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Poly[hydronium [dysprosium(III)-μ_3-(ethylenediaminetetraacetato-$\kappa^8N,N',O,O',O'',O''':O'''':O''''')$] monohydrate]

Xiu-Li You[a] and Seik Weng Ng[b]*

[a]Institute of Organic Chemistry, Jiangxi Science and Technology Normal University, Nanchang 330013, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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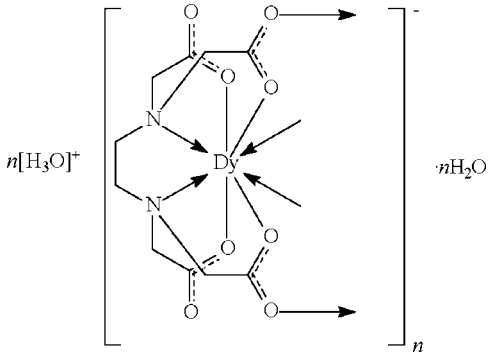
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(O–C) = 0.004 Å; H-atom completeness 71%; disorder in main residue; R factor = 0.017; wR factor = 0.050; data-to-parameter ratio = 10.5.

The Dy^{III} atom in the title compound, $(H_3O)[Dy(C_{10}H_{12}N_2O_8)]\cdot H_2O$, is N,N',O,O',O'',O'''-chelated by the edta tetraanion; it is also linked to the O atoms of two other tetraaanions in the polyanionic layer. The metal atom (site symmetry m) exists in a square-antiprismatic DyO_6N_2 geometry. The tetraanion is disordered over a mirror plane. The oxonium cation and water molecule are disordered, in a 2:1 ratio, and these occupy the space between adjacent layers. They probably interact with the layers by way of O—H···O hydrogen bonds, but the H atoms could not be located.

Related literature

For the isostructural erbium(III) and holmium(III) analogs, see: You *et al.* (2007*a*,*b*).



Experimental

Crystal data

$(H_3O)[Dy(C_{10}H_{12}N_2O_8)]\cdot H_2O$
M_r = 487.76
Orthorhombic, *Pbcm*
a = 6.6271 (3) Å
b = 12.9233 (6) Å
c = 18.5496 (9) Å
V = 1588.6 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.76 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.425, T_{max} = 0.648
13726 measured reflections
1873 independent reflections
1784 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.050
S = 1.05
1873 reflections
178 parameters
127 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected bond lengths (Å).

Dy1—O1	2.331 (2)	Dy1—O3′	2.313 (3)
Dy1—O1^{i}	2.331 (2)	Dy1—O4′^{iii}	2.318 (3)
Dy1—O3	2.324 (3)	Dy1—N1	2.592 (4)
Dy1—O4^{ii}	2.339 (3)	Dy1—N1′	2.617 (4)

Symmetry codes: (i) $x, y, -z+\frac{1}{2}$; (ii) $x-1, y, z$; (iii) $-x, y-\frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

We thank Jiangxi Science and Technology Normal University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2422).

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supplementary materials

Acta Cryst. (2007). E**63**, m1819 [**doi:10.1107/S1600536807025044**]

Poly[hydronium [dysprosium(III)-μ_3-(ethylenediaminetetraacetato-$\kappa^8N,N',O,O',O'',O''':O''''':O''''')$] monohydrate]

X.-L. You and S. W. Ng

Comment

The erbium(III) and holonium(III) derivatives of edta have recently been reported (You *et al.*, 2007*a*, b). The dysprosium analog described here is isostructural.

Experimental

Dysprosium(III) oxide (0.162 g, 0.5 mmol), ethylenediaminetetraacetic acid (edta) (0.286 g, 0.8 mmol), perchloric acid (0.385 mmol) and oxalic acid (0.042 g, 0.175 mmol) were dissolved in a mixture of methanol (5 ml) and water (5 ml). This solution was sealed in a Teflon-lined, stainless-steel autoclave (20 ml capacity) and heated to 433 K for 4 days. It was cooled to room temperature at 5 K h^{-1} to obtain colorless blocks of (I).

