Electronic Supplementary Material (ESI) for Chemical Communications.
This journal is © The Royal Society of Chemistry 2014

Supplementary information

Enhancing the Effective Energy Barrier of a Dy(III) SMM Using a Diamagnetic Bridged Zn(II) ion

Apoorva Upadhyay,[a] Saurabh Kumar Singh,[a] Chinmoy Das,[a] Ranajit Mondal,[a] Stuart K. Langley,[b] Keith S. Murray,[b] Gopalan Rajaraman[a] *, and Maheswaran Shanmugam[a] *

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]

Synthesis of **1**:

NaOH (0.0528g, 1.3 mmol) was added to a methanolic solution containing the Schiff base ligand (0.3 g, 1.3 mmol) allowing for deprotonation of the ligand. Into this solution; $Dy(NO_3)_3 \cdot 5H_2O$ (0.2898 g, 0.065mmol) was added and was stirred for 15-20 minutes, after which $Zn(CH_3COO)_2 \cdot 2H_2O$ (0.29 g, 1.3 mmol) was added. Upon addition of the zinc salt the colour of the solution changes from orange to yellow. The reaction mixture was then allowed to stir for 8 hours at room temperature. The solvent was then removed under reduced pressure and the product of interest was extracted with DCM. The residue obtained after removal of the DCM was recrystallized from methanol whilst standing in fridge at 4-5°C. This resulted in X-ray quality light yellow block shaped crystals, which were obtained in 2-3 days. IR: (KBr pellet), 2925 cm^{-1}(s,(Ar-H)),1618 cm^{-1}(s,(C=N)).

Synthesis of **2:**

The ligand HL (0.3 g, 1.3 mmol)) and $Dy(NO_3)_3.5H_2O$ (0.2898 g, 0.6 mmol) 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, giving X-ray suitable single crystals in the 3-4 days. IR: (KBr pellet), 3424.28 cm^{-1}(b,(NH)), 2942.20 cm^{-1}(s,(Ar-H)),1630.42 cm^{-1}(s,(C=N)).

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

	1	**2**
Formula	$Zn_1Dy_1C_{32}H_{27}O_{14}N_4$	$Dy_1C_{28}H_{26}N_5O_{13}$
Size	0.41× 0.21× 0.07	0.2 × 0.2 × 0.2
System	Triclinic	Orthorhombic
Space group	*P-1*	*Aba2*
a [Å]	11.132(5)	17.654(3)
b [Å]	12.522(6)	54.092(9)
c [Å]	13.219(6)	9.550(16)
α [°]	105.888(10)	90
β [°]	91.753(5)	90
γ [°]	94.464(6)	90
V [Å^3]	1764.3(14)	9120(3)
Z	2	12
ρ_{calcd}[g/cm^{-3}]	1.731	1.755
$2\Theta_{max}$	58.34	58.34
Radiation	MoK_α	MoK_α
λ [Å]	0.71073	0.71073
T [K]	100	100
Reflns	29756	33334
Ind. Reflns	9054	11627
reflns with >2σ(I)	8566	9529
R1	0.0348	0.0494
wR2	0.0910	0.1015

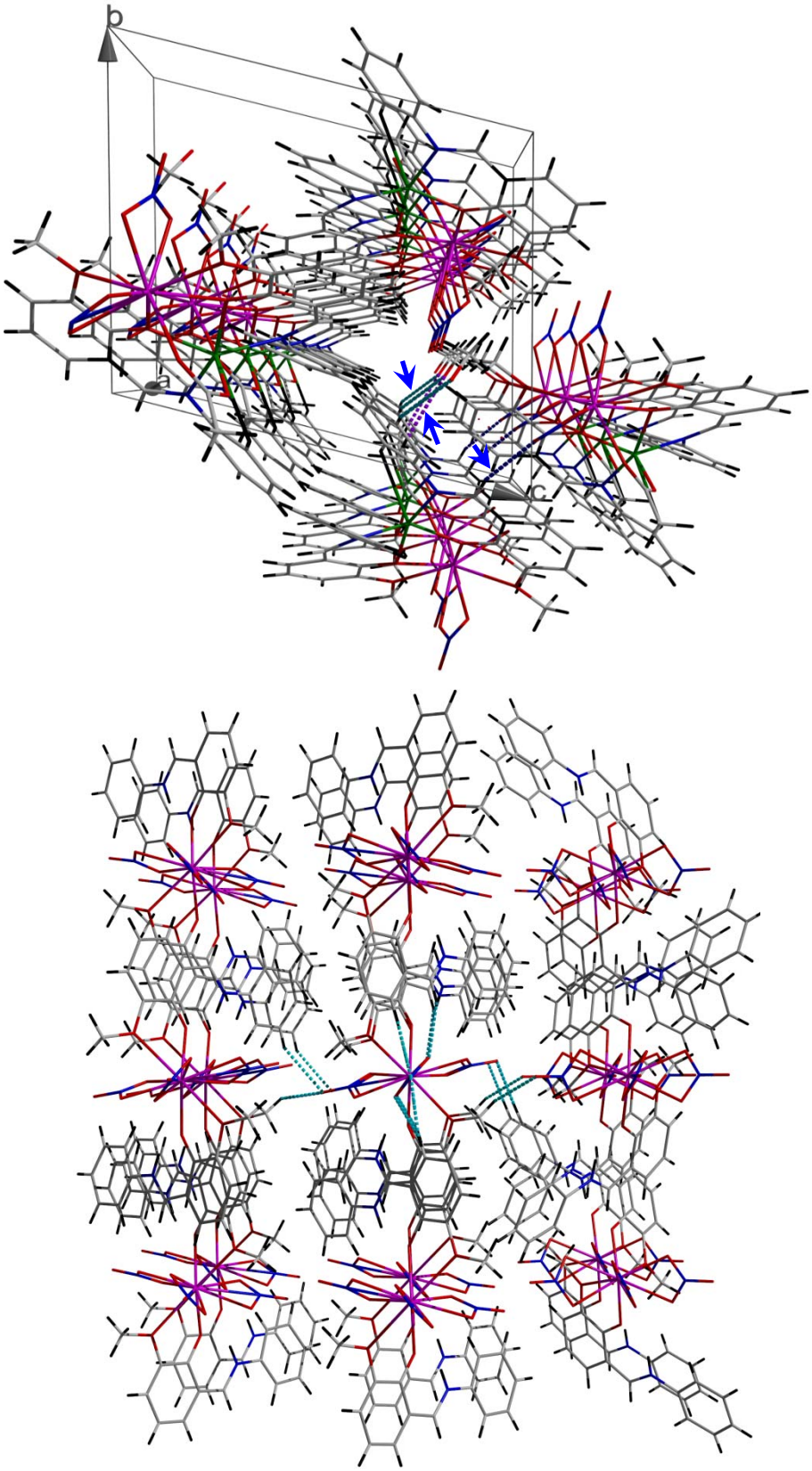


Figure S1. Packing diagram, highlighting the intermolecular hydrogen bonding interactions between the molecules in **1** (top) and **2** (bottom).

Table S2. Selected bond lengths and angles for **1** and **2**.

Bond lengths

Dy(1)-O(6)	2.296(2)
Dy(1)-O(12)	2.296(2)
Dy(1)-O(11)	2.325(3)
Dy(1)-O(15)	2.394(3)
Dy(1)-O(9)	2.416(3)
Dy(1)-O(10)	2.466(3)
Dy(1)-O(13)	2.495(3)
Dy(1)-O(20)	2.516(3)
Dy(1)-O(7)	2.562(2)
Dy(1)-N(27)	2.779(4)
Dy(1)-N(4)	2.886(3)
Dy(1)-Zn(2)	3.4312(10)
Zn(2)-O(8)	1.997(2)
Zn(2)-O(6)	2.010(2)
Zn(2)-N(18)	2.071(3)
Zn(2)-N(16)	2.096(3)
Zn(2)-O(12)	2.107(2)

Bond angles

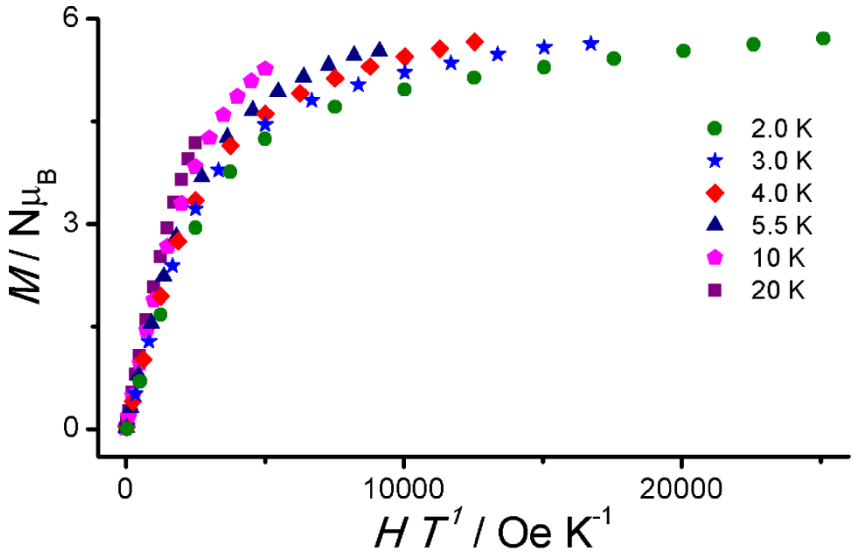
Zn(2)-O(6)-Dy(1)	105.47(9)
Zn(2)-O(12)-Dy(1)	102.32(10)

Selected bond lengths for **2a**.

Dy(1)-O(11)	2.272(4)
Dy(1)-O(31)	2.308(4)
Dy(1)-O(62)	2.434(6)
Dy(1)-O(52)	2.453(5)
Dy(1)-O(42)	2.465(6)
Dy(1)-O(51)	2.465(5)
Dy(1)-O(41)	2.495(4)
Dy(1)-O(61)	2.498(5)
Dy(1)-O(12)	2.702(4)
Dy(1)-O(32)	2.719(4)

Selected bond lengths for **2b**.

Dy(2)-O(111)#1	2.271(4)
Dy(2)-O(111)	2.271(4)
Dy(2)-O(141)	2.463(4)
Dy(2)-O(141)#1	2.463(4)
Dy(2)-O(151)	2.505(4)
Dy(2)-O(151)#1	2.505(4)
Dy(2)-O(142)	2.527(4)
Dy(2)-O(142)#1	2.527(4)
Dy(2)-O(112)	2.548(4)
Dy(2)-O(112)#1	2.548(4)



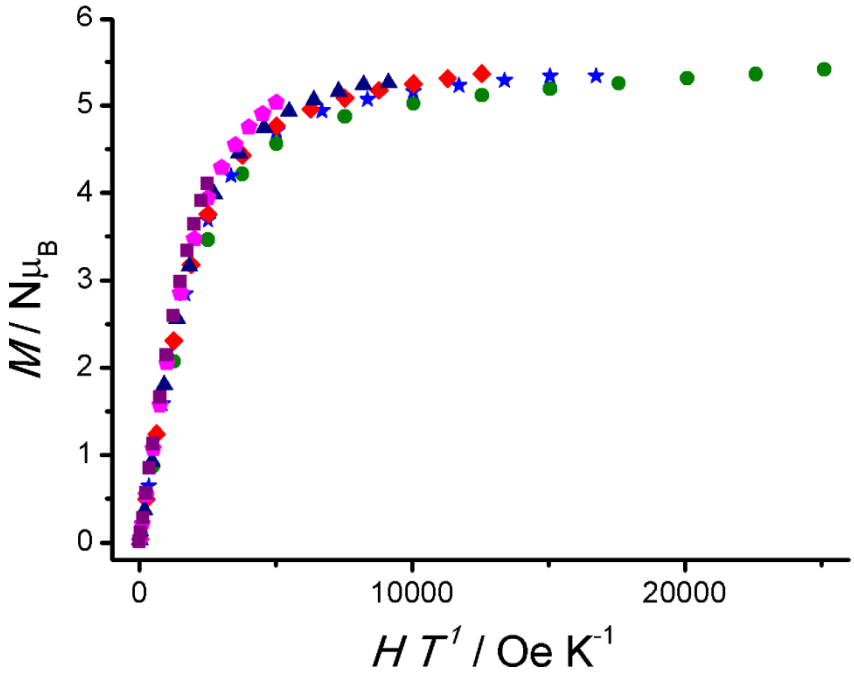


Figure S2. Reduced magnetization plots for **1** (top) and **2** (bottom)

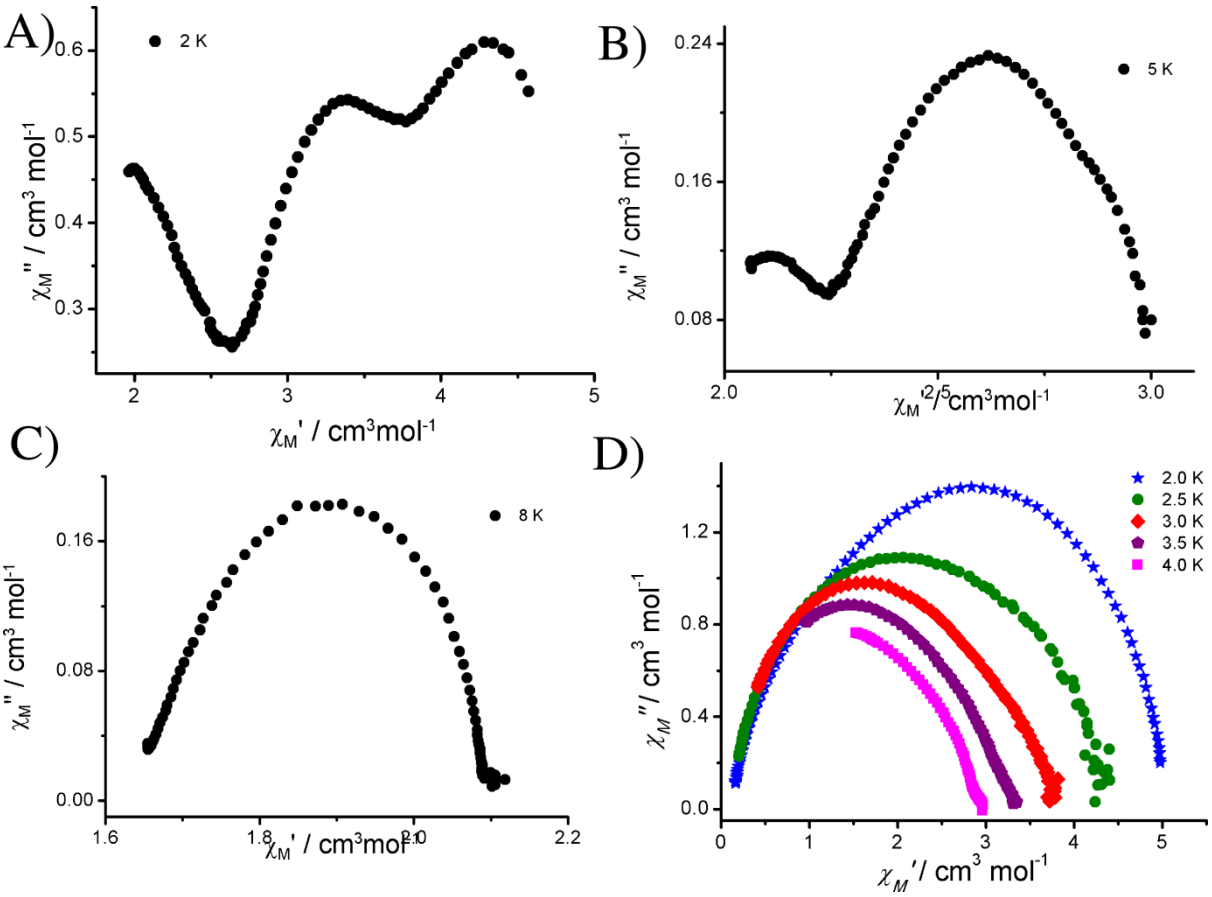


Figure S3. Cole-Cole plot for **1** at 2.0 K (A), 5.0 K (B) and 8.0 K (C); and the Cole-Cole plot for **2** at the indicated temperatures (D).

Ab initio Calculations

Ab initio calculations have been carried out on the both the parent complex **1** and **2a/2b** to compute and g-tensors and the relative energies of the ground state Kramer's doublets (KDs). All the calculations have been performed with MOLCAS 7.8.[2] quantum chemistry package. In this multi-configurational approach, relativistic effect are treated using Douglas-Kroll Hamiltonian. We have employed atomic natural (ANO-RCC) basis set for the calculation of the g-tensors. The following contraction scheme has been employed [8s7p5d3f2g1h] for Dy, [5s4p2d1f] for Zn, [3s2p1d] for N, [3s2p1d.] for O, [3s2p] for C and [2s] for H. The ground state atomic multiplicity of Dy^{III} is $^6H_{15/2}$ which results in eight low-lying Kramer's doublets. The CASSCF calculation comprises an active space of nine active electrons in seven active orbitals (CAS(9,7)). The CASSCF calculations have been performed with 21 sextets which arises from (^{6}H, ^{6}F and ^{6}P) multiplets. In the next step we have mixed these CASSCF computed spin-free states via the RASSI module to obtain the spin-orbit states. Here we have performed RASSI calculations with 21 sextet states which arise from (^{6}H, ^{6}F and ^{6}P) multiplets and extracted the relative energies of the KDs. In the last step we have used the SINGLE_ANISO code implemented in the MOLCAS to compute the g-tensors. In previous studies Luzon et al. have explored that 21 roots are good enough to obtain the *g*-tensors in Dy(III) complexes, thus this methodology has been employed throughout. [3] Furthermore our computed molar magnetic susceptibility and molar magnetization are in the excellent agreement with experimental observations adding confidence to the computed parameters.

DFT Calculations

Density functional calculations have been performed using the G09 code[4] to analyse the spin density and Mulliken charge on complexes **1** and **2a/2b**. We have employed UB3LYP[5] functional along with a double-zeta quality basis set employing the Cundari-Stevens (CS) relativistic effective core potential[6] on the Dy atom and the TZV basis set[7] on the rest of atoms. A tight SCF ($1x10^{-8}E_h$) has been employed throughout the calculations.

Table S3. Energies of the low-lying Kramer's doublets for complex **1**, the computed g-tensors and the angle between the main anisotropy axis and the excited state anisotropic axes.

Energies (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ	Sign of $g_x \cdot g_y \cdot g_z$	Magnitude of $g_x \cdot g_y \cdot g_z$
0.000	0.0225	0.0446	18.8867	0	+	9.511
91.070	11.1583	6.7744	1.2847	104.42	+	2.210
106.866	2.3233	4.3693	11.9998	70.99	-	6.761
178.486	1.8937	3.4470	11.8294	21.82	+	6.241
208.041	0.7158	1.5069	16.3630	48.94	+	4.446
229.567	1.4932	4.2892	10.0403	49.01	+	4.666
290.967	1.6938	2.9913	14.5177	88.44	+	8.305
396.140	0.1272	0.2420	18.9402	94.06	+	10.072

Table S4. Energies of low-lying Kramer's doublets for the mononuclear Dy complex **2a**, the computed g-tensors and the angle between the main anisotropy axis and the excited state anisotropic axes.

Energies (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ	Sign of $g_x \cdot g_y \cdot g_z$	Magnitude of $g_x \cdot g_y \cdot g_z$
0.000	0.0202	0.0362	19.4436	0	+	10.852
76.753	0.0446	0.0946	16.4140	6.12	+	7.743
184.268	1.4020	1.9475	13.1898	14.02	+	9.495
263.951	3.8376	6.0597	9.3941	40.30	+	5.949
301.404	0.8589	3.4604	13.3133	62.10	+	3.304
349.486	0.0741	2.3324	10.8657	107.96	+	0.345
413.726	1.3743	2.9837	12.9447	87.54	+	5.962
559.709	0.0370	0.2431	18.8295	72.81	+	2.870

Table S5. Energies of low-lying Kramer's doublets for the mononuclear Dy complex **2b**, the computed g-tensors and the angle between the main anisotropy axis and the excited state anisotropic axes.

Energies (cm^{-1})	g_{xx}	g_{yy}	g_{zz}	θ	Sign of $g_x \cdot g_y \cdot g_z$	Magnitude of $g_x \cdot g_y \cdot g_z$
0.000	0.0811	0.1209	19.0927	0	+	10.2948
46.103	0.0135	0.0887	16.8808	169.26	-	2.5765
152.959	2.4148	3.0563	12.5085	179.50	+	9.8834
207.872	1.5512	5.2612	9.1200	117.20	+	11.9097
271.244	8.0238	7.0413	1.1984	126.10	+	1.3657
332.877	1.6747	2.7763	15.0649	55.22	+	9.0874
399.793	0.9314	2.8809	13.8687	89.94	+	4.4839
455.800	0.5489	2.1600	17.6667	89.95	+	4.4898

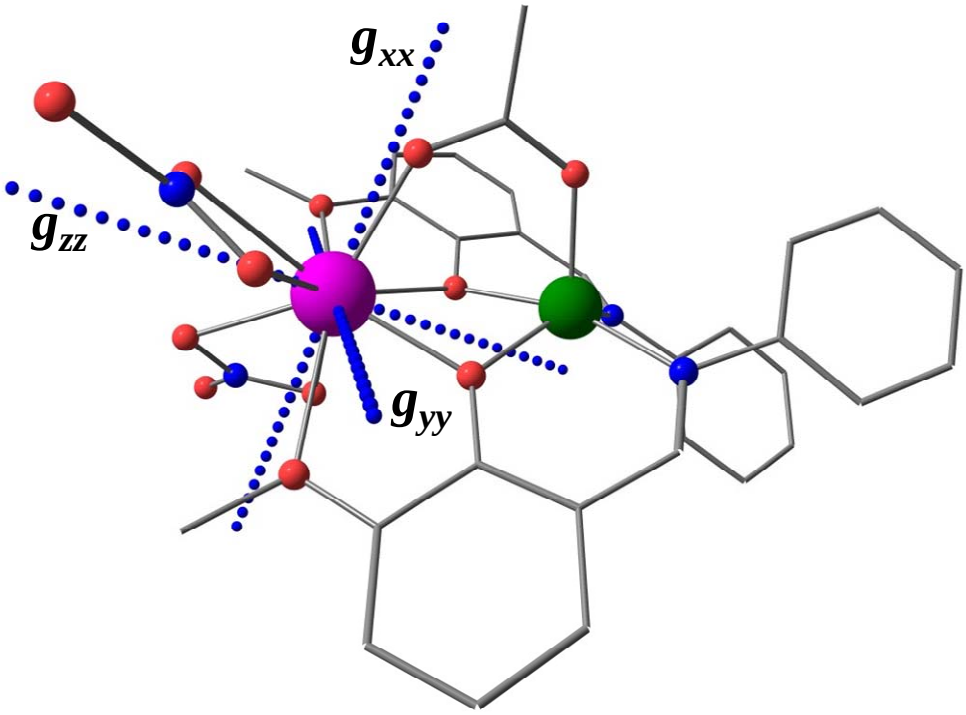


Figure S4. *Ab-initio* computed orientation of the g-tensor for complex **1**.

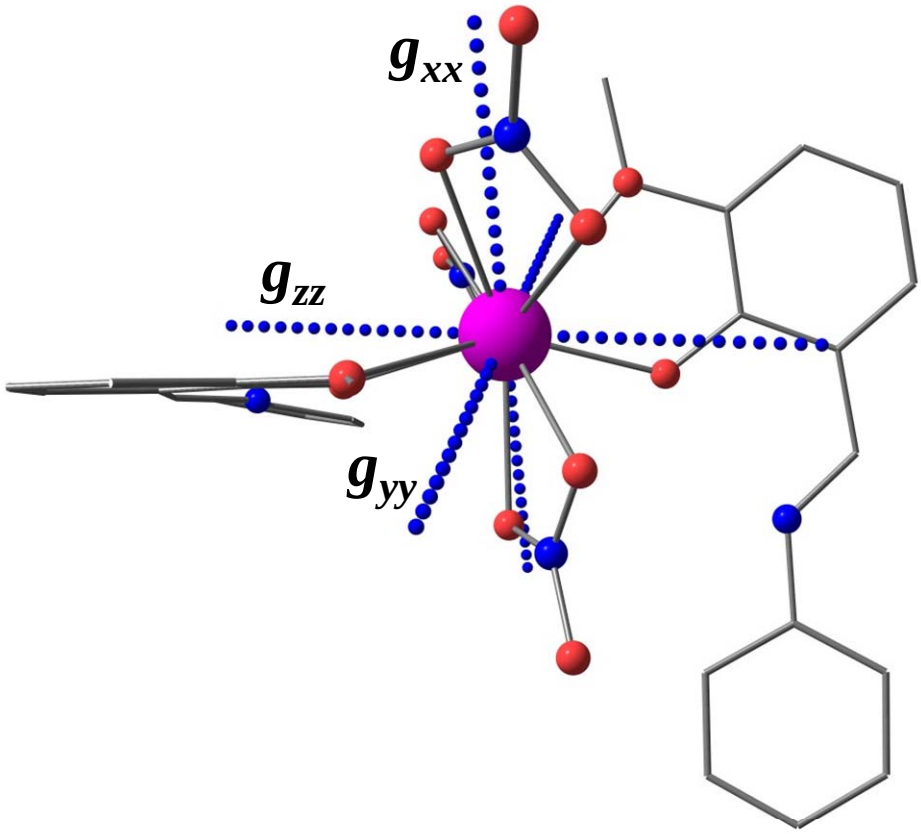


Figure S5. *Ab initio* computed orientation of the g-tensor for complex **2a**.

