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ISSN 2414-3146

Acetyl α -D-2,3,4-triacetyllyxopyranoside

Shawn Culver and Jonathan S. Rhoad*

Missouri Western State University, 4525 Downs Dr, Saint Joseph, MO 64507, USA. *Correspondence e-mail: jrhead1@missouriwestern.edu

Received 6 January 2025

Accepted 8 January 2025

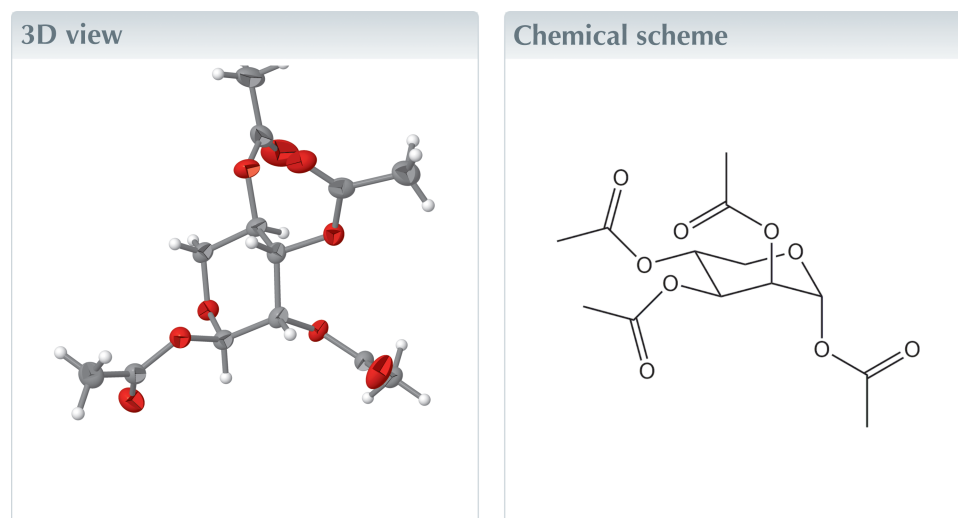
Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

Keywords: crystal structure; carbohydrate; anomeric effect; chair conformation.

CCDC reference: 2415464

Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title compound, $C_{13}H_{18}O_9$, has monoclinic ($P2_1$) symmetry. It is of interest with respect to stereochemistry and the anomeric effect. Two acetyl substituents adopt equatorial orientations and two are axial. The extended structure displays C—H \cdots O hydrogen bonding.



Structure description

The anomeric effect is of interest to aid our understanding of conformational preferences and stereocontrol of reaction of carbohydrates and carbohydrate-like molecules (Juaristi, 2024; Alabugin *et al.*, 2021). Our interest is in carbohydrate and carbohydrate analog ring conformations, leading to the synthesis of common carbohydrate derivatives. Recent methods have been used to try to evaluate the energy of the anomeric and related effects (Custodio Castro *et al.* 2024; Matamoros *et al.*, 2024) using complex techniques to deconvolute steric effects from electronic effects.

The crystal structure of the title compound, $C_{13}H_{18}O_9$ (aLyx) (Fig. 1), is of interest because the two chair conformations each have two acetate groups in axial orientations and two acetate groups equatorial, with the acetate groups at positions 2 and 3 *cis*, so that in the chair conformations, they are always *gauche*. This means that the total energy of the steric interactions for each chair conformation is equal, so any difference in energy is due to the electronic interaction at the acetal group. In the solid state, aLyx is in the 4C_1 conformation, with Cremer & Pople (1975) puckering parameters of $\varphi = 263(3)^\circ$, $\theta = 4.3(2)^\circ$ and $Q = 0.543(2) \text{ \AA}$. Since θ is close to 0° , it is in a nearly perfect chair conformation, while the Q parameter is lower than average, so the chair is a little flattened. The flattening is to be expected with two acetate groups in the axial position, as flattening the ring decreases *gauche* interactions of axial groups with the ring. The acetate substituent at the anomeric (C1) position is axial, indicating the influence of the anomeric effect. The key torsion angles are $O1-C1-C2-O2 = 169.73(14)^\circ$ and $O3-C3-C4-O4 = -71.1(2)^\circ$. The configurations of the stereogenic centers are C1 *R*, C2 *S*, C3 *R* and C4 *R*, as expected for the lyxose starting material. This structure will be the starting point for calculations to quantify the anomeric effect in this sterically

