_theta_full 29.12
_diffrn_measured_fraction_theta_full 0.997
_refine_diff_density_max 1.185

_refine_diff_density_min -2.024
_refine_diff_density_rms 0.103

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