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[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),2,9,11,13,15(30),16,23,25,27-decaene-29,30-diol-$\kappa^5N^3,N^6,N^9,O^{29},O^{30}$]bis(nitrato-$\kappa^2O,O'$)dysprosium(III) nitrate monohydrate

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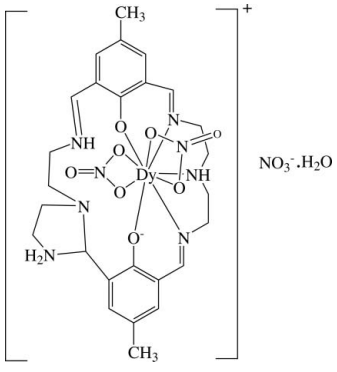
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.051; wR factor = 0.115; data-to-parameter ratio = 16.5.

The asymmetric unit of the title complex, $[Dy(C_{26}H_{34}N_6O_2)(NO_3)_2]NO_3\cdot H_2O$, comprises two cations and two anions, together with two water molecules. The Dy atom exhibits a nine-coordinate distorted tricapped trigonal-prismatic coordination geometry. The water molecules are disordered over five positions, each with a site-occupation factor of 0.4. The crystal structure involves N—H···O and N—H···N hydrogen bonds.

Related literature

For a general discussion of macrocyclic lanthanide complexes, see Bunzli & Piguet (2002). Some examples of symmetric macrocyclic lanthanide complexes are given in Hu *et al.* (2005). The Gd^{III} and Lu^{III} analogues of the title complex have been reported recently (Hu, Qiu *et al.*, 2007; Hu, Chen *et al.*, 2007).



Experimental

Crystal data

$[Dy(C_{26}H_{34}N_6O_2)(NO_3)_2]NO_3\cdot H_2O$
M_r = 829.14
Triclinic, $P\overline{1}$
a = 14.005 (3) Å
b = 14.045 (3) Å
c = 21.896 (4) Å
α = 96.386 (3)°
β = 99.094 (3)°
γ = 118.217 (3)°
V = 3661.0 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.11 mm^{-1}
T = 292 (2) K
0.30 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.58, T_{max} = 0.66
36705 measured reflections
14395 independent reflections
10889 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.115
S = 1.04
14395 reflections
872 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −1.42 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N14—H14A···O20	0.91	2.23	3.118 (6)	166
N12—H12B···O10	0.90	1.99	2.696 (6)	134
N12—H12A···N17	0.90	2.50	3.332 (7)	155
N12—H12A···O17	0.90	2.34	2.972 (7)	127
N12—H12A···O18	0.90	1.91	2.786 (6)	164
N5—H5B···O2	0.90	1.97	2.684 (6)	135
N5—H5A···N18	0.90	2.45	3.348 (7)	177
N5—H5A···O21	0.90	2.21	3.015 (7)	149
N5—H5A···O20	0.90	1.96	2.809 (6)	156
N1—H1A···O1	0.86	1.98	2.610 (5)	130
N10—H10A···O9	0.86	1.99	2.620 (5)	129
N3—H3A···O17^{i}	0.91	2.18	3.008 (5)	151

Symmetry code: (i) $x+1, y+1, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was surpported by Hubei Normal University, People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2193).

References

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Hu, X.-L., Qiu, L., Yuan, J. & Pan, Z.-Q. (2007). *Acta Cryst.* E**63**, m1438.

  doi:10.1107/S160053680702795X

supplementary materials

Acta Cryst. (2007). E**63**, m1910 [**doi:10.1107/S160053680702795X**]

[13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta-1(29),2,9,11,13,15(30),16,23,25,27-decaene-29,30-diol-$\kappa^5N^3,N^6,N^9,O^{29},O^{30}$]bis(nitrato-$\kappa^2O,O'$)dysprosium(III) nitrate monohydrate

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Comment

Lanthanide macrocyclic complexes have received much attention due to their unique properties and many valuable applications such as fluorescent probes in biological systems, material science and chemical processes (Bunzli & Piguet, 2002). Generally, the syntheses of lanthanide macrocyclic complexes are carried out in the presence of a suitable lanthanide ion which acts as a template for macrocycle formation, Most of them are symmetric (Hu *et al.*, 2005). There have been few reports of asymmetric lanthanide complexes.

Recently, Hu *et al.* (Hu, Qiu *et al.*, 2007; Hu, Chen *et al.*, 2007) have reported the crystal structures of Gd^{III} and Lu^{III} complexes with a macrocyclic ligand derived from 2,6-diformyl-4-methylphenol and 1,5-diamino-3-azapentane: $[Gd(C_{26}H_{34}N_6O_2)(NO_3)_2]^+(NO_3)^-\cdot H_2O$ and $[Lu(C_{26}H_{34}N_6O_2)(NO_3)_2]^+(NO_3)^-\cdot 0.5H_2O\cdot 0.25CH_3COOC_2H_5$. In these complexes, the central lanthanide ion is nine-coordinate, being bound to five donor atoms from the cyclic polydentate ligand and to four O of two bidentate nitrate anions. Reported here is a new Dy^{III} analogue $[Dy(III)(C_{26}H_{34}N_6O_2)(NO_3)_2]^+(NO_3)^-\cdot H_2O$, which exhibits a similar nine-coordinate distorted tricapped trigonal prismatic coordination geometry (Fig. 1 & Fig. 2). The title complex is not isostructural with its Gd^{III} and Lu^{III} analogues. (space groups *Cc* and *C2/c*, respectively).

Experimental

To a methanolic solution (20 ml) of 2,6-diformyl-4-methylphenol (1 mmol) and $Dy(NO_3)_3\cdot 6H_2O$ (0.5 mmol), 1,5-diamino-3-azapentane (1 mmol) was added dropwise. After refluxing for 3 h, the solvent was removed. The resulting yellow solid was recrystallized from CH_3CN, yielding yellow block crystals suitable for X-ray analysis.

Refinement

H atoms bound to C atoms were placed geometrically (C—H 0.93 to 0.97 Å) and were allowed to ride during refinement with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bound to N atoms were visible in difference Fourier maps, but were placed geometrically with N—H = 0.90 or 0.91 Å for N(sp^3) and 0.86 Å for N(sp^2), and allowed to ride during refinement with $U_{iso}(H) = 1.2U_{eq}(N)$. H atoms of the water molecules were located in difference Fourier maps, then their O—H distances were normalized to 0.85 Å and they were refined as riding with $U_{iso}(H) = 1.2U_{eq}(O)$.

Figures

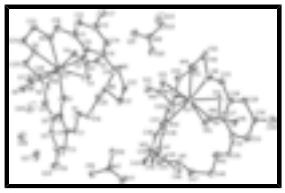


Fig. 1. The asymmetric unit of the title complex showing displacement ellipsoids at the 30% probability level. H atoms are omitted.

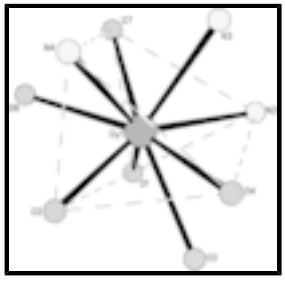


Fig. 2. Distorted tricapped trigonal prismatic coordination environment of Dy^{III}.

