

Poly[[diaquabis(2,2'-bipyridine- κ^2N,N')(μ_3 -5-hydroxyisophthalato- $\kappa^5O^1,O^1':O^3,O^3':O^3')$ (μ_3 -5-hydroxyisophthalato- $\kappa^4O^1,O^1':O^3:O^3')$ (μ_2 -5-hydroxyisophthalato- $\kappa^3O^1,O^1':O^3$)di-dysprosium(III)] dihydrate]

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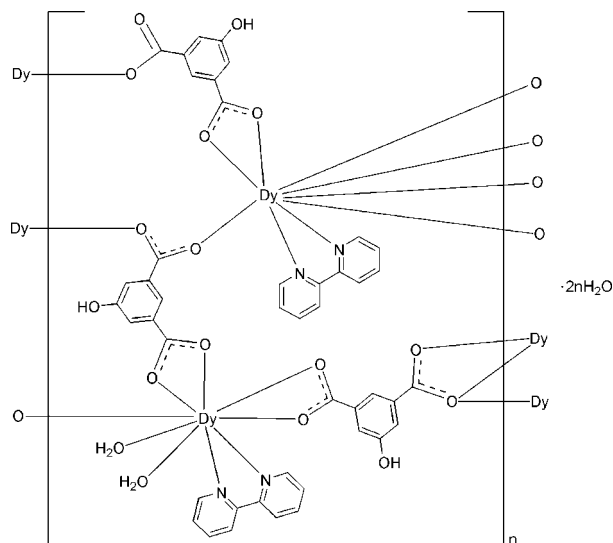
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.010$ Å; R factor = 0.035; wR factor = 0.094; data-to-parameter ratio = 12.9.

The polymeric title compound, $\{[Dy_2(C_8H_4O_5)_3(C_{10}H_8N_2)_2 \cdot (H_2O)_2] \cdot 2H_2O\}_n$, contains two independent Dy^{III} ions, both of which are nine-coordinated in a distorted tricapped trigonal-prismatic geometry. One Dy^{III} ion is coordinated by five 5-hydroxyisophthalate (hip) ligands and one 2,2'-bipyridine (bpy) ligand and the other by three hip ligands, one bpy ligand and two water molecules. The Dy^{III} ions are bridged by the carboxylate groups of the hip ligands, forming a three-dimensional framework. $O-H \cdots O$ hydrogen bonds are present in the crystal structure.

Related literature

For related structures, see: Li *et al.* (2007); Plater *et al.* (2001); Zhuo *et al.* (2006a,b).



Experimental

Crystal data

$[Dy_2(C_8H_4O_5)_3(C_{10}H_8N_2)_2 \cdot (H_2O)_2] \cdot 2H_2O$

$M_r = 1249.77$

Triclinic, $P\bar{1}$

$a = 11.3736$ (5) Å

$b = 12.0349$ (6) Å

$c = 17.8360$ (8) Å

$\alpha = 91.310$ (1)°

$\beta = 103.187$ (1)°

$\gamma = 106.505$ (1)°

$V = 2269.00$ (18) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 3.35$ mm⁻¹

$T = 298$ K

$0.25 \times 0.24 \times 0.21$ mm

Data collection

Bruker APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{min} = 0.488$, $T_{max} = 0.540$

11732 measured reflections

8024 independent reflections

7052 reflections with $I > 2\sigma(I)$

$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.094$

$S = 1.06$

8024 reflections

624 parameters

252 restraints

H-atom parameters constrained

$\Delta\rho_{max} = 2.65$ e Å⁻³

$\Delta\rho_{min} = -1.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O5—H5 \cdots O4W ⁱ	0.82	2.15	2.910 (11)	154
O10—H10A \cdots O2 ⁱⁱ	0.82	1.95	2.761 (6)	168
O15—H15 \cdots O1 ⁱⁱⁱ	0.82	1.92	2.718 (6)	163
O1W—H1WA \cdots O8 ^{iv}	0.85	1.84	2.609 (6)	150
O1W—H1WB \cdots O3W ⁱⁱⁱ	0.85	2.01	2.717 (7)	141
O2W—H2WA \cdots O11	0.85	2.15	2.676 (6)	120
O2W—H2WB \cdots O7 ⁱⁱ	0.85	1.86	2.689 (6)	164
O3W—H3WA \cdots O4W ⁱⁱⁱ	0.85	1.99	2.744 (9)	147
O3W—H3WB \cdots O8 ^v	0.85	2.03	2.832 (9)	156
O4W—H4WA \cdots O6 ^{vi}	0.85	1.96	2.809 (8)	175
O4W—H4WB \cdots O12	0.85	2.20	2.801 (8)	128

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 2, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $x + 1, y, z + 1$; (v) $x + 1, y, z$; (vi) $-x, -y + 1, -z + 1$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999) and *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2467).

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supporting information

Acta Cryst. (2011). E67, m1473–m1474 [https://doi.org/10.1107/S1600536811039080]

Poly[[diaquabis(2,2'-bipyridine- κ^2N,N')(μ_3 -5-hydroxyisophthalato- $\kappa^5O^1,O^1':O^3,O^3':O^3'$)(μ_3 -5-hydroxyisophthalato- $\kappa^4O^1,O^1':O^3:O^3'$)(μ_2 -5-hydroxyisophthalato- $\kappa^3O^1,O^1':O^3$)didysprosium(III)] dihydrate]

Yan-Lin Zhang

S1. Comment

In recent years, *in situ* metal/ligand reactions have been widely investigated for the discovery of new organic reactions and the elucidation of reaction mechanism, as well as the generation of novel coordination polymers. There is currently much interest in employing polycarboxylate ligands with O donors and bipyridine ligands with N donors to design metal coordination polymers with intriguing structures and potential applications. Particular attention has been paid to 5-hydroxyisophthalate and 2,2'-bipyridine ligands; they have five O coordination sites and two N coordination sites, respectively, and thus can potentially afford different coordination modes in multicoordinated ways with transition metal ions (Li *et al.*, 2007; Plater *et al.*, 2001; Zhuo *et al.*, 2006a,b) to form new metal coordination polymers with various structures and interesting properties. In this paper, we report the crystal structure of the title compound, which was synthesized under hydrothermal conditions.