Refinement

The edta tetraanion is disordered about a mirror plane; only the O1, O2 and C1 atoms of the molecule have full occupany, the other atoms being given 0.5 occupancy. For the disordered atoms, the C–O distances were restrained to 1.25±0.01 Å, the C–N distances to 1.45±0.01 Å and the C–C distances to 1.50±0.01 Å. The vibration of the ordered and disordered C, N and O atoms were restrained to be nearly isotropic.

Along with the [($C_{10}H_{12}N_2O_8$)Dy] monoanion, the formula unit should have one hydronium ion and one water molecule; their respective O atoms are disordered and the sum of their occupancies should be unity. As the occupancy refined to 0.67 (1):0.33 (1), the occupancies were then fixed at this ratio. The 'o' and 'w' labels are arbitrary and do not mean that the O3o is the hydronium and the O1w the water O atoms. Their H atoms could not be placed with any confidence.

The carbon-bound H atoms were placed at calculated positions (C–H 0.97 Å), and they were included in the refinement in the riding model approximation with U(H) set to 1.2U_{eq}(C).

Figures

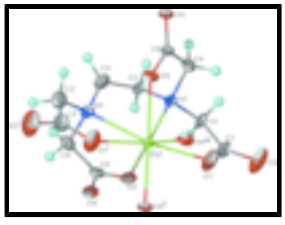


Fig. 1. View of a portion of the polyanionic structure of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radius. Symmetry codes are as given in Table 1. The disordered hydronium and water species are not shown.

Poly[hydronium [dysprosium(III)-μ$_3$-(ethylenediaminetetraacetato-\ κ^8*N*,*N*',*O*,*O*',*O*'',*O*''':*O*'''':*O*''''')] monohydrate]

Crystal data

$(H_3O)[Dy(C_{10}H_{12}N_2O_8)]\cdot H_2O$	F_{000} = 948
M_r = 487.76	D_x = 2.039 Mg m^{-3}
Orthorhombic, *Pbcm*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2c 2b	Cell parameters from 8499 reflections
a = 6.6271 (3) Å	θ = 3.1–27.5º
b = 12.9233 (6) Å	μ = 4.76 mm^{-1}
c = 18.5496 (9) Å	*T* = 295 (2) K
V = 1588.6 (1) Å^3	Block, colorless
Z = 4	0.30 × 0.20 × 0.10 mm