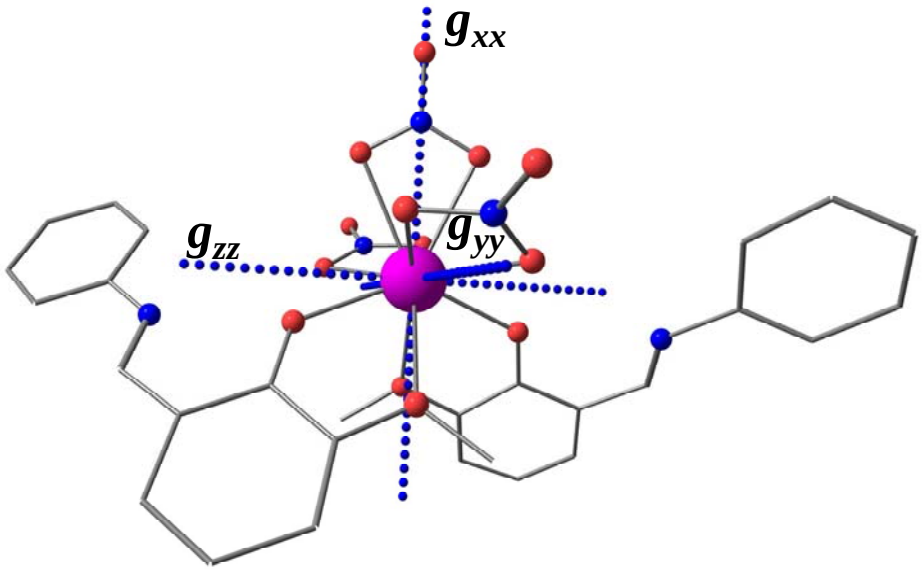


Figure S6. *Ab initio* computed orientation of the g-tensor for complex **2b**.

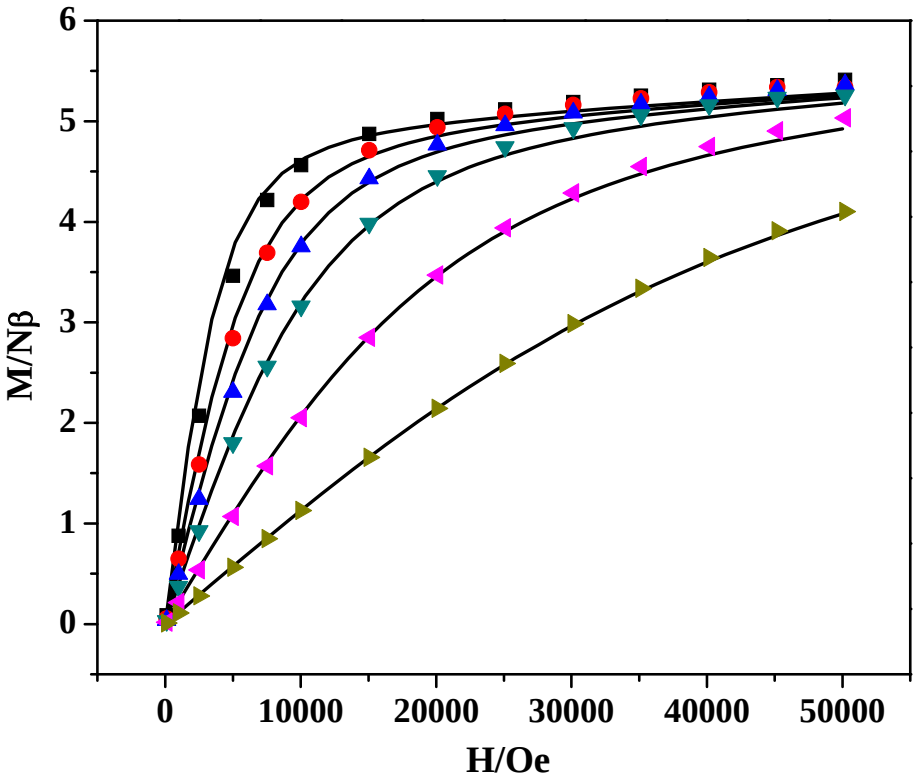


Figure S7: Field dependent magnetization measured on a polycrystalline sample of **2** at various temperatures (black squares at 2K, red circles at 3K, blue triangle at 4K, ocean blue triangle at 5.5 K, pink triangles at 10 K and light green at 20 K). The solid lines represent the calculated (using SINGLE_ANISO code) magnetization from the coordinates of **2**. Excellent

agreement between the computed and experimental data reveals the reliability of the extracted parameters from calculations.

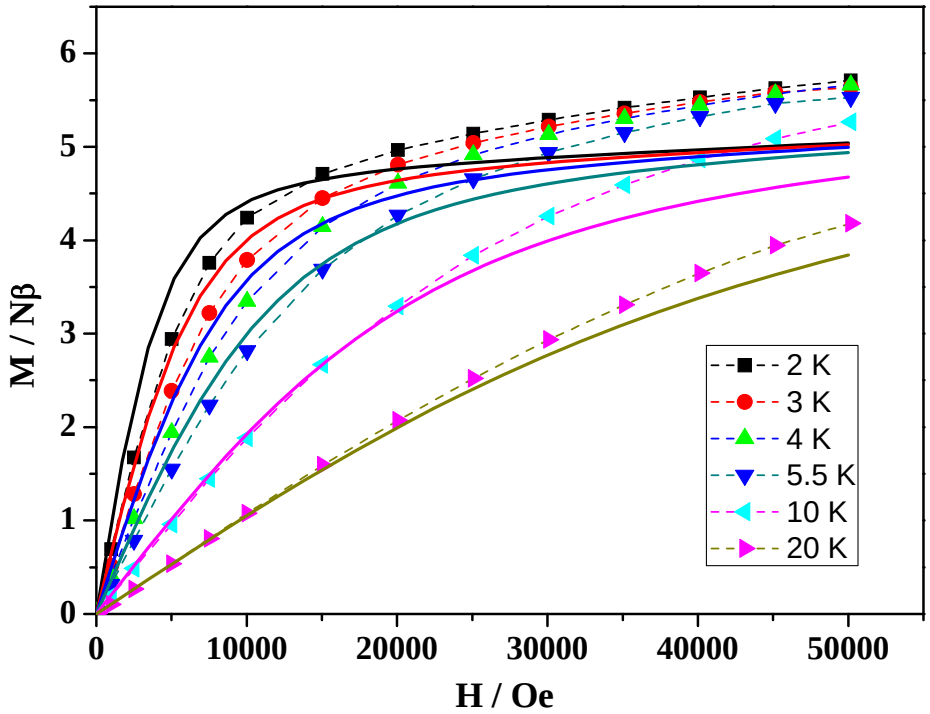


Figure S8: Field dependent magnetization measured on a polycrystalline sample of **1** at various temperatures (black squares at 2K, red circles at 3K, green triangle at 4K, blue triangle at 5.5 K, ocean blue triangles at 10 K and pink triangles at 20 K. The solid line represents the best fit obtained using the computed magnetization using SINGLE_ANISO code to the experimental magnetization data.

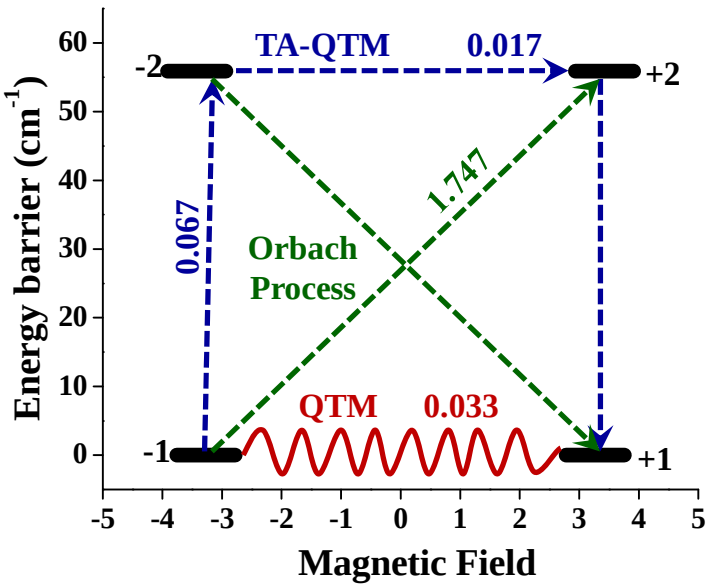


Figure S9: *Ab initio* computed matrix elements between the connecting pairs (ground state and first excited state) in complex **2b**. The thick black line indicates the Kramer's doublets (KDs) as a function of magnetic moment. The dotted green lines show the possible pathway of the Orbach process. The zig-zag lines connecting the ground state KDs represent the QTM. The dotted blues lines show the thermally activated-QTM via the first excited state.

Table S6: *Ab initio* calculated crystal field parameters for complexes **1**, **2a** and **2b**.

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

		B_q^k parameters		
k	q	Complex **1**	Complex **2a**	Complex **2b**
2	-2	1.20	-0.633×10^{-1}	0.29×10^{-2}
	-1	2.98×10^{-1}	1.94	1.56
	0	**-1.24**	**-2.39**	**-2.18**
	1	6.75×10^{-1}	-0.64	0.01
	2	-7.44×10^{-1}	-0.75	1.10
4	-4	$\mathbf{1.02 \times 10^{-2}}$	4.01×10^{-3}	-4.42×10^{-5}
	-3	$\mathbf{-2.63 \times 10^{-2}}$	-4.30×10^{-3}	6.53×10^{-3}
	-2	-6.06×10^{-4}	-0.279×10^{-3}	-2.44×10^{-5}
	-1	-6.85×10^{-3}	$\mathbf{-3.05 \times 10^{-2}}$	-5.30×10^{-4}
	0	-2.08×10^{-4}	-8.28×10^{-4}	-2.82×10^{-4}
	1	-8.36×10^{-3}	1.83×10^{-3}	-2.95×10^{-5}
	2	$\mathbf{1.73 \times 10^{-2}}$	5.93×10^{-3}	-8.11×10^{-3}
	3	$\mathbf{2.55 \times 10^{-2}}$	8.42×10^{-3}	9.79×10^{-6}
	4	-7.90×10^{-3}	5.47×10^{-3}	-6.16×10^{-3}
6	-6	-1.22×10^{-4}	-0.167×10^{-4}	-1.13×10^{-6}
	-5	1.97×10^{-4}	-3.22×10^{-5}	$\mathbf{1.30 \times 10^{-3}}$
	-4	7.71×10^{-6}	3.11×10^{-4}	2.73×10^{-6}
	-3	1.68×10^{-4}	2.55×10^{-4}	-9.18×10^{-5}
	-2	2.35×10^{-4}	-9.71×10^{-6}	1.43×10^{-6}
	-1	-5.02×10^{-5}	2.27×10^{-4}	-2.47×10^{-4}
	0	-1.73×10^{-5}	1.55×10^{-5}	1.36×10^{-5}
	1	2.20×10^{-4}	3.27×10^{-5}	9.35×10^{-7}
	2	-1.17×10^{-5}	8.47×10^{-5}	3.10×10^{-4}
	3	3.33×10^{-4}	-4.50×10^{-4}	1.70×10^{-7}
	4	9.07×10^{-5}	4.33×10^{-5}	3.29×10^{-4}
	5	2.00×10^{-4}	$\mathbf{1.37 \times 10^{-3}}$	-1.33×10^{-5}
	6	-2.57×10^{-6}	7.66×10^{-5}	-5.46×10^{-5}

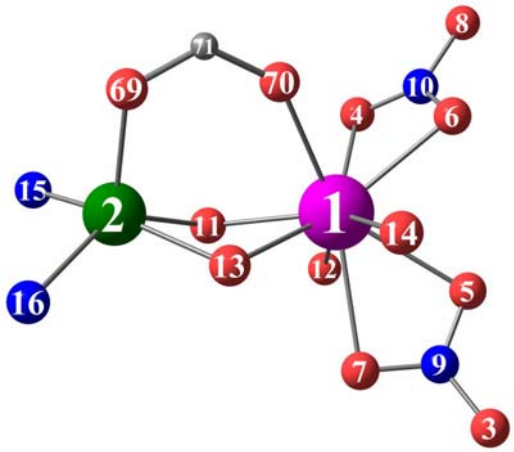


Figure S10. Labelled core structure of **1** which can be directly compared to the numbering scheme used in the DFT calculated parameters given in Table S7, below.

Table S7: DFT computed Mulliken charges on the donor atoms of complex **1** (with the hydrogen's summed in to heavy atoms)

1	Dy	1.585752	28	C	-0.158094
2	Zn	1.552638	29	C	0.249460
3	O	-0.131490	31	C	0.017817
4	O	-0.190835	33	C	-0.216479
5	O	-0.299307	34	C	0.065392
6	O	-0.152187	36	C	-0.041291
7	O	-0.228921	38	C	-0.170282
8	O	-0.269425	40	C	-0.212417
9	N	0.038965	41	C	0.170044
10	N	0.037350	43	C	0.177266
11	O	-0.735974	45	C	0.019365
12	O	-0.269220	47	C	-0.098496
13	O	-0.606043	49	C	-0.142316
14	O	-0.328604	51	C	0.024997
15	N	-0.173888	53	C	0.144515
16	N	-0.215378	55	C	-0.086307
17	C	-0.050217	57	C	0.206861

19 C 0.503204	61 C 0.230424
20 C -0.079621	65 C 0.241814
21 C 0.465307	67 C -0.063736
22 C -0.043196	69 O -0.509947
24 C -0.160386	70 O -0.403975
25 C 0.271701	71 C 0.254657
27 C -0.210728	72 C -0.008769

1 Dy 1.419736	31 C 0.074403

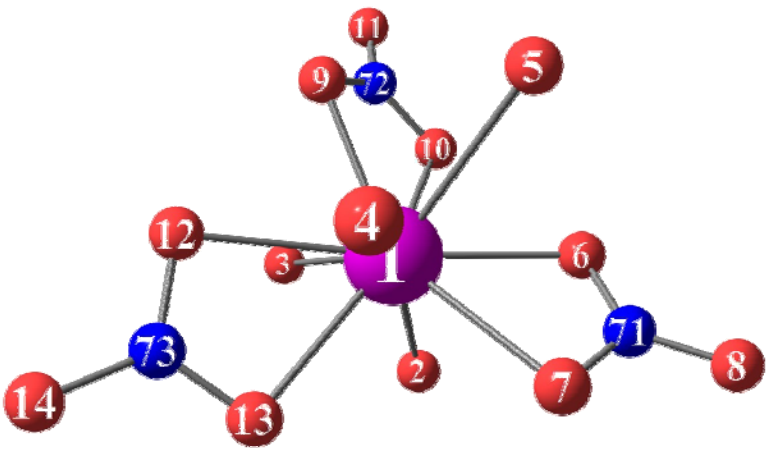


Figure S11. Labelled core structure of **2a** which can be directly compared to the numbering scheme used in the DFT calculated parameters given in Table S8, below.

Table S8: DFT computed Mulliken charges on the donor atoms of complex **2a** (with the hydrogen's summed in to heavy atoms)

2	O	-0.545689	33	C	-0.036540
3	O	-0.261270	35	C	0.195978
4	O	-0.536477	37	C	0.288781
5	O	-0.242812	41	C	-0.095152
6	O	-0.213243	42	C	0.271425
7	O	-0.263967	43	C	-0.135910
8	O	-0.143050	44	C	0.214098
9	O	-0.205109	46	C	0.014762
10	O	-0.278023	48	C	-0.013345
11	O	-0.131039	50	C	0.033558
12	O	-0.217054	52	C	-0.107711
13	O	-0.258188	53	C	0.132945
14	O	-0.141340	55	C	-0.015042
15	C	-0.141484	57	C	0.016562
16	C	0.342541	59	C	0.018319
17	C	-0.171014	61	C	0.126918
18	C	0.228448	63	C	0.286019
20	C	-0.005117	67	N	0.230989
22	C	0.043788	69	N	0.247370
24	C	-0.001194	71	N	-0.006802
26	C	-0.190404	72	N	0.000568
27	C	0.254133	73	N	0.004168
29	C	-0.088533			
1	Dy	1.543299	37	C	0.122974

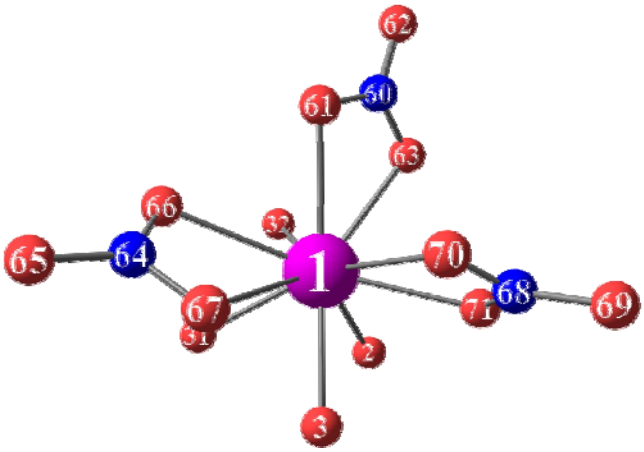


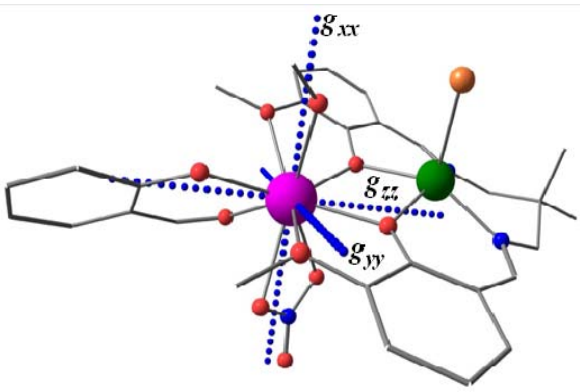
Figure S12. Labelled core structure of **2b** which can be directly compared to the numbering scheme used in the DFT calculated parameters given in Table S9, below.

Table S9: DFT computed Mulliken charges on the donor atoms of complex **2b** (with the hydrogen's summed in to heavy atoms)

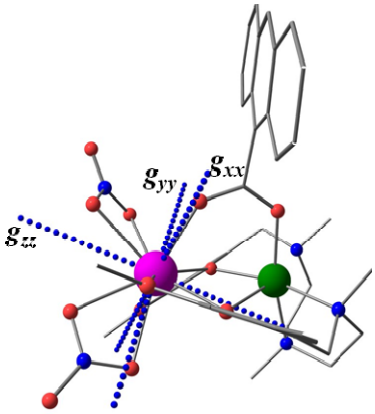
2	O	-0.269801	39	C	0.042437
3	O	-0.303712	41	C	0.228514
4	N	0.336286	43	C	-0.409656
5	C	-0.132264	45	C	-0.472147
6	C	0.205393	46	C	0.147803
7	C	0.117533	48	C	0.015635
8	C	0.082739	50	C	0.052543
10	C	0.037885	52	C	-0.021126
12	C	0.248076	54	C	0.259133
14	C	-0.418457	56	C	0.225719
16	C	-0.444310	60	N	0.030995
17	C	0.115996	61	O	-0.226798
19	C	0.057035	62	O	-0.142786
21	C	0.012760	63	O	-0.292574
23	C	0.014057	64	N	0.048163
25	C	0.252959	65	O	-0.145336
27	C	0.247478	66	O	-0.258735
31	O	-0.231675	67	O	-0.292638
32	O	-0.329656	68	N	0.008496
33	N	0.360251	69	O	-0.112333
34	C	-0.134407	70	O	-0.256021
35	C	0.238985	71	O	-0.248707
36	C	0.089996			

Table S10: *Ab initio* computed list of ZnDy complexes which are structurally related to complex **1** available in Cambridge structural database (CSD).

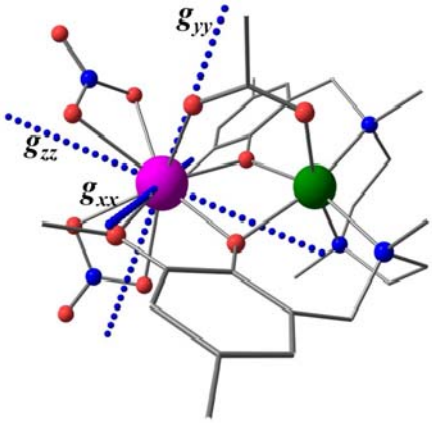
S. No	Molecular formula	Coordination number of Dy^{III}	RefCode	U_{eff} (applied field) cm^{-1}		*Computed Ground State g-tensor values*			Reference
				Experimental	**Calculated**	g_{xx}	g_{yy}	g_{zz}	
1	$ZnBr(Hsal)(L)Dy(NO_3)(CH_3OH)$	9	EWEPAY	231, 63	193.909	0.0019	0.0026	19.9391	[8]
2	$[Zn(\mu\text{-}L)(\mu\text{-}9\text{-}An)Dy(NO_3)_2]$	9	TISZAY	46.18 (0.1 Tesla)	82.654	0.0231	0.0408	18.8101	[9]
3	$[Zn(\mu\text{-}L)(\mu\text{-}OAc)Dy(NO_3)_2]$	9	ICAFEZ	--	99.967	0.0317	0.0477	19.1094	[10]
5	Complex **1** $[ZnDy(L)_2(NO_3)_2(OAc)]$	9	this paper	83.0 (0.35 Tesla)	91.070	0.0225	0.0446	18.8867	this paper
4	$[LZnDy(OAc)_3]$	9	YUWQEN	--	121.258	0.0300	0.0379	19.3960	[11]



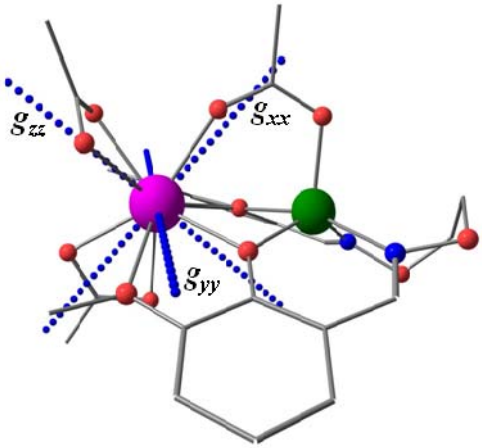
Ref Code: **EWEPAY**



Ref Code: **TISZAY**



Ref Code: **ICAFEZ**



Ref Code: **YUWQEN**

Figure S13. *Ab initio* computed orientation of the *g*-tensors for the structurally related complexes that are listed in Table S10.