Table 1

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>
C1—H1...O8 ⁱ	0.97 (3)	2.47 (3)	3.198 (3)	132 (2)
C5—H5B...O7 ⁱ	0.94 (3)	2.63 (3)	3.528 (3)	160 (2)
C9—H9C...O5 ⁱⁱ	0.97 (3)	2.57 (3)	3.434 (3)	149 (3)
C11—H11C...O6 ⁱⁱⁱ	1.07 (4)	2.39 (4)	3.331 (3)	145 (3)
C13—H13C...O6 ⁱⁱⁱ	0.92 (5)	2.66 (5)	3.554 (4)	162 (4)

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

balanced molecule. In the crystal, weak C—H...O interactions (Table 1) link the molecules.

Synthesis and crystallization

100 mg (6.7 mmol) of lyxose and 10 mg of sodium acetate were dissolved in approximately 2 ml of acetic anhydride. The solution was heated to reflux for 2 h. After cooling the reaction mixture to room temperature, the solution was poured over crushed ice. After the ice melted, the resulting oil was separated from the water and dissolved in minimal boiling ethanol. A few grains of activated charcoal were added to the ethanol and the solution was boiled as before. This was then passed through a cotton filter and eluted through a silica gel column with a 80:20 hexane-to-dichloromethane mobile phase. Upon evaporation, fine crystals were formed. The crystals were dissolved in a minimal amount of ether and allowed to evaporate overnight to form rectangular parallelepipeds of aLyx.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

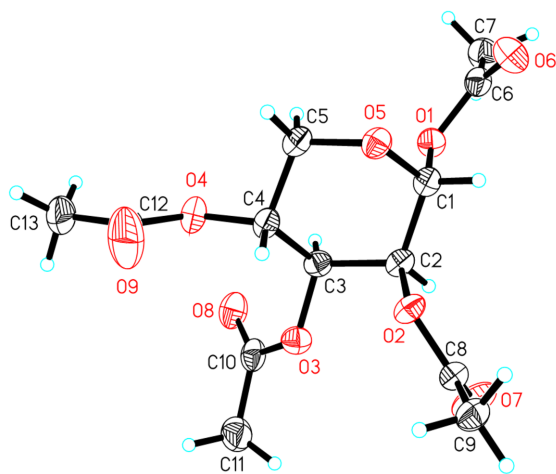


Figure 1

The molecular structure of aLyx showing 50% displacement ellipsoids.

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₃ H ₁₈ O ₉
<i>M_r</i>	318.27
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁
Temperature (K)	200
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.1174 (3), 9.5597 (4), 10.2580 (4)
β (°)	109.7341 (14)
<i>V</i> (Å ³)	749.27 (5)
<i>Z</i>	2
Radiation type	Cu Kα
μ (mm ⁻¹)	1.05
Crystal size (mm)	0.20 × 0.08 × 0.05
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.650, 0.753
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	5524, 2107, 2081
<i>R_{int}</i>	0.025
(sin θ/λ) _{max} (Å ⁻¹)	0.610
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.032, 0.076, 1.11
No. of reflections	2107
No. of parameters	270
No. of restraints	1
H-atom treatment	Only H-atom displacement parameters refined
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.30, -0.25
Absolute structure	Flack <i>x</i> determined using 630 quotients [(<i>I</i> ⁺ - <i>I</i> ⁻)] / [(<i>I</i> ⁺ + <i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.08 (7)

Computer programs: *APEX2* (Bruker, 2017), *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick 2008) and *SHELXL2019/1* (Sheldrick, 2015).

