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

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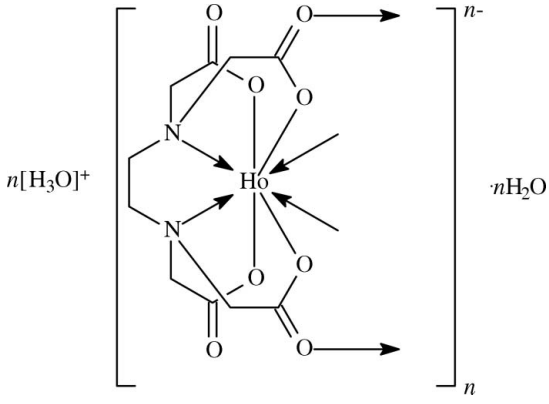
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(O–C) = 0.004 Å; H-atom completeness 71%; disorder in main residue; R factor = 0.017; wR factor = 0.045; data-to-parameter ratio = 10.4.

The holmium(III) atom in the title compound, $\{(H_3O)[Ho(C_{10}H_{12}N_2O_8)]\cdot nH_2O\}_n$, is N,N',O,O',O'',O'''-chelated by the ethylenediaminetetraacetate tetraanion. It is also linked to the O atoms of two other tetraaanions in the polyanionic layer. The metal atom, which lies on a special position of site symmetry m, exists in a square-antiprismatic geometry. The tetraanion is disordered across a mirror plane. The oxonium cation and water molecule are disordered in a ratio of 2:1. The title compound is isostructural with the erbium compound reported in the preceding paper.

Related literature

For the structure of the erbium complex, see: You *et al.* (2007).



Experimental

Crystal data

$(H_3O)[Ho(C_{10}H_{12}N_2O_8)]\cdot H_2O$
M_r = 490.19
Orthorhombic, *Pbcm*
a = 6.5924 (1) Å
b = 12.8450 (1) Å
c = 18.4246 (2) Å
V = 1560.18 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.13 mm^{-1}
T = 295 (2) K
0.31 × 0.28 × 0.17 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.253, T_{max} = 0.475
(expected range = 0.223–0.418)
11214 measured reflections
1852 independent reflections
1763 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.045
S = 0.99
1852 reflections
178 parameters
127 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ho1—O1	2.315 (2)	Ho1—O4$'^{ii}$	2.304 (3)
Ho1—O3	2.307 (3)	Ho1—N1	2.582 (4)
Ho1—O4^{i}	2.322 (3)	Ho1—N1$'$	2.601 (4)
Ho1—O3$'$	2.306 (3)		

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

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).

The authors 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: WN2140).

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  doi:10.1107/S1600536807024373

supplementary materials

Acta Cryst. (2007). E**63**, m1714 [**doi:10.1107/S1600536807024373**]

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

X.-L. You, L.-H. Wang and S. W. Ng

Comment

The preceding paper (You *et al.*, 2007) describes the structure of n[H_3O][($C_{10}H_{12}N_2O_8$)Er]$_n$.nH_2O. The present holmium analogue is isostructural (Table, Fig. 1). The coordination geometry is square-antiprismatic.

Experimental

Holmium(III) oxide (0.150 g, 0.5 mmol), edta (0.286 g, 0.8 mol) and perchloric acid (0.385 mmol) were dissolved in methanol (5 ml) and water (5 ml). The 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 block-shaped crystals. The CH&N elemental analysis corresponded to the expected formulation.

Refinement

The edta tetraanion is disordered across a mirror plane; only atoms O1, O2 and C1 have full site occupany, the other atoms having 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 displacement parameters of the ordered and disordered C, N and O atoms were restrained to be nearly isotropic.

Together with the [($C_{10}H_{12}N_2O_8$)Ho] monoanion, the formula unit has one hydronium ion and one water molecule. Because *Z* is 4, as well as the fact that O3o and O1w both lie on general positions, these two O atoms are disordered; the sum of their site occupancies should be unity. The occupancies refined to 0.67 (1) and 0.33 (1), and were then fixed at these values. The 'o' and 'w' labels are arbitrary and do not imply that O3o is the hydronium and O1w the water O atoms. Their H atoms could not be placed in any chemically sensible positions.