Table S11: List of several dysprosium(III) monomeric complexes (field induced Single ion magnets) reported in literature, along with their effective energy barrier

S. No	Molecular formula	Coordination number of Dy^{III}	U_{eff} (applied field) cm^{-1}	Reference
1	$[Dy(H_2L)(NO_3)_3]$	9	6, 22 (0.1 Tesla)	[12]
2	$[Dy(hmb)(NO_3)_2(DMF)_2]$	9	23.6 (0.18 Tesla)	[13]
3	$[Dy(paaH)_2(NO_3)_2(MeOH)][NO_3]$	9	44.0 (0.2 Tesla)	[14]
4	$[Dy(9\ Accm)_2\text{-}(NO_3)(dmf)_2]$	8	16.0 (0.1 Tesla)	[15]
5	$[Dy(NTA)_3L]$	8	21.0 (0.2 Tesla)	[16]
6	[Dy(trensal)]	7	42.0 (0.09 Tesla)	[17]
7	$[K(DME)_2][Y(tmtaa)_2]_{0.95}[Dy(tmtaa)_2]_{0.05}$	8	19.7 (0.1 Tesla)	[18]
8	$[K(DME)\text{-}(18\text{-crown-}6)]\ [Y(tmtaa)_2]_{0.95}\ [Dy(tmtaa)_2]_{0.05}$	8	24 (0.01 Tesla)	[18]
9	$[Dy(TTA)_3(L_3)]$	8	28.5 (0.2 Tesla)	[19]
10	$Dy\text{-}(H_2BPz_{Me22})_3$	6	17 (0.1 Tesla)	[20]

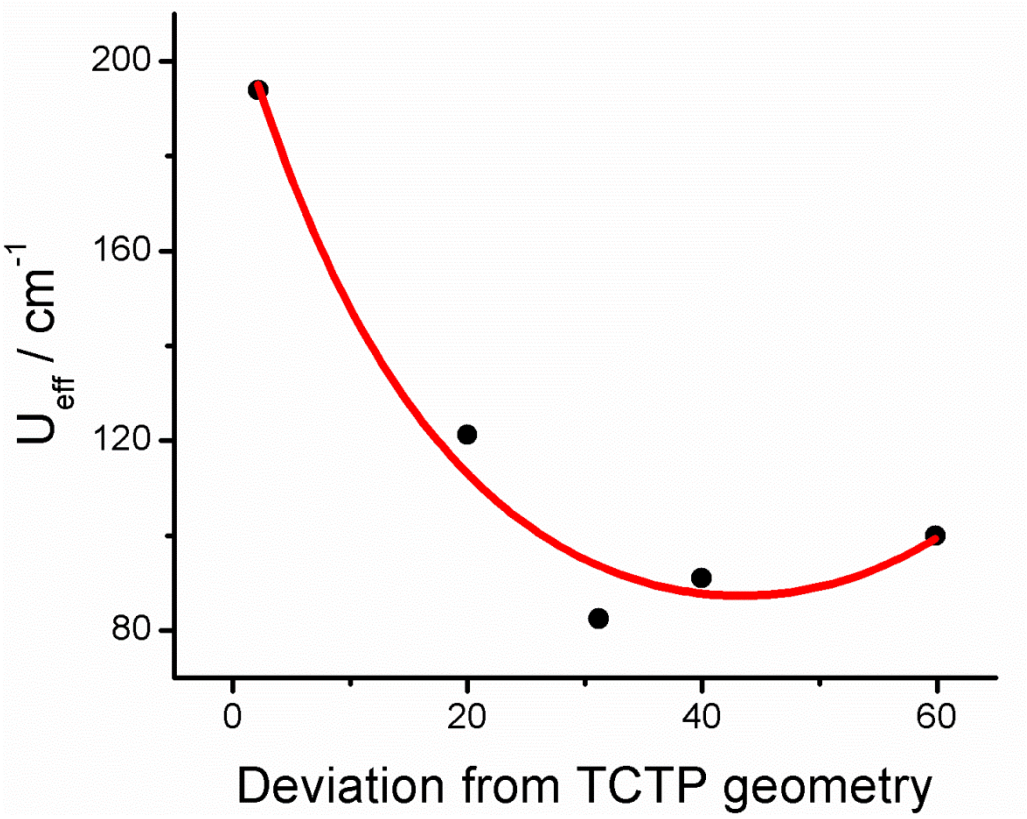


Fig S14. Plot of computed energy barrier for the complexes listed in Table S10 against the deviation from the ideal tricapped trigonal prism (TCTP) geometry calculated using continuous shape measurement software.

Crystallographic information file for 1.

```
data_shelxl

_audit_creation_method           SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common            ?
_chemical_melting_point          ?
_chemical_formula_moiety         ?
_chemical_formula_sum
 'C32 H27 Dy N4 O14 Zn'
_chemical_formula_weight         919.45

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Dy'  'Dy'  -0.1892   4.4098
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Zn'  'Zn'   0.2839   1.4301
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting           Triclinic
_symmetry_space_group_name_H-M    P-1

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                   11.132(5)
_cell_length_b                   12.522(6)
_cell_length_c                   13.219(6)
_cell_angle_alpha                105.8880(10)
_cell_angle_beta                 91.753(5)
_cell_angle_gamma                94.464(6)
_cell_volume                     1764.3(14)
_cell_formula_units_Z            2
```

```
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     3658
_cell_measurement_theta_min       3.1
_cell_measurement_theta_max       29.2

_exptl_crystal_description        Block
_exptl_crystal_colour             Yellow
_exptl_crystal_size_max           0.41
_exptl_crystal_size_mid           0.21
_exptl_crystal_size_min           0.07
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.731
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              910
_exptl_absorpt_coefficient_mu     2.854
_exptl_absorpt_correction_type    'Numerical'
_exptl_absorpt_correction_T_min   0.3874
_exptl_absorpt_correction_T_max   0.8252
_exptl_absorpt_process_details    ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       100(2)
_diffrn_radiation_wavelength      0.71075
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type
;
Rigaku Saturn724+ (4x4 bin mode)
;
_diffrn_measurement_method        'profile data from \w-scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_reflns_number             29756
_diffrn_reflns_av_R_equivalents   0.0361
_diffrn_reflns_av_sigmaI/netI     0.0340
_diffrn_reflns_limit_h_min        -14
_diffrn_reflns_limit_h_max        15
_diffrn_reflns_limit_k_min        -13
_diffrn_reflns_limit_k_max        17
_diffrn_reflns_limit_l_min        -18
_diffrn_reflns_limit_l_max        17
_diffrn_reflns_theta_min          3.08
_diffrn_reflns_theta_max          29.17
_reflns_number_total              9054
_reflns_number_gt                 8566
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection
;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
;
```

```
_computing_cell_refinement
;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
;
_computing_data_reduction
;
CrystalClear-SM Expert 2.1 b24 (Rigaku, 2012)
;
_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

_refine_special_details
;
 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.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0547P)^2^+10.5826P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          9054
_refine_ls_number_parameters      469
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0370
_refine_ls_R_factor_gt            0.0348
_refine_ls_wR_factor_ref          0.0910
_refine_ls_wR_factor_gt           0.0889
_refine_ls_goodness_of_fit_ref    0.802
_refine_ls_restrained_S_all       0.802
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
```

```
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Dy1 Dy 0.282026(12) 0.304209(13) 0.170280(11) 0.01731(5) Uani 1 1 d . . .
Zn2 Zn 0.49520(3) 0.19006(3) 0.29115(3) 0.01625(8) Uani 1 1 d . . .
O5 O 0.2966(3) 0.6405(3) 0.2061(3) 0.0432(8) Uani 1 1 d . . .
O6 O 0.4549(2) 0.2134(2) 0.14994(17) 0.0189(4) Uani 1 1 d . . .
O7 O 0.3994(2) 0.3084(2) 0.00752(18) 0.0201(5) Uani 1 1 d . . .
O8 O 0.3544(2) 0.1021(2) 0.32837(18) 0.0194(4) Uani 1 1 d . . .
O9 O 0.1942(2) 0.1607(2) 0.0186(2) 0.0261(5) Uani 1 1 d . . .
O10 O 0.2141(2) 0.4707(2) 0.1284(2) 0.0264(5) Uani 1 1 d . . .
O11 O 0.2111(2) 0.1610(2) 0.2396(2) 0.0231(5) Uani 1 1 d . . .
O12 O 0.3987(2) 0.3328(2) 0.32316(18) 0.0187(4) Uani 1 1 d . . .
O13 O 0.1922(2) 0.4157(2) 0.3319(2) 0.0228(5) Uani 1 1 d . . .
O15 O 0.0723(2) 0.2718(2) 0.1153(2) 0.0251(5) Uani 1 1 d . . .
O20 O 0.3915(2) 0.4954(2) 0.2071(2) 0.0297(6) Uani 1 1 d . . .
O37 O 0.8509(3) 0.3575(3) 0.1637(2) 0.0462(9) Uani 1 1 d . . .
O46 O -0.0196(4) 0.1258(5) -0.0302(4) 0.0815(15) Uani 1 1 d . . .
O49 O 0.9309(4) 0.2760(3) -0.1911(3) 0.0576(10) Uani 1 1 d . . .
N4 N 0.3020(3) 0.5382(3) 0.1806(3) 0.0272(6) Uani 1 1 d . . .
N16 N 0.6070(2) 0.0674(2) 0.2184(2) 0.0171(5) Uani 1 1 d . . .
N18 N 0.5951(2) 0.2728(2) 0.4288(2) 0.0179(5) Uani 1 1 d . . .
N27 N 0.0880(3) 0.1884(3) 0.0379(3) 0.0351(8) Uani 1 1 d . . .
C3 C 0.9163(3) 0.2359(3) 0.3739(3) 0.0293(8) Uani 1 1 d . . .
H3 H 0.9690 0.2373 0.3190 0.035 Uiso 1 1 calc R . .
C14 C 0.5136(3) 0.1831(3) 0.0624(2) 0.0156(5) Uani 1 1 d . . .
C17 C 0.6007(3) 0.1063(3) 0.0457(2) 0.0168(6) Uani 1 1 d . . .
C19 C 0.2467(3) 0.1012(3) 0.2953(2) 0.0184(6) Uani 1 1 d . . .
C21 C 0.3612(3) 0.3728(3) 0.4178(3) 0.0180(6) Uani 1 1 d . . .
C22 C 0.6551(3) 0.0776(3) -0.0527(2) 0.0187(6) Uani 1 1 d . . .
H22 H 0.7126 0.0239 -0.0654 0.022 Uiso 1 1 calc R . .
C23 C 0.4277(3) 0.3749(3) 0.5107(3) 0.0195(6) Uani 1 1 d . . .
C24 C 0.5812(3) -0.0333(3) 0.3506(3) 0.0211(6) Uani 1 1 d . . .
H24 H 0.5041 -0.0059 0.3625 0.025 Uiso 1 1 calc R . .
C25 C 0.6535(3) -0.0027(3) 0.2772(2) 0.0180(6) Uani 1 1 d . . .
C26 C 0.7179(3) 0.2508(3) 0.4430(3) 0.0204(6) Uani 1 1 d . . .
C28 C 0.5393(3) 0.2052(3) -0.1136(2) 0.0206(6) Uani 1 1 d . . .
H28 H 0.5190 0.2392 -0.1670 0.025 Uiso 1 1 calc R . .
C29 C 0.6250(3) 0.1270(3) -0.1300(2) 0.0208(6) Uani 1 1 d . . .
H29 H 0.6630 0.1078 -0.1951 0.025 Uiso 1 1 calc R . .
C30 C 0.2486(3) 0.4201(3) 0.4285(3) 0.0207(6) Uani 1 1 d . . .
C31 C 0.7349(3) -0.1429(3) 0.3906(3) 0.0273(7) Uani 1 1 d . . .
H31 H 0.7618 -0.1922 0.4280 0.033 Uiso 1 1 calc R . .
C32 C 0.3819(3) 0.4247(3) 0.6101(3) 0.0239(7) Uani 1 1 d . . .
H32 H 0.4286 0.4291 0.6727 0.029 Uiso 1 1 calc R . .
C33 C 0.6359(3) 0.0487(3) 0.1212(2) 0.0172(6) Uani 1 1 d . . .
H33 H 0.6863 -0.0099 0.0967 0.021 Uiso 1 1 calc R . .
C34 C 0.1548(3) 0.0189(3) 0.3215(3) 0.0236(7) Uani 1 1 d . . .
H34A H 0.0752 0.0256 0.2914 0.028 Uiso 1 1 calc R . .
H34B H 0.1520 0.0346 0.3982 0.028 Uiso 1 1 calc R . .
H34C H 0.1777 -0.0570 0.2921 0.028 Uiso 1 1 calc R . .
C35 C 0.4850(3) 0.2320(3) -0.0193(2) 0.0178(6) Uani 1 1 d . . .
```

C36 C 0.7690(3) -0.0388(3) 0.2634(3) 0.0227(6) Uani 1 1 d . . .
H36 H 0.8202 -0.0152 0.2160 0.027 Uiso 1 1 calc R . .
C38 C 0.7596(3) 0.2254(3) 0.5337(3) 0.0264(7) Uani 1 1 d . . .
H38 H 0.7063 0.2194 0.5870 0.032 Uiso 1 1 calc R . .
C39 C 0.9587(4) 0.2151(3) 0.4651(4) 0.0328(8) Uani 1 1 d . . .
H39 H 1.0417 0.2049 0.4738 0.039 Uiso 1 1 calc R . .
C40 C 0.5473(3) 0.3363(3) 0.5087(3) 0.0203(6) Uani 1 1 d . . .
H40 H 0.5955 0.3601 0.5727 0.024 Uiso 1 1 calc R . .
C41 C 0.6222(3) -0.1040(3) 0.4064(3) 0.0250(7) Uani 1 1 d . . .
H41 H 0.5723 -0.1257 0.4558 0.030 Uiso 1 1 calc R . .
C42 C 0.2709(4) 0.4666(3) 0.6169(3) 0.0277(7) Uani 1 1 d . . .
H42 H 0.2399 0.4969 0.6839 0.033 Uiso 1 1 calc R . .
C43 C 0.7850(4) 0.3742(3) 0.0787(3) 0.0296(8) Uani 1 1 d . . .
C44 C 0.7950(3) 0.2551(3) 0.3628(3) 0.0214(6) Uani 1 1 d . . .
H44 H 0.7653 0.2709 0.3008 0.026 Uiso 1 1 calc R . .
C45 C 0.8085(3) -0.1098(3) 0.3198(3) 0.0274(7) Uani 1 1 d . . .
H45 H 0.8864 -0.1357 0.3097 0.033 Uiso 1 1 calc R . .
C47 C 0.3619(4) 0.3557(4) -0.0744(3) 0.0313(8) Uani 1 1 d . . .
H47A H 0.3017 0.4083 -0.0482 0.038 Uiso 1 1 calc R . .
H47B H 0.3265 0.2961 -0.1349 0.038 Uiso 1 1 calc R . .
H47C H 0.4319 0.3949 -0.0960 0.038 Uiso 1 1 calc R . .
C48 C 0.0848(3) 0.4737(3) 0.3356(3) 0.0265(7) Uani 1 1 d . . .
H48A H 0.0530 0.4658 0.2637 0.032 Uiso 1 1 calc R . .
H48B H 0.1045 0.5529 0.3718 0.032 Uiso 1 1 calc R . .
H48C H 0.0240 0.4419 0.3737 0.032 Uiso 1 1 calc R . .
C54 C 0.2040(3) 0.4645(3) 0.5253(3) 0.0257(7) Uani 1 1 d . . .
H54 H 0.1276 0.4939 0.5299 0.031 Uiso 1 1 calc R . .
C55 C 0.8819(4) 0.2091(3) 0.5442(3) 0.0323(8) Uani 1 1 d . . .
H55 H 0.9124 0.1936 0.6061 0.039 Uiso 1 1 calc R . .
C58 C 1.0285(5) 0.3579(5) -0.1473(5) 0.0574(14) Uani 1 1 d . . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Dy1 0.01501(8) 0.02107(9) 0.01714(8) 0.00647(6) 0.00172(5) 0.00484(5)
Zn2 0.01645(16) 0.02044(19) 0.01321(16) 0.00576(14) 0.00223(12) 0.00529(13)
O5 0.058(2) 0.0261(15) 0.0485(19) 0.0155(14) 0.0096(16) 0.0008(14)
O6 0.0194(10) 0.0270(12) 0.0131(10) 0.0080(9) 0.0052(8) 0.0094(9)
O7 0.0199(11) 0.0265(12) 0.0177(10) 0.0103(10) 0.0030(8) 0.0093(9)
O8 0.0183(10) 0.0234(12) 0.0182(10) 0.0079(9) 0.0032(8) 0.0037(9)
O9 0.0225(12) 0.0301(14) 0.0231(12) 0.0014(11) 0.0035(9) 0.0060(10)
O10 0.0253(12) 0.0274(13) 0.0305(13) 0.0132(11) 0.0037(10) 0.0063(10)
O11 0.0194(11) 0.0264(13) 0.0256(12) 0.0109(10) -0.0003(9) 0.0018(9)
O12 0.0182(10) 0.0223(12) 0.0158(10) 0.0043(9) 0.0031(8) 0.0057(9)
O13 0.0210(11) 0.0252(13) 0.0219(11) 0.0040(10) 0.0037(9) 0.0095(9)
O15 0.0216(11) 0.0248(13) 0.0272(12) 0.0032(10) -0.0023(9) 0.0071(9)
O20 0.0277(13) 0.0316(14) 0.0312(14) 0.0123(12) -0.0029(10) 0.0001(11)
O37 0.0365(16) 0.081(3) 0.0250(14) 0.0147(16) 0.0031(12) 0.0262(16)
O46 0.053(3) 0.086(3) 0.089(4) 0.000(3) -0.018(2) -0.006(2)
O49 0.060(2) 0.053(2) 0.056(2) 0.0087(19) -0.0106(19) 0.0104(18)

N4 0.0350(16) 0.0247(16) 0.0241(14) 0.0100(13) 0.0072(12) 0.0014(12)
N16 0.0163(11) 0.0191(13) 0.0171(12) 0.0065(10) 0.0008(9) 0.0040(10)
N18 0.0171(12) 0.0201(13) 0.0179(12) 0.0077(11) 0.0009(9) 0.0012(10)
N27 0.0338(17) 0.040(2) 0.0329(18) 0.0123(16) -0.0017(14) 0.0028(15)
C3 0.0238(17) 0.0247(18) 0.035(2) 0.0037(16) 0.0013(14) -0.0043(13)
C14 0.0148(13) 0.0186(15) 0.0127(12) 0.0034(11) 0.0013(10) 0.0012(11)
C17 0.0146(13) 0.0206(15) 0.0154(13) 0.0055(12) -0.0005(10) 0.0010(11)
C19 0.0235(15) 0.0177(15) 0.0140(13) 0.0031(12) 0.0055(11) 0.0049(12)
C21 0.0193(14) 0.0153(14) 0.0188(14) 0.0031(12) 0.0042(11) 0.0023(11)
C22 0.0186(14) 0.0204(15) 0.0151(13) 0.0015(12) 0.0022(11) 0.0024(11)
C23 0.0210(14) 0.0175(15) 0.0188(14) 0.0034(12) 0.0023(11) -0.0002(11)
C24 0.0259(16) 0.0219(16) 0.0163(14) 0.0057(13) 0.0001(12) 0.0057(12)
C25 0.0198(14) 0.0172(15) 0.0164(13) 0.0037(12) -0.0030(11) 0.0036(11)
C26 0.0198(14) 0.0177(15) 0.0226(15) 0.0048(13) -0.0031(12) -0.0001(11)
C28 0.0222(15) 0.0257(17) 0.0144(13) 0.0065(13) 0.0004(11) 0.0015(12)
C29 0.0212(14) 0.0258(17) 0.0137(13) 0.0027(13) 0.0021(11) 0.0017(12)
C30 0.0200(14) 0.0184(15) 0.0233(15) 0.0046(13) 0.0037(12) 0.0019(12)
C31 0.0323(18) 0.0241(17) 0.0274(17) 0.0113(15) -0.0105(14) 0.0028(14)
C32 0.0308(17) 0.0228(17) 0.0166(14) 0.0024(13) 0.0051(12) 0.0023(13)
C33 0.0152(13) 0.0186(15) 0.0178(14) 0.0050(12) -0.0015(10) 0.0024(11)
C34 0.0227(15) 0.0237(17) 0.0246(16) 0.0080(14) 0.0049(12) -0.0015(12)
C35 0.0172(13) 0.0211(15) 0.0155(13) 0.0057(12) -0.0016(11) 0.0035(11)
C36 0.0193(15) 0.0257(17) 0.0246(16) 0.0084(14) 0.0001(12) 0.0054(12)
C38 0.0287(17) 0.0252(18) 0.0265(17) 0.0105(15) -0.0054(13) 0.0006(14)
C39 0.0240(17) 0.0233(18) 0.048(2) 0.0041(17) -0.0075(16) 0.0054(14)
C40 0.0243(15) 0.0204(16) 0.0163(14) 0.0056(12) -0.0003(11) 0.0000(12)
C41 0.0292(17) 0.0267(18) 0.0208(15) 0.0101(14) -0.0023(13) 0.0025(14)
C42 0.0323(18) 0.0270(18) 0.0198(15) -0.0010(14) 0.0085(13) 0.0021(14)
C43 0.0292(18) 0.0297(19) 0.0316(19) 0.0113(16) -0.0054(15) 0.0049(14)
C44 0.0205(15) 0.0158(15) 0.0269(16) 0.0043(13) 0.0027(12) 0.0009(11)
C45 0.0259(17) 0.0261(18) 0.0319(18) 0.0100(15) -0.0048(14) 0.0085(14)
C47 0.0354(19) 0.045(2) 0.0234(17) 0.0209(17) 0.0063(14) 0.0194(17)
C48 0.0198(15) 0.0233(17) 0.0362(19) 0.0051(15) 0.0058(14) 0.0095(13)
C54 0.0238(16) 0.0231(17) 0.0279(17) 0.0014(14) 0.0083(13) 0.0052(13)
C55 0.0332(19) 0.0267(19) 0.037(2) 0.0102(16) -0.0124(16) 0.0056(15)
C58 0.045(3) 0.060(4) 0.067(4) 0.019(3) -0.005(3) 0.006(2)

_geom_special_details
;
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.
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
Dy1 O6 2.296(2) . ?
Dy1 O12 2.296(2) . ?

Dy1 O11 2.325(3) . ?
Dy1 O15 2.394(3) . ?
Dy1 O9 2.416(3) . ?
Dy1 O10 2.466(3) . ?
Dy1 O13 2.495(3) . ?
Dy1 O20 2.516(3) . ?
Dy1 O7 2.562(2) . ?
Dy1 N27 2.779(4) . ?
Dy1 N4 2.886(3) . ?
Dy1 Zn2 3.4312(10) . ?
Zn2 O8 1.997(2) . ?
Zn2 O6 2.010(2) . ?
Zn2 N18 2.071(3) . ?
Zn2 N16 2.096(3) . ?
Zn2 O12 2.107(2) . ?
O5 N4 1.238(4) . ?
O6 C14 1.325(4) . ?
O7 C35 1.389(4) . ?
O7 C47 1.435(4) . ?
O8 C19 1.262(4) . ?
O9 N27 1.271(4) . ?
O10 N4 1.288(4) . ?
O11 C19 1.260(4) . ?
O12 C21 1.309(4) . ?
O13 C30 1.392(4) . ?
O13 C48 1.442(4) . ?
O15 N27 1.274(5) . ?
O20 N4 1.252(4) . ?
O37 C43 1.396(5) . ?
O46 N27 1.504(6) . ?
O49 C58 1.425(7) . ?
N16 C33 1.297(4) . ?
N16 C25 1.437(4) . ?
N18 C40 1.292(5) . ?
N18 C26 1.432(4) . ?
C3 C39 1.378(6) . ?
C3 C44 1.400(5) . ?
C3 H3 0.9500 . ?
C14 C17 1.398(4) . ?
C14 C35 1.420(4) . ?
C17 C22 1.419(4) . ?
C17 C33 1.444(4) . ?
C19 C34 1.511(5) . ?
C21 C23 1.407(4) . ?
C21 C30 1.421(4) . ?
C22 C29 1.376(4) . ?
C22 H22 0.9500 . ?
C23 C32 1.420(5) . ?
C23 C40 1.451(5) . ?
C24 C25 1.391(5) . ?
C24 C41 1.392(4) . ?
C24 H24 0.9500 . ?
C25 C36 1.396(4) . ?
C26 C44 1.393(5) . ?
C26 C38 1.397(5) . ?

C28 C35 1.370(4) . ?
C28 C29 1.400(5) . ?
C28 H28 0.9500 . ?
C29 H29 0.9500 . ?
C30 C54 1.373(5) . ?
C31 C41 1.382(5) . ?
C31 C45 1.387(6) . ?
C31 H31 0.9500 . ?
C32 C42 1.375(5) . ?
C32 H32 0.9500 . ?
C33 H33 0.9500 . ?
C34 H34A 0.9800 . ?
C34 H34B 0.9800 . ?
C34 H34C 0.9800 . ?
C36 C45 1.393(5) . ?
C36 H36 0.9500 . ?
C38 C55 1.401(5) . ?
C38 H38 0.9500 . ?
C39 C55 1.385(7) . ?
C39 H39 0.9500 . ?
C40 H40 0.9500 . ?
C41 H41 0.9500 . ?
C42 C54 1.395(5) . ?
C42 H42 0.9500 . ?
C44 H44 0.9500 . ?
C45 H45 0.9500 . ?
C47 H47A 0.9800 . ?
C47 H47B 0.9800 . ?
C47 H47C 0.9800 . ?
C48 H48A 0.9800 . ?
C48 H48B 0.9800 . ?
C48 H48C 0.9800 . ?
C54 H54 0.9500 . ?
C55 H55 0.9500 . ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O6 Dy1 O12 65.85(8) . . ?
O6 Dy1 O11 83.91(9) . . ?
O12 Dy1 O11 75.86(9) . . ?
O6 Dy1 O15 140.04(9) . . ?
O12 Dy1 O15 137.78(9) . . ?
O11 Dy1 O15 75.97(9) . . ?
O6 Dy1 O9 87.54(9) . . ?
O12 Dy1 O9 142.91(9) . . ?
O11 Dy1 O9 76.04(10) . . ?
O15 Dy1 O9 54.42(9) . . ?
O6 Dy1 O10 135.67(8) . . ?
O12 Dy1 O10 117.07(9) . . ?