As shown in Fig. 1, both Dy^{III} ions exhibit a distorted tricapped trigonal prismatic geometry. One Dy^{III} ion is coordinated by five 5-hydroxyisophthalate (hip) ligands and one 2,2'-bipyridine (bpy) ligand and the other is by three hip ligands, one bpy ligand and two water molecules. The Dy—O bond lengths range from 2.287 (4) to 2.818 (4) Å and the Dy—N bond lengths range from 2.545 (5) to 2.628 (5) Å. In the crystal, the Dy^{III} ions are bridged by the carboxylate groups of the hip ligands, forming a three-dimensional framework (Fig. 2). O—H...O hydrogen bonds are present (Table 1).

S2. Experimental

A mixture of Dy₂O₃ (0.363 g, 1 mmol), 5-hydroxyisophthalic acid (0.182 g, 1 mmol), 2,2'-bipyridine (0.132 g, 1 mmol) and water (10 ml) in the presence of HClO₄ (0.039 g, 0.385 mmol) was stirred vigorously for 30 min and then sealed in a 20 ml Teflon-lined stainless-steel autoclave. The autoclave was heated and maintained at 433 K for 50 h and then cooled to room temperature at 5 K h⁻¹. Colorless block crystals were obtained.

S3. Refinement

H atoms of water molecules and hydroxyl groups were tentatively located in difference Fourier maps and refined as riding atoms, with O—H = 0.82 (hydroxyl) and 0.85 (water) Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest residual electron density was found at 2.58 Å from H33 atom and the deepest hole at 0.51 Å from O4W atom.

Poly[[diaquabis(2,2'-bipyridine- κ^2N,N')(μ_3 -5-hydroxyisophthalato- $\kappa^5O^1,O^1':O^3,O^3':O^3$)(μ_3 -5-hydroxyisophthalato- $\kappa^4O^1,O^1':O^3:O^3$)(μ_2 -5-hydroxyisophthalato- $\kappa^3O^1,O^1':O^3$)didysprosium(III)] dihydrate]

Crystal data

[Dy₂(C₈H₄O₅)₃(C₁₀H₈N₂)₂(H₂O)₂] \cdot 2H₂O
M_r = 1249.77
 Triclinic, *P* $\bar{1}$
 Hall symbol: -P 1
a = 11.3736 (5) Å
b = 12.0349 (6) Å
c = 17.8360 (8) Å
 α = 91.310 (1)°
 β = 103.187 (1)°
 γ = 106.505 (1)°
V = 2269.00 (18) Å³

Z = 2
F(000) = 1224
D_x = 1.829 Mg m⁻³
 Mo *K* α radiation, λ = 0.71073 Å
 Cell parameters from 7036 reflections
 θ = 2.3–25.2°
 μ = 3.35 mm⁻¹
T = 298 K
 Block, colourless
 0.25 \times 0.24 \times 0.21 mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2001)
T_{min} = 0.488, *T_{max}* = 0.540

11732 measured reflections
 8024 independent reflections
 7052 reflections with *I* > 2 σ (*I*)
R_{int} = 0.020
 θ_{\max} = 25.2°, θ_{\min} = 1.8°
h = -11→13
k = -14→12
l = -21→14

Refinement

Refinement on *F*²
 Least-squares matrix: full
R [*F*² > 2 σ (*F*²)] = 0.035
wR(*F*²) = 0.094
S = 1.06
 8024 reflections
 624 parameters
 252 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
w = 1/[$\sigma^2(F_o^2) + (0.0438P)^2 + 9.6294P$]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} = 0.001
 $\Delta\rho_{\max}$ = 2.65 e Å⁻³
 $\Delta\rho_{\min}$ = -1.25 e Å⁻³

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i> */ <i>U_{eq}</i>
C1	0.4251 (5)	0.8899 (5)	0.7503 (3)	0.0251 (8)
C2	0.3246 (5)	0.8628 (5)	0.6840 (3)	0.0239 (8)
H2	0.3093	0.7969	0.6508	0.029*
C3	0.2482 (5)	0.9350 (5)	0.6685 (3)	0.0244 (8)
C4	0.2704 (5)	1.0328 (5)	0.7175 (3)	0.0293 (9)
H4	0.2188	1.0809	0.7064	0.035*
C5	0.3692 (6)	1.0599 (6)	0.7831 (4)	0.0322 (9)
C6	0.4462 (6)	0.9871 (5)	0.7995 (4)	0.0302 (9)
H6	0.5120	1.0043	0.8440	0.036*
C7	0.5145 (5)	0.8182 (5)	0.7643 (3)	0.0238 (10)
C8	0.1446 (5)	0.9091 (5)	0.5952 (3)	0.0234 (9)