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_{iso}(H) set equal to 1.2U_{eq}(C).

Figures

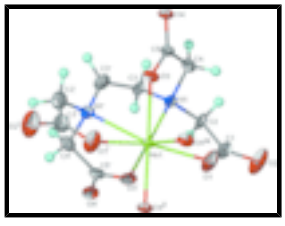


Fig. 1. A view of a portion of the polyanionic structure (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radius. Symmetry codes are as given in the Table. The disordered hydronium ion and water molecule are not shown.

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

Crystal data

$(H_3O)[Ho(C_{10}H_{12}N_2O_8)]\cdot H_2O$	$F_{000} = 952$
$M_r = 490.19$	$D_x = 2.087$ Mg m^{-3}
Orthorhombic, *Pbcm*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2c 2b	Cell parameters from 7966 reflections
$a = 6.5924$ (1) Å	θ = 3.1–27.5º
$b = 12.8450$ (1) Å	μ = 5.13 mm^{-1}
$c = 18.4246$ (2) Å	$T = 295$ (2) K
$V = 1560.18$ (3) Å^3	Block, colourless
$Z = 4$	0.31 × 0.28 × 0.17 mm

Data collection

Bruker APEXII diffractometer	1852 independent reflections
Radiation source: medium-focus sealed tube	1763 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 295$(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 3.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7\rightarrow8$
$T_{min} = 0.253$, $T_{max} = 0.475$	$k = -16\rightarrow16$
11214 measured reflections	$l = -19\rightarrow23$

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
$wR(F^2) = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2 + 0.6337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} = 0.001$
1852 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
178 parameters	$\Delta\rho_{min} = -0.76$ 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)

