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# 2-*C*-Cyclohexyl-2,3-*O*-isopropylidene-erythrofuranose

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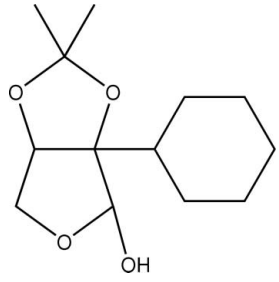
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.046; $wR$ factor = 0.124; data-to-parameter ratio = 14.3.

In the title compound, $C_{13}H_{22}O_4$, the acetonide ring adopts an envelope conformation with one of the O atoms as the flap atom, whereas a twisted conformation is found for the furanose ring. Centrosymmetric eight-membered $\{\cdots OCOH\}_2$ synthons involving the hydroxy H and acetonide O atoms are found in the crystal structure. These are linked into a supramolecular chain in the *a*-axis direction *via* C—H···O contacts.

## Related literature

For the dihydroxylation of the olefin portion of 1,2-dioxines, see: Robinson *et al.* (2006, 2009); Valente *et al.* (2009); Pedersen *et al.* (2009).




## Experimental

### *Crystal data*

$C_{13}H_{22}O_4$
$M_r$ = 242.31
Triclinic, $P\overline{1}$
$a$ = 5.454 (3) Å
$b$ = 9.908 (3) Å
$c$ = 12.442 (5) Å
$\alpha$ = 93.29 (3)°
$\beta$ = 94.95 (4)°
$\gamma$ = 102.94 (3)°
$V$ = 650.8 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 153 K
0.24 × 0.15 × 0.13 mm

### *Data collection*

Rigaku AFC12K/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.789, $T_{max}$ = 1
4992 measured reflections
2224 independent reflections
2064 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.124
$S$ = 1.09
2224 reflections
156 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H40···O3$^{i}$ | 0.84 | 1.95 | 2.787 (2) | 173 |
| C2—H2···O1$^{ii}$ | 1.00 | 2.43 | 3.350 (3) | 152 |

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We are grateful to the Australian Research Council for financial support. TVR thanks the Commonwealth Government of Australia for a postgraduate scholarship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2594).

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# supporting information

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## 2-*C*-Cyclohexyl-2,3-*O*-isopropylideneerythrofuranose

**Tony V. Robinson, Dennis K. Taylor and Edward R. T. Tiekink**

### S1. Comment

Recently we examined the dihydroxylation of the olefin portion of 1,2-dioxines, which provided access to a range of polyhydroxylated core structures upon selective manipulation of the peroxide linkage (Robinson *et al.*, 2006; Robinson *et al.*, 2009; Valente *et al.*, 2009). This methodology was extended to include the synthesis of erythrono-*γ*-lactones (Pedersen *et al.*, 2009), during the course of which the title compound, (I), was prepared.

The molecular structure of (I), Fig. 1, comprises two fused five-membered rings linked by the C2—C3 bond. The acetonide ring adopts an envelope conformation with the O2 atom being the flap atom. A twisted conformation is found for the furanose ring whereby the O3 atom is *endo* and the C4 atom is *exo*. The cyclohexyl group is in the chair conformation. The crystal structure comprises centrosymmetric dimers held by $\{\cdots OCOH\}_2$ synthons arising from the interaction between the O4-hydroxyl group and the ether-O3 atom, Fig. 2 and Table 1. The resultant eight-membered ring has an elongated chair conformation. The dimeric aggregates are linked into supramolecular chains *via* C—H···O interactions, Fig. 2 and Table 1. The topology of the supramolecular chain is linear, and is aligned along the *a* direction.

### S2. Experimental

For full synthetic procedures and characterization data see Pedersen *et al.* (2009) and Robinson *et al.* (2009). To a stirred solution of $Co(salen)_2$ (27 mg, 0.08 mmol) in THF (5 ml) at ambient temperature was added (3aR,7aS)-3a-cyclohexyl-tetrahydro-2,2-dimethyl-[1,3]dioxolo[4,5-*d*][1,2]dioxine (803 mg, 3.31 mmol). The reaction left to stir until complete by TLC (~16 h). All volatiles were removed *in vacuo* giving a crude mixture of regioisomers in a 43:57 ratio. The isomers were completely separated by flash chromatography giving a combined total yield of 779 mg (97%). Compound (I) was isolated as a colourless solid (337 mg), and the pure material was recrystallized by slowly evaporating a 1:1 mixture of dichloromethane/heptane to give colourless prisms, m. pt. 391–394 K. The compound was found to exist solely in its cyclic hemi-acetal form(*s*) both as a solid indicated by IR (absence of carbonyl signal), and in $CDCl_3$ solution which revealed a 94:6 anomeric ratio.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.98–1.00 Å) and were included in the refinement in the riding model approximation with $U_{iso}$(H) set to 1.2–1.5$U_{eq}$(C). A rotating group model was used for the methyl groups. The O–bound H-atom was located in a difference Fourier map and was refined with an O–H restraint of 0.840±0.001 Å, and with $U_{iso}$(H) = 1.5$U_{eq}$(O).