(13,27-Dimethyl-3,6,9,17,20,23-hexaazatricyclo[23.3.1.1^{11,15}]triaconta- 1(29),2,9,11,13,15 (30),16,23,25,27-decaene-29,30-diol- κ^5*N*^{3},*N*^{6},*N*^{9},*O*^{29},*O*^{30})bis(nitrato-κ^2*O*,*O*')dysprosium(III) nitrate monohydrate

Crystal data

$[Dy(C_{26}H_{34}N_6O_2)(NO_3)_2]NO_3{\cdot}H_2O$	$Z = 4$
$M_r = 829.14$	$F_{000} = 1668$
Triclinic, $P\bar{1}$	$D_x = 1.504$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 14.005$ (3) Å	Cell parameters from 6195 reflections
$b = 14.045$ (3) Å	$\theta = 2.5$–22.7º
$c = 21.896$ (4) Å	$\mu = 2.11$ mm^{-1}
$\alpha = 96.386$ (3)º	$T = 292$ (2) K
$\beta = 99.094$ (3)º	Block, yellow
$\gamma = 118.217$ (3)º	0.30 × 0.22 × 0.20 mm
$V = 3661.0$ (13) Å^3	

Data collection

Bruker SMART CCD diffractometer	14395 independent reflections
Radiation source: sealed tube	10889 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
$T = 292(2)$ K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.0$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -17\rightarrow17$
$T_{min} = 0.58$, $T_{max} = 0.66$	$k = -17\rightarrow17$
36705 measured reflections	$l = -27\rightarrow27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full with fixed elements per cycle	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
14395 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
872 parameters	$\Delta\rho_{min} = -1.42$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. 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 $F^2 > \sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.47785 (19)	0.8435 (3)	0.33060 (16)	0.0424 (11)	
C2	0.3861 (3)	0.7491 (2)	0.33767 (16)	0.0457 (11)	
C3	0.2811 (2)	0.7395 (2)	0.32526 (17)	0.0501 (12)	
H3	0.2197	0.6763	0.3300	0.060*	
C4	0.2679 (2)	0.8243 (3)	0.30578 (16)	0.0487 (12)	
C5	0.3597 (3)	0.9188 (2)	0.29872 (17)	0.0518 (12)	
H5	0.3509	0.9755	0.2857	0.062*	
C6	0.4647 (2)	0.9284 (2)	0.31113 (17)	0.0626 (15)	
C7	0.3928 (4)	0.6602 (4)	0.3563 (2)	0.0423 (11)	
H7	0.3267	0.5988	0.3580	0.051*	
C8	0.1511 (5)	0.8098 (5)	0.2895 (3)	0.0620 (15)	
H8A	0.1469	0.8625	0.3192	0.093*	
H8B	0.0972	0.7363	0.2915	0.093*	
H8C	0.1357	0.8214	0.2475	0.093*	
C9	0.5574 (5)	1.0360 (5)	0.3046 (3)	0.0622 (14)	
H9	0.5392	1.0901	0.2970	0.075*	
C10	0.8457 (3)	0.7694 (3)	0.34372 (15)	0.0533 (13)	
C11	0.9485 (3)	0.83720 (19)	0.38639 (15)	0.0465 (11)	

C12	1.0079 (2)	0.7912 (2)	0.41481 (14)	0.0528 (13)
H12	1.0767	0.8365	0.4434	0.063*
C13	0.9645 (3)	0.6774 (2)	0.40058 (15)	0.0461 (11)
C14	0.8618 (3)	0.60959 (19)	0.35791 (16)	0.0528 (13)
H14	0.8327	0.5334	0.3484	0.063*
C15	0.8024 (2)	0.6556 (2)	0.32948 (14)	0.0560 (13)
C16	1.0050 (5)	0.9589 (5)	0.4031 (2)	0.0616 (15)
H16	1.0794	0.9956	0.4254	0.074*
C17	1.0299 (4)	0.6233 (5)	0.4289 (2)	0.0531 (13)
H17A	1.0693	0.6117	0.3994	0.080*
H17B	0.9788	0.5536	0.4371	0.080*
H17C	1.0823	0.6711	0.4677	0.080*
C18	0.6876 (5)	0.5791 (5)	0.2826 (2)	0.0580 (14)
H18	0.6739	0.5032	0.2730	0.070*
C19	0.4863 (4)	0.5560 (4)	0.3875 (3)	0.0500 (12)
H19A	0.4148	0.4912	0.3668	0.060*
H19B	0.4963	0.5611	0.4328	0.060*
C20	0.5788 (5)	0.5432 (5)	0.3666 (3)	0.0619 (15)
H20A	0.6477	0.5863	0.3992	0.074*
H20B	0.5595	0.4662	0.3604	0.074*
C21	0.4973 (4)	0.5106 (5)	0.2517 (3)	0.0616 (16)
H21A	0.4337	0.5200	0.2547	0.074*
H21B	0.4751	0.4330	0.2476	0.074*
C22	0.5480 (4)	0.5575 (4)	0.1967 (2)	0.0515 (13)
H22A	0.5254	0.6091	0.1837	0.062*
H22B	0.5255	0.4986	0.1605	0.062*
C23	1.0414 (4)	1.1413 (5)	0.4118 (3)	0.0549 (14)
H23A	1.0911	1.1567	0.4524	0.066*
H23B	1.0865	1.1675	0.3816	0.066*
C24	0.9790 (4)	1.1999 (4)	0.4176 (2)	0.0549 (14)
H24A	1.0294	1.2791	0.4253	0.066*
H24B	0.9446	1.1842	0.4531	0.066*
C25	0.8306 (4)	1.2242 (5)	0.3592 (2)	0.0531 (13)
H25A	0.8800	1.3012	0.3592	0.064*
H25B	0.8029	1.2212	0.3973	0.064*
C26	0.7338 (5)	1.1730 (5)	0.3014 (3)	0.0654 (15)
H26A	0.6969	1.2165	0.2990	0.078*
H26B	0.7599	1.1696	0.2632	0.078*
C27	0.2983 (4)	−0.1020 (4)	0.1215 (2)	0.0450 (11)
C28	0.3961 (4)	−0.1080 (5)	0.1358 (2)	0.0473 (12)
C29	0.3941 (4)	−0.2033 (4)	0.1516 (2)	0.0446 (11)
H29	0.4603	−0.2049	0.1612	0.054*
C30	0.2948 (4)	−0.2947 (4)	0.1532 (2)	0.0450 (11)
C31	0.1949 (5)	−0.2905 (5)	0.1391 (3)	0.0565 (13)
H31	0.1278	−0.3508	0.1405	0.068*
C32	0.1965 (5)	−0.1951 (4)	0.1228 (3)	0.0531 (12)
C33	0.5050 (4)	−0.0196 (5)	0.1327 (2)	0.0498 (12)
H33	0.5624	−0.0360	0.1379	0.060*
C34	0.2921 (5)	−0.3957 (5)	0.1720 (3)	0.0557 (13)