C9	0.0136 (5)	0.8915 (5)	0.1828 (3)	0.0245 (8)
C10	0.1249 (5)	0.9454 (5)	0.1611 (3)	0.0249 (8)
H10	0.1973	0.9860	0.1983	0.030*
C11	0.1270 (5)	0.9381 (5)	0.0836 (3)	0.0249 (8)
C12	0.0188 (5)	0.8775 (5)	0.0280 (3)	0.0249 (8)
H12	0.0204	0.8723	-0.0238	0.030*
C13	-0.0921 (5)	0.8246 (5)	0.0506 (3)	0.0259 (8)
C14	-0.0937 (5)	0.8305 (5)	0.1277 (3)	0.0258 (8)
H14	-0.1673	0.7932	0.1425	0.031*
C15	0.0150 (5)	0.9011 (5)	0.2669 (3)	0.0241 (10)
C16	-0.2103 (5)	0.7609 (5)	-0.0104 (3)	0.0274 (10)
C17	0.5160 (5)	0.4159 (5)	0.6023 (3)	0.0211 (7)
C18	0.3978 (5)	0.3324 (5)	0.5900 (3)	0.0212 (8)
H18	0.3485	0.3307	0.6253	0.025*
C19	0.3540 (5)	0.2526 (5)	0.5257 (3)	0.0201 (7)
C20	0.4278 (5)	0.2559 (5)	0.4717 (3)	0.0216 (8)
H20	0.4007	0.1998	0.4297	0.026*
C21	0.5417 (5)	0.3438 (5)	0.4819 (3)	0.0222 (8)
C22	0.5862 (5)	0.4218 (5)	0.5472 (3)	0.0229 (8)
H22	0.6638	0.4788	0.5544	0.028*
C23	0.2276 (5)	0.1624 (5)	0.5137 (3)	0.0203 (9)
C24	0.5688 (5)	0.4978 (5)	0.6744 (3)	0.0220 (9)
C25	1.0000 (8)	0.7669 (10)	0.8074 (5)	0.0683 (16)
H25	0.9747	0.8291	0.7869	0.082*
C26	1.1267 (8)	0.7756 (10)	0.8224 (6)	0.0719 (14)
H26	1.1856	0.8417	0.8129	0.086*
C27	1.1621 (9)	0.6827 (10)	0.8517 (6)	0.0729 (13)
H27	1.2463	0.6840	0.8608	0.087*
C28	1.0729 (8)	0.5862 (9)	0.8679 (5)	0.0685 (13)
H28	1.0970	0.5233	0.8883	0.082*
C29	0.9474 (8)	0.5858 (8)	0.8531 (5)	0.0610 (12)
C30	0.8518 (8)	0.4909 (8)	0.8756 (5)	0.0602 (12)
C31	0.8801 (9)	0.3964 (8)	0.9129 (5)	0.0648 (12)
H31	0.9610	0.3886	0.9213	0.078*
C32	0.7869 (9)	0.3161 (8)	0.9366 (6)	0.0685 (13)
H32	0.8057	0.2552	0.9631	0.082*
C33	0.6694 (9)	0.3243 (8)	0.9220 (5)	0.0684 (14)
H33	0.6055	0.2697	0.9375	0.082*
C34	0.6460 (9)	0.4171 (8)	0.8831 (5)	0.0661 (16)
H34	0.5638	0.4221	0.8719	0.079*
C35	0.3302 (6)	0.9129 (6)	0.3933 (4)	0.0425 (12)
H35	0.3510	0.9844	0.4219	0.051*
C36	0.4133 (7)	0.8951 (6)	0.3514 (4)	0.0439 (11)
H36	0.4897	0.9515	0.3535	0.053*
C37	0.3786 (7)	0.7913 (6)	0.3068 (4)	0.0416 (10)
H37	0.4285	0.7779	0.2750	0.050*
C38	0.2695 (6)	0.7073 (6)	0.3096 (4)	0.0380 (10)
H38	0.2461	0.6358	0.2807	0.046*