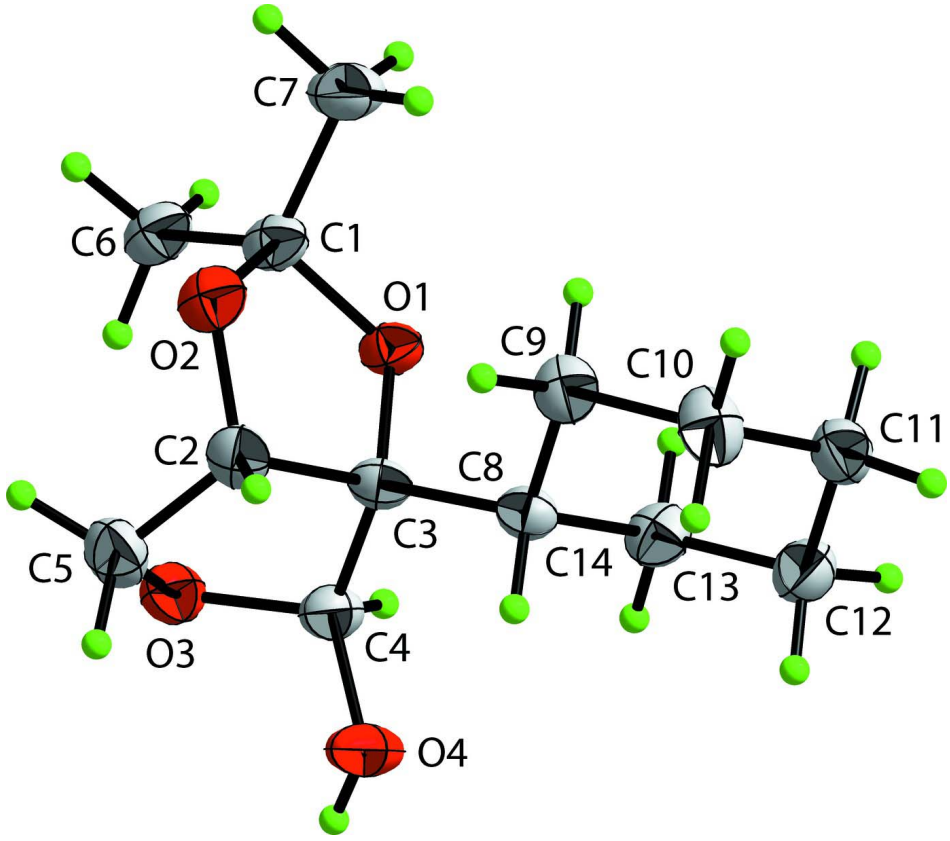


**Figure 1**

Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

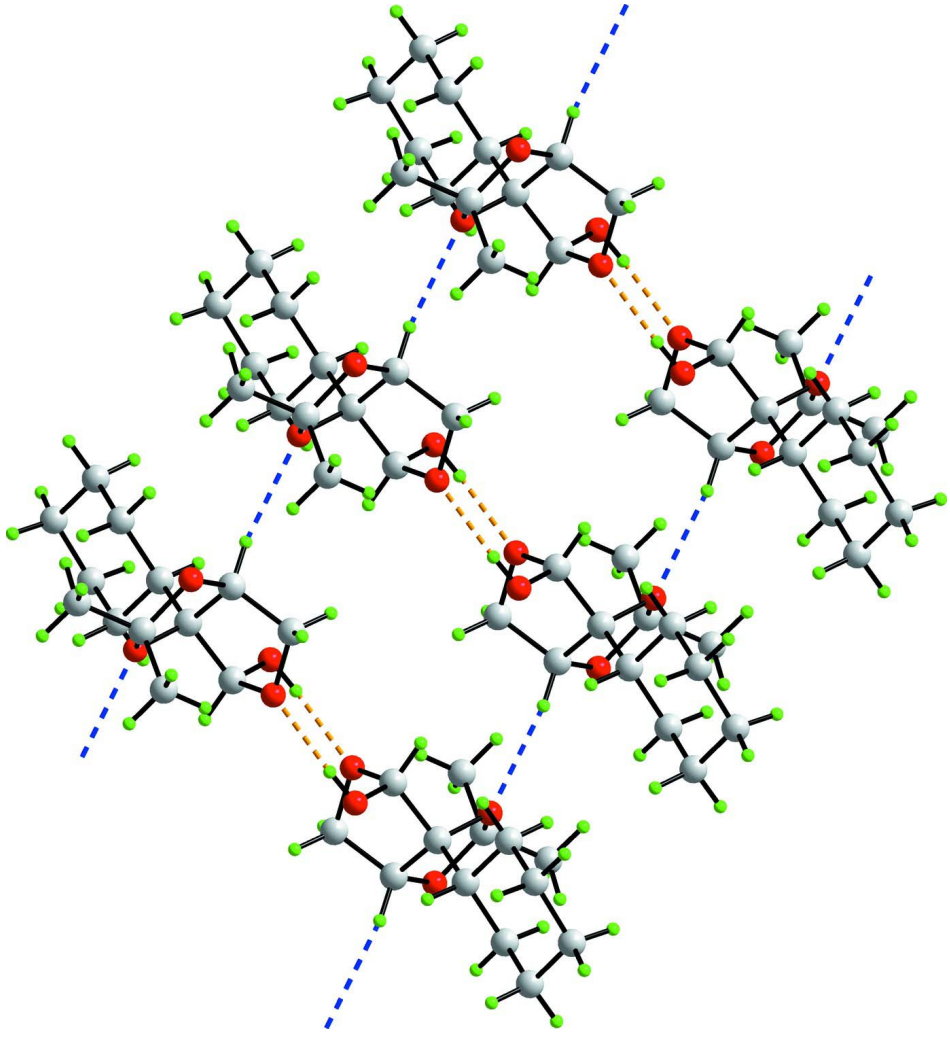

**Figure 2**

Supramolecular chain formation along the *a* axis in (I) mediated by O—H···O hydrogen bonds (orange dashed lines) and C—H···O contacts (blue dashed lines).

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*Crystal data*

$C_{13}H_{22}O_4$
$M_r = 242.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.454$ (3) Å
$b = 9.908$ (3) Å
$c = 12.442$ (5) Å
$\alpha = 93.29$ (3)°
$\beta = 94.95$ (4)°
$\gamma = 102.94$ (3)°
$V = 650.8$ (5) Å$^3$
$Z = 2$
$F(000) = 264$
$D_x = 1.237$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 657 reflections
$\theta = 2.1$–30.2°
$\mu = 0.09$ mm$^{-1}$
$T = 153$ K
Needle, colourless
0.24 × 0.15 × 0.13 mm

*Data collection*

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.789, $T_{max}$ = 1
4992 measured reflections
2224 independent reflections
2064 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.1°
$h$ = −6→5
$k$ = −11→11
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.124
$S$ = 1.09
2224 reflections
156 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.1734P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.69690 (18) | 0.26256 (11) | 0.70713 (8) | 0.0281 (3) |
| O2 | 1.0523 (2) | 0.34466 (12) | 0.62499 (9) | 0.0352 (3) |
| O3 | 0.9937 (2) | 0.48884 (11) | 0.85907 (9) | 0.0377 (3) |
| O4 | 1.0310 (3) | 0.31604 (12) | 0.97416 (9) | 0.0439 (4) |
| H4O | 1.0281 | 0.3703 | 1.0282 | 0.066* |
| C1 | 0.7854 (3) | 0.33328 (17) | 0.61509 (12) | 0.0312 (4) |
| C2 | 1.1367 (3) | 0.33878 (16) | 0.73567 (13) | 0.0320 (4) |
| H2 | 1.2783 | 0.2898 | 0.7425 | 0.038* |
| C3 | 0.9031 (3) | 0.25734 (15) | 0.78511 (12) | 0.0270 (4) |
| C4 | 0.8885 (3) | 0.35109 (16) | 0.88634 (12) | 0.0327 (4) |
| H4 | 0.7088 | 0.3415 | 0.9019 | 0.039* |
| C5 | 1.2089 (3) | 0.47939 (18) | 0.80110 (15) | 0.0410 (4) |
| H5A | 1.3609 | 0.4853 | 0.8524 | 0.049* |
| H5B | 1.2450 | 0.5556 | 0.7526 | 0.049* |
| C6 | 0.7237 (3) | 0.47484 (18) | 0.61632 (14) | 0.0366 (4) |
| H6A | 0.5397 | 0.4637 | 0.6085 | 0.055* |