Data collection

Bruker APEX II CCD diffractometer	1873 independent reflections
Radiation source: medium-focus sealed tube	1784 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −8→7
T_{min} = 0.425, T_{max} = 0.648	*k* = −16→16
13726 measured reflections	*l* = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.017	H-atom parameters constrained
$wR(F^2)$ = 0.050	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.7002P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
1873 reflections	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
178 parameters	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
127 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Dy1	0.10881 (2)	0.052175 (11)	0.2500	0.01807 (8)	
O1	0.0672 (5)	0.0318 (2)	0.12603 (13)	0.0541 (7)	
O2	0.1160 (4)	0.0739 (3)	0.01246 (15)	0.0666 (9)	
O3O	−0.2534 (15)	0.2034 (7)	−0.0555 (4)	0.188 (4)	0.67
O1W	0.477 (2)	0.0661 (9)	−0.0728 (7)	0.104 (4)	0.33
C1	0.1473 (5)	0.0859 (3)	0.07918 (16)	0.0388 (6)	
O3	0.4405 (5)	0.0077 (3)	0.27636 (19)	0.0268 (7)	0.50
O4	0.7680 (4)	0.0071 (2)	0.2593 (8)	0.025 (2)	0.50
N1	0.3675 (6)	0.1575 (3)	0.1752 (2)	0.0227 (8)	0.50
C2	0.301 (4)	0.1750 (15)	0.1018 (5)	0.027 (3)	0.50
H2A	0.4157	0.1749	0.0695	0.033*	0.50
H2B	0.2346	0.2418	0.0983	0.033*	0.50
C3	0.426 (2)	0.2566 (10)	0.2083 (7)	0.015 (3)	0.50
H3A	0.3314	0.3100	0.1940	0.018*	0.50
H3B	0.5590	0.2764	0.1913	0.018*	0.50
C4	0.5509 (7)	0.0924 (4)	0.1699 (3)	0.0284 (10)	0.50
H4A	0.6661	0.1361	0.1593	0.034*	0.50
H4B	0.5351	0.0440	0.1304	0.034*	0.50
C5	0.5907 (6)	0.0330 (3)	0.2389 (5)	0.022 (2)	0.50
O3'	−0.0529 (6)	0.2069 (2)	0.22572 (19)	0.0298 (9)	0.50
O4'	−0.1173 (4)	0.3735 (2)	0.2400 (8)	0.027 (2)	0.50
N1'	0.2516 (6)	0.2061 (3)	0.3261 (2)	0.0230 (8)	0.50
C2'	0.274 (4)	0.1684 (15)	0.3997 (5)	0.033 (5)	0.50
H2'1	0.4130	0.1465	0.4061	0.040*	0.50
H2'2	0.2509	0.2259	0.4322	0.040*	0.50
C3'	0.429 (2)	0.2477 (13)	0.2885 (9)	0.039 (6)	0.50
H3'1	0.5432	0.2049	0.3015	0.047*	0.50
H3'2	0.4544	0.3162	0.3078	0.047*	0.50
C4'	0.0925 (7)	0.2865 (4)	0.3286 (3)	0.0279 (11)	0.50
H4'1	0.1551	0.3535	0.3359	0.033*	0.50
H4'2	0.0049	0.2731	0.3694	0.033*	0.50
C5'	−0.0331 (6)	0.2898 (3)	0.2608 (5)	0.0240 (19)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy1	0.01006 (11)	0.01040 (10)	0.03376 (12)	−0.00049 (4)	0.000	0.000
O1	0.0714 (17)	0.0513 (14)	0.0395 (12)	−0.0385 (13)	−0.0086 (11)	−0.0020 (10)
O2	0.089 (2)	0.0727 (18)	0.0382 (13)	−0.0347 (14)	−0.0185 (12)	−0.0018 (13)
O3O	0.176 (7)	0.184 (7)	0.205 (6)	0.055 (6)	−0.056 (6)	0.042 (6)
O1W	0.118 (8)	0.109 (7)	0.085 (6)	0.051 (6)	0.027 (6)	0.014 (5)
C1	0.0443 (17)	0.0365 (15)	0.0358 (14)	−0.0062 (13)	−0.0085 (12)	−0.0046 (12)
O3	0.0142 (16)	0.0209 (16)	0.0454 (19)	−0.0004 (13)	0.0003 (13)	0.0086 (13)
O4	0.0123 (12)	0.0225 (12)	0.039 (7)	0.0004 (10)	−0.0009 (18)	−0.0005 (19)

N1	0.021 (2)	0.019 (2)	0.0284 (19)	−0.0039 (16)	−0.0030 (14)	0.0010 (16)
C2	0.023 (5)	0.024 (4)	0.035 (5)	−0.016 (4)	−0.008 (3)	−0.006 (3)
C3	0.021 (5)	0.009 (4)	0.016 (4)	−0.008 (3)	−0.004 (3)	0.004 (3)
C4	0.020 (2)	0.029 (2)	0.037 (3)	0.000 (2)	0.006 (2)	−0.001 (2)
C5	0.0141 (19)	0.0139 (15)	0.039 (6)	−0.0026 (12)	0.000 (2)	−0.003 (2)
O3'	0.0194 (14)	0.0153 (15)	0.055 (2)	0.0032 (12)	−0.0113 (14)	−0.0050 (12)
O4'	0.0225 (14)	0.0111 (12)	0.048 (7)	0.0018 (9)	−0.0040 (18)	−0.0006 (19)
N1'	0.021 (2)	0.0184 (18)	0.0290 (19)	−0.0022 (17)	0.0016 (16)	0.0023 (15)
C2'	0.034 (8)	0.039 (7)	0.027 (5)	−0.010 (5)	0.004 (3)	−0.007 (4)
C3'	0.032 (7)	0.033 (7)	0.051 (8)	−0.012 (5)	−0.006 (5)	−0.002 (5)
C4'	0.028 (3)	0.018 (2)	0.037 (3)	0.0006 (17)	0.0060 (19)	−0.005 (2)
C5'	0.0150 (16)	0.0134 (16)	0.044 (6)	−0.0012 (13)	0.004 (2)	−0.002 (2)