C39	0.1949 (6)	0.7292 (5)	0.3553 (4)	0.0339 (9)
C40	0.0846 (6)	0.6358 (6)	0.3694 (4)	0.0356 (9)
C41	0.0697 (7)	0.5191 (6)	0.3519 (4)	0.0409 (10)
H41	0.1247	0.4972	0.3274	0.049*
C42	-0.0277 (7)	0.4353 (6)	0.3710 (5)	0.0464 (11)
H42	-0.0391	0.3565	0.3601	0.056*
C43	-0.1078 (7)	0.4720 (6)	0.4069 (5)	0.0460 (11)
H43	-0.1743	0.4182	0.4206	0.055*
C44	-0.0871 (6)	0.5902 (6)	0.4219 (4)	0.0422 (12)
H44	-0.1419	0.6141	0.4457	0.051*
Dy1	0.04319 (2)	0.89445 (2)	0.429009 (13)	0.01643 (8)
Dy2	0.67367 (2)	0.67220 (2)	0.800601 (14)	0.01969 (8)
N1	0.9105 (5)	0.6742 (5)	0.8207 (3)	0.0390 (13)
N2	0.7338 (6)	0.4996 (5)	0.8606 (3)	0.0407 (13)
N3	0.0070 (4)	0.6719 (4)	0.4043 (3)	0.0238 (10)
N4	0.2227 (5)	0.8338 (4)	0.3947 (3)	0.0298 (11)
O1	0.4947 (4)	0.7273 (4)	0.7207 (2)	0.0282 (9)
O2	0.6118 (4)	0.8495 (3)	0.8205 (2)	0.0267 (9)
O3	0.0652 (4)	0.9668 (4)	0.5843 (3)	0.0312 (10)
O4	0.1422 (4)	0.8342 (4)	0.5450 (2)	0.0324 (10)
O5	0.3955 (6)	1.1574 (5)	0.8318 (3)	0.072 (2)
H5	0.3461	1.1943	0.8150	0.108*
O6	-0.0618 (4)	0.8244 (4)	0.2938 (2)	0.0256 (9)
O7	0.0951 (4)	0.9848 (4)	0.3114 (2)	0.0307 (9)
O8	-0.3077 (5)	0.7129 (6)	0.0117 (3)	0.0632 (18)
O9	-0.2044 (4)	0.7600 (4)	-0.0800 (2)	0.0281 (9)
O10	0.2343 (4)	0.9872 (4)	0.0599 (2)	0.0352 (10)
H10A	0.2877	1.0299	0.0958	0.053*
O11	0.6748 (4)	0.5741 (4)	0.6827 (2)	0.0324 (10)
O12	0.5103 (4)	0.4909 (4)	0.7272 (2)	0.0283 (9)
O13	0.1492 (3)	0.1884 (3)	0.5452 (2)	0.0263 (9)
O14	0.2080 (3)	0.0689 (3)	0.4735 (2)	0.0247 (8)
O15	0.6135 (4)	0.3572 (4)	0.4296 (2)	0.0368 (11)
H15	0.5706	0.3213	0.3881	0.055*
O1W	0.5317 (4)	0.6243 (4)	0.8801 (2)	0.0377 (11)
H1WA	0.5604	0.6566	0.9261	0.057*
H1WB	0.4515	0.6014	0.8712	0.057*
O2W	0.7608 (4)	0.8059 (4)	0.7123 (2)	0.0337 (10)
H2WA	0.7579	0.7565	0.6765	0.051*
H2WB	0.7932	0.8733	0.6996	0.051*
O3W	0.6892 (5)	0.5249 (5)	0.1047 (4)	0.0671 (17)
H3WA	0.7242	0.5719	0.1452	0.101*
H3WB	0.6780	0.5651	0.0666	0.101*
O4W	0.2982 (7)	0.3417 (7)	0.7652 (4)	0.106 (3)
H4WA	0.2287	0.2884	0.7480	0.160*
H4WB	0.3365	0.3533	0.7291	0.160*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0205 (15)	0.0297 (16)	0.0218 (15)	0.0061 (13)	0.0008 (13)	-0.0021 (14)
C2	0.0201 (16)	0.0278 (17)	0.0217 (16)	0.0068 (14)	0.0016 (14)	-0.0009 (15)
C3	0.0198 (15)	0.0278 (16)	0.0231 (15)	0.0061 (13)	0.0017 (13)	-0.0006 (14)
C4	0.0235 (16)	0.0319 (17)	0.0287 (17)	0.0084 (15)	-0.0007 (15)	-0.0053 (15)
C5	0.0252 (17)	0.0354 (18)	0.0304 (18)	0.0085 (15)	-0.0025 (15)	-0.0083 (16)
C6	0.0234 (16)	0.0344 (18)	0.0274 (17)	0.0074 (15)	-0.0021 (15)	-0.0064 (16)
C7	0.0196 (19)	0.029 (2)	0.0202 (19)	0.0057 (17)	0.0013 (17)	-0.0010 (17)
C8	0.0201 (19)	0.026 (2)	0.021 (2)	0.0038 (17)	0.0030 (17)	0.0034 (17)
C9	0.0239 (15)	0.0292 (16)	0.0168 (15)	0.0044 (13)	0.0027 (13)	-0.0021 (14)
C10	0.0239 (16)	0.0295 (17)	0.0171 (16)	0.0040 (15)	0.0021 (14)	-0.0030 (15)
C11	0.0244 (17)	0.0298 (17)	0.0176 (16)	0.0050 (15)	0.0041 (14)	-0.0023 (15)
C12	0.0256 (16)	0.0295 (17)	0.0171 (16)	0.0057 (14)	0.0040 (14)	-0.0024 (15)
C13	0.0255 (15)	0.0303 (16)	0.0179 (15)	0.0043 (14)	0.0027 (13)	-0.0020 (14)
C14	0.0248 (16)	0.0306 (17)	0.0177 (16)	0.0034 (14)	0.0029 (14)	-0.0013 (15)
C15	0.0237 (19)	0.028 (2)	0.0172 (19)	0.0051 (17)	0.0024 (17)	-0.0017 (17)
C16	0.025 (2)	0.032 (2)	0.020 (2)	0.0041 (17)	0.0021 (17)	-0.0024 (18)
C17	0.0192 (14)	0.0225 (15)	0.0186 (15)	0.0031 (13)	0.0032 (13)	-0.0030 (13)
C18	0.0193 (15)	0.0234 (16)	0.0182 (16)	0.0024 (14)	0.0046 (13)	-0.0039 (14)
C19	0.0180 (14)	0.0230 (15)	0.0169 (14)	0.0032 (13)	0.0033 (12)	-0.0035 (13)
C20	0.0190 (15)	0.0245 (16)	0.0176 (16)	0.0024 (14)	0.0029 (14)	-0.0051 (14)
C21	0.0196 (16)	0.0256 (17)	0.0183 (16)	0.0028 (14)	0.0040 (14)	-0.0030 (14)
C22	0.0199 (16)	0.0253 (17)	0.0193 (16)	0.0013 (14)	0.0036 (14)	-0.0027 (14)
C23	0.0183 (18)	0.0230 (19)	0.0164 (18)	0.0027 (16)	0.0027 (16)	-0.0019 (17)
C24	0.0203 (19)	0.0223 (19)	0.0193 (19)	0.0034 (16)	0.0011 (16)	-0.0022 (17)
C25	0.043 (3)	0.104 (4)	0.063 (3)	0.024 (3)	0.019 (3)	0.021 (3)
C26	0.047 (2)	0.105 (3)	0.067 (3)	0.024 (2)	0.018 (2)	0.020 (3)
C27	0.050 (2)	0.102 (3)	0.070 (3)	0.028 (2)	0.015 (2)	0.017 (2)
C28	0.052 (2)	0.093 (3)	0.068 (3)	0.034 (2)	0.012 (2)	0.015 (2)
C29	0.052 (2)	0.080 (3)	0.061 (2)	0.038 (2)	0.011 (2)	0.010 (2)
C30	0.058 (2)	0.070 (3)	0.061 (2)	0.039 (2)	0.007 (2)	0.007 (2)
C31	0.066 (2)	0.065 (3)	0.067 (3)	0.035 (2)	0.002 (2)	0.008 (2)
C32	0.073 (3)	0.058 (3)	0.070 (3)	0.027 (2)	-0.001 (2)	0.009 (2)
C33	0.074 (3)	0.053 (3)	0.068 (3)	0.020 (2)	-0.003 (2)	0.011 (2)
C34	0.073 (3)	0.050 (3)	0.066 (3)	0.019 (3)	-0.003 (3)	0.010 (3)
C35	0.037 (2)	0.036 (2)	0.060 (3)	0.008 (2)	0.026 (2)	0.004 (2)
C36	0.039 (2)	0.039 (2)	0.058 (2)	0.0082 (18)	0.0248 (19)	0.0066 (19)
C37	0.039 (2)	0.038 (2)	0.054 (2)	0.0111 (17)	0.0248 (18)	0.0069 (18)
C38	0.0384 (19)	0.0341 (19)	0.048 (2)	0.0124 (16)	0.0220 (17)	0.0056 (17)
C39	0.0349 (19)	0.0294 (18)	0.044 (2)	0.0120 (16)	0.0201 (17)	0.0049 (17)
C40	0.0352 (19)	0.0289 (18)	0.047 (2)	0.0100 (16)	0.0192 (17)	0.0001 (17)
C41	0.0390 (19)	0.0305 (19)	0.056 (2)	0.0086 (16)	0.0196 (18)	-0.0044 (18)
C42	0.042 (2)	0.0324 (19)	0.064 (2)	0.0049 (17)	0.0189 (19)	-0.0042 (18)
C43	0.039 (2)	0.032 (2)	0.066 (2)	0.0034 (18)	0.020 (2)	-0.001 (2)
C44	0.035 (2)	0.030 (2)	0.064 (3)	0.005 (2)	0.021 (2)	-0.001 (2)
Dy1	0.01444 (13)	0.01919 (14)	0.01331 (14)	0.00240 (10)	0.00243 (10)	-0.00233 (10)