| | | | | |
|---|---|---|---|---|
| H6B | 0.7959 | 0.5243 | 0.5562 | 0.055* |
| H6C | 0.7954 | 0.5282 | 0.6850 | 0.055* |
| C7 | 0.6697 (4) | 0.2440 (2) | 0.51267 (14) | 0.0446 (5) |
| H7A | 0.4850 | 0.2278 | 0.5085 | 0.067* |
| H7B | 0.7193 | 0.1549 | 0.5134 | 0.067* |
| H7C | 0.7299 | 0.2916 | 0.4497 | 0.067* |
| C8 | 0.9010 (3) | 0.10690 (15) | 0.80714 (12) | 0.0281 (4) |
| H8 | 1.0454 | 0.1086 | 0.8629 | 0.034* |
| C9 | 0.9368 (3) | 0.01889 (16) | 0.70736 (14) | 0.0353 (4) |
| H9A | 0.7968 | 0.0159 | 0.6504 | 0.042* |
| H9B | 1.0973 | 0.0623 | 0.6788 | 0.042* |
| C10 | 0.9421 (3) | −0.12889 (17) | 0.73441 (16) | 0.0410 (4) |
| H10A | 0.9581 | −0.1844 | 0.6677 | 0.049* |
| H10B | 1.0915 | −0.1265 | 0.7863 | 0.049* |
| C11 | 0.7028 (3) | −0.19803 (17) | 0.78331 (14) | 0.0363 (4) |
| H11A | 0.5557 | −0.2117 | 0.7280 | 0.044* |
| H11B | 0.7179 | −0.2905 | 0.8053 | 0.044* |
| C12 | 0.6588 (3) | −0.11062 (17) | 0.88099 (14) | 0.0376 (4) |
| H12A | 0.7936 | −0.1083 | 0.9402 | 0.045* |
| H12B | 0.4948 | −0.1539 | 0.9067 | 0.045* |
| C13 | 0.6576 (3) | 0.03762 (17) | 0.85399 (13) | 0.0343 (4) |
| H13A | 0.6391 | 0.0929 | 0.9204 | 0.041* |
| H13B | 0.5107 | 0.0361 | 0.8010 | 0.041* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0218 (5) | 0.0379 (6) | 0.0252 (6) | 0.0082 (4) | 0.0014 (4) | 0.0048 (4) |
| O2 | 0.0277 (6) | 0.0454 (7) | 0.0345 (6) | 0.0098 (5) | 0.0089 (5) | 0.0062 (5) |
| O3 | 0.0485 (7) | 0.0307 (6) | 0.0335 (7) | 0.0112 (5) | −0.0019 (5) | −0.0002 (5) |
| O4 | 0.0662 (8) | 0.0383 (7) | 0.0279 (6) | 0.0212 (6) | −0.0115 (6) | −0.0033 (5) |
| C1 | 0.0266 (8) | 0.0414 (9) | 0.0262 (8) | 0.0078 (6) | 0.0047 (6) | 0.0051 (6) |
| C2 | 0.0240 (8) | 0.0352 (8) | 0.0373 (9) | 0.0082 (6) | 0.0009 (6) | 0.0041 (7) |
| C3 | 0.0234 (7) | 0.0332 (8) | 0.0250 (8) | 0.0095 (6) | −0.0009 (6) | −0.0001 (6) |
| C4 | 0.0413 (9) | 0.0312 (8) | 0.0264 (8) | 0.0125 (7) | −0.0015 (7) | 0.0008 (6) |
| C5 | 0.0334 (9) | 0.0370 (9) | 0.0483 (10) | 0.0027 (7) | −0.0044 (7) | 0.0023 (8) |
| C6 | 0.0343 (9) | 0.0440 (10) | 0.0337 (9) | 0.0121 (7) | 0.0037 (7) | 0.0100 (7) |
| C7 | 0.0490 (11) | 0.0548 (11) | 0.0272 (9) | 0.0082 (8) | −0.0003 (8) | 0.0005 (8) |
| C8 | 0.0260 (8) | 0.0313 (8) | 0.0272 (8) | 0.0084 (6) | 0.0005 (6) | 0.0000 (6) |
| C9 | 0.0347 (9) | 0.0351 (9) | 0.0373 (9) | 0.0079 (7) | 0.0124 (7) | −0.0006 (7) |