Geometric parameters (Å, °)

Dy1—O1	2.331 (2)	C3—H3A	0.9700
Dy1—O1^{i}	2.331 (2)	C3—H3B	0.9700
Dy1—O3	2.324 (3)	C4—C5	1.516 (7)
Dy1—O4^{ii}	2.339 (3)	C4—H4A	0.9700
Dy1—O3'	2.313 (3)	C4—H4B	0.9700
Dy1—O4'^{iii}	2.318 (3)	O3'—C5'	1.260 (6)
Dy1—N1	2.592 (4)	O4'—C5'	1.276 (6)
Dy1—N1'	2.617 (4)	O4'—Dy1^{iv}	2.318 (3)
O1—C1	1.235 (4)	N1'—C2'	1.457 (9)
O2—C1	1.265 (4)	N1'—C3'	1.466 (9)
C1—C2'^{i}	1.41 (2)	N1'—C4'	1.481 (5)
C1—C2	1.59 (2)	C2'—C1^{i}	1.41 (2)
O3—C5	1.257 (6)	C2'—H2'1	0.9700
O4—C5	1.279 (6)	C2'—H2'2	0.9700
N1—C2	1.451 (9)	C3'—H3'1	0.9700
N1—C3	1.471 (8)	C3'—H3'2	0.9700
N1—C4	1.481 (5)	C4'—C5'	1.509 (8)
C2—H2A	0.9700	C4'—H4'1	0.9700
C2—H2B	0.9700	C4'—H4'2	0.9700
C3—C3'	1.493 (7)		
O3'^{i}—Dy1—O3'	22.46 (17)	C1—O1—Dy1	125.4 (2)
O3'^{i}—Dy1—O4'^{v}	149.0 (2)	O1—C1—O2	123.2 (3)
O3'—Dy1—O4'^{v}	152.68 (14)	O1—C1—C2'^{i}	119.2 (5)
O3'^{i}—Dy1—O4'^{iii}	152.68 (14)	O2—C1—C2'^{i}	117.5 (6)
O3'—Dy1—O4'^{iii}	149.0 (2)	O1—C1—C2	119.9 (5)
O4'^{v}—Dy1—O4'^{iii}	9.2 (7)	O2—C1—C2	116.8 (5)
O3'^{i}—Dy1—O3	127.66 (13)	C2'^{i}—C1—C2	3.2 (14)
O3'—Dy1—O3	133.86 (12)	C5—O3—Dy1	124.6 (3)
O4'^{v}—Dy1—O3	73.36 (12)	C5—O4—Dy1^{vii}	143.1 (6)
O4'^{iii}—Dy1—O3	75.36 (14)	C2—N1—C3	109.7 (10)
O3'^{i}—Dy1—O3^{i}	133.86 (12)	C2—N1—C4	106.0 (8)