O11 Dy1 O10 140.38(9) . . ?
O15 Dy1 O10 70.48(9) . . ?
O9 Dy1 O10 100.00(10) . . ?
O6 Dy1 O13 130.88(8) . . ?
O12 Dy1 O13 65.23(8) . . ?
O11 Dy1 O13 80.40(9) . . ?
O15 Dy1 O13 79.55(9) . . ?
O9 Dy1 O13 131.92(9) . . ?
O10 Dy1 O13 73.44(9) . . ?
O6 Dy1 O20 94.48(9) . . ?
O12 Dy1 O20 73.09(9) . . ?
O11 Dy1 O20 146.53(9) . . ?
O15 Dy1 O20 121.05(9) . . ?
O9 Dy1 O20 137.40(9) . . ?
O10 Dy1 O20 51.48(9) . . ?
O13 Dy1 O20 75.54(9) . . ?
O6 Dy1 O7 63.65(7) . . ?
O12 Dy1 O7 115.03(8) . . ?
O11 Dy1 O7 133.14(9) . . ?
O15 Dy1 O7 107.19(9) . . ?
O9 Dy1 O7 70.02(9) . . ?
O10 Dy1 O7 77.99(8) . . ?
O13 Dy1 O7 146.42(8) . . ?
O20 Dy1 O7 72.96(9) . . ?
O6 Dy1 N27 113.81(10) . . ?
O12 Dy1 N27 149.16(10) . . ?
O11 Dy1 N27 73.52(10) . . ?
O15 Dy1 N27 27.24(10) . . ?
O9 Dy1 N27 27.20(10) . . ?
O10 Dy1 N27 85.42(10) . . ?
O13 Dy1 N27 105.72(10) . . ?
O20 Dy1 N27 135.41(10) . . ?
O7 Dy1 N27 89.01(10) . . ?
O6 Dy1 N4 117.98(9) . . ?
O12 Dy1 N4 92.97(9) . . ?
O11 Dy1 N4 149.22(9) . . ?
O15 Dy1 N4 95.45(9) . . ?
O9 Dy1 N4 123.10(9) . . ?
O10 Dy1 N4 26.37(9) . . ?
O13 Dy1 N4 68.93(9) . . ?
O20 Dy1 N4 25.64(9) . . ?
O7 Dy1 N4 77.62(8) . . ?
N27 Dy1 N4 111.74(10) . . ?
O6 Dy1 Zn2 34.36(6) . . ?
O12 Dy1 Zn2 36.87(6) . . ?
O11 Dy1 Zn2 63.87(6) . . ?
O15 Dy1 Zn2 139.48(7) . . ?
O9 Dy1 Zn2 107.82(7) . . ?
O10 Dy1 Zn2 148.08(6) . . ?
O13 Dy1 Zn2 98.09(6) . . ?
O20 Dy1 Zn2 96.73(7) . . ?
O7 Dy1 Zn2 96.86(6) . . ?
N27 Dy1 Zn2 126.26(8) . . ?
N4 Dy1 Zn2 121.73(7) . . ?
O8 Zn2 O6 107.77(10) . . ?

O8 Zn2 N18 108.14(10) . . ?
O6 Zn2 N18 138.38(11) . . ?
O8 Zn2 N16 103.25(11) . . ?
O6 Zn2 N16 89.24(10) . . ?
N18 Zn2 N16 102.28(11) . . ?
O8 Zn2 O12 90.38(10) . . ?
O6 Zn2 O12 74.59(9) . . ?
N18 Zn2 O12 84.82(10) . . ?
N16 Zn2 O12 161.53(10) . . ?
O8 Zn2 Dy1 84.87(7) . . ?
O6 Zn2 Dy1 40.16(6) . . ?
N18 Zn2 Dy1 124.96(8) . . ?
N16 Zn2 Dy1 127.10(8) . . ?
O12 Zn2 Dy1 40.82(6) . . ?
C14 O6 Zn2 128.21(19) . . ?
C14 O6 Dy1 126.31(18) . . ?
Zn2 O6 Dy1 105.47(9) . . ?
C35 O7 C47 115.4(3) . . ?
C35 O7 Dy1 116.19(18) . . ?
C47 O7 Dy1 125.6(2) . . ?
C19 O8 Zn2 124.8(2) . . ?
N27 O9 Dy1 92.5(2) . . ?
N4 O10 Dy1 95.36(19) . . ?
C19 O11 Dy1 140.7(2) . . ?
C21 O12 Zn2 119.3(2) . . ?
C21 O12 Dy1 124.5(2) . . ?
Zn2 O12 Dy1 102.32(10) . . ?
C30 O13 C48 116.3(3) . . ?
C30 O13 Dy1 117.28(19) . . ?
C48 O13 Dy1 126.4(2) . . ?
N27 O15 Dy1 93.4(2) . . ?
N4 O20 Dy1 94.0(2) . . ?
O5 N4 O20 121.6(3) . . ?
O5 N4 O10 121.5(3) . . ?
O20 N4 O10 116.9(3) . . ?
O5 N4 Dy1 165.2(3) . . ?
O20 N4 Dy1 60.39(18) . . ?
O10 N4 Dy1 58.27(16) . . ?
C33 N16 C25 116.9(3) . . ?
C33 N16 Zn2 123.8(2) . . ?
C25 N16 Zn2 119.3(2) . . ?
C40 N18 C26 117.3(3) . . ?
C40 N18 Zn2 122.2(2) . . ?
C26 N18 Zn2 120.2(2) . . ?
O9 N27 O15 119.6(3) . . ?
O9 N27 O46 121.3(4) . . ?
O15 N27 O46 119.1(4) . . ?
O9 N27 Dy1 60.32(19) . . ?
O15 N27 Dy1 59.32(18) . . ?
O46 N27 Dy1 177.8(3) . . ?
C39 C3 C44 119.6(4) . . ?
C39 C3 H3 120.2 . . ?
C44 C3 H3 120.2 . . ?
O6 C14 C17 124.3(3) . . ?
O6 C14 C35 117.2(3) . . ?

C17 C14 C35 118.4(3) . . ?
C14 C17 C22 119.3(3) . . ?
C14 C17 C33 124.0(3) . . ?
C22 C17 C33 116.6(3) . . ?
O11 C19 O8 125.1(3) . . ?
O11 C19 C34 117.9(3) . . ?
O8 C19 C34 117.0(3) . . ?
O12 C21 C23 123.7(3) . . ?
O12 C21 C30 118.7(3) . . ?
C23 C21 C30 117.6(3) . . ?
C29 C22 C17 120.5(3) . . ?
C29 C22 H22 119.8 . . ?
C17 C22 H22 119.8 . . ?
C21 C23 C32 119.6(3) . . ?
C21 C23 C40 121.9(3) . . ?
C32 C23 C40 118.3(3) . . ?
C25 C24 C41 119.8(3) . . ?
C25 C24 H24 120.1 . . ?
C41 C24 H24 120.1 . . ?
C24 C25 C36 120.0(3) . . ?
C24 C25 N16 118.4(3) . . ?
C36 C25 N16 121.6(3) . . ?
C44 C26 C38 120.8(3) . . ?
C44 C26 N18 117.8(3) . . ?
C38 C26 N18 121.5(3) . . ?
C35 C28 C29 119.1(3) . . ?
C35 C28 H28 120.5 . . ?
C29 C28 H28 120.5 . . ?
C22 C29 C28 120.7(3) . . ?
C22 C29 H29 119.6 . . ?
C28 C29 H29 119.6 . . ?
C54 C30 O13 125.5(3) . . ?
C54 C30 C21 121.9(3) . . ?
O13 C30 C21 112.6(3) . . ?
C41 C31 C45 119.8(3) . . ?
C41 C31 H31 120.1 . . ?
C45 C31 H31 120.1 . . ?
C42 C32 C23 121.0(3) . . ?
C42 C32 H32 119.5 . . ?
C23 C32 H32 119.5 . . ?
N16 C33 C17 127.8(3) . . ?
N16 C33 H33 116.1 . . ?
C17 C33 H33 116.1 . . ?
C19 C34 H34A 109.5 . . ?
C19 C34 H34B 109.5 . . ?
H34A C34 H34B 109.5 . . ?
C19 C34 H34C 109.5 . . ?
H34A C34 H34C 109.5 . . ?
H34B C34 H34C 109.5 . . ?
C28 C35 O7 125.1(3) . . ?
C28 C35 C14 121.9(3) . . ?
O7 C35 C14 113.0(3) . . ?
C45 C36 C25 119.4(3) . . ?
C45 C36 H36 120.3 . . ?
C25 C36 H36 120.3 . . ?

C26 C38 C55 118.5(4) . . ?
C26 C38 H38 120.8 . . ?
C55 C38 H38 120.8 . . ?
C3 C39 C55 120.8(4) . . ?
C3 C39 H39 119.6 . . ?
C55 C39 H39 119.6 . . ?
N18 C40 C23 126.8(3) . . ?
N18 C40 H40 116.6 . . ?
C23 C40 H40 116.6 . . ?
C31 C41 C24 120.5(3) . . ?
C31 C41 H41 119.8 . . ?
C24 C41 H41 119.8 . . ?
C32 C42 C54 119.8(3) . . ?
C32 C42 H42 120.1 . . ?
C54 C42 H42 120.1 . . ?
C26 C44 C3 119.8(3) . . ?
C26 C44 H44 120.1 . . ?
C3 C44 H44 120.1 . . ?
C31 C45 C36 120.5(3) . . ?
C31 C45 H45 119.7 . . ?
C36 C45 H45 119.7 . . ?
O7 C47 H47A 109.5 . . ?
O7 C47 H47B 109.5 . . ?
H47A C47 H47B 109.5 . . ?
O7 C47 H47C 109.5 . . ?
H47A C47 H47C 109.5 . . ?
H47B C47 H47C 109.5 . . ?
O13 C48 H48A 109.5 . . ?
O13 C48 H48B 109.5 . . ?
H48A C48 H48B 109.5 . . ?
O13 C48 H48C 109.5 . . ?
H48A C48 H48C 109.5 . . ?
H48B C48 H48C 109.5 . . ?
C30 C54 C42 120.0(3) . . ?
C30 C54 H54 120.0 . . ?
C42 C54 H54 120.0 . . ?
C39 C55 C38 120.6(4) . . ?
C39 C55 H55 119.7 . . ?
C38 C55 H55 119.7 . . ?

loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
O6 Dy1 Zn2 O8 -125.55(13) . . . . ?
O12 Dy1 Zn2 O8 96.56(12) . . . . ?
O11 Dy1 Zn2 O8 -5.01(10) . . . . ?
O15 Dy1 Zn2 O8 -13.29(12) . . . . ?

O9 Dy1 Zn2 O8 -68.91(10) . . . . ?
O10 Dy1 Zn2 O8 141.64(14) . . . . ?
O13 Dy1 Zn2 O8 70.07(10) . . . . ?
O20 Dy1 Zn2 O8 146.35(10) . . . . ?
O7 Dy1 Zn2 O8 -140.08(9) . . . . ?
N27 Dy1 Zn2 O8 -46.26(12) . . . . ?
N4 Dy1 Zn2 O8 140.26(10) . . . . ?
O12 Dy1 Zn2 O6 -137.89(15) . . . . ?
O11 Dy1 Zn2 O6 120.54(13) . . . . ?
O15 Dy1 Zn2 O6 112.26(15) . . . . ?
O9 Dy1 Zn2 O6 56.64(13) . . . . ?
O10 Dy1 Zn2 O6 -92.81(16) . . . . ?
O13 Dy1 Zn2 O6 -164.38(13) . . . . ?
O20 Dy1 Zn2 O6 -88.10(13) . . . . ?
O7 Dy1 Zn2 O6 -14.53(13) . . . . ?
N27 Dy1 Zn2 O6 79.29(15) . . . . ?
N4 Dy1 Zn2 O6 -94.19(13) . . . . ?
O6 Dy1 Zn2 N18 125.86(14) . . . . ?
O12 Dy1 Zn2 N18 -12.03(13) . . . . ?
O11 Dy1 Zn2 N18 -113.59(12) . . . . ?
O15 Dy1 Zn2 N18 -121.88(13) . . . . ?
O9 Dy1 Zn2 N18 -177.50(11) . . . . ?
O10 Dy1 Zn2 N18 33.05(15) . . . . ?
O13 Dy1 Zn2 N18 -38.51(11) . . . . ?
O20 Dy1 Zn2 N18 37.77(11) . . . . ?
O7 Dy1 Zn2 N18 111.33(11) . . . . ?
N27 Dy1 Zn2 N18 -154.85(13) . . . . ?
N4 Dy1 Zn2 N18 31.67(12) . . . . ?
O6 Dy1 Zn2 N16 -22.80(15) . . . . ?
O12 Dy1 Zn2 N16 -160.69(13) . . . . ?
O11 Dy1 Zn2 N16 97.74(12) . . . . ?
O15 Dy1 Zn2 N16 89.46(14) . . . . ?
O9 Dy1 Zn2 N16 33.84(12) . . . . ?
O10 Dy1 Zn2 N16 -115.61(15) . . . . ?
O13 Dy1 Zn2 N16 172.82(11) . . . . ?
O20 Dy1 Zn2 N16 -110.90(12) . . . . ?
O7 Dy1 Zn2 N16 -37.33(11) . . . . ?
N27 Dy1 Zn2 N16 56.49(14) . . . . ?
N4 Dy1 Zn2 N16 -116.99(12) . . . . ?
O6 Dy1 Zn2 O12 137.89(15) . . . . ?
O11 Dy1 Zn2 O12 -101.57(12) . . . . ?
O15 Dy1 Zn2 O12 -109.85(14) . . . . ?
O9 Dy1 Zn2 O12 -165.47(12) . . . . ?
O10 Dy1 Zn2 O12 45.08(15) . . . . ?
O13 Dy1 Zn2 O12 -26.48(11) . . . . ?
O20 Dy1 Zn2 O12 49.79(12) . . . . ?
O7 Dy1 Zn2 O12 123.36(11) . . . . ?
N27 Dy1 Zn2 O12 -142.82(14) . . . . ?
N4 Dy1 Zn2 O12 43.70(12) . . . . ?
O8 Zn2 O6 C14 -121.4(3) . . . . ?
N18 Zn2 O6 C14 90.1(3) . . . . ?
N16 Zn2 O6 C14 -17.7(3) . . . . ?
O12 Zn2 O6 C14 153.3(3) . . . . ?
Dy1 Zn2 O6 C14 -179.7(3) . . . . ?
O8 Zn2 O6 Dy1 58.31(13) . . . . ?

N18 Zn2 O6 Dy1 -90.23(16) . . . . ?
N16 Zn2 O6 Dy1 161.99(11) . . . . ?
O12 Zn2 O6 Dy1 -27.04(10) . . . . ?
O12 Dy1 O6 C14 -154.2(3) . . . . ?
O11 Dy1 O6 C14 128.6(3) . . . . ?
O15 Dy1 O6 C14 69.1(3) . . . . ?
O9 Dy1 O6 C14 52.4(3) . . . . ?
O10 Dy1 O6 C14 -49.4(3) . . . . ?
O13 Dy1 O6 C14 -159.7(2) . . . . ?
O20 Dy1 O6 C14 -84.9(3) . . . . ?
O7 Dy1 O6 C14 -16.5(2) . . . . ?
N27 Dy1 O6 C14 59.7(3) . . . . ?
N4 Dy1 O6 C14 -74.2(3) . . . . ?
Zn2 Dy1 O6 C14 179.7(3) . . . . ?
O12 Dy1 O6 Zn2 26.16(10) . . . . ?
O11 Dy1 O6 Zn2 -51.04(11) . . . . ?
O15 Dy1 O6 Zn2 -110.60(14) . . . . ?
O9 Dy1 O6 Zn2 -127.26(12) . . . . ?
O10 Dy1 O6 Zn2 130.92(11) . . . . ?
O13 Dy1 O6 Zn2 20.65(16) . . . . ?
O20 Dy1 O6 Zn2 95.37(11) . . . . ?
O7 Dy1 O6 Zn2 163.86(14) . . . . ?
N27 Dy1 O6 Zn2 -120.01(12) . . . . ?
N4 Dy1 O6 Zn2 106.14(11) . . . . ?
O6 Dy1 O7 C35 15.6(2) . . . . ?
O12 Dy1 O7 C35 58.3(2) . . . . ?
O11 Dy1 O7 C35 -35.6(3) . . . . ?
O15 Dy1 O7 C35 -122.3(2) . . . . ?
O9 Dy1 O7 C35 -81.8(2) . . . . ?
O10 Dy1 O7 C35 172.7(2) . . . . ?
O13 Dy1 O7 C35 140.6(2) . . . . ?
O20 Dy1 O7 C35 119.7(2) . . . . ?
N27 Dy1 O7 C35 -101.7(2) . . . . ?
N4 Dy1 O7 C35 145.7(2) . . . . ?
Zn2 Dy1 O7 C35 24.7(2) . . . . ?
O6 Dy1 O7 C47 175.5(3) . . . . ?
O12 Dy1 O7 C47 -141.9(3) . . . . ?
O11 Dy1 O7 C47 124.2(3) . . . . ?
O15 Dy1 O7 C47 37.6(3) . . . . ?
O9 Dy1 O7 C47 78.1(3) . . . . ?
O10 Dy1 O7 C47 -27.4(3) . . . . ?
O13 Dy1 O7 C47 -59.5(3) . . . . ?
O20 Dy1 O7 C47 -80.5(3) . . . . ?
N27 Dy1 O7 C47 58.1(3) . . . . ?
N4 Dy1 O7 C47 -54.4(3) . . . . ?
Zn2 Dy1 O7 C47 -175.4(3) . . . . ?
O6 Zn2 O8 C19 -26.4(3) . . . . ?
N18 Zn2 O8 C19 132.2(3) . . . . ?
N16 Zn2 O8 C19 -119.9(3) . . . . ?
O12 Zn2 O8 C19 47.5(3) . . . . ?
Dy1 Zn2 O8 C19 7.0(3) . . . . ?
O6 Dy1 O9 N27 165.4(2) . . . . ?
O12 Dy1 O9 N27 122.8(2) . . . . ?
O11 Dy1 O9 N27 81.0(2) . . . . ?
O15 Dy1 O9 N27 -1.5(2) . . . . ?

O10 Dy1 O9 N27 -58.6(2) . . . . ?
O13 Dy1 O9 N27 18.0(3) . . . . ?
O20 Dy1 O9 N27 -100.7(2) . . . . ?
O7 Dy1 O9 N27 -131.8(2) . . . . ?
N4 Dy1 O9 N27 -72.5(2) . . . . ?
Zn2 Dy1 O9 N27 137.2(2) . . . . ?
O6 Dy1 O10 N4 -56.4(2) . . . . ?
O12 Dy1 O10 N4 25.8(2) . . . . ?
O11 Dy1 O10 N4 126.6(2) . . . . ?
O15 Dy1 O10 N4 160.4(2) . . . . ?
O9 Dy1 O10 N4 -153.22(19) . . . . ?
O13 Dy1 O10 N4 75.8(2) . . . . ?
O20 Dy1 O10 N4 -8.64(18) . . . . ?
O7 Dy1 O10 N4 -86.3(2) . . . . ?
N27 Dy1 O10 N4 -176.3(2) . . . . ?
Zn2 Dy1 O10 N4 -2.7(3) . . . . ?
O6 Dy1 O11 C19 36.6(4) . . . . ?
O12 Dy1 O11 C19 -29.9(3) . . . . ?
O15 Dy1 O11 C19 -178.2(4) . . . . ?
O9 Dy1 O11 C19 125.6(4) . . . . ?
O10 Dy1 O11 C19 -145.5(3) . . . . ?
O13 Dy1 O11 C19 -96.6(4) . . . . ?
O20 Dy1 O11 C19 -52.3(4) . . . . ?
O7 Dy1 O11 C19 81.3(4) . . . . ?
N27 Dy1 O11 C19 153.7(4) . . . . ?
N4 Dy1 O11 C19 -101.4(4) . . . . ?
Zn2 Dy1 O11 C19 7.4(3) . . . . ?
O8 Zn2 O12 C21 60.3(2) . . . . ?
O6 Zn2 O12 C21 168.7(2) . . . . ?
N18 Zn2 O12 C21 -47.9(2) . . . . ?
N16 Zn2 O12 C21 -161.6(3) . . . . ?
Dy1 Zn2 O12 C21 142.0(3) . . . . ?
O8 Zn2 O12 Dy1 -81.69(10) . . . . ?
O6 Zn2 O12 Dy1 26.65(9) . . . . ?
N18 Zn2 O12 Dy1 170.13(11) . . . . ?
N16 Zn2 O12 Dy1 56.4(3) . . . . ?
O6 Dy1 O12 C21 -163.9(3) . . . . ?
O11 Dy1 O12 C21 -74.2(2) . . . . ?
O15 Dy1 O12 C21 -24.8(3) . . . . ?
O9 Dy1 O12 C21 -116.0(2) . . . . ?
O10 Dy1 O12 C21 65.5(3) . . . . ?
O13 Dy1 O12 C21 11.6(2) . . . . ?
O20 Dy1 O12 C21 93.1(2) . . . . ?
O7 Dy1 O12 C21 154.4(2) . . . . ?
N27 Dy1 O12 C21 -67.4(3) . . . . ?
N4 Dy1 O12 C21 76.7(2) . . . . ?
Zn2 Dy1 O12 C21 -139.3(3) . . . . ?
O6 Dy1 O12 Zn2 -24.51(9) . . . . ?
O11 Dy1 O12 Zn2 65.10(10) . . . . ?
O15 Dy1 O12 Zn2 114.59(12) . . . . ?
O9 Dy1 O12 Zn2 23.33(18) . . . . ?
O10 Dy1 O12 Zn2 -155.14(9) . . . . ?
O13 Dy1 O12 Zn2 150.91(12) . . . . ?
O20 Dy1 O12 Zn2 -127.56(11) . . . . ?
O7 Dy1 O12 Zn2 -66.24(11) . . . . ?

N27 Dy1 O12 Zn2 71.9(2) . . . . ?
N4 Dy1 O12 Zn2 -143.96(10) . . . . ?
O6 Dy1 O13 C30 -4.9(3) . . . . ?
O12 Dy1 O13 C30 -10.4(2) . . . . ?
O11 Dy1 O13 C30 68.3(2) . . . . ?
O15 Dy1 O13 C30 145.7(2) . . . . ?
O9 Dy1 O13 C30 129.6(2) . . . . ?
O10 Dy1 O13 C30 -141.8(2) . . . . ?
O20 Dy1 O13 C30 -88.2(2) . . . . ?
O7 Dy1 O13 C30 -108.9(2) . . . . ?
N27 Dy1 O13 C30 138.0(2) . . . . ?
N4 Dy1 O13 C30 -114.3(2) . . . . ?
Zn2 Dy1 O13 C30 6.7(2) . . . . ?
O6 Dy1 O13 C48 177.2(2) . . . . ?
O12 Dy1 O13 C48 171.6(3) . . . . ?
O11 Dy1 O13 C48 -109.6(3) . . . . ?
O15 Dy1 O13 C48 -32.2(3) . . . . ?
O9 Dy1 O13 C48 -48.3(3) . . . . ?
O10 Dy1 O13 C48 40.3(3) . . . . ?
O20 Dy1 O13 C48 93.9(3) . . . . ?
O7 Dy1 O13 C48 73.2(3) . . . . ?
N27 Dy1 O13 C48 -39.9(3) . . . . ?
N4 Dy1 O13 C48 67.8(3) . . . . ?
Zn2 Dy1 O13 C48 -171.2(3) . . . . ?
O6 Dy1 O15 N27 -19.1(3) . . . . ?
O12 Dy1 O15 N27 -130.6(2) . . . . ?
O11 Dy1 O15 N27 -81.2(2) . . . . ?
O9 Dy1 O15 N27 1.5(2) . . . . ?
O10 Dy1 O15 N27 120.2(2) . . . . ?
O13 Dy1 O15 N27 -163.8(2) . . . . ?
O20 Dy1 O15 N27 130.3(2) . . . . ?
O7 Dy1 O15 N27 50.2(2) . . . . ?
N4 Dy1 O15 N27 128.9(2) . . . . ?
Zn2 Dy1 O15 N27 -73.5(2) . . . . ?
O6 Dy1 O20 N4 157.6(2) . . . . ?
O12 Dy1 O20 N4 -139.3(2) . . . . ?
O11 Dy1 O20 N4 -116.7(2) . . . . ?
O15 Dy1 O20 N4 -3.2(2) . . . . ?
O9 Dy1 O20 N4 66.3(2) . . . . ?
O10 Dy1 O20 N4 8.87(18) . . . . ?
O13 Dy1 O20 N4 -71.3(2) . . . . ?
O7 Dy1 O20 N4 96.9(2) . . . . ?
N27 Dy1 O20 N4 26.6(3) . . . . ?
Zn2 Dy1 O20 N4 -167.95(19) . . . . ?
Dy1 O20 N4 O5 163.0(3) . . . . ?
Dy1 O20 N4 O10 -15.0(3) . . . . ?
Dy1 O10 N4 O5 -162.7(3) . . . . ?
Dy1 O10 N4 O20 15.3(3) . . . . ?
O6 Dy1 N4 O5 -127.5(11) . . . . ?
O12 Dy1 N4 O5 -63.3(11) . . . . ?
O11 Dy1 N4 O5 3.6(12) . . . . ?
O15 Dy1 N4 O5 75.2(11) . . . . ?
O9 Dy1 N4 O5 125.8(11) . . . . ?
O10 Dy1 N4 O5 93.8(11) . . . . ?
O13 Dy1 N4 O5 -1.4(11) . . . . ?