Dy2	0.01911 (14)	0.02153 (15)	0.01423 (14)	0.00364 (10)	-0.00064 (10)	-0.00393 (10)
N1	0.031 (3)	0.056 (4)	0.028 (3)	0.014 (3)	0.003 (2)	-0.008 (3)
N2	0.047 (3)	0.036 (3)	0.036 (3)	0.015 (3)	-0.002 (3)	0.002 (3)
N3	0.022 (2)	0.021 (2)	0.027 (3)	0.0041 (19)	0.007 (2)	-0.002 (2)
N4	0.025 (3)	0.028 (3)	0.039 (3)	0.007 (2)	0.015 (2)	0.001 (2)
O1	0.028 (2)	0.032 (2)	0.020 (2)	0.0113 (18)	-0.0043 (17)	-0.0067 (17)
O2	0.021 (2)	0.031 (2)	0.023 (2)	0.0085 (17)	-0.0051 (16)	-0.0102 (17)
O3	0.023 (2)	0.033 (2)	0.038 (2)	0.0123 (18)	0.0013 (18)	0.0082 (19)
O4	0.038 (2)	0.034 (2)	0.022 (2)	0.016 (2)	-0.0039 (18)	-0.0002 (18)
O5	0.074 (4)	0.069 (4)	0.063 (4)	0.047 (3)	-0.032 (3)	-0.047 (3)
O6	0.026 (2)	0.033 (2)	0.0132 (19)	0.0030 (17)	0.0032 (16)	0.0001 (16)
O7	0.035 (2)	0.032 (2)	0.015 (2)	-0.0036 (18)	0.0041 (17)	-0.0036 (17)
O8	0.033 (3)	0.103 (5)	0.024 (3)	-0.023 (3)	0.005 (2)	-0.006 (3)
O9	0.028 (2)	0.036 (2)	0.0140 (19)	0.0053 (18)	-0.0009 (16)	-0.0052 (17)
O10	0.027 (2)	0.045 (3)	0.027 (2)	-0.0024 (19)	0.0107 (19)	-0.009 (2)
O11	0.028 (2)	0.031 (2)	0.028 (2)	-0.0036 (18)	0.0046 (18)	-0.0111 (18)
O12	0.030 (2)	0.029 (2)	0.022 (2)	0.0026 (17)	0.0078 (17)	-0.0076 (17)
O13	0.0190 (19)	0.027 (2)	0.030 (2)	0.0000 (16)	0.0095 (17)	-0.0094 (17)
O14	0.0198 (19)	0.023 (2)	0.026 (2)	-0.0008 (16)	0.0057 (16)	-0.0103 (17)
O15	0.024 (2)	0.054 (3)	0.024 (2)	-0.004 (2)	0.0114 (18)	-0.012 (2)
O1W	0.027 (2)	0.049 (3)	0.025 (2)	-0.006 (2)	0.0046 (18)	-0.008 (2)
O2W	0.042 (3)	0.027 (2)	0.028 (2)	0.0007 (19)	0.011 (2)	0.0007 (18)
O3W	0.062 (4)	0.058 (4)	0.064 (4)	-0.007 (3)	0.014 (3)	-0.003 (3)
O4W	0.095 (5)	0.122 (7)	0.056 (4)	-0.047 (5)	0.030 (4)	-0.019 (4)