O3'—Dy1—O3^{i}	127.66 (13)	C3—N1—C4	107.8 (6)
O4'^{v}—Dy1—O3^{i}	75.36 (14)	C2—N1—Dy1	112.4 (10)
O4'^{iii}—Dy1—O3^{i}	73.36 (12)	C3—N1—Dy1	114.1 (7)
O3—Dy1—O3^{i}	24.29 (17)	C4—N1—Dy1	106.3 (3)
O3'^{i}—Dy1—O1^{i}	81.42 (11)	N1—C2—C1	109.3 (13)
O3'—Dy1—O1^{i}	103.60 (12)	N1—C2—H2A	109.8
O4'^{v}—Dy1—O1^{i}	79.1 (3)	C1—C2—H2A	109.8
O4'^{iii}—Dy1—O1^{i}	88.2 (3)	N1—C2—H2B	109.8
O3—Dy1—O1^{i}	82.89 (11)	C1—C2—H2B	109.8
O3^{i}—Dy1—O1^{i}	106.94 (12)	H2A—C2—H2B	108.3
O3'^{i}—Dy1—O1	103.60 (12)	N1—C3—C3'	110.6 (15)
O3'—Dy1—O1	81.42 (11)	N1—C3—H3A	109.5
O4'^{v}—Dy1—O1	88.2 (4)	C3'—C3—H3A	109.5
O4'^{iii}—Dy1—O1	79.1 (3)	N1—C3—H3B	109.5
O3—Dy1—O1	106.94 (12)	C3'—C3—H3B	109.5
O3^{i}—Dy1—O1	82.89 (11)	H3A—C3—H3B	108.1
O1^{i}—Dy1—O1	161.18 (12)	N1—C4—C5	112.0 (4)
O3'^{i}—Dy1—O4^{vi}	77.44 (14)	N1—C4—H4A	109.2
O3'—Dy1—O4^{vi}	75.74 (14)	C5—C4—H4A	109.2
O4'^{v}—Dy1—O4^{vi}	77.36 (11)	N1—C4—H4B	109.2
O4'^{iii}—Dy1—O4^{vi}	76.67 (10)	C5—C4—H4B	109.2
O3—Dy1—O4^{vi}	150.15 (16)	H4A—C4—H4B	107.9
O3^{i}—Dy1—O4^{vi}	146.7 (2)	O3—C5—O4	119.6 (7)
O1^{i}—Dy1—O4^{vi}	86.0 (4)	O3—C5—C4	117.5 (4)
O1—Dy1—O4^{vi}	77.6 (4)	O4—C5—C4	122.9 (7)
O3'^{i}—Dy1—O4^{ii}	75.74 (14)	C5'—O3'—Dy1	125.9 (3)
O3'—Dy1—O4^{ii}	77.44 (14)	C5'—O4'—Dy1^{iv}	144.0 (6)
O4'^{v}—Dy1—O4^{ii}	76.67 (10)	C2'—N1'—C3'	119.1 (13)
O4'^{iii}—Dy1—O4^{ii}	77.36 (11)	C2'—N1'—C4'	106.2 (8)
O3—Dy1—O4^{ii}	146.7 (2)	C3'—N1'—C4'	109.1 (8)
O3^{i}—Dy1—O4^{ii}	150.15 (16)	C2'—N1'—Dy1	106.7 (9)
O1^{i}—Dy1—O4^{ii}	77.6 (4)	C3'—N1'—Dy1	108.1 (8)
O1—Dy1—O4^{ii}	86.0 (4)	C4'—N1'—Dy1	107.0 (3)
O4^{vi}—Dy1—O4^{ii}	8.5 (7)	C1^{i}—C2'—N1'	116.9 (15)
O3'^{i}—Dy1—N1^{i}	75.41 (13)	C1^{i}—C2'—H2'1	108.1
O3'—Dy1—N1^{i}	87.50 (12)	N1'—C2'—H2'1	108.1
O4'^{v}—Dy1—N1^{i}	117.7 (2)	C1^{i}—C2'—H2'2	108.1
O4'^{iii}—Dy1—N1^{i}	123.4 (2)	N1'—C2'—H2'2	108.1
O3—Dy1—N1^{i}	52.53 (12)	H2'1—C2'—H2'2	107.3
O3^{i}—Dy1—N1^{i}	67.47 (12)	N1'—C3'—C3	119.6 (17)
O1^{i}—Dy1—N1^{i}	67.02 (10)	N1'—C3'—H3'1	107.4