Acknowledgements

The authors would like to thank Dr Victor Day and acknowledge the NSF-MRI grant (CHE-0923449) that was used to purchase the X-ray diffractometer and software used in this study.

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full crystallographic data

IUCrData (2025). **10**, x250016 [<https://doi.org/10.1107/S2414314625000161>]

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Acetyl α -D-2,3,4-triacetyllyxopyranoside*Crystal data*

$C_{13}H_{18}O_9$

$M_r = 318.27$

Monoclinic, $P2_1$

$a = 8.1174$ (3) Å

$b = 9.5597$ (4) Å

$c = 10.2580$ (4) Å

$\beta = 109.7341$ (14)°

$V = 749.27$ (5) Å³

$Z = 2$

$F(000) = 336$

$D_x = 1.411$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 5073 reflections

$\theta = 6.5$ – 70.0°

$\mu = 1.05$ mm⁻¹

$T = 200$ K

Rectangular parallelepiped, colourless

$0.20 \times 0.08 \times 0.05$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.650$, $T_{\max} = 0.753$

5524 measured reflections

2107 independent reflections

2081 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 70.1^\circ$, $\theta_{\min} = 6.5^\circ$

$h = -9 \rightarrow 8$

$k = -11 \rightarrow 8$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.076$

$S = 1.11$

2107 reflections

270 parameters

1 restraint

Hydrogen site location: difference Fourier map

Only H-atom displacement parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.0979P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.30$ e Å⁻³

$\Delta\rho_{\min} = -0.24$ e Å⁻³

Extinction correction: *SHELXL2019/1*

(Sheldrick, 2015),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.028 (3)

Absolute structure: Flack x determined using

630 quotients $[(I^-) - (I)] / [(I^+) + (I)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.08 (7)