Ho1	0.11085 (2)	0.053681 (10)	0.2500	0.01692 (7)	
O1	0.0688 (4)	0.03224 (19)	0.12617 (13)	0.0504 (7)	
O2	0.1161 (4)	0.0744 (2)	0.01229 (16)	0.0700 (10)	
O3O	−0.2554 (17)	0.2003 (8)	−0.0534 (5)	0.218 (4)	0.67
O1W	0.471 (3)	0.0632 (9)	−0.0720 (8)	0.129 (5)	0.33
C1	0.1483 (5)	0.0865 (3)	0.07919 (18)	0.0376 (7)	
O3	0.4421 (5)	0.0094 (3)	0.27598 (19)	0.0259 (8)	0.50
O4	0.7705 (4)	0.0082 (2)	0.2575 (15)	0.028 (3)	0.50
N1	0.3678 (6)	0.1596 (3)	0.1743 (2)	0.0214 (8)	0.50
C2	0.290 (3)	0.1783 (16)	0.1009 (5)	0.025 (4)	0.50
H2A	0.4021	0.1832	0.0669	0.029*	0.50
H2B	0.2155	0.2433	0.0996	0.029*	0.50
C3	0.426 (3)	0.2592 (11)	0.2076 (11)	0.021 (4)	0.50
H3A	0.3300	0.3126	0.1935	0.026*	0.50
H3B	0.5591	0.2796	0.1899	0.026*	0.50
C4	0.5516 (7)	0.0943 (4)	0.1686 (3)	0.0270 (11)	0.50
H4A	0.6673	0.1383	0.1577	0.032*	0.50
H4B	0.5353	0.0454	0.1290	0.032*	0.50
C5	0.5927 (6)	0.0350 (3)	0.2378 (4)	0.020 (2)	0.50
O3'	−0.0522 (5)	0.2087 (2)	0.22602 (19)	0.0278 (10)	0.50
O4'	−0.1192 (4)	0.3749 (2)	0.2407 (11)	0.029 (3)	0.50
N1'	0.2545 (6)	0.2074 (3)	0.3262 (2)	0.0212 (8)	0.50
C2'	0.289 (3)	0.1668 (16)	0.3990 (6)	0.041 (6)	0.50
H2'1	0.4258	0.1389	0.4015	0.049*	0.50
H2'2	0.2805	0.2238	0.4333	0.049*	0.50
C3'	0.432 (3)	0.2508 (14)	0.2886 (12)	0.029 (5)	0.50
H3'1	0.5485	0.2088	0.3016	0.035*	0.50
H3'2	0.4554	0.3201	0.3079	0.035*	0.50
C4'	0.0938 (7)	0.2875 (4)	0.3294 (3)	0.0265 (11)	0.50
H4'1	0.1557	0.3551	0.3373	0.032*	0.50
H4'2	0.0058	0.2731	0.3704	0.032*	0.50
C5'	−0.0318 (7)	0.2914 (3)	0.2613 (5)	0.025 (2)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ho1	0.01070 (10)	0.01106 (9)	0.02899 (11)	−0.00052 (4)	0.000	0.000
O1	0.0675 (17)	0.0506 (13)	0.0330 (13)	−0.0357 (12)	−0.0075 (11)	−0.0024 (10)
O2	0.097 (3)	0.0776 (19)	0.0349 (15)	−0.0431 (15)	−0.0163 (13)	−0.0033 (13)
O3O	0.210 (7)	0.216 (8)	0.228 (8)	0.065 (6)	−0.055 (7)	0.039 (6)
O1W	0.143 (8)	0.129 (8)	0.116 (8)	0.056 (7)	0.023 (8)	0.015 (6)
C1	0.0439 (18)	0.0377 (15)	0.0312 (16)	−0.0093 (13)	−0.0062 (13)	−0.0050 (13)
O3	0.0157 (16)	0.0208 (16)	0.041 (2)	−0.0004 (13)	0.0013 (13)	0.0078 (13)
O4	0.0130 (13)	0.0225 (12)	0.048 (9)	−0.0005 (10)	−0.003 (3)	0.001 (3)
N1	0.021 (2)	0.0180 (19)	0.025 (2)	−0.0017 (16)	−0.0046 (16)	0.0000 (17)
C2	0.030 (6)	0.019 (4)	0.025 (7)	−0.013 (3)	−0.008 (4)	0.003 (3)
C3	0.029 (7)	0.017 (5)	0.019 (5)	−0.004 (4)	0.000 (4)	0.000 (4)
C4	0.018 (2)	0.029 (2)	0.034 (3)	0.001 (2)	0.007 (2)	−0.003 (2)

C5	0.0125 (19)	0.0121 (15)	0.036 (7)	−0.0026 (12)	−0.002 (2)	−0.004 (2)
O3'	0.0193 (14)	0.0155 (15)	0.049 (3)	0.0024 (12)	−0.0107 (14)	−0.0044 (12)
O4'	0.0245 (15)	0.0097 (12)	0.052 (9)	0.0049 (9)	−0.002 (2)	0.005 (2)
N1'	0.023 (2)	0.0176 (18)	0.023 (2)	−0.0026 (17)	0.0023 (17)	0.0007 (15)
C2'	0.050 (9)	0.042 (9)	0.030 (8)	−0.010 (6)	−0.003 (6)	0.002 (5)
C3'	0.025 (7)	0.025 (6)	0.036 (7)	−0.016 (5)	0.000 (5)	−0.008 (4)
C4'	0.028 (3)	0.017 (2)	0.035 (3)	−0.0004 (17)	0.006 (2)	−0.005 (2)
C5'	0.0141 (17)	0.0139 (16)	0.048 (6)	0.0012 (13)	0.006 (3)	−0.001 (2)

Geometric parameters (Å, °)