| C10 | 0.0407 (10) | 0.0329 (9) | 0.0506 (11) | 0.0097 (7) | 0.0137 (8) | −0.0047 (7) |
| C11 | 0.0380 (9) | 0.0314 (8) | 0.0378 (9) | 0.0050 (7) | 0.0042 (7) | −0.0006 (7) |
| C12 | 0.0432 (10) | 0.0365 (9) | 0.0340 (9) | 0.0088 (7) | 0.0070 (7) | 0.0061 (7) |
| C13 | 0.0369 (9) | 0.0369 (9) | 0.0319 (9) | 0.0119 (7) | 0.0107 (7) | 0.0027 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C3 | 1.4328 (18) | C7—H7A | 0.9800 |
| O1—C1 | 1.4392 (19) | C7—H7B | 0.9800 |
| O2—C2 | 1.423 (2) | C7—H7C | 0.9800 |
| O2—C1 | 1.429 (2) | C8—C9 | 1.528 (2) |
| O3—C4 | 1.429 (2) | C8—C13 | 1.531 (2) |
| O3—C5 | 1.447 (2) | C8—H8 | 1.0000 |
| O4—C4 | 1.392 (2) | C9—C10 | 1.527 (2) |
| O4—H4O | 0.8399 | C9—H9A | 0.9900 |
| C1—C7 | 1.512 (2) | C9—H9B | 0.9900 |
| C1—C6 | 1.513 (2) | C10—C11 | 1.526 (2) |
| C2—C5 | 1.526 (2) | C10—H10A | 0.9900 |
| C2—C3 | 1.544 (2) | C10—H10B | 0.9900 |
| C2—H2 | 1.0000 | C11—C12 | 1.519 (2) |
| C3—C8 | 1.529 (2) | C11—H11A | 0.9900 |
| C3—C4 | 1.540 (2) | C11—H11B | 0.9900 |
| C4—H4 | 1.0000 | C12—C13 | 1.527 (2) |
| C5—H5A | 0.9900 | C12—H12A | 0.9900 |
| C5—H5B | 0.9900 | C12—H12B | 0.9900 |
| C6—H6A | 0.9800 | C13—H13A | 0.9900 |
| C6—H6B | 0.9800 | C13—H13B | 0.9900 |
| C6—H6C | 0.9800 | | |
| | | | |
| C3—O1—C1 | 111.24 (11) | C1—C7—H7B | 109.5 |
| C2—O2—C1 | 108.79 (12) | H7A—C7—H7B | 109.5 |
| C4—O3—C5 | 105.95 (12) | C1—C7—H7C | 109.5 |
| C4—O4—H4O | 108.8 | H7A—C7—H7C | 109.5 |
| O2—C1—O1 | 105.26 (12) | H7B—C7—H7C | 109.5 |
| O2—C1—C7 | 108.62 (14) | C9—C8—C3 | 113.25 (13) |
| O1—C1—C7 | 109.15 (13) | C9—C8—C13 | 109.62 (13) |
| O2—C1—C6 | 111.35 (13) | C3—C8—C13 | 111.20 (12) |
| O1—C1—C6 | 110.47 (13) | C9—C8—H8 | 107.5 |
| C7—C1—C6 | 111.76 (14) | C3—C8—H8 | 107.5 |
| O2—C2—C5 | 114.39 (14) | C13—C8—H8 | 107.5 |
| O2—C2—C3 | 104.95 (12) | C10—C9—C8 | 111.22 (14) |
| C5—C2—C3 | 104.74 (13) | C10—C9—H9A | 109.4 |
| O2—C2—H2 | 110.8 | C8—C9—H9A | 109.4 |
| C5—C2—H2 | 110.8 | C10—C9—H9B | 109.4 |
| C3—C2—H2 | 110.8 | C8—C9—H9B | 109.4 |
| O1—C3—C8 | 110.40 (12) | H9A—C9—H9B | 108.0 |
| O1—C3—C4 | 108.10 (12) | C11—C10—C9 | 111.32 (14) |
| C8—C3—C4 | 114.24 (13) | C11—C10—H10A | 109.4 |
| O1—C3—C2 | 103.39 (12) | C9—C10—H10A | 109.4 |
| C8—C3—C2 | 116.55 (12) | C11—C10—H10B | 109.4 |
| C4—C3—C2 | 103.27 (12) | C9—C10—H10B | 109.4 |
| O4—C4—O3 | 111.08 (13) | H10A—C10—H10B | 108.0 |
| O4—C4—C3 | 109.45 (12) | C12—C11—C10 | 111.32 (14) |