Special details

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

Refinement. The ring and methyl hydrogen atoms were initially located in difference-Fourier maps and refined as individual isotropic atoms.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	−0.12797 (18)	0.61079 (17)	0.65441 (14)	0.0265 (4)
O2	0.18123 (17)	0.40848 (17)	0.55297 (15)	0.0261 (4)
O3	0.05956 (18)	0.56065 (17)	0.31122 (15)	0.0278 (4)
O4	−0.2996 (2)	0.45517 (19)	0.21466 (16)	0.0335 (4)
O5	−0.14941 (18)	0.37458 (16)	0.58585 (15)	0.0267 (4)
O6	−0.1547 (2)	0.5135 (2)	0.84634 (17)	0.0396 (4)
O7	0.4179 (2)	0.5469 (2)	0.5983 (2)	0.0458 (5)
O8	−0.1219 (2)	0.7203 (2)	0.17276 (16)	0.0374 (4)
O9	−0.2878 (4)	0.2352 (3)	0.1434 (2)	0.0698 (7)
C1	−0.0355 (3)	0.4874 (2)	0.6386 (2)	0.0249 (5)
H1	0.038 (3)	0.457 (3)	0.730 (3)	0.025 (6)*
C2	0.0676 (2)	0.5270 (2)	0.5439 (2)	0.0237 (4)
H2	0.138 (3)	0.606 (3)	0.571 (3)	0.020 (5)*
C3	−0.0509 (3)	0.5479 (2)	0.3942 (2)	0.0244 (4)
H3	−0.117 (3)	0.631 (3)	0.386 (2)	0.018 (5)*
C4	−0.1710 (3)	0.4228 (3)	0.3476 (2)	0.0260 (5)
H4	−0.103 (3)	0.344 (3)	0.343 (2)	0.020 (6)*
C5	−0.2688 (3)	0.3961 (3)	0.4481 (2)	0.0273 (5)
H5A	−0.342 (3)	0.470 (3)	0.446 (2)	0.017 (6)*
H5B	−0.336 (3)	0.315 (3)	0.427 (3)	0.021 (6)*
C6	−0.1753 (3)	0.6122 (3)	0.7703 (2)	0.0285 (5)
C7	−0.2522 (4)	0.7496 (3)	0.7883 (3)	0.0381 (6)
H7A	−0.211 (2)	0.7748 (15)	0.880 (5)	0.075 (12)*
H7B	−0.232 (7)	0.826 (6)	0.730 (6)	0.093 (15)*
H7C	−0.369 (8)	0.738 (7)	0.761 (6)	0.104 (18)*
C8	0.3551 (3)	0.4327 (3)	0.5903 (2)	0.0267 (5)
C9	0.4529 (3)	0.2978 (3)	0.6181 (2)	0.0305 (5)
H9A	0.414 (4)	0.237 (4)	0.535 (4)	0.050 (9)*
H9B	0.428 (4)	0.251 (4)	0.691 (3)	0.034 (7)*
H9C	0.579 (4)	0.312 (4)	0.648 (3)	0.045 (8)*
C10	0.0097 (3)	0.6518 (3)	0.2030 (2)	0.0301 (5)
C11	0.1387 (4)	0.6508 (4)	0.1280 (3)	0.0423 (6)
H11A	0.246 (5)	0.623 (5)	0.185 (4)	0.051 (9)*
H11B	0.141 (7)	0.742 (7)	0.088 (6)	0.092 (15)*
H11C	0.090 (5)	0.577 (5)	0.045 (4)	0.060 (10)*
C12	−0.3453 (3)	0.3515 (3)	0.1204 (2)	0.0394 (6)
C13	−0.4761 (4)	0.4017 (5)	−0.0120 (3)	0.0540 (9)
H13A	−0.544 (7)	0.482 (7)	0.009 (5)	0.092 (16)*
H13B	−0.546 (6)	0.333 (6)	−0.055 (5)	0.074 (13)*
H13C	−0.410 (6)	0.421 (6)	−0.067 (5)	0.074 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0271 (7)	0.0251 (8)	0.0268 (6)	0.0027 (6)	0.0085 (5)	-0.0005 (6)
O2	0.0187 (7)	0.0230 (8)	0.0344 (7)	0.0007 (6)	0.0060 (5)	-0.0024 (6)
O3	0.0275 (7)	0.0268 (8)	0.0305 (7)	0.0011 (6)	0.0117 (6)	0.0024 (6)
O4	0.0309 (7)	0.0349 (10)	0.0273 (7)	-0.0029 (7)	0.0000 (6)	-0.0030 (7)
O5	0.0260 (7)	0.0231 (8)	0.0294 (7)	-0.0025 (6)	0.0073 (6)	0.0005 (6)
O6	0.0494 (9)	0.0388 (11)	0.0336 (8)	0.0015 (8)	0.0179 (7)	0.0031 (8)
O7	0.0252 (8)	0.0303 (10)	0.0781 (12)	-0.0055 (7)	0.0126 (8)	-0.0029 (10)
O8	0.0374 (9)	0.0336 (10)	0.0333 (8)	0.0012 (8)	0.0015 (6)	0.0044 (7)
O9	0.0903 (17)	0.0519 (16)	0.0528 (12)	0.0004 (14)	0.0051 (11)	-0.0247 (12)
C1	0.0236 (9)	0.0231 (11)	0.0262 (9)	0.0010 (8)	0.0061 (7)	-0.0016 (8)
C2	0.0208 (9)	0.0187 (11)	0.0306 (10)	0.0001 (8)	0.0071 (7)	-0.0019 (9)
C3	0.0228 (9)	0.0224 (11)	0.0282 (9)	0.0017 (9)	0.0090 (8)	-0.0006 (9)
C4	0.0227 (9)	0.0254 (11)	0.0265 (10)	0.0005 (9)	0.0038 (7)	-0.0025 (9)
C5	0.0222 (10)	0.0260 (12)	0.0310 (10)	-0.0018 (10)	0.0056 (8)	-0.0024 (9)
C6	0.0267 (10)	0.0316 (13)	0.0263 (9)	-0.0029 (9)	0.0075 (7)	-0.0049 (9)
C7	0.0417 (14)	0.0378 (15)	0.0361 (12)	0.0055 (11)	0.0146 (10)	-0.0067 (11)
C8	0.0212 (9)	0.0320 (12)	0.0262 (9)	-0.0009 (9)	0.0071 (7)	-0.0011 (9)
C9	0.0234 (10)	0.0325 (14)	0.0334 (11)	0.0029 (9)	0.0067 (8)	0.0030 (10)
C10	0.0326 (11)	0.0274 (12)	0.0259 (10)	-0.0081 (10)	0.0042 (8)	-0.0036 (9)
C11	0.0424 (14)	0.0515 (17)	0.0327 (12)	-0.0114 (12)	0.0124 (10)	0.0015 (12)
C12	0.0392 (12)	0.0507 (18)	0.0303 (11)	-0.0095 (12)	0.0144 (9)	-0.0103 (11)
C13	0.0473 (15)	0.084 (3)	0.0263 (11)	-0.0197 (18)	0.0065 (10)	-0.0040 (15)