H34A	0.2948	−0.4404	0.1366	0.084*
H34B	0.2246	−0.4377	0.1852	0.084*
H34C	0.3553	−0.3734	0.2064	0.084*
C35	0.0938 (4)	−0.2017 (4)	0.1077 (2)	0.0420 (11)
H35	0.0314	−0.2654	0.1109	0.050*
C36	0.2392 (4)	0.2650 (4)	0.1082 (3)	0.0543 (13)
C37	0.2605 (4)	0.3269 (4)	0.0600 (2)	0.0492 (12)
C38	0.1853 (4)	0.3658 (4)	0.0384 (3)	0.0514 (13)
H38	0.1995	0.4079	0.0076	0.062*
C39	0.0952 (5)	0.3430 (4)	0.0615 (3)	0.0572 (15)
C40	0.0692 (5)	0.2750 (4)	0.1055 (2)	0.0539 (13)
H40	0.0034	0.2540	0.1187	0.065*
C41	0.1393 (4)	0.2397 (4)	0.1287 (2)	0.0433 (11)
C42	0.3492 (4)	0.3483 (4)	0.0306 (2)	0.0421 (10)
H42A	0.3568	0.3914	0.0004	0.050*
C43	0.0218 (4)	0.3921 (4)	0.0331 (2)	0.0550 (14)
H43A	0.0479	0.4641	0.0582	0.083*
H43B	−0.0547	0.3442	0.0333	0.083*
H43C	0.0274	0.3979	−0.0097	0.083*
C44	0.1037 (5)	0.1637 (4)	0.1756 (3)	0.0586 (14)
H44	0.0403	0.1628	0.1897	0.070*
C45	0.1679 (4)	0.0949 (5)	0.2612 (2)	0.0517 (12)
H45A	0.2276	0.0775	0.2676	0.062*
H45B	0.1478	0.1033	0.3011	0.062*
C46	0.0712 (4)	0.0098 (5)	0.2122 (2)	0.0463 (11)
H46A	0.0727	−0.0589	0.2058	0.056*
H46B	0.0021	−0.0040	0.2232	0.056*
C47	−0.0090 (4)	−0.0068 (4)	0.1010 (3)	0.0521 (13)
H47A	0.0066	0.0308	0.0662	0.062*
H47B	−0.0762	−0.0110	0.1103	0.062*
C48	−0.0293 (4)	−0.1248 (4)	0.0808 (2)	0.0458 (11)
H48A	−0.0734	−0.1719	0.1065	0.055*
H48B	−0.0705	−0.1552	0.0369	0.055*
C49	0.6479 (4)	0.1487 (4)	0.1208 (2)	0.0435 (11)
H49A	0.6855	0.1059	0.1196	0.052*
H49B	0.6874	0.2086	0.1580	0.052*
C50	0.6474 (4)	0.1958 (4)	0.0607 (2)	0.0470 (11)
H50A	0.7235	0.2443	0.0584	0.056*
H50B	0.6116	0.1358	0.0236	0.056*
C51	0.5600 (4)	0.2838 (5)	−0.0015 (2)	0.0520 (13)
H51A	0.5052	0.2163	−0.0318	0.062*
H51B	0.6265	0.3184	−0.0175	0.062*
C52	0.5134 (4)	0.3620 (4)	0.0067 (2)	0.0483 (12)
H52A	0.5722	0.4342	0.0310	0.058*
H52B	0.4850	0.3707	−0.0344	0.058*
Dy1	0.75925 (2)	0.95316 (2)	0.336610 (11)	0.05113 (8)
Dy2	0.407500 (18)	0.16379 (2)	0.100570 (12)	0.04739 (8)
N1	0.4865 (4)	0.6566 (4)	0.3717 (2)	0.0529 (11)
H1A	0.5490	0.7138	0.3725	0.063*

N2	0.6562 (4)	1.0606 (4)	0.3082 (2)	0.0573 (12)	
N3	0.8918 (4)	1.1639 (3)	0.3585 (2)	0.0463 (10)	
H3A	0.9267	1.1785	0.3262	0.056*	
N4	0.9631 (4)	1.0184 (4)	0.3904 (2)	0.0538 (11)	
N5	0.6776 (4)	0.6179 (4)	0.2258 (2)	0.0601 (12)	
H5A	0.7121	0.5997	0.1992	0.072*	
H5B	0.7072	0.6918	0.2342	0.072*	
N6	0.5944 (3)	0.5815 (4)	0.3070 (2)	0.0537 (11)	
N7	0.7380 (4)	0.9146 (4)	0.1990 (2)	0.0596 (12)	
N8	0.7392 (4)	0.9437 (4)	0.4685 (2)	0.0592 (13)	
N9	0.5318 (4)	0.0781 (4)	0.1236 (2)	0.0586 (12)	
N10	0.0796 (3)	−0.1221 (4)	0.0888 (2)	0.0480 (10)	
H10A	0.1353	−0.0669	0.0810	0.058*	
N11	0.0828 (3)	0.0565 (3)	0.15591 (19)	0.0438 (9)	
N12	0.2046 (4)	0.2077 (4)	0.2318 (2)	0.0575 (12)	
H12A	0.2115	0.2641	0.2597	0.069*	
H12B	0.2686	0.2291	0.2192	0.069*	
N13	0.4212 (4)	0.3152 (4)	0.0404 (2)	0.0567 (12)	
N14	0.5880 (3)	0.2569 (3)	0.06133 (18)	0.0430 (9)	
H14A	0.6345	0.3227	0.0891	0.052*	
N15	0.5202 (4)	0.2597 (3)	0.2372 (2)	0.0504 (11)	
N16	0.2567 (3)	0.0129 (3)	−0.01617 (18)	0.0423 (9)	
N17	0.1430 (4)	0.3787 (3)	0.3121 (2)	0.0550 (12)	
N18	0.8148 (4)	0.5559 (4)	0.1309 (2)	0.0554 (11)	
O1	0.5778 (3)	0.8473 (3)	0.33876 (17)	0.0556 (9)	
O2	0.7896 (3)	0.8106 (3)	0.31100 (18)	0.0645 (11)	
O3	0.6560 (3)	0.8534 (3)	0.22214 (19)	0.0638 (11)	
O4	0.8157 (3)	0.9962 (3)	0.23469 (16)	0.0511 (9)	
O5	0.7318 (3)	0.8909 (3)	0.14592 (18)	0.0582 (10)	
O6	0.7480 (3)	0.8677 (3)	0.43658 (16)	0.0534 (9)	
O7	0.7562 (3)	1.0260 (3)	0.44466 (17)	0.0566 (10)	
O8	0.7203 (3)	0.9337 (3)	0.52032 (18)	0.0593 (10)	
O9	0.2978 (3)	−0.0141 (3)	0.10996 (16)	0.0466 (8)	
O10	0.3063 (3)	0.2363 (3)	0.13515 (16)	0.0457 (8)	
O11	0.4298 (3)	0.1682 (3)	0.21994 (16)	0.0539 (9)	
O12	0.5602 (3)	0.3048 (3)	0.19477 (16)	0.0469 (8)	
O13	0.5665 (3)	0.3021 (3)	0.29462 (19)	0.0620 (10)	
O14	0.3596 (2)	0.0465 (3)	−0.00753 (15)	0.0410 (7)	
O15	0.2248 (3)	0.0671 (3)	0.01518 (15)	0.0483 (8)	
O16	0.1887 (3)	−0.0741 (3)	−0.05426 (17)	0.0627 (11)	
O17	0.0664 (3)	0.2836 (3)	0.28828 (18)	0.0665 (12)	
O18	0.2305 (3)	0.4028 (3)	0.29827 (19)	0.0637 (11)	
O19	0.1357 (3)	0.4538 (3)	0.34430 (18)	0.0616 (10)	
O20	0.7317 (3)	0.5001 (3)	0.13864 (19)	0.0686 (12)	
O21	0.8556 (4)	0.6503 (4)	0.15550 (19)	0.0661 (11)	
O22	0.8672 (3)	0.5325 (4)	0.09746 (18)	0.0649 (11)	
O23	0.9291 (9)	0.4352 (9)	0.2281 (5)	0.071 (3)	0.40
H23D	0.9409	0.4081	0.2593	0.085*	0.40
H23E	0.8911	0.3836	0.1953	0.085*	0.40