O20 Dy1 N4 O5 -102.0(12) . . . . ?
O7 Dy1 N4 O5 -178.3(11) . . . . ?
N27 Dy1 N4 O5 97.8(11) . . . . ?
Zn2 Dy1 N4 O5 -87.9(11) . . . . ?
O6 Dy1 N4 O20 -25.5(2) . . . . ?
O12 Dy1 N4 O20 38.6(2) . . . . ?
O11 Dy1 N4 O20 105.6(2) . . . . ?
O15 Dy1 N4 O20 177.2(2) . . . . ?
O9 Dy1 N4 O20 -132.3(2) . . . . ?
O10 Dy1 N4 O20 -164.2(3) . . . . ?
O13 Dy1 N4 O20 100.6(2) . . . . ?
O7 Dy1 N4 O20 -76.4(2) . . . . ?
N27 Dy1 N4 O20 -160.2(2) . . . . ?
Zn2 Dy1 N4 O20 14.1(2) . . . . ?
O6 Dy1 N4 O10 138.75(19) . . . . ?
O12 Dy1 N4 O10 -157.13(19) . . . . ?
O11 Dy1 N4 O10 -90.1(2) . . . . ?
O15 Dy1 N4 O10 -18.5(2) . . . . ?
O9 Dy1 N4 O10 32.0(2) . . . . ?
O13 Dy1 N4 O10 -95.1(2) . . . . ?
O20 Dy1 N4 O10 164.2(3) . . . . ?
O7 Dy1 N4 O10 87.9(2) . . . . ?
N27 Dy1 N4 O10 4.0(2) . . . . ?
Zn2 Dy1 N4 O10 178.35(16) . . . . ?
O8 Zn2 N16 C33 117.6(3) . . . . ?
O6 Zn2 N16 C33 9.6(3) . . . . ?
N18 Zn2 N16 C33 -130.1(3) . . . . ?
O12 Zn2 N16 C33 -19.0(5) . . . . ?
Dy1 Zn2 N16 C33 24.0(3) . . . . ?
O8 Zn2 N16 C25 -61.0(2) . . . . ?
O6 Zn2 N16 C25 -169.1(2) . . . . ?
N18 Zn2 N16 C25 51.3(2) . . . . ?
O12 Zn2 N16 C25 162.4(3) . . . . ?
Dy1 Zn2 N16 C25 -154.59(19) . . . . ?
O8 Zn2 N18 C40 -53.8(3) . . . . ?
O6 Zn2 N18 C40 94.7(3) . . . . ?
N16 Zn2 N18 C40 -162.3(2) . . . . ?
O12 Zn2 N18 C40 34.9(3) . . . . ?
Dy1 Zn2 N18 C40 42.8(3) . . . . ?
O8 Zn2 N18 C26 118.8(2) . . . . ?
O6 Zn2 N18 C26 -92.7(3) . . . . ?
N16 Zn2 N18 C26 10.3(2) . . . . ?
O12 Zn2 N18 C26 -152.4(2) . . . . ?
Dy1 Zn2 N18 C26 -144.6(2) . . . . ?
Dy1 O9 N27 O15 2.7(3) . . . . ?
Dy1 O9 N27 O46 -178.3(4) . . . . ?
Dy1 O15 N27 O9 -2.7(4) . . . . ?
Dy1 O15 N27 O46 178.2(4) . . . . ?
O6 Dy1 N27 O9 -16.0(2) . . . . ?
O12 Dy1 N27 O9 -98.4(3) . . . . ?
O11 Dy1 N27 O9 -91.5(2) . . . . ?
O15 Dy1 N27 O9 177.3(4) . . . . ?
O10 Dy1 N27 O9 122.5(2) . . . . ?
O13 Dy1 N27 O9 -166.2(2) . . . . ?
O20 Dy1 N27 O9 108.7(2) . . . . ?

O7 Dy1 N27 O9 44.5(2) . . . . ?
N4 Dy1 N27 O9 120.7(2) . . . . ?
Zn2 Dy1 N27 O9 -53.3(2) . . . . ?
O6 Dy1 N27 O15 166.73(19) . . . . ?
O12 Dy1 N27 O15 84.4(3) . . . . ?
O11 Dy1 N27 O15 91.3(2) . . . . ?
O9 Dy1 N27 O15 -177.3(4) . . . . ?
O10 Dy1 N27 O15 -54.8(2) . . . . ?
O13 Dy1 N27 O15 16.6(2) . . . . ?
O20 Dy1 N27 O15 -68.6(3) . . . . ?
O7 Dy1 N27 O15 -132.8(2) . . . . ?
N4 Dy1 N27 O15 -56.6(2) . . . . ?
Zn2 Dy1 N27 O15 129.41(18) . . . . ?
O6 Dy1 N27 O46 121(8) . . . . ?
O12 Dy1 N27 O46 39(8) . . . . ?
O11 Dy1 N27 O46 46(8) . . . . ?
O15 Dy1 N27 O46 -46(8) . . . . ?
O9 Dy1 N27 O46 137(8) . . . . ?
O10 Dy1 N27 O46 -100(8) . . . . ?
O13 Dy1 N27 O46 -29(8) . . . . ?
O20 Dy1 N27 O46 -114(8) . . . . ?
O7 Dy1 N27 O46 -178(100) . . . . ?
N4 Dy1 N27 O46 -102(8) . . . . ?
Zn2 Dy1 N27 O46 84(8) . . . . ?
Zn2 O6 C14 C17 15.3(5) . . . . ?
Dy1 O6 C14 C17 -164.4(2) . . . . ?
Zn2 O6 C14 C35 -165.1(2) . . . . ?
Dy1 O6 C14 C35 15.3(4) . . . . ?
O6 C14 C17 C22 178.0(3) . . . . ?
C35 C14 C17 C22 -1.7(5) . . . . ?
O6 C14 C17 C33 1.2(5) . . . . ?
C35 C14 C17 C33 -178.5(3) . . . . ?
Dy1 O11 C19 O8 -5.0(6) . . . . ?
Dy1 O11 C19 C34 177.2(2) . . . . ?
Zn2 O8 C19 O11 -4.9(5) . . . . ?
Zn2 O8 C19 C34 172.8(2) . . . . ?
Zn2 O12 C21 C23 37.4(4) . . . . ?
Dy1 O12 C21 C23 170.5(2) . . . . ?
Zn2 O12 C21 C30 -144.6(2) . . . . ?
Dy1 O12 C21 C30 -11.5(4) . . . . ?
C14 C17 C22 C29 1.8(5) . . . . ?
C33 C17 C22 C29 178.8(3) . . . . ?
O12 C21 C23 C32 177.1(3) . . . . ?
C30 C21 C23 C32 -0.9(5) . . . . ?
O12 C21 C23 C40 2.6(5) . . . . ?
C30 C21 C23 C40 -175.4(3) . . . . ?
C41 C24 C25 C36 -3.0(5) . . . . ?
C41 C24 C25 N16 178.0(3) . . . . ?
C33 N16 C25 C24 -144.0(3) . . . . ?
Zn2 N16 C25 C24 34.7(4) . . . . ?
C33 N16 C25 C36 37.0(4) . . . . ?
Zn2 N16 C25 C36 -144.3(3) . . . . ?
C40 N18 C26 C44 -136.6(3) . . . . ?
Zn2 N18 C26 C44 50.4(4) . . . . ?
C40 N18 C26 C38 43.7(5) . . . . ?

Zn2 N18 C26 C38 -129.3(3) . . . . ?
C17 C22 C29 C28 -0.9(5) . . . . ?
C35 C28 C29 C22 -0.1(5) . . . . ?
C48 O13 C30 C54 7.1(5) . . . . ?
Dy1 O13 C30 C54 -171.0(3) . . . . ?
C48 O13 C30 C21 -172.8(3) . . . . ?
Dy1 O13 C30 C21 9.1(3) . . . . ?
O12 C21 C30 C54 -179.4(3) . . . . ?
C23 C21 C30 C54 -1.3(5) . . . . ?
O12 C21 C30 O13 0.5(4) . . . . ?
C23 C21 C30 O13 178.6(3) . . . . ?
C21 C23 C32 C42 2.9(5) . . . . ?
C40 C23 C32 C42 177.6(3) . . . . ?
C25 N16 C33 C17 179.6(3) . . . . ?
Zn2 N16 C33 C17 0.9(5) . . . . ?
C14 C17 C33 N16 -9.6(5) . . . . ?
C22 C17 C33 N16 173.5(3) . . . . ?
C29 C28 C35 O7 179.5(3) . . . . ?
C29 C28 C35 C14 0.3(5) . . . . ?
C47 O7 C35 C28 4.1(5) . . . . ?
Dy1 O7 C35 C28 166.1(3) . . . . ?
C47 O7 C35 C14 -176.5(3) . . . . ?
Dy1 O7 C35 C14 -14.6(3) . . . . ?
O6 C14 C35 C28 -179.0(3) . . . . ?
C17 C14 C35 C28 0.7(5) . . . . ?
O6 C14 C35 O7 1.6(4) . . . . ?
C17 C14 C35 O7 -178.7(3) . . . . ?
C24 C25 C36 C45 3.1(5) . . . . ?
N16 C25 C36 C45 -177.9(3) . . . . ?
C44 C26 C38 C55 2.7(5) . . . . ?
N18 C26 C38 C55 -177.6(3) . . . . ?
C44 C3 C39 C55 2.3(6) . . . . ?
C26 N18 C40 C23 176.1(3) . . . . ?
Zn2 N18 C40 C23 -11.1(5) . . . . ?
C21 C23 C40 N18 -18.2(5) . . . . ?
C32 C23 C40 N18 167.2(3) . . . . ?
C45 C31 C41 C24 1.1(6) . . . . ?
C25 C24 C41 C31 0.9(5) . . . . ?
C23 C32 C42 C54 -2.6(6) . . . . ?
C38 C26 C44 C3 -1.3(5) . . . . ?
N18 C26 C44 C3 179.0(3) . . . . ?
C39 C3 C44 C26 -1.2(5) . . . . ?
C41 C31 C45 C36 -0.9(6) . . . . ?
C25 C36 C45 C31 -1.2(6) . . . . ?
O13 C30 C54 C42 -178.3(3) . . . . ?
C21 C30 C54 C42 1.6(5) . . . . ?
C32 C42 C54 C30 0.4(6) . . . . ?
C3 C39 C55 C38 -0.9(6) . . . . ?
C26 C38 C55 C39 -1.6(6) . . . . ?

_diffrn_measured_fraction_theta_max 0.950
_diffrn_reflns_theta_full 29.17
_diffrn_measured_fraction_theta_full 0.950
_refine_diff_density_max 1.256
_refine_diff_density_min -1.835

_refine_diff_density_rms 0.127

checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.
THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: shelxl

Bond precision: C-C = 0.0051 A Wavelength=0.71075
Cell: a=11.132(5) b=12.522(6) c=13.219(6)
alpha=105.888(1) beta=91.753(5) gamma=94.464(6)
Temperature: 100 K

	Calculated	Reported
Volume	1764.3(14)	1764.3(14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C30 H27 Dy N4 O12 Zn, 2(C O)	?
Sum formula	C32 H27 Dy N4 O14 Zn	C32 H27 Dy N4 O14 Zn
Mr	919.47	919.45
Dx,g cm-3	1.731	1.731
Z	2	2
Mu (mm-1)	2.854	2.854
F000	910.0	910.0
F000'	910.62	
h,k,lmax	15,17,18	15,17,18
Nref	9522	9054
Tmin,Tmax	0.492,0.819	0.387,0.825
Tmin'	0.307	

Correction method= NUMERICAL
Data completeness= 0.951 Theta(max)= 29.170
R(reflections)= 0.0348(8566) wR2(reflections)= 0.0910(9054)
S = 0.802 Npar= 469

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low 0.950
PLAT220_ALERT_2_B Large Non-Solvent O Ueq(max)/Ueq(min) ... 4.4 Ratio
PLAT230_ALERT_2_B Hirshfeld Test Diff for O9 -- N27 .. 8.0 su

PLAT230_ALERT_2_B Hirshfeld Test Diff for O15 -- N27 ..
8.5 su

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Numerical
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .....
O37 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .....
O49 Check

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF
Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.
10.58
PLAT344_ALERT_2_G Check sp? Angle Range in Solvent/Ion for ...
C43
PLAT344_ALERT_2_G Check sp? Angle Range in Solvent/Ion for ...
C58
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....
C34 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #
293 Do !
O6 -DY1 -N27 -O46 121.00 8.00 1.555 1.555 1.555
1.555
And 10 other PLAT710 Alerts
More ...
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #
3
C O

0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or
oversight
17 **ALERT level G** = General information/check it is not something
unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing
data
8 ALERT type 2 Indicator that the structure model may be wrong or
deficient
1 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may

appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

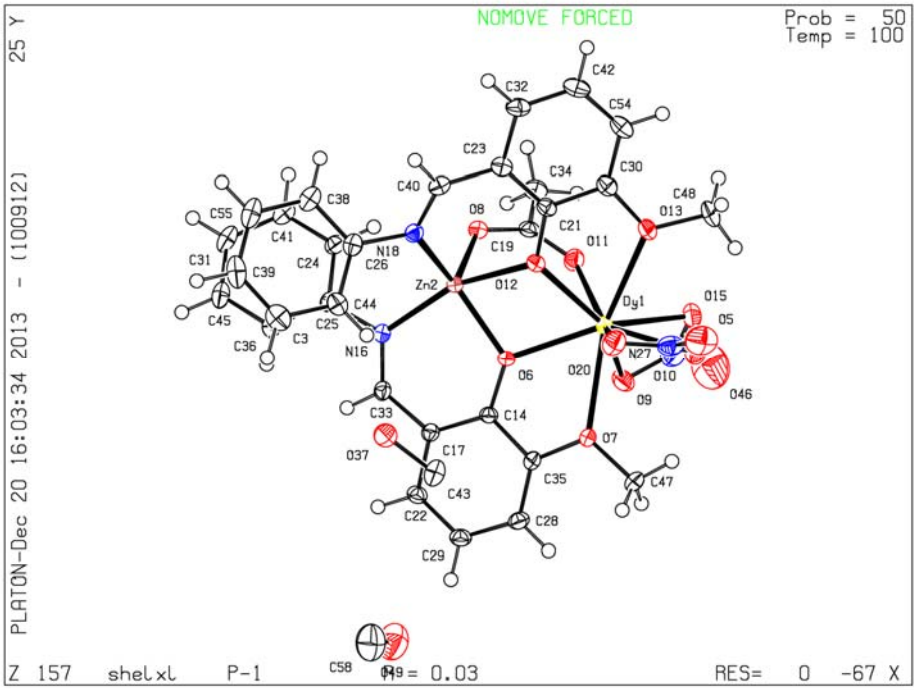
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/09/2013; check.def file version of 12/09/2013

Datablock shelxl - ellipsoid plot

Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry



Crystallographic information file for complex 2

```
data_shelxl

_audit_creation_method           SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common            ?
_chemical_melting_point          ?
_chemical_formula_moiety         ?
_chemical_formula_sum
 'C28 H26 Dy N5 O13'
_chemical_formula_weight         803.04

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Dy'  'Dy'  -0.1892   4.4098
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting           Orthorhombic
_symmetry_space_group_name_H-M    Aba2

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, y+1/2, z'
 'x+1/2, -y+1/2, z'
 '-x, -y, z'
 'x, y+1/2, z+1/2'
 '-x+1/2, y+1, z+1/2'
 'x+1/2, -y+1, z+1/2'
 '-x, -y+1/2, z+1/2'

_cell_length_a                   17.654(3)
```

```
_cell_length_b                    54.092(9)
_cell_length_c                    9.5502(16)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      9120(3)
_cell_formula_units_Z             12
_cell_measurement_temperature     100(2)
_cell_measurement_reflns_used     ?
_cell_measurement_theta_min       3.01
_cell_measurement_theta_max       29.17

_exptl_crystal_description        Block
_exptl_crystal_colour             'Orange red'
_exptl_crystal_size_max           0.20
_exptl_crystal_size_mid           0.20
_exptl_crystal_size_min           0.20
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.755
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              4788
_exptl_absorpt_coefficient_mu     2.534
_exptl_absorpt_correction_type    Numerical
_exptl_absorpt_correction_T_min   0.6312
_exptl_absorpt_correction_T_max   0.6312
_exptl_absorpt_process_details    ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       100(2)
_diffrn_radiation_wavelength      0.71075
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean  ?
_diffrn_reflns_number             33334
_diffrn_reflns_av_R_equivalents   0.0510
_diffrn_reflns_av_sigmaI/netI     0.0633
_diffrn_reflns_limit_h_min        -20
_diffrn_reflns_limit_h_max        24
_diffrn_reflns_limit_k_min        -74
_diffrn_reflns_limit_k_max        74
_diffrn_reflns_limit_l_min        -12
_diffrn_reflns_limit_l_max        12
_diffrn_reflns_theta_min          3.01
```

```
_diffrn_reflns_theta_max          29.17
_reflns_number_total              11627
_reflns_number_gt                 9529
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        ?
_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 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.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0342P)^2^+19.6649P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_abs_structure_details
 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    -0.008(11)
_refine_ls_number_reflns          11627
_refine_ls_number_parameters      632
_refine_ls_number_restraints      25
_refine_ls_R_factor_all           0.0628
_refine_ls_R_factor_gt            0.0494
_refine_ls_wR_factor_ref          0.1015
_refine_ls_wR_factor_gt           0.0941
_refine_ls_goodness_of_fit_ref    1.067
_refine_ls_restrained_S_all       1.067
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000
```

```
loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Dy1 Dy 0.503158(12) -0.166199(6) 0.63036(3) 0.01758(8) Uani 1 1 d . . .
Dy2 Dy 0.5000 0.0000 0.43114(5) 0.01227(10) Uani 1 2 d S . .
O11 O 0.6265(2) -0.16465(7) 0.6974(4) 0.0180(9) Uani 1 1 d . . .
O12 O 0.6002(2) -0.19826(7) 0.5084(5) 0.0206(9) Uani 1 1 d . . .
O31 O 0.3834(2) -0.16780(7) 0.7267(5) 0.0175(9) Uani 1 1 d . . .
O32 O 0.3970(2) -0.13373(7) 0.5369(4) 0.0188(9) Uani 1 1 d . . .
O41 O 0.5421(2) -0.12187(8) 0.6269(6) 0.0303(10) Uani 1 1 d . . .
O42 O 0.5049(2) -0.13639(9) 0.8256(7) 0.0296(11) Uani 1 1 d . . .
O43 O 0.5383(3) -0.09737(9) 0.8079(6) 0.0416(14) Uani 1 1 d . . .
O51 O 0.4547(3) -0.17747(9) 0.3969(5) 0.0327(12) Uani 1 1 d U . .
O52 O 0.5464(3) -0.15168(9) 0.4006(5) 0.0335(11) Uani 1 1 d U . .
O53 O 0.5007(2) -0.16550(15) 0.2014(6) 0.054(2) Uani 1 1 d U . .
O61 O 0.4533(3) -0.20935(10) 0.6166(8) 0.0610(19) Uani 1 1 d . . .
O62 O 0.5095(3) -0.19764(14) 0.8124(8) 0.056(2) Uani 1 1 d . . .
O63 O 0.4653(5) -0.23516(12) 0.7911(10) 0.114(4) Uani 1 1 d . . .
O112 O 0.4739(2) 0.02648(7) 0.6465(5) 0.0195(9) Uani 1 1 d . . .
O141 O 0.5597(2) -0.03777(7) 0.3387(5) 0.0244(10) Uani 1 1 d . . .
O142 O 0.4436(2) -0.04264(7) 0.4029(5) 0.0229(10) Uani 1 1 d . . .
O143 O 0.4996(3) -0.07190(11) 0.2875(6) 0.046(2) Uani 1 1 d . . .
O151 O 0.4456(2) -0.00887(8) 0.1941(5) 0.0230(10) Uani 1 1 d . . .
O153 O 0.5000 0.0000 -0.0030(7) 0.040(2) Uani 1 2 d S . .
C11 C 0.7615(3) -0.16840(10) 0.6735(7) 0.0186(13) Uani 1 1 d . . .
C12 C 0.6861(3) -0.17493(9) 0.6386(6) 0.0118(10) Uani 1 1 d . . .
C13 C 0.6760(3) -0.19313(10) 0.5346(7) 0.0154(12) Uani 1 1 d . . .
C14 C 0.7360(3) -0.20392(11) 0.4687(7) 0.0190(13) Uani 1 1 d . . .
H14A H 0.7274 -0.2160 0.3982 0.023 Uiso 1 1 calc R . .
C15 C 0.8118(3) -0.19722(11) 0.5051(7) 0.0222(14) Uani 1 1 d . . .
H15A H 0.8538 -0.2048 0.4602 0.027 Uiso 1 1 calc R . .
C16 C 0.8227(3) -0.17965(10) 0.6058(7) 0.0192(14) Uani 1 1 d . . .
H16A H 0.8728 -0.1750 0.6303 0.023 Uiso 1 1 calc R . .
C17 C 0.7755(3) -0.15025(11) 0.7797(6) 0.0173(14) Uani 1 1 d . . .
H17A H 0.8264 -0.1458 0.8001 0.021 Uiso 1 1 calc R . .
C18 C 0.7254(3) -0.12116(10) 0.9555(6) 0.0171(12) Uani 1 1 d . . .
C19 C 0.6581(4) -0.11487(12) 1.0203(8) 0.0289(15) Uani 1 1 d . . .
H19A H 0.6122 -0.1229 0.9952 0.035 Uiso 1 1 calc R . .
C20 C 0.6585(4) -0.09647(12) 1.1235(8) 0.0336(16) Uani 1 1 d . . .
```

H20A H 0.6126 -0.0917 1.1680 0.040 Uiso 1 1 calc R . .
C21 C 0.7261(4) -0.08524(11) 1.1605(8) 0.0336(17) Uani 1 1 d . . .
H21A H 0.7265 -0.0726 1.2296 0.040 Uiso 1 1 calc R . .
C22 C 0.7934(4) -0.09237(11) 1.0968(7) 0.0268(15) Uani 1 1 d . . .
H22A H 0.8396 -0.0848 1.1244 0.032 Uiso 1 1 calc R . .
C23 C 0.7940(4) -0.11038(11) 0.9932(7) 0.0239(14) Uani 1 1 d . . .
H23A H 0.8399 -0.1152 0.9493 0.029 Uiso 1 1 calc R . .
C24 C 0.5844(3) -0.21802(11) 0.4098(7) 0.0228(14) Uani 1 1 d . . .
H24A H 0.6318 -0.2263 0.3843 0.034 Uiso 1 1 calc R . .
H24B H 0.5608 -0.2111 0.3256 0.034 Uiso 1 1 calc R . .
H24C H 0.5499 -0.2300 0.4530 0.034 Uiso 1 1 calc R . .
C31 C 0.2484(3) -0.16631(10) 0.7266(7) 0.0191(13) Uani 1 1 d . . .
C32 C 0.3204(3) -0.15858(10) 0.6780(6) 0.0162(12) Uani 1 1 d . . .
C33 C 0.3240(3) -0.14003(9) 0.5741(6) 0.0128(11) Uani 1 1 d . . .
C34 C 0.2596(3) -0.12991(10) 0.5200(6) 0.0166(12) Uani 1 1 d . . .
H34A H 0.2630 -0.1174 0.4506 0.020 Uiso 1 1 calc R . .
C35 C 0.1876(3) -0.13802(11) 0.5668(7) 0.0219(14) Uani 1 1 d . . .
H35A H 0.1429 -0.1312 0.5271 0.026 Uiso 1 1 calc R . .
C36 C 0.1824(3) -0.15528(11) 0.6668(6) 0.0172(13) Uani 1 1 d . . .
H36A H 0.1338 -0.1603 0.6987 0.021 Uiso 1 1 calc R . .
C37 C 0.2413(3) -0.18387(10) 0.8357(7) 0.0166(12) Uani 1 1 d . . .
H37A H 0.1922 -0.1887 0.8657 0.020 Uiso 1 1 calc R . .
C38 C 0.3015(3) -0.21135(10) 1.0062(7) 0.0203(13) Uani 1 1 d . . .
C39 C 0.3723(3) -0.21574(11) 1.0671(7) 0.0232(14) Uani 1 1 d . . .
H39A H 0.4161 -0.2074 1.0337 0.028 Uiso 1 1 calc R . .
C40 C 0.3780(4) -0.23245(11) 1.1770(7) 0.0268(15) Uani 1 1 d . . .
H40A H 0.4256 -0.2353 1.2204 0.032 Uiso 1 1 calc R . .
C41 C 0.3148(4) -0.24497(12) 1.2235(8) 0.0346(17) Uani 1 1 d . . .
H41A H 0.3191 -0.2565 1.2981 0.041 Uiso 1 1 calc R . .
C42 C 0.2451(4) -0.24080(12) 1.1620(8) 0.0349(18) Uani 1 1 d . . .
H42A H 0.2019 -0.2497 1.1929 0.042 Uiso 1 1 calc R . .
C43 C 0.2381(4) -0.22338(12) 1.0539(7) 0.0255(15) Uani 1 1 d . . .
H43A H 0.1900 -0.2199 1.0141 0.031 Uiso 1 1 calc R . .
C44 C 0.4063(3) -0.11355(10) 0.4397(7) 0.0234(13) Uani 1 1 d . . .
H44A H 0.3575 -0.1052 0.4259 0.035 Uiso 1 1 calc R . .
H44B H 0.4246 -0.1199 0.3498 0.035 Uiso 1 1 calc R . .
H44C H 0.4431 -0.1017 0.4773 0.035 Uiso 1 1 calc R . .
C111 C 0.2797(3) 0.00599(9) 0.6764(6) 0.0128(11) Uani 1 1 d . . .
C112 C 0.3547(3) 0.00919(9) 0.6281(7) 0.0128(10) Uani 1 1 d . . .
C113 C 0.4016(3) 0.02575(10) 0.7025(6) 0.0146(12) Uani 1 1 d . . .
C114 C 0.3760(4) 0.03894(10) 0.8151(7) 0.0197(13) Uani 1 1 d . . .
H11A H 0.4089 0.0500 0.8631 0.024 Uiso 1 1 calc R . .
C115 C 0.3000(3) 0.03597(10) 0.8593(6) 0.0201(13) Uani 1 1 d . . .
H11B H 0.2820 0.0452 0.9373 0.024 Uiso 1 1 calc R . .
C116 C 0.2519(4) 0.02008(11) 0.7918(6) 0.0182(14) Uani 1 1 d . . .
H11C H 0.2008 0.0185 0.8214 0.022 Uiso 1 1 calc R . .
C117 C 0.2313(3) -0.01233(9) 0.6166(6) 0.0139(11) Uani 1 1 d . . .
H11D H 0.1803 -0.0134 0.6472 0.017 Uiso 1 1 calc R . .
C118 C 0.2168(3) -0.04817(10) 0.4600(7) 0.0151(12) Uani 1 1 d . . .
C119 C 0.2522(3) -0.05973(10) 0.3480(6) 0.0189(13) Uani 1 1 d . . .