Geometric parameters (Å, °)

O1—C6	1.367 (3)	C4—C5	1.520 (3)
O1—C1	1.437 (3)	C4—H4	0.95 (3)
O2—C8	1.352 (3)	C5—H5A	0.92 (3)
O2—C2	1.444 (2)	C5—H5B	0.94 (3)
O3—C10	1.361 (3)	C6—C7	1.493 (4)
O3—C3	1.435 (2)	C7—H7A	0.91 (5)
O4—C12	1.346 (3)	C7—H7B	0.99 (6)
O4—C4	1.443 (2)	C7—H7C	0.90 (6)
O5—C1	1.405 (3)	C8—C9	1.491 (3)
O5—C5	1.433 (2)	C9—H9A	0.99 (4)
O6—C6	1.199 (3)	C9—H9B	0.95 (3)
O7—C8	1.196 (3)	C9—H9C	0.97 (3)
O8—C10	1.201 (3)	C10—C11	1.494 (3)
O9—C12	1.198 (4)	C11—H11A	0.91 (4)
C1—C2	1.528 (3)	C11—H11B	0.96 (7)
C1—H1	0.97 (3)	C11—H11C	1.07 (4)
C2—C3	1.525 (3)	C12—C13	1.493 (4)
C2—H2	0.94 (3)	C13—H13A	1.01 (6)
C3—C4	1.515 (3)	C13—H13B	0.89 (6)
C3—H3	0.94 (3)	C13—H13C	0.92 (5)