O24	0.2786 (8)	0.5461 (8)	0.5132 (4)	0.058 (2)	0.40
H24C	0.2583	0.4991	0.5366	0.069*	0.40
H24E	0.2217	0.5358	0.4866	0.069*	0.40
O25	0.6348 (8)	0.7333 (8)	0.5865 (4)	0.065 (3)	0.40
H25D	0.6597	0.6894	0.5920	0.078*	0.40
H25E	0.6646	0.7713	0.5603	0.078*	0.40
O26	0.4610 (10)	0.8251 (10)	0.5315 (6)	0.087 (4)	0.40
H26E	0.5163	0.8174	0.5460	0.105*	0.40
H26D	0.4735	0.8536	0.4993	0.105*	0.40
O27	0.3462 (10)	0.6915 (12)	0.5223 (5)	0.097 (5)	0.40
H27C	0.3388	0.6655	0.5556	0.117*	0.40
H27A	0.2893	0.6967	0.5076	0.117*	0.40

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.039 (2)	0.056 (3)	0.043 (2)	0.033 (2)	0.0094 (19)	0.007 (2)
C2	0.036 (2)	0.037 (3)	0.072 (3)	0.024 (2)	0.012 (2)	0.013 (2)
C3	0.041 (3)	0.052 (3)	0.050 (3)	0.017 (2)	0.016 (2)	0.008 (2)
C4	0.040 (3)	0.047 (3)	0.061 (3)	0.021 (2)	0.016 (2)	0.016 (2)
C5	0.051 (3)	0.054 (3)	0.052 (3)	0.027 (3)	0.014 (2)	0.008 (2)
C6	0.060 (3)	0.065 (4)	0.048 (3)	0.019 (3)	0.018 (3)	0.009 (3)
C7	0.040 (2)	0.032 (2)	0.038 (2)	0.009 (2)	0.0065 (18)	−0.0072 (18)
C8	0.064 (4)	0.055 (3)	0.058 (3)	0.021 (3)	0.019 (3)	0.012 (3)
C9	0.051 (3)	0.051 (3)	0.076 (4)	0.019 (3)	0.014 (3)	0.014 (3)
C10	0.050 (3)	0.062 (3)	0.031 (2)	0.016 (3)	0.009 (2)	0.004 (2)
C11	0.040 (3)	0.039 (3)	0.052 (3)	0.012 (2)	0.013 (2)	0.013 (2)
C12	0.056 (3)	0.037 (3)	0.041 (2)	0.007 (2)	0.005 (2)	0.008 (2)
C13	0.041 (3)	0.054 (3)	0.044 (2)	0.021 (2)	0.016 (2)	0.019 (2)
C14	0.053 (3)	0.031 (3)	0.061 (3)	0.009 (2)	0.017 (2)	0.009 (2)
C15	0.056 (3)	0.047 (3)	0.053 (3)	0.017 (3)	0.013 (2)	0.006 (2)
C16	0.056 (3)	0.059 (4)	0.045 (3)	0.013 (3)	0.006 (2)	0.002 (2)
C17	0.044 (3)	0.051 (3)	0.047 (3)	0.012 (2)	0.006 (2)	0.010 (2)
C18	0.051 (3)	0.059 (3)	0.044 (3)	0.021 (3)	0.000 (2)	−0.016 (2)
C19	0.041 (3)	0.046 (3)	0.055 (3)	0.015 (2)	0.009 (2)	0.015 (2)
C20	0.042 (3)	0.059 (4)	0.066 (3)	0.010 (3)	0.019 (3)	0.006 (3)
C21	0.038 (3)	0.062 (4)	0.056 (3)	0.019 (3)	−0.016 (2)	−0.025 (3)
C22	0.043 (3)	0.040 (3)	0.047 (3)	0.013 (2)	−0.013 (2)	−0.012 (2)
C23	0.030 (2)	0.066 (4)	0.051 (3)	0.010 (2)	0.013 (2)	0.007 (3)
C24	0.048 (3)	0.033 (3)	0.055 (3)	0.000 (2)	0.006 (2)	0.006 (2)
C25	0.045 (3)	0.049 (3)	0.050 (3)	0.010 (2)	0.010 (2)	0.022 (2)
C26	0.061 (4)	0.065 (4)	0.067 (4)	0.029 (3)	0.014 (3)	0.017 (3)
C27	0.048 (3)	0.045 (3)	0.033 (2)	0.019 (2)	0.0073 (19)	−0.0041 (19)
C28	0.045 (3)	0.053 (3)	0.039 (2)	0.027 (2)	−0.004 (2)	−0.001 (2)
C29	0.037 (2)	0.046 (3)	0.045 (2)	0.022 (2)	0.0017 (19)	−0.007 (2)
C30	0.052 (3)	0.039 (3)	0.045 (2)	0.030 (2)	−0.002 (2)	−0.001 (2)
C31	0.057 (3)	0.042 (3)	0.065 (3)	0.020 (3)	0.010 (3)	0.022 (3)
C32	0.049 (3)	0.041 (3)	0.057 (3)	0.017 (2)	0.006 (2)	0.003 (2)