H11E H 0.2998 -0.0539 0.3154 0.023 Uiso 1 1 calc R . .
C120 C 0.2179(4) -0.07971(11) 0.2841(6) 0.0194(14) Uani 1 1 d . . .
H12A H 0.2420 -0.0879 0.2081 0.023 Uiso 1 1 calc R . .
C121 C 0.1475(3) -0.08782(10) 0.3321(7) 0.0199(13) Uani 1 1 d . . .
H12B H 0.1229 -0.1012 0.2866 0.024 Uiso 1 1 calc R . .
C122 C 0.1138(3) -0.07664(11) 0.4441(7) 0.0223(14) Uani 1 1 d . . .
H12C H 0.0667 -0.0827 0.4778 0.027 Uiso 1 1 calc R . .
C123 C 0.1478(3) -0.05640(11) 0.5097(7) 0.0174(12) Uani 1 1 d . . .
H12D H 0.1239 -0.0485 0.5867 0.021 Uiso 1 1 calc R . .
C124 C 0.5275(3) 0.04156(11) 0.7248(8) 0.0241(14) Uani 1 1 d . . .
H12E H 0.5014 0.0496 0.8030 0.036 Uiso 1 1 calc R . .
H12F H 0.5492 0.0542 0.6629 0.036 Uiso 1 1 calc R . .
H12G H 0.5682 0.0310 0.7613 0.036 Uiso 1 1 calc R . .
N11 N 0.7209(2) -0.13959(8) 0.8495(5) 0.0160(10) Uani 1 1 d . . .
H11F H 0.6748 -0.1445 0.8279 0.019 Uiso 1 1 calc R . .
N31 N 0.3006(3) -0.19366(8) 0.8964(5) 0.0162(10) Uani 1 1 d . . .
H31A H 0.3450 -0.1887 0.8656 0.019 Uiso 1 1 calc R . .
N41 N 0.5278(3) -0.11802(10) 0.7551(7) 0.0271(13) Uani 1 1 d . . .
N51 N 0.5003(3) -0.16556(13) 0.3291(9) 0.0299(14) Uani 1 1 d U . .
N61 N 0.4782(5) -0.21461(13) 0.7395(13) 0.058(2) Uani 1 1 d . . .
N111 N 0.2555(2) -0.02755(9) 0.5211(5) 0.0144(10) Uani 1 1 d . . .
H11G H 0.3017 -0.0248 0.4900 0.017 Uiso 1 1 calc R . .
N141 N 0.4994(3) -0.05155(10) 0.3430(7) 0.0273(13) Uani 1 1 d . . .
N151 N 0.5000 0.0000 0.1312(9) 0.0056(12) Uani 1 2 d S . .
O111 O 0.3813(2) -0.00320(6) 0.5212(4) 0.0123(8) Uiso 1 1 d . . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Dy1 0.01000(12) 0.02234(14) 0.02040(18) 0.00056(11) 0.00008(17) -0.00134(10)
Dy2 0.00852(18) 0.01428(18) 0.0140(2) 0.000 0.000 -0.00125(13)
O11 0.0080(18) 0.022(2) 0.024(2) -0.0060(18) -0.0002(16) 0.0013(15)
O12 0.019(2) 0.017(2) 0.025(3) -0.0056(18) -0.0031(19) -0.0038(16)
O31 0.0076(17) 0.023(2) 0.022(2) 0.0130(19) -0.0001(17) -0.0008(15)
O32 0.0168(19) 0.019(2) 0.021(2) 0.0101(18) 0.0046(18) 0.0025(16)
O41 0.033(2) 0.027(2) 0.030(3) 0.001(2) -0.004(3) -0.0048(18)
O42 0.021(2) 0.024(2) 0.044(3) -0.004(3) 0.003(2) 0.0007(18)
O43 0.033(3) 0.029(3) 0.062(4) -0.017(3) -0.012(3) 0.001(2)
O51 0.023(2) 0.042(3) 0.034(3) -0.016(2) -0.012(2) 0.008(2)
O52 0.025(2) 0.041(3) 0.034(3) 0.010(2) 0.005(2) 0.000(2)
O53 0.021(3) 0.111(6) 0.030(3) -0.029(4) 0.002(2) 0.022(3)
O61 0.069(4) 0.032(3) 0.083(6) -0.004(4) 0.037(4) -0.012(3)
O62 0.018(3) 0.077(5) 0.074(5) 0.047(4) 0.007(3) 0.009(3)
O63 0.151(7) 0.030(4) 0.160(9) 0.039(4) 0.117(7) 0.037(4)
O112 0.0129(17) 0.0204(19) 0.025(3) -0.0100(19) -0.0002(19) -0.0033(15)

O141 0.021(2) 0.020(2) 0.032(3) 0.000(2) 0.012(2) 0.0031(17)
O142 0.017(2) 0.018(2) 0.033(3) -0.0031(19) 0.015(2) -0.0022(16)
O143 0.056(4) 0.016(3) 0.066(6) -0.014(2) 0.027(3) -0.005(2)
O151 0.021(2) 0.024(2) 0.024(3) 0.0004(19) -0.0074(19) -0.0016(18)
O153 0.073(6) 0.038(4) 0.008(4) 0.000 0.000 0.006(4)
C11 0.015(3) 0.018(3) 0.022(4) 0.005(3) 0.002(2) -0.002(2)
C12 0.016(2) 0.009(2) 0.010(3) -0.002(2) 0.003(3) 0.0031(18)
C13 0.010(2) 0.015(3) 0.021(3) 0.003(2) -0.003(2) 0.003(2)
C14 0.022(3) 0.017(3) 0.018(4) -0.002(2) 0.001(2) 0.000(2)
C15 0.021(3) 0.023(3) 0.023(4) 0.005(3) 0.006(3) 0.006(2)
C16 0.013(2) 0.013(2) 0.031(4) 0.004(2) -0.001(3) 0.0024(19)
C17 0.010(3) 0.021(3) 0.021(4) 0.007(2) -0.003(2) -0.001(2)
C18 0.018(3) 0.018(3) 0.015(3) -0.004(2) -0.005(2) 0.000(2)
C19 0.031(4) 0.027(3) 0.029(4) -0.002(3) -0.008(3) 0.005(3)
C20 0.040(4) 0.029(3) 0.032(4) -0.010(3) -0.009(4) 0.015(3)
C21 0.055(5) 0.020(3) 0.026(4) -0.001(3) -0.008(3) 0.010(3)
C22 0.035(3) 0.024(3) 0.021(4) -0.004(3) -0.012(3) -0.005(3)
C23 0.028(3) 0.025(3) 0.019(4) 0.004(3) -0.011(3) -0.004(3)
C24 0.022(3) 0.021(3) 0.026(4) -0.001(3) -0.005(3) -0.002(2)
C31 0.016(3) 0.015(3) 0.026(4) -0.006(3) 0.003(3) 0.000(2)
C32 0.014(3) 0.020(3) 0.015(3) 0.003(2) 0.000(2) 0.003(2)
C33 0.012(2) 0.009(2) 0.018(3) -0.005(2) 0.002(2) -0.0015(19)
C34 0.019(3) 0.016(3) 0.015(3) 0.004(2) -0.003(3) 0.000(2)
C35 0.013(3) 0.020(3) 0.033(4) -0.006(3) -0.002(3) 0.008(2)
C36 0.009(2) 0.028(3) 0.014(3) -0.007(2) 0.004(2) -0.003(2)
C37 0.010(3) 0.020(3) 0.020(3) -0.003(3) 0.009(3) -0.004(2)
C38 0.028(3) 0.015(3) 0.018(3) -0.001(2) 0.004(3) 0.000(2)
C39 0.024(3) 0.021(3) 0.025(4) -0.003(3) 0.005(3) 0.005(2)
C40 0.041(4) 0.025(3) 0.015(3) -0.001(3) 0.001(3) 0.008(3)
C41 0.060(5) 0.021(3) 0.023(4) 0.005(3) 0.006(4) -0.005(3)
C42 0.051(4) 0.022(3) 0.032(5) -0.001(3) 0.014(4) -0.017(3)
C43 0.036(4) 0.026(3) 0.015(4) -0.005(3) 0.007(3) -0.001(3)
C44 0.024(3) 0.020(3) 0.026(4) 0.009(3) 0.004(3) 0.001(2)
C111 0.017(3) 0.012(2) 0.009(3) 0.002(2) 0.004(2) 0.006(2)
C112 0.018(2) 0.011(2) 0.009(3) 0.004(2) -0.001(3) -0.0011(19)
C113 0.012(3) 0.014(2) 0.018(3) 0.001(2) -0.003(2) 0.002(2)
C114 0.032(3) 0.017(3) 0.011(3) -0.005(2) -0.009(3) 0.004(2)
C115 0.029(3) 0.019(3) 0.013(3) -0.002(2) 0.003(3) 0.009(3)
C116 0.016(3) 0.019(3) 0.019(4) 0.003(2) 0.010(2) 0.006(2)
C117 0.014(2) 0.010(2) 0.018(3) 0.001(2) 0.005(2) -0.0003(18)
C118 0.009(2) 0.012(2) 0.024(4) 0.005(2) -0.002(2) 0.003(2)
C119 0.016(2) 0.019(3) 0.022(4) 0.004(2) 0.003(3) 0.000(2)
C120 0.019(3) 0.016(3) 0.023(4) -0.003(2) -0.008(2) 0.003(2)
C121 0.020(3) 0.014(3) 0.025(4) -0.002(3) -0.007(3) 0.000(2)
C122 0.012(3) 0.024(3) 0.031(4) 0.001(3) -0.006(3) -0.004(2)
C123 0.011(3) 0.025(3) 0.016(3) 0.007(3) 0.003(2) 0.007(2)
C124 0.020(3) 0.022(3) 0.030(4) -0.011(3) -0.007(3) -0.008(2)
N11 0.013(2) 0.018(2) 0.017(3) -0.001(2) -0.005(2) -0.0023(18)
N31 0.017(2) 0.016(2) 0.016(3) -0.0005(19) 0.006(2) -0.0035(19)
N41 0.028(3) 0.015(3) 0.038(4) -0.003(2) -0.002(3) 0.001(2)

N51 0.015(3) 0.048(3) 0.027(3) -0.011(3) 0.004(2) 0.016(2)
N61 0.067(5) 0.016(3) 0.092(7) 0.007(4) 0.049(6) 0.012(4)
N111 0.008(2) 0.018(2) 0.017(3) 0.006(2) -0.001(2) -0.0054(17)
N141 0.036(3) 0.020(3) 0.026(4) 0.003(2) 0.020(3) -0.003(2)
N151 0.006(3) 0.010(3) 0.001(3) 0.000 0.000 0.0007(19)

_geom_special_details
;
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.
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
Dy1 O11 2.272(4) . ?
Dy1 O31 2.308(4) . ?
Dy1 O62 2.434(6) . ?
Dy1 O52 2.453(5) . ?
Dy1 O42 2.465(6) . ?
Dy1 O51 2.465(5) . ?
Dy1 O41 2.495(4) . ?
Dy1 O61 2.498(5) . ?
Dy1 O12 2.702(4) . ?
Dy1 O32 2.719(4) . ?
Dy1 N61 2.853(7) . ?
Dy1 N51 2.878(9) . ?
Dy2 O111 2.271(4) 4_655 ?
Dy2 O111 2.271(4) . ?
Dy2 O141 2.463(4) . ?
Dy2 O141 2.463(4) 4_655 ?
Dy2 O151 2.505(4) . ?
Dy2 O151 2.505(4) 4_655 ?
Dy2 O142 2.527(4) . ?
Dy2 O142 2.527(4) 4_655 ?
Dy2 O112 2.548(4) . ?
Dy2 O112 2.548(4) 4_655 ?
Dy2 N151 2.865(9) . ?
Dy2 N141 2.913(6) 4_655 ?
O11 C12 1.316(6) . ?
O12 C13 1.388(6) . ?
O12 C24 1.451(7) . ?
O31 C32 1.305(6) . ?

O32 C33 1.380(6) . ?
O32 C44 1.442(7) . ?
O41 N41 1.268(8) . ?
O42 N41 1.266(8) . ?
O43 N41 1.239(7) . ?
O51 N51 1.218(8) . ?
O52 N51 1.300(8) . ?
O53 N51 1.219(10) . ?
O61 N61 1.284(12) . ?
O62 N61 1.278(12) . ?
O63 N61 1.237(9) . ?
O112 C113 1.385(6) . ?
O112 C124 1.457(7) . ?
O141 N141 1.301(6) . ?
O142 N141 1.238(6) . ?
O143 N141 1.221(8) . ?
O151 N151 1.230(6) . ?
O153 N151 1.281(11) . ?
C11 C16 1.398(8) . ?
C11 C12 1.416(7) . ?
C11 C17 1.433(8) . ?
C12 C13 1.410(8) . ?
C13 C14 1.363(8) . ?
C14 C15 1.429(8) . ?
C14 H14A 0.9500 . ?
C15 C16 1.366(9) . ?
C15 H15A 0.9500 . ?
C16 H16A 0.9500 . ?
C17 N11 1.306(7) . ?
C17 H17A 0.9500 . ?
C18 C19 1.383(9) . ?
C18 C23 1.391(8) . ?
C18 N11 1.423(7) . ?
C19 C20 1.401(9) . ?
C19 H19A 0.9500 . ?
C20 C21 1.385(9) . ?
C20 H20A 0.9500 . ?
C21 C22 1.390(9) . ?
C21 H21A 0.9500 . ?
C22 C23 1.389(8) . ?
C22 H22A 0.9500 . ?
C23 H23A 0.9500 . ?
C24 H24A 0.9800 . ?
C24 H24B 0.9800 . ?
C24 H24C 0.9800 . ?
C31 C37 1.415(8) . ?
C31 C32 1.416(7) . ?
C31 C36 1.427(8) . ?
C32 C33 1.413(8) . ?
C33 C34 1.364(7) . ?

C34 C35 1.417(8) . ?
C34 H34A 0.9500 . ?
C35 C36 1.339(8) . ?
C35 H35A 0.9500 . ?
C36 H36A 0.9500 . ?
C37 N31 1.308(7) . ?
C37 H37A 0.9500 . ?
C38 C43 1.372(8) . ?
C38 C39 1.399(8) . ?
C38 N31 1.420(7) . ?
C39 C40 1.389(8) . ?
C39 H39A 0.9500 . ?
C40 C41 1.379(9) . ?
C40 H40A 0.9500 . ?
C41 C42 1.381(10) . ?
C41 H41A 0.9500 . ?
C42 C43 1.403(9) . ?
C42 H42A 0.9500 . ?
C43 H43A 0.9500 . ?
C44 H44A 0.9800 . ?
C44 H44B 0.9800 . ?
C44 H44C 0.9800 . ?
C111 C112 1.412(7) . ?
C111 C116 1.426(8) . ?
C111 C117 1.427(7) . ?
C112 O111 1.309(7) . ?
C112 C113 1.412(7) . ?
C113 C114 1.367(8) . ?
C114 C115 1.416(8) . ?
C114 H11A 0.9500 . ?
C115 C116 1.370(8) . ?
C115 H11B 0.9500 . ?
C116 H11C 0.9500 . ?
C117 N111 1.300(7) . ?
C117 H11D 0.9500 . ?
C118 C123 1.381(7) . ?
C118 C119 1.388(8) . ?
C118 N111 1.433(7) . ?
C119 C120 1.381(8) . ?
C119 H11E 0.9500 . ?
C120 C121 1.395(8) . ?
C120 H12A 0.9500 . ?
C121 C122 1.366(9) . ?
C121 H12B 0.9500 . ?
C122 C123 1.397(8) . ?
C122 H12C 0.9500 . ?
C123 H12D 0.9500 . ?
C124 H12E 0.9800 . ?
C124 H12F 0.9800 . ?
C124 H12G 0.9800 . ?

N11 H11F 0.8800 . ?
N31 H31A 0.8800 . ?
N111 H11G 0.8800 . ?
N151 O151 1.230(6) 4_655 ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O11 Dy1 O31 140.12(16) . . ?
O11 Dy1 O62 77.30(17) . . ?
O31 Dy1 O62 74.42(15) . . ?
O11 Dy1 O52 86.67(15) . . ?
O31 Dy1 O52 130.85(15) . . ?
O62 Dy1 O52 148.0(2) . . ?
O11 Dy1 O42 75.58(14) . . ?
O31 Dy1 O42 74.58(15) . . ?
O62 Dy1 O42 85.2(2) . . ?
O52 Dy1 O42 117.60(18) . . ?
O11 Dy1 O51 126.65(15) . . ?
O31 Dy1 O51 91.91(16) . . ?
O62 Dy1 O51 119.3(2) . . ?
O52 Dy1 O51 51.53(18) . . ?
O42 Dy1 O51 148.23(16) . . ?
O11 Dy1 O41 72.78(14) . . ?
O31 Dy1 O41 107.10(14) . . ?
O62 Dy1 O41 131.9(2) . . ?
O52 Dy1 O41 66.08(18) . . ?
O42 Dy1 O41 51.53(18) . . ?
O51 Dy1 O41 108.75(18) . . ?
O11 Dy1 O61 112.77(19) . . ?
O31 Dy1 O61 70.31(16) . . ?
O62 Dy1 O61 53.2(3) . . ?
O52 Dy1 O61 111.2(2) . . ?
O42 Dy1 O61 130.9(2) . . ?
O51 Dy1 O61 66.4(2) . . ?
O41 Dy1 O61 174.0(2) . . ?
O11 Dy1 O12 62.43(13) . . ?
O31 Dy1 O12 136.80(13) . . ?
O62 Dy1 O12 80.2(2) . . ?
O52 Dy1 O12 67.81(15) . . ?
O42 Dy1 O12 137.57(13) . . ?
O51 Dy1 O12 70.82(14) . . ?
O41 Dy1 O12 115.86(14) . . ?
O61 Dy1 O12 66.49(15) . . ?
O11 Dy1 O32 136.84(13) . . ?

O31 Dy1 O32 61.56(12) . . ?
O62 Dy1 O32 135.86(15) . . ?
O52 Dy1 O32 73.37(14) . . ?
O42 Dy1 O32 80.46(15) . . ?
O51 Dy1 O32 67.88(14) . . ?
O41 Dy1 O32 64.20(13) . . ?
O61 Dy1 O32 110.10(19) . . ?
O12 Dy1 O32 135.24(14) . . ?
O11 Dy1 N61 94.5(2) . . ?
O31 Dy1 N61 71.24(17) . . ?
O62 Dy1 N61 26.5(3) . . ?
O52 Dy1 N61 132.0(2) . . ?
O42 Dy1 N61 109.0(3) . . ?
O51 Dy1 N61 92.9(3) . . ?
O41 Dy1 N61 158.4(3) . . ?
O61 Dy1 N61 26.7(3) . . ?
O12 Dy1 N61 70.50(17) . . ?
O32 Dy1 N61 127.3(2) . . ?
O11 Dy1 N51 107.34(15) . . ?
O31 Dy1 N51 112.54(15) . . ?
O62 Dy1 N51 136.3(3) . . ?
O52 Dy1 N51 26.74(16) . . ?
O42 Dy1 N51 138.5(2) . . ?
O51 Dy1 N51 24.85(16) . . ?
O41 Dy1 N51 88.8(2) . . ?
O61 Dy1 N51 87.3(2) . . ?
O12 Dy1 N51 65.65(15) . . ?
O32 Dy1 N51 69.63(14) . . ?
N61 Dy1 N51 111.9(3) . . ?
O111 Dy2 O111 135.5(2) 4_655 . ?
O111 Dy2 O141 78.71(14) 4_655 . ?
O111 Dy2 O141 117.87(13) . . ?
O111 Dy2 O141 117.87(13) 4_655 4_655 ?
O111 Dy2 O141 78.72(14) . 4_655 ?
O141 Dy2 O141 138.0(2) . 4_655 ?
O111 Dy2 O151 135.26(14) 4_655 . ?
O111 Dy2 O151 88.53(14) . . ?
O141 Dy2 O151 71.40(15) . . ?
O141 Dy2 O151 70.78(15) 4_655 . ?
O111 Dy2 O151 88.53(14) 4_655 4_655 ?
O111 Dy2 O151 135.26(14) . 4_655 ?
O141 Dy2 O151 70.78(15) . 4_655 ?
O141 Dy2 O151 71.40(15) 4_655 4_655 ?
O151 Dy2 O151 50.7(2) . 4_655 ?
O111 Dy2 O142 118.27(13) 4_655 . ?
O111 Dy2 O142 66.87(12) . . ?
O141 Dy2 O142 51.20(13) . . ?
O141 Dy2 O142 123.38(14) 4_655 . ?
O151 Dy2 O142 65.02(14) . . ?
O151 Dy2 O142 103.27(14) 4_655 . ?

O111 Dy2 O142 66.87(12) 4_655 4_655 ?
O111 Dy2 O142 118.28(13) . 4_655 ?
O141 Dy2 O142 123.37(14) . 4_655 ?
O141 Dy2 O142 51.20(13) 4_655 4_655 ?
O151 Dy2 O142 103.26(15) . 4_655 ?
O151 Dy2 O142 65.02(14) 4_655 4_655 ?
O142 Dy2 O142 167.7(2) . 4_655 ?
O111 Dy2 O112 79.53(13) 4_655 . ?
O111 Dy2 O112 64.54(13) . . ?
O141 Dy2 O112 146.42(15) . . ?
O141 Dy2 O112 75.27(15) 4_655 . ?
O151 Dy2 O112 140.14(13) . . ?
O151 Dy2 O112 133.71(14) 4_655 . ?
O142 Dy2 O112 121.85(13) . . ?
O142 Dy2 O112 69.18(14) 4_655 . ?
O111 Dy2 O112 64.54(13) 4_655 4_655 ?
O111 Dy2 O112 79.53(13) . 4_655 ?
O141 Dy2 O112 75.27(15) . 4_655 ?
O141 Dy2 O112 146.42(15) 4_655 4_655 ?
O151 Dy2 O112 133.71(14) . 4_655 ?
O151 Dy2 O112 140.14(13) 4_655 4_655 ?
O142 Dy2 O112 69.17(14) . 4_655 ?
O142 Dy2 O112 121.85(13) 4_655 4_655 ?
O112 Dy2 O112 72.4(2) . 4_655 ?
O111 Dy2 N151 112.26(10) 4_655 . ?
O111 Dy2 N151 112.27(10) . . ?
O141 Dy2 N151 68.98(12) . . ?
O141 Dy2 N151 68.98(12) 4_655 . ?
O151 Dy2 N151 25.36(10) . . ?
O151 Dy2 N151 25.36(10) 4_655 . ?
O142 Dy2 N151 83.87(11) . . ?
O142 Dy2 N151 83.87(11) 4_655 . ?
O112 Dy2 N151 143.81(10) . . ?
O112 Dy2 N151 143.81(10) 4_655 . ?
O111 Dy2 N141 91.90(13) 4_655 4_655 ?
O111 Dy2 N141 100.71(14) . 4_655 ?
O141 Dy2 N141 133.54(16) . 4_655 ?
O141 Dy2 N141 26.33(13) 4_655 4_655 ?
O151 Dy2 N141 85.61(15) . 4_655 ?
O151 Dy2 N141 63.52(17) 4_655 4_655 ?
O142 Dy2 N141 147.61(15) . 4_655 ?
O142 Dy2 N141 25.03(13) 4_655 4_655 ?
O112 Dy2 N141 72.29(16) . 4_655 ?
O112 Dy2 N141 140.41(16) 4_655 4_655 ?
N151 Dy2 N141 73.20(13) . 4_655 ?
C12 O11 Dy1 129.1(4) . . ?
C13 O12 C24 116.7(4) . . ?
C13 O12 Dy1 113.9(3) . . ?
C24 O12 Dy1 129.0(3) . . ?
C32 O31 Dy1 128.6(4) . . ?