Ho1—O1	2.315 (2)	C3—C3'	1.498 (6)
Ho1—O1^{i}	2.315 (2)	C3—H3A	0.9700
Ho1—O3	2.307 (3)	C3—H3B	0.9700
Ho1—O4^{ii}	2.322 (3)	C4—C5	1.509 (7)
Ho1—O3'	2.306 (3)	C4—H4A	0.9700
Ho1—O4'^{iii}	2.304 (3)	C4—H4B	0.9700
Ho1—N1	2.582 (4)	O3'—C5'	1.253 (6)
Ho1—N1'	2.601 (4)	O4'—C5'	1.275 (7)
O1—C1	1.229 (4)	O4'—Ho1^{v}	2.304 (3)
O2—C1	1.260 (4)	N1'—C2'	1.458 (9)
C1—C2'^{i}	1.44 (2)	N1'—C3'	1.468 (10)
C1—C2	1.56 (2)	N1'—C4'	1.479 (5)
O3—C5	1.260 (6)	C2'—C1^{i}	1.44 (2)
O4—C5	1.275 (8)	C2'—H2'1	0.9700
O4—Ho1^{iv}	2.322 (3)	C2'—H2'2	0.9700
N1—C3	1.470 (9)	C3'—H3'1	0.9700
N1—C2	1.466 (9)	C3'—H3'2	0.9700
N1—C4	1.477 (5)	C4'—C5'	1.504 (8)
C2—H2A	0.9700	C4'—H4'1	0.9700
C2—H2B	0.9700	C4'—H4'2	0.9700
O3'—Ho1—O3'^{i}	22.10 (17)	N1^{i}—Ho1—N1	65.43 (18)
O3'—Ho1—O3^{i}	127.93 (12)	C1—O1—Ho1	125.2 (2)
O3'^{i}—Ho1—O3^{i}	133.96 (12)	O1—C1—O2	123.2 (3)
O3'—Ho1—O3	133.96 (12)	O1—C1—C2'^{i}	118.9 (6)
O3'^{i}—Ho1—O3	127.93 (12)	O2—C1—C2'^{i}	117.9 (6)
O3^{i}—Ho1—O3	23.95 (17)	O1—C1—C2	120.3 (5)
O3'—Ho1—O4'^{iii}	149.1 (3)	O2—C1—C2	116.4 (5)
O3'^{i}—Ho1—O4'^{iii}	152.43 (17)	C5—O3—Ho1	124.4 (3)
O3^{i}—Ho1—O4'^{iii}	73.50 (14)	C5—O4—Ho1^{iv}	143.5 (10)
O3—Ho1—O4'^{iii}	75.33 (16)	C3—N1—C2	109.5 (12)
O3'—Ho1—O4'^{vi}	152.43 (17)	C3—N1—C4	107.9 (8)
O3'^{i}—Ho1—O4'^{vi}	149.1 (3)	C2—N1—C4	108.4 (7)
O3^{i}—Ho1—O4'^{vi}	75.33 (16)	C3—N1—Ho1	113.9 (9)
O3—Ho1—O4'^{vi}	73.50 (14)	C2—N1—Ho1	110.9 (9)