C33	0.029 (2)	0.062 (3)	0.045 (3)	0.019 (2)	−0.0042 (19)	−0.005 (2)
C34	0.047 (3)	0.067 (4)	0.054 (3)	0.029 (3)	0.011 (2)	0.015 (3)
C35	0.030 (2)	0.021 (2)	0.060 (3)	0.0082 (18)	0.0037 (19)	−0.0158 (19)
C36	0.041 (3)	0.039 (3)	0.062 (3)	0.008 (2)	0.008 (2)	−0.001 (2)
C37	0.042 (3)	0.040 (3)	0.052 (3)	0.016 (2)	0.000 (2)	−0.005 (2)
C38	0.043 (3)	0.032 (3)	0.058 (3)	0.014 (2)	−0.012 (2)	−0.012 (2)
C39	0.060 (3)	0.033 (3)	0.060 (3)	0.025 (3)	−0.018 (3)	−0.021 (2)
C40	0.059 (3)	0.036 (3)	0.044 (3)	0.018 (2)	−0.009 (2)	−0.019 (2)
C41	0.039 (2)	0.040 (3)	0.049 (3)	0.022 (2)	0.005 (2)	−0.006 (2)
C42	0.043 (3)	0.034 (2)	0.055 (3)	0.023 (2)	0.012 (2)	0.009 (2)
C43	0.046 (3)	0.042 (3)	0.050 (3)	0.014 (2)	−0.021 (2)	−0.010 (2)
C44	0.055 (3)	0.035 (3)	0.071 (4)	0.011 (2)	0.008 (3)	0.020 (3)
C45	0.041 (3)	0.049 (3)	0.051 (3)	0.012 (2)	0.011 (2)	0.009 (2)
C46	0.038 (2)	0.054 (3)	0.049 (3)	0.021 (2)	0.016 (2)	0.019 (2)
C47	0.040 (3)	0.043 (3)	0.054 (3)	0.014 (2)	−0.010 (2)	−0.001 (2)
C48	0.043 (3)	0.038 (3)	0.050 (3)	0.017 (2)	0.007 (2)	0.005 (2)
C49	0.031 (2)	0.040 (3)	0.052 (3)	0.008 (2)	0.023 (2)	0.005 (2)
C50	0.054 (3)	0.030 (2)	0.047 (3)	0.013 (2)	0.014 (2)	0.006 (2)
C51	0.038 (3)	0.056 (3)	0.052 (3)	0.015 (2)	0.012 (2)	0.010 (2)
C52	0.043 (3)	0.045 (3)	0.057 (3)	0.017 (2)	0.017 (2)	0.031 (2)
Dy1	0.04810 (14)	0.04859 (15)	0.04748 (14)	0.01280 (12)	0.01949 (11)	0.01889 (11)
Dy2	0.02832 (11)	0.04888 (15)	0.05916 (15)	0.01496 (10)	0.01314 (10)	0.00690 (11)
N1	0.048 (2)	0.037 (2)	0.060 (3)	0.008 (2)	0.011 (2)	0.027 (2)
N2	0.071 (3)	0.052 (3)	0.045 (2)	0.019 (2)	0.032 (2)	0.027 (2)
N3	0.055 (3)	0.036 (2)	0.049 (2)	0.020 (2)	0.0164 (19)	0.0164 (18)
N4	0.049 (3)	0.053 (3)	0.063 (3)	0.025 (2)	0.021 (2)	0.014 (2)
N5	0.057 (3)	0.053 (3)	0.048 (2)	0.019 (2)	−0.005 (2)	−0.009 (2)
N6	0.032 (2)	0.057 (3)	0.046 (2)	0.011 (2)	−0.0042 (17)	−0.013 (2)
N7	0.057 (3)	0.058 (3)	0.048 (3)	0.019 (3)	0.010 (2)	0.007 (2)
N8	0.053 (3)	0.053 (3)	0.046 (2)	0.014 (2)	0.005 (2)	−0.015 (2)
N9	0.043 (2)	0.045 (3)	0.066 (3)	0.006 (2)	0.010 (2)	0.009 (2)
N10	0.038 (2)	0.048 (3)	0.057 (2)	0.0151 (19)	0.0163 (19)	0.029 (2)
N11	0.035 (2)	0.044 (2)	0.049 (2)	0.0150 (18)	0.0192 (17)	0.0096 (18)
N12	0.054 (3)	0.051 (3)	0.044 (2)	0.016 (2)	−0.0008 (19)	−0.0120 (19)
N13	0.043 (2)	0.050 (3)	0.057 (3)	0.009 (2)	0.011 (2)	0.008 (2)
N14	0.045 (2)	0.037 (2)	0.0387 (19)	0.0139 (18)	0.0148 (16)	0.0022 (16)
N15	0.050 (3)	0.034 (2)	0.049 (2)	0.016 (2)	−0.005 (2)	−0.0042 (19)
N16	0.040 (2)	0.030 (2)	0.045 (2)	0.0095 (18)	0.0063 (17)	0.0066 (17)
N17	0.063 (3)	0.024 (2)	0.053 (2)	0.002 (2)	0.015 (2)	0.0093 (18)
N18	0.055 (3)	0.054 (3)	0.049 (2)	0.019 (3)	0.015 (2)	0.013 (2)
O1	0.056 (2)	0.044 (2)	0.053 (2)	0.0139 (18)	0.0120 (17)	0.0167 (16)
O2	0.056 (2)	0.058 (3)	0.052 (2)	0.016 (2)	−0.0029 (18)	−0.0034 (18)
O3	0.048 (2)	0.052 (2)	0.066 (2)	0.0084 (19)	0.0002 (18)	0.0196 (19)
O4	0.048 (2)	0.043 (2)	0.0514 (19)	0.0108 (17)	0.0169 (16)	0.0214 (17)
O5	0.056 (2)	0.052 (2)	0.051 (2)	0.0130 (19)	0.0194 (17)	0.0093 (17)
O6	0.056 (2)	0.045 (2)	0.0489 (19)	0.0133 (18)	0.0217 (17)	0.0146 (16)
O7	0.049 (2)	0.047 (2)	0.049 (2)	0.0067 (18)	0.0152 (16)	−0.0047 (17)
O8	0.046 (2)	0.058 (2)	0.060 (2)	0.0141 (18)	0.0161 (17)	0.0123 (19)
O9	0.0417 (18)	0.043 (2)	0.0535 (19)	0.0170 (16)	0.0133 (15)	0.0192 (16)

O10	0.051 (2)	0.0321 (17)	0.060 (2)	0.0260 (16)	0.0118 (16)	0.0098 (15)
O11	0.064 (2)	0.044 (2)	0.0434 (18)	0.0184 (19)	0.0120 (16)	0.0125 (15)
O12	0.0435 (19)	0.044 (2)	0.0459 (18)	0.0181 (16)	0.0133 (15)	−0.0010 (15)
O13	0.059 (2)	0.040 (2)	0.067 (2)	0.0138 (19)	0.0045 (19)	0.0006 (18)
O14	0.0268 (15)	0.0415 (18)	0.0496 (17)	0.0160 (14)	0.0104 (13)	−0.0058 (14)
O15	0.0468 (19)	0.045 (2)	0.0423 (17)	0.0196 (17)	0.0039 (15)	−0.0036 (15)
O16	0.045 (2)	0.059 (2)	0.052 (2)	0.0145 (19)	−0.0167 (17)	−0.0159 (18)
O17	0.059 (2)	0.046 (2)	0.053 (2)	−0.0071 (19)	0.0226 (18)	−0.0012 (17)
O18	0.050 (2)	0.059 (3)	0.064 (2)	0.018 (2)	0.0196 (18)	−0.0154 (19)
O19	0.059 (2)	0.053 (2)	0.057 (2)	0.017 (2)	0.0195 (18)	−0.0032 (18)
O20	0.053 (2)	0.052 (2)	0.060 (2)	−0.001 (2)	0.0174 (19)	−0.0151 (19)
O21	0.070 (3)	0.056 (3)	0.061 (2)	0.020 (2)	0.019 (2)	0.020 (2)
O22	0.061 (2)	0.065 (3)	0.053 (2)	0.019 (2)	0.0144 (19)	0.0162 (19)
O23	0.068 (7)	0.054 (6)	0.067 (6)	0.019 (5)	−0.012 (5)	0.021 (5)
O24	0.052 (5)	0.054 (6)	0.042 (4)	0.008 (5)	0.006 (4)	0.016 (4)
O25	0.065 (6)	0.054 (6)	0.057 (5)	0.022 (5)	−0.015 (5)	0.024 (5)
O26	0.064 (7)	0.077 (8)	0.084 (8)	0.007 (6)	0.032 (6)	−0.005 (6)
O27	0.078 (8)	0.112 (11)	0.066 (7)	0.046 (8)	−0.028 (6)	−0.046 (7)

Geometric parameters (Å, °)

C1—O1	1.358 (4)	C39—C43	1.576 (5)
C1—C2	1.390	C40—C41	1.353 (6)
C1—C6	1.390	C40—H40	0.930
C2—C3	1.390	C41—C44	1.530 (8)
C2—C7	1.396 (6)	C42—N13	1.296 (7)
C3—C4	1.390	C42—H42A	0.930
C3—H3	0.930	C43—H43A	0.960
C4—C5	1.390	C43—H43B	0.960
C4—C8	1.526 (6)	C43—H43C	0.960
C5—C6	1.390	C44—N11	1.391 (7)
C5—H5	0.930	C44—N12	1.533 (7)
C6—C9	1.498 (6)	C44—H44	0.980
C7—N1	1.328 (5)	C45—C46	1.463 (7)
C7—H7	0.930	C45—N12	1.659 (7)
C8—H8A	0.960	C45—H45A	0.970
C8—H8B	0.960	C45—H45B	0.970
C8—H8C	0.960	C46—N11	1.455 (6)
C9—N2	1.244 (6)	C46—H46A	0.970
C9—H9	0.930	C46—H46B	0.970
C10—O2	1.346 (4)	C47—N11	1.443 (6)
C10—C11	1.390	C47—C48	1.541 (7)
C10—C15	1.390	C47—H47A	0.970
C11—C12	1.390	C47—H47B	0.970
C11—C16	1.474 (7)	C48—N10	1.490 (6)
C12—C13	1.390	C48—H48A	0.970
C12—H12	0.930	C48—H48B	0.970
C13—C14	1.390	C49—N9	1.467 (6)
C13—C17	1.542 (6)	C49—C50	1.538 (7)