C33 O32 C44 117.3(4) . . ?
C33 O32 Dy1 113.6(3) . . ?
C44 O32 Dy1 128.5(3) . . ?
N41 O41 Dy1 95.2(4) . . ?
N41 O42 Dy1 96.6(4) . . ?
N51 O51 Dy1 96.9(4) . . ?
N51 O52 Dy1 95.2(4) . . ?
N61 O61 Dy1 92.2(5) . . ?
N61 O62 Dy1 95.3(6) . . ?
C113 O112 C124 114.6(5) . . ?
C113 O112 Dy2 117.6(3) . . ?
C124 O112 Dy2 127.7(3) . . ?
N141 O141 Dy2 96.5(3) . . ?
N141 O142 Dy2 95.2(3) . . ?
N151 O151 Dy2 93.9(4) . . ?
C16 C11 C12 120.6(5) . . ?
C16 C11 C17 119.4(5) . . ?
C12 C11 C17 120.0(5) . . ?
O11 C12 C13 119.6(5) . . ?
O11 C12 C11 123.0(5) . . ?
C13 C12 C11 117.3(5) . . ?
C14 C13 O12 125.4(5) . . ?
C14 C13 C12 121.7(5) . . ?
O12 C13 C12 112.9(5) . . ?
C13 C14 C15 120.5(6) . . ?
C13 C14 H14A 119.8 . . ?
C15 C14 H14A 119.8 . . ?
C16 C15 C14 118.6(5) . . ?
C16 C15 H15A 120.7 . . ?
C14 C15 H15A 120.7 . . ?
C15 C16 C11 121.3(5) . . ?
C15 C16 H16A 119.3 . . ?
C11 C16 H16A 119.3 . . ?
N11 C17 C11 122.4(5) . . ?
N11 C17 H17A 118.8 . . ?
C11 C17 H17A 118.8 . . ?
C19 C18 C23 121.9(6) . . ?
C19 C18 N11 116.3(5) . . ?
C23 C18 N11 121.8(5) . . ?
C18 C19 C20 119.0(6) . . ?
C18 C19 H19A 120.5 . . ?
C20 C19 H19A 120.5 . . ?
C21 C20 C19 119.7(6) . . ?
C21 C20 H20A 120.1 . . ?
C19 C20 H20A 120.1 . . ?
C20 C21 C22 120.2(6) . . ?
C20 C21 H21A 119.9 . . ?
C22 C21 H21A 119.9 . . ?
C23 C22 C21 120.9(6) . . ?
C23 C22 H22A 119.6 . . ?

C21 C22 H22A 119.6 . . ?
C22 C23 C18 118.2(6) . . ?
C22 C23 H23A 120.9 . . ?
C18 C23 H23A 120.9 . . ?
O12 C24 H24A 109.5 . . ?
O12 C24 H24B 109.5 . . ?
H24A C24 H24B 109.5 . . ?
O12 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
C37 C31 C32 121.2(5) . . ?
C37 C31 C36 120.2(5) . . ?
C32 C31 C36 118.5(5) . . ?
O31 C32 C33 118.9(5) . . ?
O31 C32 C31 122.4(5) . . ?
C33 C32 C31 118.7(5) . . ?
C34 C33 O32 125.6(5) . . ?
C34 C33 C32 120.9(5) . . ?
O32 C33 C32 113.5(5) . . ?
C33 C34 C35 120.2(6) . . ?
C33 C34 H34A 119.9 . . ?
C35 C34 H34A 119.9 . . ?
C36 C35 C34 120.2(5) . . ?
C36 C35 H35A 119.9 . . ?
C34 C35 H35A 119.9 . . ?
C35 C36 C31 121.4(5) . . ?
C35 C36 H36A 119.3 . . ?
C31 C36 H36A 119.3 . . ?
N31 C37 C31 121.8(5) . . ?
N31 C37 H37A 119.1 . . ?
C31 C37 H37A 119.1 . . ?
C43 C38 C39 120.7(6) . . ?
C43 C38 N31 123.7(6) . . ?
C39 C38 N31 115.6(5) . . ?
C40 C39 C38 119.3(6) . . ?
C40 C39 H39A 120.4 . . ?
C38 C39 H39A 120.4 . . ?
C41 C40 C39 120.3(6) . . ?
C41 C40 H40A 119.8 . . ?
C39 C40 H40A 119.8 . . ?
C40 C41 C42 120.2(7) . . ?
C40 C41 H41A 119.9 . . ?
C42 C41 H41A 119.9 . . ?
C41 C42 C43 120.1(6) . . ?
C41 C42 H42A 120.0 . . ?
C43 C42 H42A 120.0 . . ?
C38 C43 C42 119.4(6) . . ?
C38 C43 H43A 120.3 . . ?
C42 C43 H43A 120.3 . . ?
O32 C44 H44A 109.5 . . ?

O32 C44 H44B 109.5 . . ?
H44A C44 H44B 109.5 . . ?
O32 C44 H44C 109.5 . . ?
H44A C44 H44C 109.5 . . ?
H44B C44 H44C 109.5 . . ?
C112 C111 C116 120.6(5) . . ?
C112 C111 C117 121.0(5) . . ?
C116 C111 C117 118.4(5) . . ?
O111 C112 C113 120.4(5) . . ?
O111 C112 C111 122.0(5) . . ?
C113 C112 C111 117.6(5) . . ?
C114 C113 O112 126.4(5) . . ?
C114 C113 C112 122.3(5) . . ?
O112 C113 C112 111.4(5) . . ?
C113 C114 C115 119.2(6) . . ?
C113 C114 H11A 120.4 . . ?
C115 C114 H11A 120.4 . . ?
C116 C115 C114 121.2(6) . . ?
C116 C115 H11B 119.4 . . ?
C114 C115 H11B 119.4 . . ?
C115 C116 C111 119.1(6) . . ?
C115 C116 H11C 120.4 . . ?
C111 C116 H11C 120.4 . . ?
N111 C117 C111 121.6(5) . . ?
N111 C117 H11D 119.2 . . ?
C111 C117 H11D 119.2 . . ?
C123 C118 C119 121.1(6) . . ?
C123 C118 N111 122.1(5) . . ?
C119 C118 N111 116.7(5) . . ?
C120 C119 C118 119.7(6) . . ?
C120 C119 H11E 120.1 . . ?
C118 C119 H11E 120.1 . . ?
C119 C120 C121 119.4(6) . . ?
C119 C120 H12A 120.3 . . ?
C121 C120 H12A 120.3 . . ?
C122 C121 C120 120.4(5) . . ?
C122 C121 H12B 119.8 . . ?
C120 C121 H12B 119.8 . . ?
C121 C122 C123 120.7(5) . . ?
C121 C122 H12C 119.6 . . ?
C123 C122 H12C 119.6 . . ?
C118 C123 C122 118.5(6) . . ?
C118 C123 H12D 120.7 . . ?
C122 C123 H12D 120.7 . . ?
O112 C124 H12E 109.5 . . ?
O112 C124 H12F 109.5 . . ?
H12E C124 H12F 109.5 . . ?
O112 C124 H12G 109.5 . . ?
H12E C124 H12G 109.5 . . ?
H12F C124 H12G 109.5 . . ?

C17 N11 C18 129.1(5) . . ?
C17 N11 H11F 115.4 . . ?
C18 N11 H11F 115.4 . . ?
C37 N31 C38 127.6(5) . . ?
C37 N31 H31A 116.2 . . ?
C38 N31 H31A 116.2 . . ?
O43 N41 O42 122.6(7) . . ?
O43 N41 O41 120.7(6) . . ?
O42 N41 O41 116.6(6) . . ?
O43 N41 Dy1 179.7(6) . . ?
O42 N41 Dy1 57.7(4) . . ?
O41 N41 Dy1 59.0(3) . . ?
O51 N51 O53 122.4(7) . . ?
O51 N51 O52 116.1(7) . . ?
O53 N51 O52 121.4(7) . . ?
O51 N51 Dy1 58.2(4) . . ?
O53 N51 Dy1 178.6(4) . . ?
O52 N51 Dy1 58.1(4) . . ?
O63 N61 O62 120.5(12) . . ?
O63 N61 O61 120.0(11) . . ?
O62 N61 O61 119.1(7) . . ?
O63 N61 Dy1 177.2(6) . . ?
O62 N61 Dy1 58.2(4) . . ?
O61 N61 Dy1 61.0(4) . . ?
C117 N111 C118 128.5(5) . . ?
C117 N111 H11G 115.8 . . ?
C118 N111 H11G 115.8 . . ?
O143 N141 O142 123.6(5) . . ?
O143 N141 O141 120.0(5) . . ?
O142 N141 O141 116.3(5) . . ?
O143 N141 Dy2 171.1(5) . . ?
O142 N141 Dy2 59.8(3) . . ?
O141 N141 Dy2 57.1(3) . . ?
O151 N151 O151 121.4(8) . 4_655 ?
O151 N151 O153 119.3(4) . . ?
O151 N151 O153 119.3(4) 4_655 . ?
O151 N151 Dy2 60.7(4) . . ?
O151 N151 Dy2 60.7(4) 4_655 . ?
O153 N151 Dy2 180.0 . . ?
C112 O111 Dy2 126.0(3) . . ?

loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3

_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
O31 Dy1 O11 C12 144.1(4) . . . . ?
O62 Dy1 O11 C12 98.4(5) . . . . ?
O52 Dy1 O11 C12 -53.7(4) . . . . ?
O42 Dy1 O11 C12 -173.3(5) . . . . ?
O51 Dy1 O11 C12 -18.8(5) . . . . ?
O41 Dy1 O11 C12 -119.7(5) . . . . ?
O61 Dy1 O11 C12 58.0(5) . . . . ?
O12 Dy1 O11 C12 13.0(4) . . . . ?
O32 Dy1 O11 C12 -114.9(4) . . . . ?
N61 Dy1 O11 C12 78.2(5) . . . . ?
N51 Dy1 O11 C12 -36.5(5) . . . . ?
O11 Dy1 O12 C13 -11.5(4) . . . . ?
O31 Dy1 O12 C13 -146.7(4) . . . . ?
O62 Dy1 O12 C13 -92.2(4) . . . . ?
O52 Dy1 O12 C13 86.6(4) . . . . ?
O42 Dy1 O12 C13 -20.5(5) . . . . ?
O51 Dy1 O12 C13 141.9(4) . . . . ?
O41 Dy1 O12 C13 39.8(4) . . . . ?
O61 Dy1 O12 C13 -146.2(5) . . . . ?
O32 Dy1 O12 C13 118.4(4) . . . . ?
N61 Dy1 O12 C13 -117.7(5) . . . . ?
N51 Dy1 O12 C13 115.7(4) . . . . ?
O11 Dy1 O12 C24 175.5(5) . . . . ?
O31 Dy1 O12 C24 40.4(5) . . . . ?
O62 Dy1 O12 C24 94.8(5) . . . . ?
O52 Dy1 O12 C24 -86.3(5) . . . . ?
O42 Dy1 O12 C24 166.5(4) . . . . ?
O51 Dy1 O12 C24 -31.0(4) . . . . ?
O41 Dy1 O12 C24 -133.1(4) . . . . ?
O61 Dy1 O12 C24 40.8(5) . . . . ?
O32 Dy1 O12 C24 -54.5(5) . . . . ?
N61 Dy1 O12 C24 69.3(5) . . . . ?
N51 Dy1 O12 C24 -57.2(5) . . . . ?
O11 Dy1 O31 C32 148.0(4) . . . . ?
O62 Dy1 O31 C32 -165.7(5) . . . . ?
O52 Dy1 O31 C32 -8.3(6) . . . . ?
O42 Dy1 O31 C32 105.1(5) . . . . ?
O51 Dy1 O31 C32 -45.7(5) . . . . ?
O41 Dy1 O31 C32 64.6(5) . . . . ?
O61 Dy1 O31 C32 -109.8(5) . . . . ?
O12 Dy1 O31 C32 -109.3(5) . . . . ?
O32 Dy1 O31 C32 17.7(4) . . . . ?
N61 Dy1 O31 C32 -138.1(6) . . . . ?
N51 Dy1 O31 C32 -31.5(5) . . . . ?
O11 Dy1 O32 C33 -149.5(3) . . . . ?
O31 Dy1 O32 C33 -15.2(3) . . . . ?
O62 Dy1 O32 C33 -20.0(5) . . . . ?
O52 Dy1 O32 C33 144.5(4) . . . . ?

O42 Dy1 O32 C33 -92.8(4) . . . . ?
O51 Dy1 O32 C33 89.9(4) . . . . ?
O41 Dy1 O32 C33 -144.5(4) . . . . ?
O61 Dy1 O32 C33 37.4(4) . . . . ?
O12 Dy1 O32 C33 113.9(4) . . . . ?
N61 Dy1 O32 C33 13.9(5) . . . . ?
N51 Dy1 O32 C33 116.5(4) . . . . ?
O11 Dy1 O32 C44 40.2(5) . . . . ?
O31 Dy1 O32 C44 174.5(5) . . . . ?
O62 Dy1 O32 C44 169.8(5) . . . . ?
O52 Dy1 O32 C44 -25.8(5) . . . . ?
O42 Dy1 O32 C44 96.9(5) . . . . ?
O51 Dy1 O32 C44 -80.4(5) . . . . ?
O41 Dy1 O32 C44 45.2(5) . . . . ?
O61 Dy1 O32 C44 -132.8(5) . . . . ?
O12 Dy1 O32 C44 -56.4(5) . . . . ?
N61 Dy1 O32 C44 -156.3(5) . . . . ?
N51 Dy1 O32 C44 -53.8(5) . . . . ?
O11 Dy1 O41 N41 -86.4(4) . . . . ?
O31 Dy1 O41 N41 51.8(4) . . . . ?
O62 Dy1 O41 N41 -32.4(4) . . . . ?
O52 Dy1 O41 N41 179.6(4) . . . . ?
O42 Dy1 O41 N41 -1.3(3) . . . . ?
O51 Dy1 O41 N41 149.9(4) . . . . ?
O61 Dy1 O41 N41 115.3(19) . . . . ?
O12 Dy1 O41 N41 -132.8(3) . . . . ?
O32 Dy1 O41 N41 97.2(4) . . . . ?
N61 Dy1 O41 N41 -30.3(7) . . . . ?
N51 Dy1 O41 N41 165.1(4) . . . . ?
O11 Dy1 O42 N41 80.6(4) . . . . ?
O31 Dy1 O42 N41 -126.2(4) . . . . ?
O62 Dy1 O42 N41 158.7(4) . . . . ?
O52 Dy1 O42 N41 2.3(4) . . . . ?
O51 Dy1 O42 N41 -58.4(5) . . . . ?
O41 Dy1 O42 N41 1.3(3) . . . . ?
O61 Dy1 O42 N41 -171.6(4) . . . . ?
O12 Dy1 O42 N41 88.9(4) . . . . ?
O32 Dy1 O42 N41 -63.2(4) . . . . ?
N61 Dy1 O42 N41 170.5(4) . . . . ?
N51 Dy1 O42 N41 -19.4(4) . . . . ?
O11 Dy1 O51 N51 -43.7(4) . . . . ?
O31 Dy1 O51 N51 147.2(4) . . . . ?
O62 Dy1 O51 N51 -139.6(4) . . . . ?
O52 Dy1 O51 N51 3.2(4) . . . . ?
O42 Dy1 O51 N51 84.0(5) . . . . ?
O41 Dy1 O51 N51 38.4(4) . . . . ?
O61 Dy1 O51 N51 -145.3(4) . . . . ?
O12 Dy1 O51 N51 -73.3(4) . . . . ?
O32 Dy1 O51 N51 89.1(4) . . . . ?
N61 Dy1 O51 N51 -141.5(4) . . . . ?

O11 Dy1 O52 N51 141.1(4) . . . . ?
O31 Dy1 O52 N51 -53.9(4) . . . . ?
O62 Dy1 O52 N51 81.7(5) . . . . ?
O42 Dy1 O52 N51 -147.0(3) . . . . ?
O51 Dy1 O52 N51 -3.0(3) . . . . ?
O41 Dy1 O52 N51 -146.2(4) . . . . ?
O61 Dy1 O52 N51 28.0(4) . . . . ?
O12 Dy1 O52 N51 79.6(4) . . . . ?
O32 Dy1 O52 N51 -77.6(3) . . . . ?
N61 Dy1 O52 N51 48.0(5) . . . . ?
O11 Dy1 O61 N61 50.0(5) . . . . ?
O31 Dy1 O61 N61 -87.2(4) . . . . ?
O62 Dy1 O61 N61 -2.3(4) . . . . ?
O52 Dy1 O61 N61 145.5(4) . . . . ?
O42 Dy1 O61 N61 -40.4(5) . . . . ?
O51 Dy1 O61 N61 171.5(5) . . . . ?
O41 Dy1 O61 N61 -152.5(18) . . . . ?
O12 Dy1 O61 N61 93.1(4) . . . . ?
O32 Dy1 O61 N61 -135.2(4) . . . . ?
N51 Dy1 O61 N61 157.7(4) . . . . ?
O11 Dy1 O62 N61 -129.3(5) . . . . ?
O31 Dy1 O62 N61 79.1(4) . . . . ?
O52 Dy1 O62 N61 -67.6(5) . . . . ?
O42 Dy1 O62 N61 154.4(5) . . . . ?
O51 Dy1 O62 N61 -4.2(5) . . . . ?
O41 Dy1 O62 N61 178.3(4) . . . . ?
O61 Dy1 O62 N61 2.3(4) . . . . ?
O12 Dy1 O62 N61 -65.6(5) . . . . ?
O32 Dy1 O62 N61 83.4(6) . . . . ?
N51 Dy1 O62 N61 -27.4(5) . . . . ?
O111 Dy2 O112 C113 -155.0(4) 4_655 . . . ?
O111 Dy2 O112 C113 -2.0(3) . . . . ?
O141 Dy2 O112 C113 -104.7(4) . . . . ?
O141 Dy2 O112 C113 82.3(4) 4_655 . . . ?
O151 Dy2 O112 C113 50.1(5) . . . . ?
O151 Dy2 O112 C113 127.3(4) 4_655 . . . ?
O142 Dy2 O112 C113 -38.1(4) . . . . ?
O142 Dy2 O112 C113 135.9(4) 4_655 . . . ?
O112 Dy2 O112 C113 -88.6(4) 4_655 . . . ?
N151 Dy2 O112 C113 91.4(4) . . . . ?
N141 Dy2 O112 C113 109.6(4) 4_655 . . . ?
O111 Dy2 O112 C124 21.1(5) 4_655 . . . ?
O111 Dy2 O112 C124 174.1(5) . . . . ?
O141 Dy2 O112 C124 71.5(5) . . . . ?
O141 Dy2 O112 C124 -101.6(5) 4_655 . . . ?
O151 Dy2 O112 C124 -133.8(4) . . . . ?
O151 Dy2 O112 C124 -56.6(5) 4_655 . . . ?
O142 Dy2 O112 C124 138.0(4) . . . . ?
O142 Dy2 O112 C124 -48.0(4) 4_655 . . . ?
O112 Dy2 O112 C124 87.5(5) 4_655 . . . ?

N151 Dy2 O112 C124 -92.5(5) . . . . ?
N141 Dy2 O112 C124 -74.3(5) 4_655 . . . ?
O111 Dy2 O141 N141 146.1(4) 4_655 . . . ?
O111 Dy2 O141 N141 10.3(4) . . . . ?
O141 Dy2 O141 N141 -94.5(4) 4_655 . . . ?
O151 Dy2 O141 N141 -67.6(4) . . . . ?
O151 Dy2 O141 N141 -121.5(4) 4_655 . . . ?
O142 Dy2 O141 N141 4.8(4) . . . . ?
O142 Dy2 O141 N141 -161.5(4) 4_655 . . . ?
O112 Dy2 O141 N141 95.6(4) . . . . ?
O112 Dy2 O141 N141 79.8(4) 4_655 . . . ?
N151 Dy2 O141 N141 -94.5(4) . . . . ?
N141 Dy2 O141 N141 -132.1(4) 4_655 . . . ?
O111 Dy2 O142 N141 -49.2(4) 4_655 . . . ?
O111 Dy2 O142 N141 -179.8(4) . . . . ?
O141 Dy2 O142 N141 -5.1(4) . . . . ?
O141 Dy2 O142 N141 122.6(4) 4_655 . . . ?
O151 Dy2 O142 N141 80.5(4) . . . . ?
O151 Dy2 O142 N141 46.3(4) 4_655 . . . ?
O142 Dy2 O142 N141 62.8(4) 4_655 . . . ?
O112 Dy2 O142 N141 -144.5(4) . . . . ?
O112 Dy2 O142 N141 -92.6(4) 4_655 . . . ?
N151 Dy2 O142 N141 62.8(4) . . . . ?
N141 Dy2 O142 N141 107.4(6) 4_655 . . . ?
O111 Dy2 O151 N151 -29.3(3) 4_655 . . . ?
O111 Dy2 O151 N151 159.9(2) . . . . ?
O141 Dy2 O151 N151 -80.0(2) . . . . ?
O141 Dy2 O151 N151 81.3(2) 4_655 . . . ?
O151 Dy2 O151 N151 0.0 4_655 . . . ?
O142 Dy2 O151 N151 -135.1(3) . . . . ?
O142 Dy2 O151 N151 41.1(2) 4_655 . . . ?
O112 Dy2 O151 N151 114.4(2) . . . . ?
O112 Dy2 O151 N151 -126.2(2) 4_655 . . . ?
N141 Dy2 O151 N151 59.0(2) 4_655 . . . ?
Dy1 O11 C12 C13 -12.9(7) . . . . ?
Dy1 O11 C12 C11 166.4(4) . . . . ?
C16 C11 C12 O11 -178.9(5) . . . . ?
C17 C11 C12 O11 1.5(9) . . . . ?
C16 C11 C12 C13 0.4(8) . . . . ?
C17 C11 C12 C13 -179.2(5) . . . . ?
C24 O12 C13 C14 4.7(9) . . . . ?
Dy1 O12 C13 C14 -169.2(5) . . . . ?
C24 O12 C13 C12 -175.8(5) . . . . ?
Dy1 O12 C13 C12 10.3(6) . . . . ?
O11 C12 C13 C14 178.6(5) . . . . ?
C11 C12 C13 C14 -0.7(8) . . . . ?
O11 C12 C13 O12 -0.9(8) . . . . ?
C11 C12 C13 O12 179.8(5) . . . . ?
O12 C13 C14 C15 -179.7(6) . . . . ?
C12 C13 C14 C15 0.8(9) . . . . ?