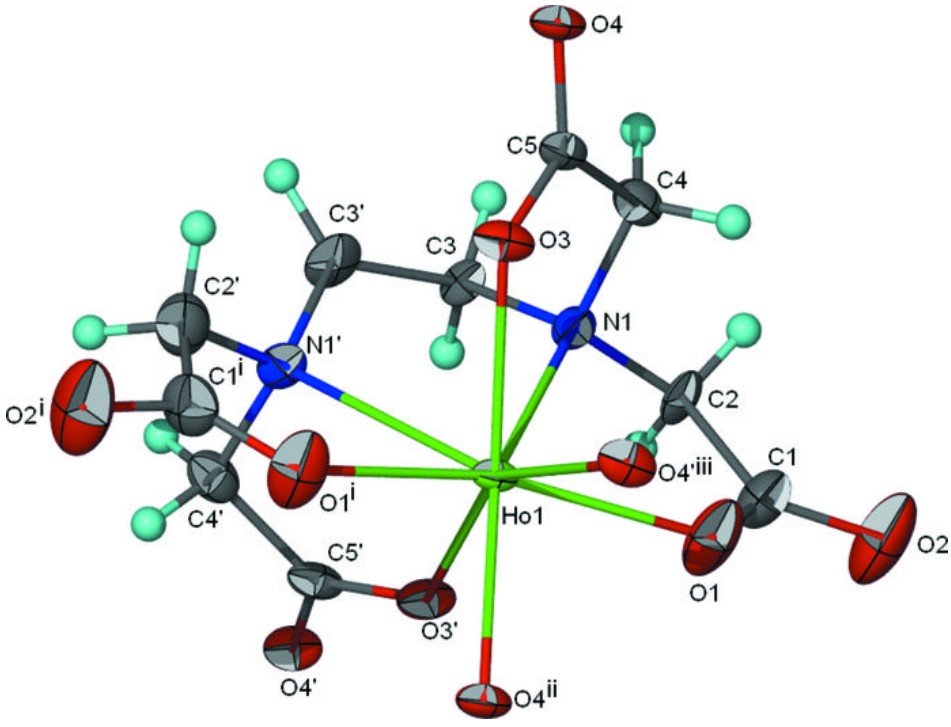
O4'^{iii}—Ho1—O4'^{vi}	8.5 (10)	C4—N1—Ho1	106.1 (3)
O3'—Ho1—O1	81.84 (11)	N1—C2—C1	108.8 (12)
O3'^{i}—Ho1—O1	103.64 (11)	N1—C2—H2A	109.9
O3^{i}—Ho1—O1	83.07 (11)	C1—C2—H2A	109.9
O3—Ho1—O1	106.76 (12)	N1—C2—H2B	109.9
O4'^{iii}—Ho1—O1	79.1 (5)	C1—C2—H2B	109.9
O4'^{vi}—Ho1—O1	87.6 (5)	H2A—C2—H2B	108.3
O3'—Ho1—O1^{i}	103.64 (11)	N1—C3—C3'	111.1 (18)
O3'^{i}—Ho1—O1^{i}	81.84 (11)	N1—C3—H3A	109.4
O3^{i}—Ho1—O1^{i}	106.76 (12)	C3'—C3—H3A	109.4
O3—Ho1—O1^{i}	83.07 (11)	N1—C3—H3B	109.4
O4'^{iii}—Ho1—O1^{i}	87.6 (5)	C3'—C3—H3B	109.4
O4'^{vi}—Ho1—O1^{i}	79.1 (5)	H3A—C3—H3B	108.0
O1—Ho1—O1^{i}	160.57 (11)	N1—C4—C5	112.0 (4)
O3'—Ho1—O4^{vii}	75.83 (17)	N1—C4—H4A	109.2
O3'^{i}—Ho1—O4^{vii}	77.18 (18)	C5—C4—H4A	109.2
O3^{i}—Ho1—O4^{vii}	147.2 (3)	N1—C4—H4B	109.2
O3—Ho1—O4^{vii}	149.9 (2)	C5—C4—H4B	109.2
O4'^{iii}—Ho1—O4^{vii}	76.60 (11)	H4A—C4—H4B	107.9
O4'^{vi}—Ho1—O4^{vii}	77.12 (13)	O3—C5—O4	119.7 (10)
O1—Ho1—O4^{vii}	78.2 (7)	O3—C5—C4	117.5 (4)