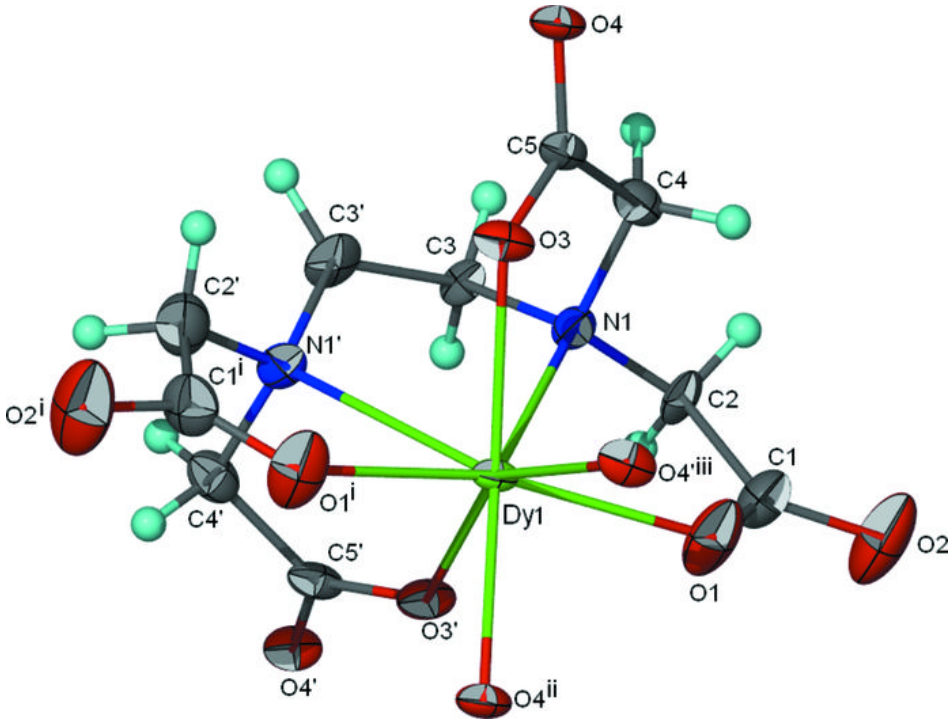
O1—Dy1—N1^{i}	131.72 (11)	C3—C3'—H3'1	107.4
O4^{vi}—Dy1—N1^{i}	144.0 (3)	N1'—C3'—H3'2	107.4
O4^{ii}—Dy1—N1^{i}	136.9 (3)	C3—C3'—H3'2	107.4
O3'^{i}—Dy1—N1	87.50 (12)	H3'1—C3'—H3'2	107.0
O3'—Dy1—N1	75.41 (13)	N1'—C4'—C5'	112.8 (4)
O4'^{v}—Dy1—N1	123.4 (2)	N1'—C4'—H4'1	109.0
O4'^{iii}—Dy1—N1	117.7 (2)	C5'—C4'—H4'1	109.0
O3—Dy1—N1	67.47 (12)	N1'—C4'—H4'2	109.0
O3^{i}—Dy1—N1	52.53 (13)	C5'—C4'—H4'2	109.0
O1^{i}—Dy1—N1	131.72 (11)	H4'1—C4'—H4'2	107.8
O1—Dy1—N1	67.02 (10)	O3'—C5'—O4'	121.2 (8)
O4^{vi}—Dy1—N1	136.9 (3)	O3'—C5'—C4'	117.6 (4)
O4^{ii}—Dy1—N1	144.0 (3)	O4'—C5'—C4'	121.2 (7)
N1^{i}—Dy1—N1	64.71 (17)		
O3'^{i}—Dy1—O1—C1	68.6 (3)	Dy1—O3—C5—O4	177.9 (5)
O3'—Dy1—O1—C1	65.0 (3)	Dy1—O3—C5—C4	−2.9 (7)
O4'^{v}—Dy1—O1—C1	−140.4 (3)	Dy1^{vii}—O4—C5—O3	−155.4 (11)
O4'^{iii}—Dy1—O1—C1	−139.3 (3)	Dy1^{vii}—O4—C5—C4	25.5 (17)
O3—Dy1—O1—C1	−68.4 (3)	N1—C4—C5—O3	30.2 (7)
O3^{i}—Dy1—O1—C1	−64.9 (3)	N1—C4—C5—O4	−150.7 (6)
O1^{i}—Dy1—O1—C1	172.1 (3)	O3'^{i}—Dy1—O3'—C5'	37.5 (5)
O4^{vi}—Dy1—O1—C1	142.1 (3)	O4'^{v}—Dy1—O3'—C5'	139.4 (8)