| | | | |
|---|---|---|---|
| O3—C4—C3 | 104.59 (13) | C12—C11—H11A | 109.4 |
| O4—C4—H4 | 110.5 | C10—C11—H11A | 109.4 |
| O3—C4—H4 | 110.5 | C12—C11—H11B | 109.4 |
| C3—C4—H4 | 110.5 | C10—C11—H11B | 109.4 |
| O3—C5—C2 | 106.01 (13) | H11A—C11—H11B | 108.0 |
| O3—C5—H5A | 110.5 | C11—C12—C13 | 111.60 (14) |
| C2—C5—H5A | 110.5 | C11—C12—H12A | 109.3 |
| O3—C5—H5B | 110.5 | C13—C12—H12A | 109.3 |
| C2—C5—H5B | 110.5 | C11—C12—H12B | 109.3 |
| H5A—C5—H5B | 108.7 | C13—C12—H12B | 109.3 |
| C1—C6—H6A | 109.5 | H12A—C12—H12B | 108.0 |
| C1—C6—H6B | 109.5 | C12—C13—C8 | 111.60 (13) |
| H6A—C6—H6B | 109.5 | C12—C13—H13A | 109.3 |
| C1—C6—H6C | 109.5 | C8—C13—H13A | 109.3 |
| H6A—C6—H6C | 109.5 | C12—C13—H13B | 109.3 |
| H6B—C6—H6C | 109.5 | C8—C13—H13B | 109.3 |
| C1—C7—H7A | 109.5 | H13A—C13—H13B | 108.0 |