O1^{i}—Ho1—O4^{vii}	85.0 (7)	O4—C5—C4	122.8 (11)
O3'—Ho1—O4^{ii}	77.18 (18)	C5'—O3'—Ho1	125.7 (4)
O3'^{i}—Ho1—O4^{ii}	75.83 (17)	C5'—O4'—Ho1^{v}	143.6 (8)
O3^{i}—Ho1—O4^{ii}	149.9 (2)	C2'—N1'—C3'	116.4 (14)
O3—Ho1—O4^{ii}	147.2 (3)	C2'—N1'—C4'	108.9 (8)
O4'^{iii}—Ho1—O4^{ii}	77.12 (13)	C3'—N1'—C4'	108.9 (8)
O4'^{vi}—Ho1—O4^{ii}	76.60 (11)	C2'—N1'—Ho1	106.4 (9)
O1—Ho1—O4^{ii}	85.0 (7)	C3'—N1'—Ho1	108.9 (9)
O1^{i}—Ho1—O4^{ii}	78.2 (7)	C4'—N1'—Ho1	106.8 (3)
O4^{vii}—Ho1—O4^{ii}	6.8 (13)	C1^{i}—C2'—N1'	114.3 (14)
O3'—Ho1—N1^{i}	87.39 (12)	C1^{i}—C2'—H2'1	108.7
O3'^{i}—Ho1—N1^{i}	75.36 (13)	N1'—C2'—H2'1	108.7
O3^{i}—Ho1—N1^{i}	67.74 (12)	C1^{i}—C2'—H2'2	108.7
O3—Ho1—N1^{i}	52.90 (13)	N1'—C2'—H2'2	108.7
O4'^{iii}—Ho1—N1^{i}	123.3 (3)	H2'1—C2'—H2'2	107.6
O4'^{vi}—Ho1—N1^{i}	118.0 (3)	N1'—C3'—C3	118.5 (19)
O1—Ho1—N1^{i}	132.37 (11)	N1'—C3'—H3'1	107.7
O1^{i}—Ho1—N1^{i}	66.95 (11)	C3—C3'—H3'1	107.7
O4^{vii}—Ho1—N1^{i}	143.0 (5)	N1'—C3'—H3'2	107.7
O4^{ii}—Ho1—N1^{i}	137.2 (6)	C3—C3'—H3'2	107.7