C14—C15	1.390	C49—H49A	0.970
C14—H14	0.930	C49—H49B	0.970
C15—C18	1.546 (5)	C50—N14	1.451 (7)
C16—N4	1.259 (7)	C50—H50A	0.970
C16—H16	0.930	C50—H50B	0.970
C17—H17A	0.960	C51—N14	1.507 (6)
C17—H17B	0.960	C51—C52	1.528 (8)
C17—H17C	0.960	C51—H51A	0.970
C18—N5	1.425 (6)	C51—H51B	0.970
C18—N6	1.501 (6)	C52—N13	1.500 (6)
C18—H18	0.980	C52—H52A	0.970
C19—N1	1.490 (5)	C52—H52B	0.970
C19—C20	1.519 (8)	Dy1—O2	2.265 (4)
C19—H19A	0.970	Dy1—O1	2.269 (4)
C19—H19B	0.970	Dy1—O7	2.486 (3)
C20—N6	1.475 (6)	Dy1—O4	2.525 (3)
C20—H20A	0.970	Dy1—O3	2.548 (4)
C20—H20B	0.970	Dy1—N4	2.569 (5)
C21—N6	1.495 (5)	Dy1—N3	2.578 (4)
C21—C22	1.548 (8)	Dy1—N2	2.595 (5)
C21—H21A	0.970	Dy1—O6	2.602 (3)
C21—H21B	0.970	Dy2—O10	2.270 (3)
C22—N5	1.575 (5)	Dy2—O9	2.287 (3)
C22—H22A	0.970	Dy2—O14	2.520 (3)
C22—H22B	0.970	Dy2—O12	2.538 (3)
C23—C24	1.467 (8)	Dy2—O15	2.555 (3)
C23—N4	1.506 (6)	Dy2—N9	2.564 (5)
C23—H23A	0.970	Dy2—N13	2.571 (5)
C23—H23B	0.970	Dy2—O11	2.573 (3)
C24—N3	1.480 (5)	Dy2—N14	2.578 (4)
C24—H24A	0.970	N1—H1A	0.860
C24—H24B	0.970	N3—H3A	0.910
C25—N3	1.463 (6)	N5—H5A	0.900
C25—C26	1.513 (8)	N5—H5B	0.900
C25—H25A	0.970	N7—O5	1.151 (6)
C25—H25B	0.970	N7—O4	1.209 (6)
C26—N2	1.475 (6)	N7—O3	1.288 (6)
C26—H26A	0.970	N8—O8	1.214 (6)
C26—H26B	0.970	N8—O7	1.257 (7)
C27—O9	1.291 (5)	N8—O6	1.275 (6)
C27—C28	1.401 (7)	N10—H10A	0.860
C27—C32	1.415 (7)	N12—H12A	0.900
C28—C29	1.408 (7)	N12—H12B	0.900
C28—C33	1.460 (7)	N14—H14A	0.910
C29—C30	1.385 (7)	N15—O12	1.240 (6)
C29—H29	0.930	N15—O13	1.252 (5)
C30—C31	1.414 (7)	N15—O11	1.265 (6)
C30—C34	1.507 (7)	N16—O16	1.231 (5)
C31—C32	1.416 (8)	N16—O15	1.246 (5)

C31—H31	0.930	N16—O14	1.259 (5)
C32—C35	1.379 (7)	N17—O18	1.206 (6)
C33—N9	1.289 (6)	N17—O17	1.233 (5)
C33—H33	0.930	N17—O19	1.257 (6)
C34—H34A	0.960	N18—O20	1.107 (6)
C34—H34B	0.960	N18—O21	1.185 (6)
C34—H34C	0.960	N18—O22	1.235 (6)
C35—N10	1.321 (5)	O23—H23D	0.850
C35—H35	0.930	O23—H23E	0.850
C36—O10	1.276 (6)	O24—H24C	0.850
C36—C37	1.421 (8)	O24—H24E	0.850
C36—C41	1.431 (6)	O25—H25D	0.850
C37—C42	1.411 (5)	O25—H25E	0.850
C37—C38	1.442 (7)	O26—H26E	0.850
C38—C39	1.343 (8)	O26—H26D	0.850
C38—H38	0.930	O27—H27C	0.850
C39—C40	1.400 (8)	O27—H27A	0.850
O1—C1—C2	118.6 (2)	N11—C47—H47B	109.2
O1—C1—C6	121.2 (2)	C48—C47—H47B	109.2
C2—C1—C6	120.0	H47A—C47—H47B	107.9
C1—C2—C3	120.0	N10—C48—C47	109.7 (4)
C1—C2—C7	123.1 (3)	N10—C48—H48A	109.7
C3—C2—C7	116.9 (3)	C47—C48—H48A	109.7
C4—C3—C2	120.0	N10—C48—H48B	109.7
C4—C3—H3	120.0	C47—C48—H48B	109.7
C2—C3—H3	120.0	H48A—C48—H48B	108.2
C3—C4—C5	120.0	N9—C49—C50	108.3 (4)
C3—C4—C8	119.1 (3)	N9—C49—H49A	110.0
C5—C4—C8	120.9 (3)	C50—C49—H49A	110.0
C6—C5—C4	120.0	N9—C49—H49B	110.0
C6—C5—H5	120.0	C50—C49—H49B	110.0
C4—C5—H5	120.0	H49A—C49—H49B	108.4
C5—C6—C1	120.0	N14—C50—C49	110.2 (4)
C5—C6—C9	114.8 (3)	N14—C50—H50A	109.6
C1—C6—C9	125.1 (3)	C49—C50—H50A	109.6
N1—C7—C2	124.9 (4)	N14—C50—H50B	109.6
N1—C7—H7	117.5	C49—C50—H50B	109.6
C2—C7—H7	117.5	H50A—C50—H50B	108.1
C4—C8—H8A	109.5	N14—C51—C52	109.6 (4)
C4—C8—H8B	109.5	N14—C51—H51A	109.7
H8A—C8—H8B	109.5	C52—C51—H51A	109.7
C4—C8—H8C	109.5	N14—C51—H51B	109.7
H8A—C8—H8C	109.5	C52—C51—H51B	109.7
H8B—C8—H8C	109.5	H51A—C51—H51B	108.2
N2—C9—C6	126.7 (5)	N13—C52—C51	109.2 (4)
N2—C9—H9	116.7	N13—C52—H52A	109.8
C6—C9—H9	116.7	C51—C52—H52A	109.8
O2—C10—C11	122.2 (2)	N13—C52—H52B	109.8
O2—C10—C15	117.6 (2)	C51—C52—H52B	109.8