Geometric parameters (Å, °)

C1—C6	1.377 (8)	C30—C31	1.409 (12)
C1—C2	1.401 (8)	C31—C32	1.371 (13)
C1—C7	1.494 (8)	C31—H31	0.9300
C2—C3	1.383 (8)	C32—C33	1.334 (13)
C2—H2	0.9300	C32—H32	0.9300
C3—C4	1.377 (8)	C33—C34	1.385 (12)
C3—C8	1.505 (8)	C33—H33	0.9300
C4—C5	1.383 (8)	C34—N2	1.336 (11)
C4—H4	0.9300	C34—H34	0.9300
C5—O5	1.362 (8)	C35—N4	1.325 (8)
C5—C6	1.397 (9)	C35—C36	1.389 (9)
C6—H6	0.9300	C35—H35	0.9300
C7—O1	1.263 (7)	C36—C37	1.371 (10)
C7—O2	1.269 (7)	C36—H36	0.9300
C8—O4	1.246 (7)	C37—C38	1.372 (9)
C8—O3	1.272 (7)	C37—H37	0.9300
C9—C14	1.381 (8)	C38—C39	1.372 (9)
C9—C10	1.393 (8)	C38—H38	0.9300
C9—C15	1.499 (7)	C39—N4	1.345 (8)
C10—C11	1.390 (8)	C39—C40	1.502 (9)
C10—H10	0.9300	C40—N3	1.346 (7)

C11—O10	1.362 (7)	C40—C41	1.386 (9)
C11—C12	1.388 (8)	C41—C42	1.384 (10)
C12—C13	1.396 (8)	C41—H41	0.9300
C12—H12	0.9300	C42—C43	1.383 (10)
C13—C14	1.380 (8)	C42—H42	0.9300
C13—C16	1.511 (8)	C43—C44	1.384 (9)
C14—H14	0.9300	C43—H43	0.9300
C15—O7	1.260 (7)	C44—N3	1.335 (8)
C15—O6	1.265 (7)	C44—H44	0.9300
C16—O8	1.249 (7)	Dy1—O13 ⁱ	2.287 (4)
C16—O9	1.260 (7)	Dy1—O3 ⁱⁱ	2.328 (4)
C17—C22	1.392 (7)	Dy1—O4	2.355 (4)
C17—C18	1.397 (7)	Dy1—O14 ⁱⁱⁱ	2.358 (4)
C17—C24	1.497 (8)	Dy1—O6	2.444 (4)
C18—C19	1.380 (7)	Dy1—O7	2.496 (4)
C18—H18	0.9300	Dy1—N4	2.545 (5)
C19—C20	1.409 (7)	Dy1—N3	2.603 (5)
C19—C23	1.502 (7)	Dy1—O3	2.818 (4)
C20—C21	1.391 (7)	Dy2—O9 ^{iv}	2.300 (4)
C20—H20	0.9300	Dy2—O1W	2.346 (4)
C21—O15	1.359 (7)	Dy2—O11	2.393 (4)
C21—C22	1.380 (8)	Dy2—O2W	2.444 (4)
C22—H22	0.9300	Dy2—O1	2.470 (4)
C23—O14	1.257 (6)	Dy2—O2	2.472 (4)
C23—O13	1.260 (6)	Dy2—O12	2.527 (4)
C24—O12	1.262 (7)	Dy2—N2	2.549 (6)
C24—O11	1.266 (7)	Dy2—N1	2.628 (5)
C25—N1	1.346 (11)	O5—H5	0.8200
C25—C26	1.377 (12)	O10—H10A	0.8200
C25—H25	0.9300	O15—H15	0.8200
C26—C27	1.367 (14)	O1W—H1WA	0.8500
C26—H26	0.9300	O1W—H1WB	0.8500
C27—C28	1.394 (14)	O2W—H2WA	0.8501
C27—H27	0.9300	O2W—H2WB	0.8500
C28—C29	1.390 (11)	O3W—H3WA	0.8500
C28—H28	0.9300	O3W—H3WB	0.8501
C29—N1	1.347 (10)	O4W—H4WA	0.8500
C29—C30	1.470 (13)	O4W—H4WB	0.8500
C30—N2	1.343 (10)		
C6—C1—C2	119.8 (5)	C42—C41—C40	119.5 (6)
C6—C1—C7	120.1 (5)	C42—C41—H41	120.2
C2—C1—C7	120.0 (5)	C40—C41—H41	120.2
C3—C2—C1	119.5 (5)	C43—C42—C41	118.2 (7)
C3—C2—H2	120.2	C43—C42—H42	120.9
C1—C2—H2	120.2	C41—C42—H42	120.9
C4—C3—C2	120.5 (5)	C42—C43—C44	118.8 (7)
C4—C3—C8	120.1 (5)	C42—C43—H43	120.6