O4^{ii}—Dy1—O1—C1	142.8 (3)	O4'^{iii}—Dy1—O3'—C5'	156.8 (7)
N1^{i}—Dy1—O1—C1	−13.9 (4)	O3—Dy1—O3'—C5'	−46.4 (5)
N1—Dy1—O1—C1	−12.7 (3)	O3^{i}—Dy1—O3'—C5'	−77.6 (5)
Dy1—O1—C1—O2	−177.9 (3)	O1^{i}—Dy1—O3'—C5'	46.8 (5)
Dy1—O1—C1—C2'^{i}	−0.6 (10)	O1—Dy1—O3'—C5'	−151.7 (5)
Dy1—O1—C1—C2	2.9 (9)	O4^{vi}—Dy1—O3'—C5'	129.1 (6)
O3'^{i}—Dy1—O3—C5	−81.4 (5)	O4^{ii}—Dy1—O3'—C5'	120.5 (6)
O3'—Dy1—O3—C5	−52.7 (5)	N1^{i}—Dy1—O3'—C5'	−18.8 (5)
O4'^{v}—Dy1—O3—C5	124.5 (6)	N1—Dy1—O3'—C5'	−83.3 (5)
O4'^{iii}—Dy1—O3—C5	115.2 (6)	O3'^{i}—Dy1—N1'—C2'	115.0 (9)
O3^{i}—Dy1—O3—C5	33.3 (4)	O3'—Dy1—N1'—C2'	135.5 (9)
O1^{i}—Dy1—O3—C5	−154.8 (5)	O4'^{v}—Dy1—N1'—C2'	−25.2 (10)
O1—Dy1—O3—C5	41.6 (5)	O4'^{iii}—Dy1—N1'—C2'	−33.2 (10)
O4^{vi}—Dy1—O3—C5	136.2 (8)	O3—Dy1—N1'—C2'	−71.1 (9)
O4^{ii}—Dy1—O3—C5	151.1 (7)	O3^{i}—Dy1—N1'—C2'	−91.7 (9)
N1^{i}—Dy1—O3—C5	−88.4 (5)	O1^{i}—Dy1—N1'—C2'	17.9 (9)
N1—Dy1—O3—C5	−13.7 (4)	O1—Dy1—N1'—C2'	−170.2 (9)
O3'^{i}—Dy1—N1—C2	−85.2 (7)	O4^{vi}—Dy1—N1'—C2'	84.0 (10)
O3'—Dy1—N1—C2	−66.1 (7)	O4^{ii}—Dy1—N1'—C2'	76.2 (10)