C11—C10—C15	120.0	H52A—C52—H52B	108.3
C12—C11—C10	120.0	O2—Dy1—O1	96.09 (15)
C12—C11—C16	115.1 (3)	O2—Dy1—O7	124.77 (15)
C10—C11—C16	124.9 (3)	O1—Dy1—O7	77.37 (13)
C11—C12—C13	120.0	O2—Dy1—O4	82.30 (14)
C11—C12—H12	120.0	O1—Dy1—O4	121.63 (12)
C13—C12—H12	120.0	O7—Dy1—O4	147.27 (13)
C12—C13—C14	120.0	O2—Dy1—O3	70.77 (14)
C12—C13—C17	121.7 (3)	O1—Dy1—O3	74.58 (13)
C14—C13—C17	118.3 (3)	O7—Dy1—O3	149.38 (13)
C15—C14—C13	120.0	O4—Dy1—O3	49.67 (12)
C15—C14—H14	120.0	O2—Dy1—N4	72.73 (14)
C13—C14—H14	120.0	O1—Dy1—N4	145.61 (14)
C14—C15—C10	120.0	O7—Dy1—N4	82.75 (14)
C14—C15—C18	119.4 (3)	O4—Dy1—N4	89.71 (13)
C10—C15—C18	120.6 (3)	O3—Dy1—N4	127.77 (14)
N4—C16—C11	126.8 (5)	O2—Dy1—N3	130.87 (14)
N4—C16—H16	116.6	O1—Dy1—N3	133.02 (14)
C11—C16—H16	116.6	O7—Dy1—N3	74.39 (13)
C13—C17—H17A	109.5	O4—Dy1—N3	73.54 (12)
C13—C17—H17B	109.5	O3—Dy1—N3	117.53 (13)
H17A—C17—H17B	109.5	N4—Dy1—N3	65.19 (14)
C13—C17—H17C	109.5	O2—Dy1—N2	149.91 (14)
H17A—C17—H17C	109.5	O1—Dy1—N2	71.76 (14)
H17B—C17—H17C	109.5	O7—Dy1—N2	80.41 (14)
N5—C18—N6	100.7 (4)	O4—Dy1—N2	81.32 (12)
N5—C18—C15	112.2 (4)	O3—Dy1—N2	79.39 (14)
N6—C18—C15	111.9 (3)	N4—Dy1—N2	132.06 (15)
N5—C18—H18	110.5	N3—Dy1—N2	67.11 (14)
N6—C18—H18	110.5	O2—Dy1—O6	75.76 (14)
C15—C18—H18	110.5	O1—Dy1—O6	70.35 (12)
N1—C19—C20	111.3 (4)	O7—Dy1—O6	50.09 (13)
N1—C19—H19A	109.4	O4—Dy1—O6	156.28 (13)
C20—C19—H19A	109.4	O3—Dy1—O6	127.74 (12)
N1—C19—H19B	109.4	N4—Dy1—O6	75.35 (13)
C20—C19—H19B	109.4	N3—Dy1—O6	114.73 (12)
H19A—C19—H19B	108.0	N2—Dy1—O6	122.36 (12)
N6—C20—C19	109.7 (5)	O10—Dy2—O9	98.05 (12)
N6—C20—H20A	109.7	O10—Dy2—O14	125.75 (11)
C19—C20—H20A	109.7	O9—Dy2—O14	74.94 (12)
N6—C20—H20B	109.7	O10—Dy2—O12	83.54 (12)
C19—C20—H20B	109.7	O9—Dy2—O12	119.82 (12)
H20A—C20—H20B	108.2	O14—Dy2—O12	147.03 (10)
N6—C21—C22	100.6 (4)	O10—Dy2—O15	76.39 (12)
N6—C21—H21A	111.7	O9—Dy2—O15	69.21 (12)
C22—C21—H21A	111.7	O14—Dy2—O15	50.44 (10)
N6—C21—H21B	111.7	O12—Dy2—O15	159.19 (11)
C22—C21—H21B	111.7	O10—Dy2—N9	149.36 (14)
H21A—C21—H21B	109.4	O9—Dy2—N9	71.61 (13)

C21—C22—N5	103.5 (3)	O14—Dy2—N9	80.44 (13)
C21—C22—H22A	111.1	O12—Dy2—N9	77.60 (13)
N5—C22—H22A	111.1	O15—Dy2—N9	122.92 (13)
C21—C22—H22B	111.1	O10—Dy2—N13	71.20 (14)
N5—C22—H22B	111.1	O9—Dy2—N13	145.54 (13)
H22A—C22—H22B	109.0	O14—Dy2—N13	85.04 (13)
C24—C23—N4	110.8 (4)	O12—Dy2—N13	92.10 (13)
C24—C23—H23A	109.5	O15—Dy2—N13	76.39 (13)
N4—C23—H23A	109.5	N9—Dy2—N13	132.80 (15)
C24—C23—H23B	109.5	O10—Dy2—O11	72.68 (13)
N4—C23—H23B	109.5	O9—Dy2—O11	73.55 (12)
H23A—C23—H23B	108.1	O14—Dy2—O11	145.53 (12)
C23—C24—N3	109.5 (4)	O12—Dy2—O11	49.39 (12)
C23—C24—H24A	109.8	O15—Dy2—O11	126.79 (12)
N3—C24—H24A	109.8	N9—Dy2—O11	76.71 (14)
C23—C24—H24B	109.8	N13—Dy2—O11	129.33 (14)
N3—C24—H24B	109.8	O10—Dy2—N14	129.84 (13)
H24A—C24—H24B	108.2	O9—Dy2—N14	132.09 (13)
N3—C25—C26	109.5 (4)	O14—Dy2—N14	75.68 (11)
N3—C25—H25A	109.8	O12—Dy2—N14	73.20 (11)
C26—C25—H25A	109.8	O15—Dy2—N14	116.04 (12)
N3—C25—H25B	109.8	N9—Dy2—N14	66.83 (14)
C26—C25—H25B	109.8	N13—Dy2—N14	66.10 (14)
H25A—C25—H25B	108.2	O11—Dy2—N14	117.08 (12)
N2—C26—C25	106.7 (4)	C7—N1—C19	121.9 (3)
N2—C26—H26A	110.4	C7—N1—H1A	119.1
C25—C26—H26A	110.4	C19—N1—H1A	119.0
N2—C26—H26B	110.4	C9—N2—C26	117.1 (4)
C25—C26—H26B	110.4	C9—N2—Dy1	130.9 (3)
H26A—C26—H26B	108.6	C26—N2—Dy1	111.7 (3)
O9—C27—C28	123.0 (4)	C25—N3—C24	112.7 (3)
O9—C27—C32	118.8 (4)	C25—N3—Dy1	111.6 (2)
C28—C27—C32	118.1 (5)	C24—N3—Dy1	110.0 (2)
C27—C28—C29	121.3 (5)	C25—N3—H3A	107.4
C27—C28—C33	123.0 (5)	C24—N3—H3A	107.4
C29—C28—C33	115.7 (4)	Dy1—N3—H3A	107.4
C30—C29—C28	121.0 (4)	C16—N4—C23	115.4 (3)
C30—C29—H29	119.5	C16—N4—Dy1	127.2 (3)
C28—C29—H29	119.5	C23—N4—Dy1	117.3 (2)
C29—C30—C31	118.8 (5)	C18—N5—C22	104.1 (3)
C29—C30—C34	121.4 (4)	C18—N5—H5A	110.9
C31—C30—C34	119.8 (5)	C22—N5—H5A	110.9
C30—C31—C32	120.4 (5)	C18—N5—H5B	110.9
C30—C31—H31	119.8	C22—N5—H5B	110.9
C32—C31—H31	119.8	H5A—N5—H5B	108.9
C35—C32—C27	124.1 (5)	C20—N6—C21	113.7 (3)
C35—C32—C31	115.5 (5)	C20—N6—C18	115.4 (3)
C27—C32—C31	120.4 (5)	C21—N6—C18	101.1 (3)
N9—C33—C28	128.5 (4)	O5—N7—O4	123.9 (5)