C13 C14 C15 C16 -0.7(9) . . . . ?
C14 C15 C16 C11 0.4(9) . . . . ?
C12 C11 C16 C15 -0.3(9) . . . . ?
C17 C11 C16 C15 179.3(6) . . . . ?
C16 C11 C17 N11 -178.0(5) . . . . ?
C12 C11 C17 N11 1.5(9) . . . . ?
C23 C18 C19 C20 2.3(10) . . . . ?
N11 C18 C19 C20 -178.7(6) . . . . ?
C18 C19 C20 C21 -1.1(10) . . . . ?
C19 C20 C21 C22 -0.8(10) . . . . ?
C20 C21 C22 C23 1.5(10) . . . . ?
C21 C22 C23 C18 -0.3(9) . . . . ?
C19 C18 C23 C22 -1.6(9) . . . . ?
N11 C18 C23 C22 179.4(5) . . . . ?
Dy1 O31 C32 C33 -18.0(8) . . . . ?
Dy1 O31 C32 C31 162.7(4) . . . . ?
C37 C31 C32 O31 2.7(9) . . . . ?
C36 C31 C32 O31 -179.7(5) . . . . ?
C37 C31 C32 C33 -176.6(5) . . . . ?
C36 C31 C32 C33 1.0(8) . . . . ?
C44 O32 C33 C34 4.6(8) . . . . ?
Dy1 O32 C33 C34 -166.8(5) . . . . ?
C44 O32 C33 C32 -175.1(5) . . . . ?
Dy1 O32 C33 C32 13.4(6) . . . . ?
O31 C32 C33 C34 179.8(5) . . . . ?
C31 C32 C33 C34 -0.9(8) . . . . ?
O31 C32 C33 O32 -0.4(8) . . . . ?
C31 C32 C33 O32 178.9(5) . . . . ?
O32 C33 C34 C35 179.9(5) . . . . ?
C32 C33 C34 C35 -0.4(9) . . . . ?
C33 C34 C35 C36 1.5(9) . . . . ?
C34 C35 C36 C31 -1.3(9) . . . . ?
C37 C31 C36 C35 177.7(6) . . . . ?
C32 C31 C36 C35 0.1(8) . . . . ?
C32 C31 C37 N31 0.2(9) . . . . ?
C36 C31 C37 N31 -177.4(5) . . . . ?
C43 C38 C39 C40 -0.1(9) . . . . ?
N31 C38 C39 C40 178.8(5) . . . . ?
C38 C39 C40 C41 1.4(9) . . . . ?
C39 C40 C41 C42 -0.6(10) . . . . ?
C40 C41 C42 C43 -1.4(11) . . . . ?
C39 C38 C43 C42 -2.0(9) . . . . ?
N31 C38 C43 C42 179.2(6) . . . . ?
C41 C42 C43 C38 2.7(10) . . . . ?
C116 C111 C112 O111 -179.0(5) . . . . ?
C117 C111 C112 O111 4.6(8) . . . . ?
C116 C111 C112 C113 3.2(8) . . . . ?
C117 C111 C112 C113 -173.1(5) . . . . ?
C124 O112 C113 C114 4.9(8) . . . . ?
Dy2 O112 C113 C114 -178.4(5) . . . . ?

C124 O112 C113 C112 -175.0(5) . . . . ?
Dy2 O112 C113 C112 1.6(6) . . . . ?
O111 C112 C113 C114 -179.6(5) . . . . ?
C111 C112 C113 C114 -1.8(8) . . . . ?
O111 C112 C113 O112 0.3(7) . . . . ?
C111 C112 C113 O112 178.1(5) . . . . ?
O112 C113 C114 C115 -179.9(5) . . . . ?
C112 C113 C114 C115 0.1(9) . . . . ?
C113 C114 C115 C116 0.3(9) . . . . ?
C114 C115 C116 C111 1.1(9) . . . . ?
C112 C111 C116 C115 -2.9(8) . . . . ?
C117 C111 C116 C115 173.6(5) . . . . ?
C112 C111 C117 N111 3.7(8) . . . . ?
C116 C111 C117 N111 -172.8(5) . . . . ?
C123 C118 C119 C120 0.4(9) . . . . ?
N111 C118 C119 C120 -179.9(5) . . . . ?
C118 C119 C120 C121 0.8(9) . . . . ?
C119 C120 C121 C122 -2.1(9) . . . . ?
C120 C121 C122 C123 2.2(9) . . . . ?
C119 C118 C123 C122 -0.3(8) . . . . ?
N111 C118 C123 C122 180.0(5) . . . . ?
C121 C122 C123 C118 -1.0(9) . . . . ?
C11 C17 N11 C18 -179.0(5) . . . . ?
C19 C18 N11 C17 -174.3(6) . . . . ?
C23 C18 N11 C17 4.7(9) . . . . ?
C31 C37 N31 C38 -180.0(5) . . . . ?
C43 C38 N31 C37 8.8(10) . . . . ?
C39 C38 N31 C37 -170.1(6) . . . . ?
Dy1 O42 N41 O43 179.9(6) . . . . ?
Dy1 O42 N41 O41 -2.3(6) . . . . ?
Dy1 O41 N41 O43 -179.9(5) . . . . ?
Dy1 O41 N41 O42 2.3(6) . . . . ?
O11 Dy1 N41 O43 103(100) . . . . ?
O31 Dy1 N41 O43 -114(100) . . . . ?
O62 Dy1 N41 O43 173(100) . . . . ?
O52 Dy1 N41 O43 17(100) . . . . ?
O42 Dy1 N41 O43 -165(100) . . . . ?
O51 Dy1 N41 O43 -21(100) . . . . ?
O41 Dy1 N41 O43 17(100) . . . . ?
O61 Dy1 N41 O43 -149(100) . . . . ?
O12 Dy1 N41 O43 79(100) . . . . ?
O32 Dy1 N41 O43 -54(100) . . . . ?
N61 Dy1 N41 O43 -178(100) . . . . ?
N51 Dy1 N41 O43 1(100) . . . . ?
O11 Dy1 N41 O42 -92.0(4) . . . . ?
O31 Dy1 N41 O42 51.1(4) . . . . ?
O62 Dy1 N41 O42 -22.5(4) . . . . ?
O52 Dy1 N41 O42 -178.0(4) . . . . ?
O51 Dy1 N41 O42 144.0(3) . . . . ?
O41 Dy1 N41 O42 -177.6(6) . . . . ?

O61 Dy1 N41 O42 15.9(7) . . . . ?
O12 Dy1 N41 O42 -116.2(3) . . . . ?
O32 Dy1 N41 O42 110.5(4) . . . . ?
N61 Dy1 N41 O42 -12.6(5) . . . . ?
N51 Dy1 N41 O42 166.1(3) . . . . ?
O11 Dy1 N41 O41 85.5(4) . . . . ?
O31 Dy1 N41 O41 -131.3(4) . . . . ?
O62 Dy1 N41 O41 155.1(3) . . . . ?
O52 Dy1 N41 O41 -0.4(4) . . . . ?
O42 Dy1 N41 O41 177.6(6) . . . . ?
O51 Dy1 N41 O41 -38.4(4) . . . . ?
O61 Dy1 N41 O41 -166.5(5) . . . . ?
O12 Dy1 N41 O41 61.3(4) . . . . ?
O32 Dy1 N41 O41 -71.9(3) . . . . ?
N61 Dy1 N41 O41 165.0(4) . . . . ?
N51 Dy1 N41 O41 -16.3(4) . . . . ?
Dy1 O51 N51 O53 178.6(5) . . . . ?
Dy1 O51 N51 O52 -5.2(6) . . . . ?
Dy1 O52 N51 O51 5.2(6) . . . . ?
Dy1 O52 N51 O53 -178.5(5) . . . . ?
O11 Dy1 N51 O51 144.5(4) . . . . ?
O31 Dy1 N51 O51 -35.9(4) . . . . ?
O62 Dy1 N51 O51 54.9(4) . . . . ?
O52 Dy1 N51 O51 -174.5(6) . . . . ?
O42 Dy1 N51 O51 -127.9(4) . . . . ?
O41 Dy1 N51 O51 -143.9(4) . . . . ?
O61 Dy1 N51 O51 31.5(4) . . . . ?
O12 Dy1 N51 O51 96.8(4) . . . . ?
O32 Dy1 N51 O51 -81.1(4) . . . . ?
N61 Dy1 N51 O51 42.1(4) . . . . ?
O11 Dy1 N51 O53 26(26) . . . . ?
O31 Dy1 N51 O53 -154(100) . . . . ?
O62 Dy1 N51 O53 -63(26) . . . . ?
O52 Dy1 N51 O53 67(26) . . . . ?
O42 Dy1 N51 O53 114(26) . . . . ?
O51 Dy1 N51 O53 -118(27) . . . . ?
O41 Dy1 N51 O53 98(26) . . . . ?
O61 Dy1 N51 O53 -87(26) . . . . ?
O12 Dy1 N51 O53 -21(26) . . . . ?
O32 Dy1 N51 O53 161(100) . . . . ?
N61 Dy1 N51 O53 -76(26) . . . . ?
O11 Dy1 N51 O52 -41.0(4) . . . . ?
O31 Dy1 N51 O52 138.6(3) . . . . ?
O62 Dy1 N51 O52 -130.6(4) . . . . ?
O42 Dy1 N51 O52 46.6(4) . . . . ?
O51 Dy1 N51 O52 174.5(6) . . . . ?
O41 Dy1 N51 O52 30.5(4) . . . . ?
O61 Dy1 N51 O52 -154.0(4) . . . . ?
O12 Dy1 N51 O52 -88.7(3) . . . . ?
O32 Dy1 N51 O52 93.4(4) . . . . ?

N61 Dy1 N51 O52 -143.4(4) . . . . ?
Dy1 O62 N61 O63 -177.1(7) . . . . ?
Dy1 O62 N61 O61 -4.1(8) . . . . ?
Dy1 O61 N61 O63 177.0(7) . . . . ?
Dy1 O61 N61 O62 4.0(7) . . . . ?
O11 Dy1 N61 O63 112(21) . . . . ?
O31 Dy1 N61 O63 -30(21) . . . . ?
O62 Dy1 N61 O63 63(21) . . . . ?
O52 Dy1 N61 O63 -159(21) . . . . ?
O42 Dy1 N61 O63 35(22) . . . . ?
O51 Dy1 N61 O63 -121(21) . . . . ?
O41 Dy1 N61 O63 59(22) . . . . ?
O61 Dy1 N61 O63 -113(22) . . . . ?
O12 Dy1 N61 O63 170(22) . . . . ?
O32 Dy1 N61 O63 -57(22) . . . . ?
N51 Dy1 N61 O63 -137(21) . . . . ?
O11 Dy1 N61 O62 49.2(5) . . . . ?
O31 Dy1 N61 O62 -92.6(5) . . . . ?
O52 Dy1 N61 O62 138.8(4) . . . . ?
O42 Dy1 N61 O62 -27.1(5) . . . . ?
O51 Dy1 N61 O62 176.3(5) . . . . ?
O41 Dy1 N61 O62 -3.4(8) . . . . ?
O61 Dy1 N61 O62 -175.9(8) . . . . ?
O12 Dy1 N61 O62 107.8(5) . . . . ?
O32 Dy1 N61 O62 -119.5(5) . . . . ?
N51 Dy1 N61 O62 160.0(4) . . . . ?
O11 Dy1 N61 O61 -134.9(4) . . . . ?
O31 Dy1 N61 O61 83.3(4) . . . . ?
O62 Dy1 N61 O61 175.9(8) . . . . ?
O52 Dy1 N61 O61 -45.3(5) . . . . ?
O42 Dy1 N61 O61 148.8(4) . . . . ?
O51 Dy1 N61 O61 -7.8(4) . . . . ?
O41 Dy1 N61 O61 172.5(4) . . . . ?
O12 Dy1 N61 O61 -76.2(4) . . . . ?
O32 Dy1 N61 O61 56.4(5) . . . . ?
N51 Dy1 N61 O61 -24.1(5) . . . . ?
C111 C117 N111 C118 173.9(5) . . . . ?
C123 C118 N111 C117 -7.7(9) . . . . ?
C119 C118 N111 C117 172.6(5) . . . . ?
Dy2 O142 N141 O143 -170.3(7) . . . . ?
Dy2 O142 N141 O141 8.4(6) . . . . ?
Dy2 O141 N141 O143 170.1(6) . . . . ?
Dy2 O141 N141 O142 -8.6(6) . . . . ?
O111 Dy2 N141 O143 -108(3) 4_655 . . . ?
O111 Dy2 N141 O143 115(3) . . . . ?
O141 Dy2 N141 O143 -74(3) . . . . ?
O141 Dy2 N141 O143 39(3) 4_655 . . . ?
O151 Dy2 N141 O143 28(3) . . . . ?
O151 Dy2 N141 O143 -20(3) 4_655 . . . ?
O142 Dy2 N141 O143 115(3) . . . . ?

O142 Dy2 N141 O143 -45(3) 4_655 . . . ?
O112 Dy2 N141 O143 166(3) . . . . ?
O112 Dy2 N141 O143 -167(3) 4_655 . . . ?
N151 Dy2 N141 O143 2(3) . . . . ?
N141 Dy2 N141 O143 2(3) 4_655 . . . ?
O111 Dy2 N141 O142 137.3(4) 4_655 . . . ?
O111 Dy2 N141 O142 0.2(4) . . . . ?
O141 Dy2 N141 O142 171.0(7) . . . . ?
O141 Dy2 N141 O142 -76.0(4) 4_655 . . . ?
O151 Dy2 N141 O142 -87.2(4) . . . . ?
O151 Dy2 N141 O142 -135.1(4) 4_655 . . . ?
O142 Dy2 N141 O142 -159.4(4) 4_655 . . . ?
O112 Dy2 N141 O142 50.8(5) . . . . ?
O112 Dy2 N141 O142 78.6(4) 4_655 . . . ?
N151 Dy2 N141 O142 -112.5(4) . . . . ?
N141 Dy2 N141 O142 -112.5(4) 4_655 . . . ?
O111 Dy2 N141 O141 -33.8(4) 4_655 . . . ?
O111 Dy2 N141 O141 -170.9(4) . . . . ?
O141 Dy2 N141 O141 112.9(5) 4_655 . . . ?
O151 Dy2 N141 O141 101.7(4) . . . . ?
O151 Dy2 N141 O141 53.9(4) 4_655 . . . ?
O142 Dy2 N141 O141 -171.0(7) . . . . ?
O142 Dy2 N141 O141 29.6(6) 4_655 . . . ?
O112 Dy2 N141 O141 -120.3(4) . . . . ?
O112 Dy2 N141 O141 -92.5(4) 4_655 . . . ?
N151 Dy2 N141 O141 76.4(4) . . . . ?
N141 Dy2 N141 O141 76.4(4) 4_655 . . . ?
Dy2 O151 N151 O151 0.0 . . . 4_655 ?
Dy2 O151 N151 O153 180.0 . . . . ?
O111 Dy2 N151 O151 158.2(2) 4_655 . . . ?
O111 Dy2 N151 O151 -21.8(2) . . . . ?
O141 Dy2 N151 O151 90.7(2) . . . . ?
O141 Dy2 N151 O151 -89.3(2) 4_655 . . . ?
O151 Dy2 N151 O151 -180.0 4_655 . . . ?
O142 Dy2 N151 O151 40.1(2) . . . . ?
O142 Dy2 N151 O151 -139.9(2) 4_655 . . . ?
O112 Dy2 N151 O151 -98.7(3) . . . . ?
O112 Dy2 N151 O151 81.3(3) 4_655 . . . ?
N141 Dy2 N151 O151 -116.8(3) 4_655 . . . ?
O111 Dy2 N151 O151 -21.8(2) 4_655 . . 4_655 ?
O111 Dy2 N151 O151 158.2(2) . . . 4_655 ?
O141 Dy2 N151 O151 -89.3(2) . . . 4_655 ?
O141 Dy2 N151 O151 90.7(2) 4_655 . . 4_655 ?
O151 Dy2 N151 O151 180.0 . . . 4_655 ?
O142 Dy2 N151 O151 -139.9(2) . . . 4_655 ?
O142 Dy2 N151 O151 40.1(2) 4_655 . . 4_655 ?
O112 Dy2 N151 O151 81.3(3) . . . 4_655 ?
O112 Dy2 N151 O151 -98.7(3) 4_655 . . 4_655 ?
N141 Dy2 N151 O151 63.2(3) 4_655 . . 4_655 ?
O111 Dy2 N151 O153 5(100) 4_655 . . . ?

O111 Dy2 N151 O153 -175(100) . . . . ?
O141 Dy2 N151 O153 -63(100) . . . . ?
O141 Dy2 N151 O153 117(100) 4_655 . . . ?
O151 Dy2 N151 O153 -153(100) . . . . ?
O151 Dy2 N151 O153 27(100) 4_655 . . . ?
O142 Dy2 N151 O153 -113(100) . . . . ?
O142 Dy2 N151 O153 67(100) 4_655 . . . ?
O112 Dy2 N151 O153 108(100) . . . . ?
O112 Dy2 N151 O153 -72(100) 4_655 . . . ?
N141 Dy2 N151 O153 90(100) 4_655 . . . ?
C113 C112 O111 Dy2 -2.5(7) . . . . ?
C111 C112 O111 Dy2 179.8(4) . . . . ?
O111 Dy2 O111 C112 41.9(4) 4_655 . . . ?
O141 Dy2 O111 C112 144.7(4) . . . . ?
O141 Dy2 O111 C112 -76.6(4) 4_655 . . . ?
O151 Dy2 O111 C112 -147.2(4) . . . . ?
O151 Dy2 O111 C112 -125.0(4) 4_655 . . . ?
O142 Dy2 O111 C112 149.4(4) . . . . ?
O142 Dy2 O111 C112 -43.0(4) 4_655 . . . ?
O112 Dy2 O111 C112 2.4(4) . . . . ?
O112 Dy2 O111 C112 77.7(4) 4_655 . . . ?
N151 Dy2 O111 C112 -138.1(4) . . . . ?
N141 Dy2 O111 C112 -62.0(4) 4_655 . . . ?

_diffrn_measured_fraction_theta_max 0.992
_diffrn_reflns_theta_full 29.17
_diffrn_measured_fraction_theta_full 0.992
_refine_diff_density_max 2.071
_refine_diff_density_min -1.099
_refine_diff_density_rms 0.131

CheckCIF/PLATON (standard) for complex 2:

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: shelxl

Bond precision: C-C = 0.0086 A Wavelength=0.71075

Cell: a=17.654(3) b=54.092(9) c=9.5502(16)
alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	9120(3)	9120(3)
Space group	A b a 2	Aba2
Hall group	A 2 -2ac	?
Moiety formula	C28 H26 Dy N5 O13	?
Sum formula	C28 H26 Dy N5 O13	C28 H26 Dy N5 O13
Mr	803.04	803.04
Dx,g cm-3	1.755	1.755
Z	12	12
Mu (mm-1)	2.534	2.534
F000	4788.0	4788.0
F000'	4788.08	
h,k,lmax	24,74,13	24,74,12
Nref	12318[6521]	11627
Tmin,Tmax	0.608,0.602	0.631,0.631
Tmin'	0.596	

Correction method= NUMERICAL

Data completeness= 1.78/0.94 Theta(max)= 29.170

R(reflections)= 0.0494(9529) wR2(reflections)= 0.1015(11627)

S = 1.067 Npar= 632

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .....
1 Why ?

PLAT220_ALERT_2_B Large Non-Solvent O Ueq(max)/Ueq(min) ...
6.5 Ratio

PLAT220_ALERT_2_B Large Non-Solvent N Ueq(max)/Ueq(min) ...
4.8 Ratio

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H14A .. H24A ..
1.78 Ang.

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H11A .. H12E ..
1.73 Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.
Absorption correction given as Numerical
PLAT213_ALERT_2_C Atom O53 has ADP max/min Ratio .....
3.5 prolat
And 4 other PLAT213 Alerts
More ...
PLAT220_ALERT_2_C Large Non-Solvent N Ueq(max)/Ueq(min) ...
3.6 Ratio
PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ...
3.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O151 -- N151 ..
5.2 su
PLAT234_ALERT_4_C Large Hirshfeld Difference O62 -- N61 ..
0.16 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for .....
O61 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for .....
O62 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....
N61 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .....
N151 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....
0.0086 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H34A .. H44A ..
1.81 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #
1
C28 H26 Dy N5 O13

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
4
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF
Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....
3 Why ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.
19.66
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #
73 Do !
O61 -DY1 -O41 -N41 115.30 1.90 1.555 1.555 1.555
1.555
And 58 other PLAT710 Alerts
More ...
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
25 Note

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully
17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
64 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
20 ALERT type 2 Indicator that the structure model may be wrong or deficient

```
  2 ALERT type 3 Indicator that the structure quality may be low
 61 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

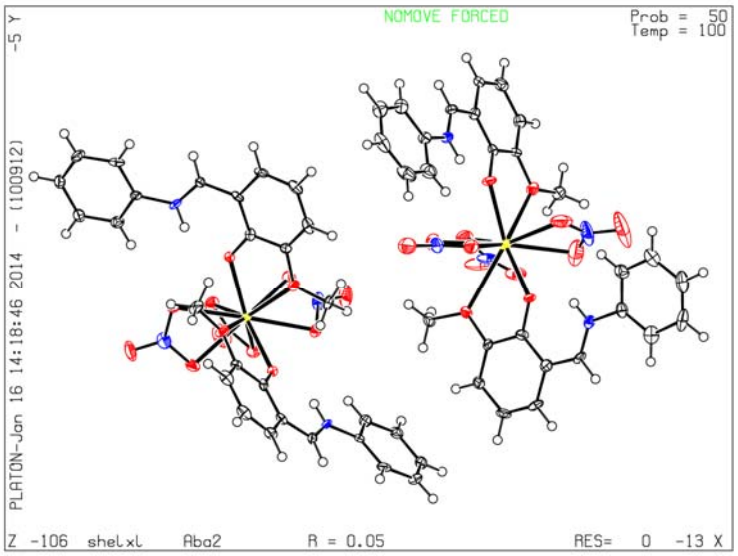
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/09/2013; check.def file version of 12/09/2013

Datablock shelxl - ellipsoid plot



References:

1 a) A. Upadhyay, S. Vaidya, V. S. Venkatasai, P. Jayapal, A. K. Srivastava, M. Shanmugam and M. Shanmugam, *Polyhedron* 2013, **66**, 87; b) A. Upadhyay, N. Komatireddy, A. Ghirri, F. Tuna, S. K. Langley, A. K. Srivastava, E. C. Sanudo, B. Moubaraki, K. S. Murray, E. J. McInnes, M. Affronte and M. Shanmugam, *Dalton Trans.* 2014, **43**, 259.

2 F. Aquilante, L. De Vico, N. Ferré, G. Ghigo, P.-å. Malmqvist, P. Neogrády, T. B. Pedersen, M. Pitoňák, M. Reiher, B. O. Roos, L. Serrano-Andrés, M. Urban, V. Veryazov and R. Lindh, *J. Comp. Chem.* 2010, **31**, 224.

3 K. Bernot, J. Luzon, L. Bogani, M. Etienne, C. Sangregorio, M. Shanmugam, A. Caneschi, R. Sessoli and D. Gatteschi, *J. Am. Chem. Soc.* 2009, **131**, 5573.

4 Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

5 A. D. Becke, *J. Chem. Phy.* 1993, **98**, 5648.

6 T. R. Cundari and W. J. Stevens, *J. Chem. Phy.* 1993, *98*, 5555-5565.

7 A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phy.* 1994, *100*, 5829-5835.

8 A. Watanabe, A. Yamashita, M. Nakano, T. Yamamura and T. Kajiwara, *Chem –Eur.J*2011, **17,** 7428.

9 M. A. Palacios, S. Titos-Padilla, J. Ruiz, J. M. Herrera, S. J. A. Pope, E. K. Brechin and E. Colacio, *Inorg. Chem.* 2014, **53**, 1465.

10 E. Colacio, J. Ruiz-Sanchez, F. J. White and E. K. Brechin, *Inorg. Chem.* 2011, **50**, 7268.

11 S. Akine, F. Utsuno, T. Taniguchi and T. Nabeshima, *Eur. J. Inorg. Chem.* 2010, 3143-3152.

12 J. Ruiz, A. J. Mota, A. Rodriguez-Dieguez, S. Titos, J. M. Herrera, E. Ruiz, E. Cremades, J. P. Costes and E. Colacio, *Chem. Commun.* 2012, **48**, 7916.

13 P. H. Lin, I. Korobkov, T. J. Burchell and M. Murugesu, *Dalton Trans.* 2012, **41**, 13649.

14 N. F. Chilton, S. K. Langley, B. Moubaraki, A. Soncini, S. R. Batten and K. S. Murray, *Chem. Sci.* 2013, **4**, 1719.

15 M. Menelaou, F. Ouharrou, L. Rodriguez, O. Roubeau, S. J. Teat and N. Aliaga-Alcalde, *Chemistry* 2012, **18**, 11545.

16 D. P. Li, X. P. Zhang, T. W. Wang, B. B. Ma, C. H. Li, Y. Z. Li and X. Z. You, *Chem. Commun.* 2011, **47**, 6867.

17 E. Lucaccini, L. Sorace, M. Perfetti, J. P. Costes and R. Sessoli, *Chem. Commun.* 2014, **50**, 1648-1651.

18 U. J. Williams, B. D. Mahoney, P. T. DeGregorio, P. J. Carroll, E. Nakamaru-Ogiso, J. M. Kikkawa and E. J. Schelter, *Chem. Commun.* 2012, **48**, 5593.

19 Y. Wang, X. L. Li, T. W. Wang, Y. Song and X. Z. You, *Inorg. Chem.* 2010, **49**, 969.

20 K. R. Meihaus, J. D. Rinehart and J. R. Long, *Inorg. Chem.* 2011, **50**, 8484.