C6—O1—C1	114.64 (16)	O6—C6—C7	125.7 (2)
C8—O2—C2	117.83 (18)	O1—C6—C7	111.6 (2)
C10—O3—C3	117.73 (17)	C6—C7—H7A	109.7
C12—O4—C4	117.2 (2)	C6—C7—H7B	114 (3)
C1—O5—C5	114.06 (16)	H7A—C7—H7B	110.1
O5—C1—O1	111.88 (15)	C6—C7—H7C	107 (4)
O5—C1—C2	112.09 (17)	H7A—C7—H7C	109.4
O1—C1—C2	106.69 (17)	H7B—C7—H7C	106 (5)
O5—C1—H1	104.6 (17)	O7—C8—O2	123.8 (2)
O1—C1—H1	108.5 (16)	O7—C8—C9	126.10 (19)
C2—C1—H1	113.1 (15)	O2—C8—C9	110.1 (2)
O2—C2—C3	109.81 (16)	C8—C9—H9A	110 (2)
O2—C2—C1	103.86 (16)	C8—C9—H9B	109 (2)
C3—C2—C1	112.22 (16)	H9A—C9—H9B	108 (3)
O2—C2—H2	107.6 (16)	C8—C9—H9C	112 (2)
C3—C2—H2	108.1 (15)	H9A—C9—H9C	110 (3)
C1—C2—H2	115.0 (15)	H9B—C9—H9C	107 (3)
O3—C3—C4	110.17 (17)	O8—C10—O3	123.6 (2)
O3—C3—C2	107.51 (15)	O8—C10—C11	126.0 (2)
C4—C3—C2	109.53 (17)	O3—C10—C11	110.4 (2)
O3—C3—H3	109.2 (15)	C10—C11—H11A	111 (2)
C4—C3—H3	110.3 (15)	C10—C11—H11B	109 (3)
C2—C3—H3	110.1 (14)	H11A—C11—H11B	113 (4)
O4—C4—C3	108.18 (18)	C10—C11—H11C	106 (2)
O4—C4—C5	107.47 (16)	H11A—C11—H11C	109 (3)
C3—C4—C5	110.29 (17)	H11B—C11—H11C	108 (4)
O4—C4—H4	111.8 (15)	O9—C12—O4	123.2 (2)
C3—C4—H4	108.6 (15)	O9—C12—C13	126.0 (3)
C5—C4—H4	110.5 (15)	O4—C12—C13	110.8 (3)
O5—C5—C4	111.03 (16)	C12—C13—H13A	109 (3)
O5—C5—H5A	110.3 (15)	C12—C13—H13B	111 (3)
C4—C5—H5A	109.7 (15)	H13A—C13—H13B	112 (4)
O5—C5—H5B	105.0 (15)	C12—C13—H13C	104 (3)
C4—C5—H5B	112.4 (15)	H13A—C13—H13C	117 (5)
H5A—C5—H5B	108 (2)	H13B—C13—H13C	104 (4)
O6—C6—O1	122.7 (2)		
C5—O5—C1—O1	64.6 (2)	C12—O4—C4—C5	-99.9 (2)
C5—O5—C1—C2	-55.2 (2)	O3—C3—C4—O4	-71.1 (2)
C6—O1—C1—O5	79.4 (2)	C2—C3—C4—O4	170.86 (16)
C6—O1—C1—C2	-157.64 (16)	O3—C3—C4—C5	171.64 (17)
C8—O2—C2—C3	114.69 (18)	C2—C3—C4—C5	53.6 (2)
C8—O2—C2—C1	-125.12 (17)	C1—O5—C5—C4	58.9 (2)
O5—C1—C2—O2	-67.48 (19)	O4—C4—C5—O5	-175.16 (18)
O1—C1—C2—O2	169.73 (14)	C3—C4—C5—O5	-57.5 (2)
O5—C1—C2—C3	51.1 (2)	C1—O1—C6—O6	-6.1 (3)
O1—C1—C2—C3	-71.7 (2)	C1—O1—C6—C7	173.50 (18)

C10—O3—C3—C4	97.3 (2)	C2—O2—C8—O7	-10.3 (3)
C10—O3—C3—C2	-143.44 (18)	C2—O2—C8—C9	170.07 (16)
O2—C2—C3—O3	-55.3 (2)	C3—O3—C10—O8	-0.8 (3)
C1—C2—C3—O3	-170.28 (18)	C3—O3—C10—C11	-179.63 (19)
O2—C2—C3—C4	64.4 (2)	C4—O4—C12—O9	1.9 (4)
C1—C2—C3—C4	-50.6 (2)	C4—O4—C12—C13	-178.94 (19)
C12—O4—C4—C3	141.0 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C1—H1 \cdots O8 ⁱ	0.97 (3)	2.47 (3)	3.198 (3)	132 (2)
C5—H5B \cdots O7 ⁱ	0.94 (3)	2.63 (3)	3.528 (3)	160 (2)
C9—H9C \cdots O5 ⁱⁱ	0.97 (3)	2.57 (3)	3.434 (3)	149 (3)
C11—H11C \cdots O6 ⁱⁱⁱ	1.07 (4)	2.39 (4)	3.331 (3)	145 (3)
C13—H13C \cdots O6 ⁱⁱⁱ	0.92 (5)	2.66 (5)	3.554 (4)	162 (4)

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