O3'—Ho1—N1	75.36 (13)	H3'1—C3'—H3'2	107.1
O3'^{i}—Ho1—N1	87.39 (12)	N1'—C4'—C5'	112.6 (4)
O3^{i}—Ho1—N1	52.90 (13)	N1'—C4'—H4'1	109.1
O3—Ho1—N1	67.74 (12)	C5'—C4'—H4'1	109.1
O4'^{iii}—Ho1—N1	118.0 (3)	N1'—C4'—H4'2	109.1
O4'^{vi}—Ho1—N1	123.3 (3)	C5'—C4'—H4'2	109.1
O1—Ho1—N1	66.95 (11)	H4'1—C4'—H4'2	107.8
O1^{i}—Ho1—N1	132.37 (11)	O3'—C5'—O4'	120.7 (9)
O4^{vii}—Ho1—N1	137.2 (6)	O3'—C5'—C4'	117.6 (4)
O4^{ii}—Ho1—N1	143.0 (5)	O4'—C5'—C4'	121.7 (8)
O3'—Ho1—O1—C1	64.8 (3)	Ho1—O3—C5—O4	178.7 (8)
O3'^{i}—Ho1—O1—C1	68.4 (3)	Ho1—O3—C5—C4	−3.0 (7)
O3^{i}—Ho1—O1—C1	−65.2 (3)	Ho1^{iv}—O4—C5—O3	−153.3 (19)
O3—Ho1—O1—C1	−68.7 (3)	Ho1^{iv}—O4—C5—C4	29 (3)
O4'^{iii}—Ho1—O1—C1	−139.6 (3)	N1—C4—C5—O3	30.3 (7)
O4'^{vi}—Ho1—O1—C1	−140.7 (3)	N1—C4—C5—O4	−151.5 (8)
O1^{i}—Ho1—O1—C1	172.9 (3)	O3'^{i}—Ho1—O3'—C5'	37.8 (5)
O4^{vii}—Ho1—O1—C1	142.0 (3)	O3^{i}—Ho1—O3'—C5'	−77.1 (5)
O4^{ii}—Ho1—O1—C1	142.6 (3)	O3—Ho1—O3'—C5'	−46.2 (5)
N1^{i}—Ho1—O1—C1	−14.0 (4)	O4'^{iii}—Ho1—O3'—C5'	156.0 (10)
N1—Ho1—O1—C1	−12.7 (3)	O4'^{vi}—Ho1—O3'—C5'	139.9 (11)
Ho1—O1—C1—O2	−177.5 (3)	O1—Ho1—O3'—C5'	−151.6 (5)
Ho1—O1—C1—C2'^{i}	3.9 (10)	O1^{i}—Ho1—O3'—C5'	47.3 (5)
Ho1—O1—C1—C2	0.0 (8)	O4^{vii}—Ho1—O3'—C5'	128.5 (8)
O3'—Ho1—O3—C5	−52.9 (5)	O4^{ii}—Ho1—O3'—C5'	121.6 (8)
O3'^{i}—Ho1—O3—C5	−81.2 (4)	N1^{i}—Ho1—O3'—C5'	−18.2 (5)
O3^{i}—Ho1—O3—C5	33.2 (4)	N1—Ho1—O3'—C5'	−83.5 (5)
O4'^{iii}—Ho1—O3—C5	115.5 (6)	O3'—Ho1—N1'—C2'	138.7 (9)
O4'^{vi}—Ho1—O3—C5	124.1 (7)	O3'^{i}—Ho1—N1'—C2'	118.7 (9)
O1—Ho1—O3—C5	41.9 (4)	O3^{i}—Ho1—N1'—C2'	−88.0 (9)
O1^{i}—Ho1—O3—C5	−155.2 (4)	O3—Ho1—N1'—C2'	−67.6 (9)
O4^{vii}—Ho1—O3—C5	137.3 (13)	O4'^{iii}—Ho1—N1'—C2'	−29.4 (10)
O4^{ii}—Ho1—O3—C5	149.3 (12)	O4'^{vi}—Ho1—N1'—C2'	−21.9 (10)
N1^{i}—Ho1—O3—C5	−89.0 (4)	O1—Ho1—N1'—C2'	−166.4 (9)
N1—Ho1—O3—C5	−13.7 (4)	O1^{i}—Ho1—N1'—C2'	21.5 (9)
O3'—Ho1—N1—C3	59.7 (8)	O4^{vii}—Ho1—N1'—C2'	86.6 (11)
O3'^{i}—Ho1—N1—C3	40.9 (8)	O4^{ii}—Ho1—N1'—C2'	80.4 (11)
O3^{i}—Ho1—N1—C3	−114.0 (8)	N1^{i}—Ho1—N1'—C2'	−64.9 (9)
O3—Ho1—N1—C3	−92.2 (8)	N1—Ho1—N1'—C2'	−139.2 (9)
O4'^{iii}—Ho1—N1—C3	−150.4 (9)	O3'—Ho1—N1'—C3'	−95.0 (9)
O4'^{vi}—Ho1—N1—C3	−142.7 (9)	O3'^{i}—Ho1—N1'—C3'	−115.1 (9)