C2—C3—C8	119.3 (5)	C44—C43—H43	120.6
C3—C4—C5	120.4 (6)	N3—C44—C43	123.6 (6)
C3—C4—H4	119.8	N3—C44—H44	118.2
C5—C4—H4	119.8	C43—C44—H44	118.2
O5—C5—C4	121.8 (6)	O13 ⁱ —Dy1—O3 ⁱⁱ	72.52 (14)
O5—C5—C6	118.7 (5)	O13 ⁱ —Dy1—O4	89.48 (15)
C4—C5—C6	119.5 (6)	O3 ⁱⁱ —Dy1—O4	127.26 (15)
C1—C6—C5	120.3 (6)	O13 ⁱ —Dy1—O14 ⁱⁱⁱ	134.77 (13)
C1—C6—H6	119.8	O3 ⁱⁱ —Dy1—O14 ⁱⁱⁱ	77.83 (14)
C5—C6—H6	119.8	O4—Dy1—O14 ⁱⁱⁱ	82.03 (15)
O1—C7—O2	119.7 (5)	O13 ⁱ —Dy1—O6	86.34 (13)
O1—C7—C1	120.7 (5)	O3 ⁱⁱ —Dy1—O6	87.44 (14)
O2—C7—C1	119.6 (5)	O4—Dy1—O6	141.71 (14)
O4—C8—O3	121.5 (5)	O14 ⁱⁱⁱ —Dy1—O6	125.92 (13)
O4—C8—C3	118.6 (5)	O13 ⁱ —Dy1—O7	129.91 (14)
O3—C8—C3	119.8 (5)	O3 ⁱⁱ —Dy1—O7	77.91 (15)
C14—C9—C10	120.3 (5)	O4—Dy1—O7	140.19 (15)
C14—C9—C15	121.7 (5)	O14 ⁱⁱⁱ —Dy1—O7	73.56 (13)
C10—C9—C15	118.1 (5)	O6—Dy1—O7	52.45 (13)
C11—C10—C9	119.6 (5)	O13 ⁱ —Dy1—N4	139.44 (15)
C11—C10—H10	120.2	O3 ⁱⁱ —Dy1—N4	145.09 (16)
C9—C10—H10	120.2	O4—Dy1—N4	76.16 (16)
O10—C11—C12	118.2 (5)	O14 ⁱⁱⁱ —Dy1—N4	81.22 (15)
O10—C11—C10	121.6 (5)	O6—Dy1—N4	82.61 (15)
C12—C11—C10	120.3 (5)	O7—Dy1—N4	69.50 (16)
C11—C12—C13	119.5 (5)	O13 ⁱ —Dy1—N3	76.12 (14)
C11—C12—H12	120.2	O3 ⁱⁱ —Dy1—N3	141.60 (15)
C13—C12—H12	120.2	O4—Dy1—N3	73.24 (15)
C14—C13—C12	120.2 (5)	O14 ⁱⁱⁱ —Dy1—N3	140.54 (14)
C14—C13—C16	120.5 (5)	O6—Dy1—N3	68.80 (14)
C12—C13—C16	119.3 (5)	O7—Dy1—N3	107.11 (14)
C13—C14—C9	120.2 (5)	N4—Dy1—N3	63.48 (15)
C13—C14—H14	119.9	O13 ⁱ —Dy1—O3	73.04 (13)
C9—C14—H14	119.9	O3 ⁱⁱ —Dy1—O3	78.01 (14)
O7—C15—O6	119.7 (5)	O4—Dy1—O3	49.26 (13)
O7—C15—C9	119.8 (5)	O14 ⁱⁱⁱ —Dy1—O3	67.89 (13)
O6—C15—C9	120.4 (5)	O6—Dy1—O3	157.51 (12)
O8—C16—O9	124.3 (5)	O7—Dy1—O3	137.87 (13)
O8—C16—C13	117.8 (5)	N4—Dy1—O3	118.94 (14)
O9—C16—C13	118.0 (5)	N3—Dy1—O3	113.26 (13)
C22—C17—C18	119.5 (5)	O9 ^{iv} —Dy2—O1W	76.99 (14)
C22—C17—C24	119.6 (5)	O9 ^{iv} —Dy2—O11	144.48 (14)
C18—C17—C24	120.9 (5)	O1W—Dy2—O11	130.31 (14)
C19—C18—C17	120.2 (5)	O9 ^{iv} —Dy2—O2W	102.70 (15)
C19—C18—H18	119.9	O1W—Dy2—O2W	147.49 (16)
C17—C18—H18	119.9	O11—Dy2—O2W	67.17 (14)
C18—C19—C20	120.1 (5)	O9 ^{iv} —Dy2—O1	126.34 (14)
C18—C19—C23	119.6 (5)	O1W—Dy2—O1	80.60 (15)