| | | | |
|---|---|---|---|
| C2—O2—C1—O1 | −24.16 (15) | C2—C3—C4—O4 | −89.45 (15) |
| C2—O2—C1—C7 | −140.95 (13) | O1—C3—C4—O3 | −79.48 (14) |
| C2—O2—C1—C6 | 95.56 (15) | C8—C3—C4—O3 | 157.20 (12) |
| C3—O1—C1—O2 | 12.78 (15) | C2—C3—C4—O3 | 29.63 (14) |
| C3—O1—C1—C7 | 129.21 (14) | C4—O3—C5—C2 | 34.96 (16) |
| C3—O1—C1—C6 | −107.53 (14) | O2—C2—C5—O3 | 99.37 (16) |
| C1—O2—C2—C5 | −88.63 (16) | C3—C2—C5—O3 | −14.97 (16) |
| C1—O2—C2—C3 | 25.58 (15) | O1—C3—C8—C9 | 62.51 (16) |
| C1—O1—C3—C8 | −122.93 (13) | C4—C3—C8—C9 | −175.42 (12) |
| C1—O1—C3—C4 | 111.46 (14) | C2—C3—C8—C9 | −55.00 (17) |
| C1—O1—C3—C2 | 2.43 (14) | O1—C3—C8—C13 | −61.44 (16) |
| O2—C2—C3—O1 | −16.78 (14) | C4—C3—C8—C13 | 60.62 (17) |
| C5—C2—C3—O1 | 104.03 (13) | C2—C3—C8—C13 | −178.95 (12) |
| O2—C2—C3—C8 | 104.51 (14) | C3—C8—C9—C10 | 178.09 (12) |
| C5—C2—C3—C8 | −134.68 (14) | C13—C8—C9—C10 | −57.09 (17) |
| O2—C2—C3—C4 | −129.38 (12) | C8—C9—C10—C11 | 56.64 (19) |
| C5—C2—C3—C4 | −8.57 (15) | C9—C10—C11—C12 | −54.5 (2) |
| C5—O3—C4—O4 | 77.45 (16) | C10—C11—C12—C13 | 53.94 (19) |
| C5—O3—C4—C3 | −40.52 (15) | C11—C12—C13—C8 | −55.52 (18) |
| O1—C3—C4—O4 | 161.44 (12) | C9—C8—C13—C12 | 56.55 (17) |
| C8—C3—C4—O4 | 38.13 (18) | C3—C8—C13—C12 | −177.46 (12) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H40···O3$^{i}$ | 0.84 | 1.95 | 2.787 (2) | 173 |
| C2—H2···O1$^{ii}$ | 1.00 | 2.43 | 3.350 (3) | 152 |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+2; (ii) *x*+1, *y*, *z*.