O1—Ho1—N1—C3	146.9 (8)	O3^{i}—Ho1—N1'—C3'	38.2 (9)
O1^{i}—Ho1—N1—C3	−35.6 (8)	O3—Ho1—N1'—C3'	58.6 (9)
O4^{vii}—Ho1—N1—C3	108.8 (9)	O4'^{iii}—Ho1—N1'—C3'	96.8 (10)
O4^{ii}—Ho1—N1—C3	103.0 (10)	O4'^{vi}—Ho1—N1'—C3'	104.4 (10)
N1^{i}—Ho1—N1—C3	−34.2 (8)	O1—Ho1—N1'—C3'	−40.1 (9)
O3'—Ho1—N1—C2	−64.4 (7)	O1^{i}—Ho1—N1'—C3'	147.8 (9)
O3'^{i}—Ho1—N1—C2	−83.2 (7)	O4^{vii}—Ho1—N1'—C3'	−147.1 (11)
O3^{i}—Ho1—N1—C2	121.9 (8)	O4^{ii}—Ho1—N1'—C3'	−153.3 (10)
O3—Ho1—N1—C2	143.7 (8)	N1^{i}—Ho1—N1'—C3'	61.4 (9)
O4'^{iii}—Ho1—N1—C2	85.6 (8)	N1—Ho1—N1'—C3'	−13.0 (9)
O4'^{vi}—Ho1—N1—C2	93.3 (9)	O3'—Ho1—N1'—C4'	22.5 (3)
O1—Ho1—N1—C2	22.9 (7)	O3'^{i}—Ho1—N1'—C4'	2.4 (3)
O1^{i}—Ho1—N1—C2	−159.6 (7)	O3^{i}—Ho1—N1'—C4'	155.7 (3)
O4^{vii}—Ho1—N1—C2	−15.3 (9)	O3—Ho1—N1'—C4'	176.1 (3)
O4^{ii}—Ho1—N1—C2	−21.0 (10)	O4'^{iii}—Ho1—N1'—C4'	−145.6 (6)
N1^{i}—Ho1—N1—C2	−158.2 (7)	O4'^{vi}—Ho1—N1'—C4'	−138.1 (5)
O3'—Ho1—N1—C4	178.2 (3)	O1—Ho1—N1'—C4'	77.4 (3)
O3'^{i}—Ho1—N1—C4	159.4 (3)	O1^{i}—Ho1—N1'—C4'	−94.7 (3)
O3^{i}—Ho1—N1—C4	4.5 (3)	O4^{vii}—Ho1—N1'—C4'	−29.6 (7)
O3—Ho1—N1—C4	26.3 (3)	O4^{ii}—Ho1—N1'—C4'	−35.8 (7)
O4'^{iii}—Ho1—N1—C4	−31.9 (5)	N1^{i}—Ho1—N1'—C4'	178.9 (5)
O4'^{vi}—Ho1—N1—C4	−24.1 (6)	N1—Ho1—N1'—C4'	104.6 (3)
O1—Ho1—N1—C4	−94.6 (3)	C3'—N1'—C2'—C1^{i}	−153.6 (13)
O1^{i}—Ho1—N1—C4	82.9 (3)	C4'—N1'—C2'—C1^{i}	82.8 (13)
O4^{vii}—Ho1—N1—C4	−132.7 (6)	Ho1—N1'—C2'—C1^{i}	−32.0 (14)
O4^{ii}—Ho1—N1—C4	−138.4 (7)	C2'—N1'—C3'—C3	159.0 (18)
N1^{i}—Ho1—N1—C4	84.3 (3)	C4'—N1'—C3'—C3	−77 (2)
C3—N1—C2—C1	−156.1 (11)	Ho1—N1'—C3'—C3	39 (2)
C4—N1—C2—C1	86.4 (10)	N1—C3—C3'—N1'	−51 (3)
Ho1—N1—C2—C1	−29.6 (11)	C2'—N1'—C4'—C5'	−148.1 (11)
O1—C1—C2—N1	22.1 (13)	C3'—N1'—C4'—C5'	83.9 (11)
O2—C1—C2—N1	−160.2 (7)	Ho1—N1'—C4'—C5'	−33.6 (5)
C2'^{i}—C1—C2—N1	−46 (15)	Ho1—O3'—C5'—O4'	175.5 (6)
C2—N1—C3—C3'	158.8 (16)	Ho1—O3'—C5'—C4'	−6.3 (8)
C4—N1—C3—C3'	−83.4 (18)	Ho1^{v}—O4'—C5'—O3'	−159.0 (13)
Ho1—N1—C3—C3'	34.0 (19)	Ho1^{v}—O4'—C5'—C4'	23 (2)
C3—N1—C4—C5	85.1 (10)	N1'—C4'—C5'—O3'	29.5 (7)
C2—N1—C4—C5	−156.4 (10)	N1'—C4'—C5'—O4'	−152.3 (7)
Ho1—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*+1, *y*, *z*; (v) −*x*, *y*+1/2, *z*; (vi) −*x*, *y*−1/2, −*z*+1/2; (vii) *x*−1, *y*, −*z*+1/2.

Fig. 1


O4
C5
C4
C3'
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O4'iii
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O1i
Ho1
C4'
C5'
O2
O1
O3'
O4'
O4ii