C20—C19—C23	120.3 (5)	O11—Dy2—O1	84.89 (14)
C21—C20—C19	119.3 (5)	O2W—Dy2—O1	73.59 (14)
C21—C20—H20	120.4	O9 ^{iv} —Dy2—O2	74.47 (14)
C19—C20—H20	120.4	O1W—Dy2—O2	74.31 (15)
O15—C21—C22	117.2 (5)	O11—Dy2—O2	129.29 (14)
O15—C21—C20	122.6 (5)	O2W—Dy2—O2	74.37 (14)
C22—C21—C20	120.3 (5)	O1—Dy2—O2	52.60 (12)
C21—C22—C17	120.5 (5)	O9 ^{iv} —Dy2—O12	145.62 (14)
C21—C22—H22	119.8	O1W—Dy2—O12	77.65 (14)
C17—C22—H22	119.8	O11—Dy2—O12	52.71 (13)
O14—C23—O13	125.5 (5)	O2W—Dy2—O12	111.16 (13)
O14—C23—C19	118.4 (5)	O1—Dy2—O12	71.06 (14)
O13—C23—C19	116.1 (5)	O2—Dy2—O12	119.80 (13)
O12—C24—O11	119.8 (5)	O9 ^{iv} —Dy2—N2	79.69 (17)
O12—C24—C17	121.1 (5)	O1W—Dy2—N2	80.15 (18)
O11—C24—C17	119.1 (5)	O11—Dy2—N2	83.40 (17)
N1—C25—C26	124.2 (10)	O2W—Dy2—N2	132.21 (18)
N1—C25—H25	117.9	O1—Dy2—N2	142.38 (17)
C26—C25—H25	117.9	O2—Dy2—N2	146.97 (16)
C27—C26—C25	117.1 (10)	O12—Dy2—N2	73.40 (16)
C27—C26—H26	121.5	O9 ^{iv} —Dy2—N1	67.91 (15)
C25—C26—H26	121.5	O1W—Dy2—N1	132.17 (17)
C26—C27—C28	120.5 (9)	O11—Dy2—N1	76.59 (15)
C26—C27—H27	119.7	O2W—Dy2—N1	73.89 (17)
C28—C27—H27	119.7	O1—Dy2—N1	146.81 (16)
C29—C28—C27	118.7 (9)	O2—Dy2—N1	122.85 (16)
C29—C28—H28	120.6	O12—Dy2—N1	115.59 (16)
C27—C28—H28	120.6	N2—Dy2—N1	62.81 (19)
N1—C29—C28	121.2 (9)	C25—N1—C29	118.1 (7)
N1—C29—C30	118.0 (7)	C25—N1—Dy2	122.0 (5)
C28—C29—C30	120.8 (8)	C29—N1—Dy2	119.5 (5)
N2—C30—C31	120.4 (9)	C34—N2—C30	117.7 (7)
N2—C30—C29	116.4 (7)	C34—N2—Dy2	118.8 (5)
C31—C30—C29	123.1 (8)	C30—N2—Dy2	123.3 (5)
C32—C31—C30	119.2 (9)	C44—N3—C40	117.4 (5)
C32—C31—H31	120.4	C44—N3—Dy1	123.9 (4)
C30—C31—H31	120.4	C40—N3—Dy1	118.7 (4)
C33—C32—C31	120.7 (9)	C35—N4—C39	118.0 (5)
C33—C32—H32	119.7	C35—N4—Dy1	120.5 (4)
C31—C32—H32	119.7	C39—N4—Dy1	118.3 (4)
C32—C33—C34	117.7 (10)	C7—O1—Dy2	93.8 (3)
C32—C33—H33	121.1	C7—O2—Dy2	93.6 (3)
C34—C33—H33	121.1	C8—O3—Dy1 ⁱⁱ	168.2 (4)
N2—C34—C33	124.2 (9)	C8—O3—Dy1	81.1 (3)
N2—C34—H34	117.9	Dy1 ⁱⁱ —O3—Dy1	101.99 (14)
C33—C34—H34	117.9	C8—O4—Dy1	103.3 (3)
N4—C35—C36	123.6 (7)	C5—O5—H5	109.5
N4—C35—H35	118.2	C15—O6—Dy1	94.6 (3)

C36—C35—H35	118.2	C15—O7—Dy1	92.3 (3)
C37—C36—C35	117.5 (6)	C16—O9—Dy2 ^v	139.1 (4)
C37—C36—H36	121.3	C11—O10—H10A	109.5
C35—C36—H36	121.3	C24—O11—Dy2	96.7 (3)
C36—C37—C38	119.3 (6)	C24—O12—Dy2	90.5 (3)
C36—C37—H37	120.4	C23—O13—Dy1 ⁱ	140.5 (4)
C38—C37—H37	120.4	C23—O14—Dy1 ^{vi}	138.4 (3)
C39—C38—C37	119.8 (7)	C21—O15—H15	109.5
C39—C38—H38	120.1	Dy2—O1W—H1WA	115.0
C37—C38—H38	120.1	Dy2—O1W—H1WB	133.5
N4—C39—C38	121.5 (6)	H1WA—O1W—H1WB	107.7
N4—C39—C40	116.2 (5)	Dy2—O2W—H2WA	99.2
C38—C39—C40	122.2 (6)	Dy2—O2W—H2WB	153.0
N3—C40—C41	122.5 (6)	H2WA—O2W—H2WB	107.7
N3—C40—C39	116.2 (5)	H3WA—O3W—H3WB	107.7
C41—C40—C39	121.2 (6)	H4WA—O4W—H4WB	107.7

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x, -y+2, -z+1$; (iii) $x, y+1, z$; (iv) $x+1, y, z+1$; (v) $x-1, y, z-1$; (vi) $x, y-1, z$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5...O4W ⁱⁱⁱ	0.82	2.15	2.910 (11)	154
O10—H10A...O2 ^{vii}	0.82	1.95	2.761 (6)	168
O15—H15...O1 ^{viii}	0.82	1.92	2.718 (6)	163
O1W—H1WA...O8 ^{iv}	0.85	1.84	2.609 (6)	150
O1W—H1WB...O3W ^{viii}	0.85	2.01	2.717 (7)	141
O2W—H2WA...O11	0.85	2.15	2.676 (6)	120
O2W—H2WB...O7 ^{vii}	0.85	1.86	2.689 (6)	164
O3W—H3WA...O4W ^{viii}	0.85	1.99	2.744 (9)	147
O3W—H3WB...O8 ^{ix}	0.85	2.03	2.832 (9)	156
O4W—H4WA...O6 ⁱ	0.85	1.96	2.809 (8)	175
O4W—H4WB...O12	0.85	2.20	2.801 (8)	128

Symmetry codes: (i) $-x, -y+1, -z+1$; (iii) $x, y+1, z$; (iv) $x+1, y, z+1$; (vii) $-x+1, -y+2, -z+1$; (viii) $-x+1, -y+1, -z+1$; (ix) $x+1, y, z$.