O4'^{v}—Dy1—N1—C2	92.0 (8)	N1^{i}—Dy1—N1'—C2'	−69.4 (10)
O4'^{iii}—Dy1—N1—C2	83.7 (8)	N1—Dy1—N1'—C2'	−142.3 (9)
O3—Dy1—N1—C2	141.9 (8)	O3'^{i}—Dy1—N1'—C3'	−115.7 (8)
O3^{i}—Dy1—N1—C2	119.6 (8)	O3'—Dy1—N1'—C3'	−95.3 (8)
O1^{i}—Dy1—N1—C2	−161.4 (7)	O4'^{v}—Dy1—N1'—C3'	104.1 (9)
O1—Dy1—N1—C2	20.7 (7)	O4'^{iii}—Dy1—N1'—C3'	96.0 (9)
O4^{vi}—Dy1—N1—C2	−16.7 (8)	O3—Dy1—N1'—C3'	58.2 (8)
O4^{ii}—Dy1—N1—C2	−23.9 (9)	O3^{i}—Dy1—N1'—C3'	37.5 (8)
N1^{i}—Dy1—N1—C2	−160.3 (7)	O1^{i}—Dy1—N1'—C3'	147.2 (8)
O3'^{i}—Dy1—N1—C3	40.5 (6)	O1—Dy1—N1'—C3'	−40.9 (8)
O3'—Dy1—N1—C3	59.7 (6)	O4^{vi}—Dy1—N1'—C3'	−146.8 (9)
O4'^{v}—Dy1—N1—C3	−142.2 (7)	O4^{ii}—Dy1—N1'—C3'	−154.5 (9)
O4'^{iii}—Dy1—N1—C3	−150.6 (6)	N1^{i}—Dy1—N1'—C3'	59.9 (9)
O3—Dy1—N1—C3	−92.3 (6)	N1—Dy1—N1'—C3'	−13.1 (8)
O3^{i}—Dy1—N1—C3	−114.6 (6)	O3'^{i}—Dy1—N1'—C4'	1.7 (3)
O1^{i}—Dy1—N1—C3	−35.7 (6)	O3'—Dy1—N1'—C4'	22.1 (3)
O1—Dy1—N1—C3	146.4 (6)	O4'^{v}—Dy1—N1'—C4'	−138.5 (4)
O4^{vi}—Dy1—N1—C3	109.1 (7)	O4'^{iii}—Dy1—N1'—C4'	−146.6 (4)
O4^{ii}—Dy1—N1—C3	101.8 (7)	O3—Dy1—N1'—C4'	175.6 (3)
N1^{i}—Dy1—N1—C3	−34.5 (6)	O3^{i}—Dy1—N1'—C4'	154.9 (3)
O3'^{i}—Dy1—N1—C4	159.2 (3)	O1^{i}—Dy1—N1'—C4'	−95.4 (3)
O3'—Dy1—N1—C4	178.3 (3)	O1—Dy1—N1'—C4'	76.5 (3)
O4'^{v}—Dy1—N1—C4	−23.6 (5)	O4^{vi}—Dy1—N1'—C4'	−29.3 (5)
O4'^{iii}—Dy1—N1—C4	−31.9 (4)	O4^{ii}—Dy1—N1'—C4'	−37.1 (4)
O3—Dy1—N1—C4	26.3 (3)	N1^{i}—Dy1—N1'—C4'	177.3 (5)
O3^{i}—Dy1—N1—C4	4.0 (3)	N1—Dy1—N1'—C4'	104.3 (3)
O1^{i}—Dy1—N1—C4	83.0 (3)	C3'—N1'—C2'—C1^{i}	−148.5 (13)
O1—Dy1—N1—C4	−94.9 (3)	C4'—N1'—C2'—C1^{i}	88.0 (12)
O4^{vi}—Dy1—N1—C4	−132.3 (4)	Dy1—N1'—C2'—C1^{i}	−25.8 (15)
O4^{ii}—Dy1—N1—C4	−139.5 (5)	C2'—N1'—C3'—C3	161.5 (16)
N1^{i}—Dy1—N1—C4	84.1 (3)	C4'—N1'—C3'—C3	−76.4 (19)
C3—N1—C2—C1	−153.6 (9)	Dy1—N1'—C3'—C3	40 (2)
C4—N1—C2—C1	90.2 (11)	N1—C3—C3'—N1'	−52 (2)
Dy1—N1—C2—C1	−25.5 (12)	C2'—N1'—C4'—C5'	−146.6 (11)
O1—C1—C2—N1	17.1 (14)	C3'—N1'—C4'—C5'	83.9 (9)
O2—C1—C2—N1	−162.1 (8)	Dy1—N1'—C4'—C5'	−32.9 (5)
C2^{i}—C1—C2—N1	94 (17)	Dy1—O3'—C5'—O4'	174.7 (5)
C2—N1—C3—C3'	161.0 (16)	Dy1—O3'—C5'—C4'	−5.8 (8)
C4—N1—C3—C3'	−84.0 (15)	Dy1^{iv}—O4'—C5'—O3'	−159.8 (10)
Dy1—N1—C3—C3'	33.8 (16)	Dy1^{iv}—O4'—C5'—C4'	20.7 (16)
C2—N1—C4—C5	−157.2 (11)	N1'—C4'—C5'—O3'	28.6 (7)
C3—N1—C4—C5	85.4 (8)	N1'—C4'—C5'—O4'	−151.9 (6)

Dy1—N1—C4—C5	−37.3 (5)

Symmetry codes: (i) *x*, *y*, −*z*+1/2; (ii) *x*−1, *y*, *z*; (iii) −*x*, *y*−1/2, *z*; (iv) −*x*, *y*+1/2, *z*; (v) −*x*, *y*−1/2, −*z*+1/2; (vi) *x*−1, *y*, −*z*+1/2; (vii) *x*+1, *y*, *z*.

Fig. 1


O4
C5
C4
C3'
C3
O3
C2'
N1
N1'
C1i
C2
O2i
O4'iii
C1
O1i
Dy1
C4'
C5'
O2
O1
O3'
O4'
O4ii