N9—C33—H33	115.7	O5—N7—O3	118.9 (5)
C28—C33—H33	115.7	O4—N7—O3	117.2 (4)
C30—C34—H34A	109.5	O8—N8—O7	125.0 (5)
C30—C34—H34B	109.5	O8—N8—O6	118.0 (5)
H34A—C34—H34B	109.5	O7—N8—O6	116.8 (4)
C30—C34—H34C	109.5	C33—N9—C49	116.4 (4)
H34A—C34—H34C	109.5	C33—N9—Dy2	129.3 (3)
H34B—C34—H34C	109.5	C49—N9—Dy2	114.2 (3)
N10—C35—C32	123.4 (4)	C35—N10—C48	122.3 (4)
N10—C35—H35	118.3	C35—N10—H10A	118.7
C32—C35—H35	118.3	C48—N10—H10A	119.0
O10—C36—C37	123.3 (5)	C44—N11—C47	113.7 (4)
O10—C36—C41	119.8 (4)	C44—N11—C46	104.9 (4)
C37—C36—C41	116.8 (5)	C47—N11—C46	115.4 (4)
C42—C37—C36	123.2 (4)	C44—N12—C45	99.6 (4)
C42—C37—C38	118.5 (5)	C44—N12—H12A	111.8
C36—C37—C38	118.3 (5)	C45—N12—H12A	111.8
C39—C38—C37	121.9 (6)	C44—N12—H12B	111.8
C39—C38—H38	119.0	C45—N12—H12B	111.8
C37—C38—H38	119.0	H12A—N12—H12B	109.6
C38—C39—C40	119.9 (5)	C42—N13—C52	115.2 (5)
C38—C39—C43	115.6 (5)	C42—N13—Dy2	126.2 (4)
C40—C39—C43	124.4 (5)	C52—N13—Dy2	118.2 (3)
C41—C40—C39	120.1 (5)	C50—N14—C51	114.0 (4)
C41—C40—H40	119.9	C50—N14—Dy2	114.4 (3)
C39—C40—H40	119.9	C51—N14—Dy2	108.1 (3)
C40—C41—C36	122.7 (4)	C50—N14—H14A	106.6
C40—C41—C44	116.9 (4)	C51—N14—H14A	106.6
C36—C41—C44	120.3 (4)	Dy2—N14—H14A	106.6
N13—C42—C37	127.9 (4)	O12—N15—O13	122.0 (4)
N13—C42—H42A	116.1	O12—N15—O11	117.0 (4)
C37—C42—H42A	116.1	O13—N15—O11	121.0 (5)
C39—C43—H43A	109.5	O16—N16—O15	120.7 (4)
C39—C43—H43B	109.5	O16—N16—O14	120.0 (4)
H43A—C43—H43B	109.5	O15—N16—O14	119.4 (4)
C39—C43—H43C	109.5	O18—N17—O17	115.5 (5)
H43A—C43—H43C	109.5	O18—N17—O19	117.9 (4)
H43B—C43—H43C	109.5	O17—N17—O19	126.3 (5)
N11—C44—C41	116.3 (5)	O20—N18—O21	115.5 (5)
N11—C44—N12	100.6 (4)	O20—N18—O22	128.0 (5)
C41—C44—N12	107.4 (4)	O21—N18—O22	116.4 (5)
N11—C44—H44	110.7	C1—O1—Dy1	143.9 (2)
C41—C44—H44	110.7	C10—O2—Dy1	133.4 (2)
N12—C44—H44	110.7	N7—O3—Dy1	94.4 (3)
C46—C45—N12	102.9 (4)	N7—O4—Dy1	97.7 (3)
C46—C45—H45A	111.2	N8—O6—Dy1	93.0 (3)
N12—C45—H45A	111.2	N8—O7—Dy1	99.0 (3)
C46—C45—H45B	111.2	C27—O9—Dy2	144.3 (2)
N12—C45—H45B	111.2	C36—O10—Dy2	134.5 (3)

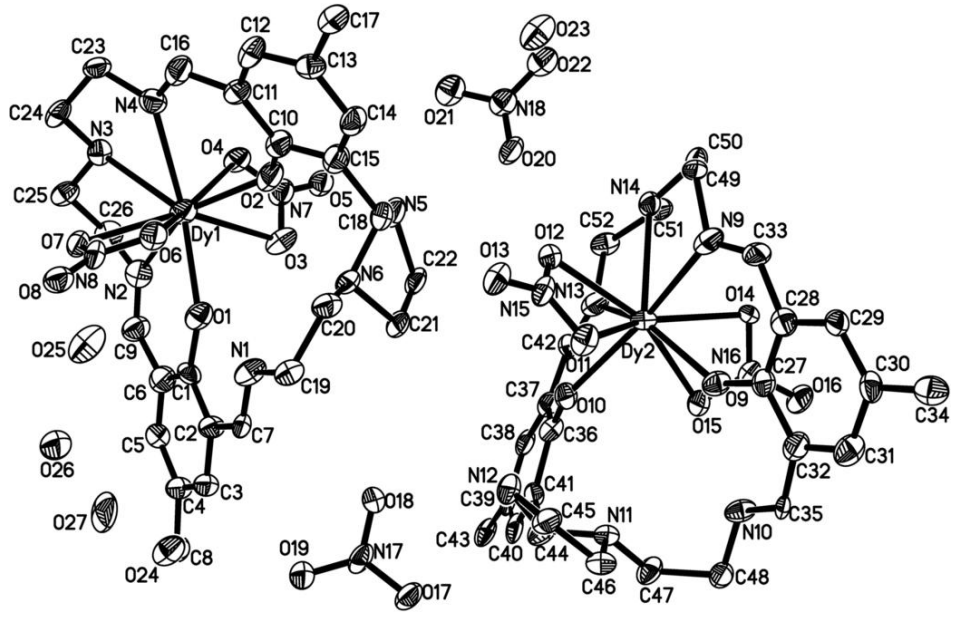
H45A—C45—H45B	109.1	N15—O11—Dy2	95.6 (3)
N11—C46—C45	103.9 (4)	N15—O12—Dy2	98.0 (3)
N11—C46—H46A	111.0	N16—O14—Dy2	93.6 (2)
C45—C46—H46A	111.0	N16—O15—Dy2	92.4 (3)
N11—C46—H46B	111.0	H23D—O23—H23E	109.5
C45—C46—H46B	111.0	H24C—O24—H24E	109.5
H46A—C46—H46B	109.0	H25D—O25—H25E	109.5
N11—C47—C48	112.1 (4)	H26E—O26—H26D	107.3
N11—C47—H47A	109.2	H27C—O27—H27A	109.8
C48—C47—H47A	109.2		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N14—H14A···O20	0.91	2.23	3.118 (6)	166
N12—H12B···O10	0.90	1.99	2.696 (6)	134
N12—H12A···N17	0.90	2.50	3.332 (7)	155
N12—H12A···O17	0.90	2.34	2.972 (7)	127
N12—H12A···O18	0.90	1.91	2.786 (6)	164
N5—H5B···O2	0.90	1.97	2.684 (6)	135
N5—H5A···N18	0.90	2.45	3.348 (7)	177
N5—H5A···O21	0.90	2.21	3.015 (7)	149
N5—H5A···O20	0.90	1.96	2.809 (6)	156
N1—H1A···O1	0.86	1.98	2.610 (5)	130
N10—H10A···O9	0.86	1.99	2.620 (5)	129
N3—H3A···O17^{i}	0.91	2.18	3.008 (5)	151

Symmetry codes: (i) *x*+1, *y*+1, *z*.

Fig. 1


C23
C16
C12
C17
C13
C24
N4
C11
C14
N3
C10
O4
C15
C25
O2
N7
O5
N5
C26
C18
O7
Dy1
O6
O3
C22
O8
N8
N2
N6
O1
C20
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O15
C31
C32
N12
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C45
N11
C35
C43
C40
C44
N10
C46
C47
C48

Fig. 2