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A monoclinic form of dendocarbin A: a borderline case of one-dimensional isostructural polymorphism

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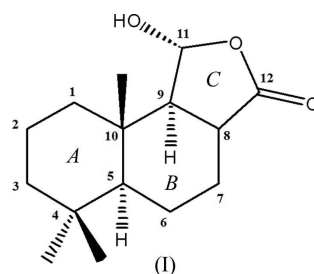
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The title compound, dendocarbin A [systematic name: (1*R*,5*aS*,9*aS*,9*bR*)-1-hydroxy-6,6,9*a*-trimethyldodecahydronaphtho[1,2-*c*]furan-3-one], C₁₅H₂₂O₃, is a sesquiterpene lactone isolated from *Drimys winteri* var *chilensis*. The monoclinic phase described herein displays an identical molecular structure to the orthorhombic phase that we reported previously [Paz Robles *et al.* (2014). *Acta Cryst. C* **70**, 1007–1010], while varying significantly in chain pitch, and can thus be considered as a borderline case of one-dimensional isostructural polymorphism.

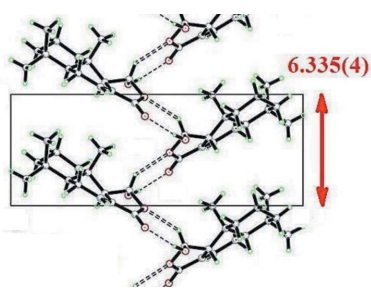
1. Introduction

Drimys winteri (Winteraceae) is a tree characterized by large and glossy green leaves, native of the Pacific side of Southern Patagonia. Due to its medicinal properties (such as antifungal, insecticidal and bactericidal) (Kubo *et al.*, 2005; Jansen & de Groot, 2004), the tree, locally called *Canelo*, was considered sacred by the native Araucanians. Drimane sesquiterpinoids, found in the bark, have been described in detail previously (Appel *et al.*, 1963). Dendocarbin A belongs to this sesquiterpinoid family but has been infrequently discussed in the literature.



The more relevant reports include extraction from nudibranchs *Dendrodoris carbunculosa* (Sakio *et al.*, 2001), *Doriopsilla pelseeneri* (Gaspar *et al.*, 2005) and from the bark of *Warburgia ugandensis* (Canellaceae) (Xu *et al.*, 2009).

As part of a series of structural characterizations of naturally occurring molecules isolated from southern Andean flora, we have recently reported the crystal structure of dendocarbin A in the orthorhombic phase (Paz Robles *et al.*, 2014), (I), which was isolated for the first time from *Drimys winteri* var *chilensis* (Winteraceae). We present herein the monoclinic phase of dendocarbin A, (II), from the same botanical origin.



2. Experimental

2.1. Synthesis and crystallization

Dendrocarbin A was extracted from 1 kg of powdered *Drimys winteri* (collected at Concepcion, VIII Region, Chile, in February 2012) by maceration in ethanol for 3 d to yield a crude solid (20 g) which was purified by column chromatography and recrystallized from methanol. The previously reported orthorhombic phase, (I) (Paz Robles *et al.*, 2014), was grown at ~ 298 K, while the present monoclinic phase, (II), was obtained at ~ 277 K.

2.2. Refinement

Crystal data collection and structure refinement details are summarized in Table 1. All H atoms were initially identified in an intermediate difference map. The hydroxy H atom was refined isotropically. The other H atoms were refined with restrained C–H distances and isotropic displacement parameters, *viz.* C–H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for tertiary H atoms, C–H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for secondary H atoms, and C–H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. The chirality of (II) was assigned based on (I) and similar compounds.

3. Results and discussion

The rigid backbone of (II) is composed of three fused rings (see Scheme and Fig. 1) and fully matches its counterpart (I) (Paz Robles *et al.*, 2014). Fig. 2 shows a least-squares fit of both molecules (r.m.s. deviation = 0.157 Å; maximum deviation = 0.303 Å for atom O2). A comparison of equivalent bond lengths [mean deviation = 0.005 (3) Å; maximum deviation = 0.012 (5) Å for C8–C12] confirms that these differences are more related to torsional rather than metrical deformations.

As in (I), ring *A* (atoms C1–C5/C10) displays a chair conformation [$\theta = 5.3$ (3)°, *cf.* $\theta = 0.00^\circ$ for an ideal chair conformation (Boeyens, 1978)], the central *B* ring (atoms C5–

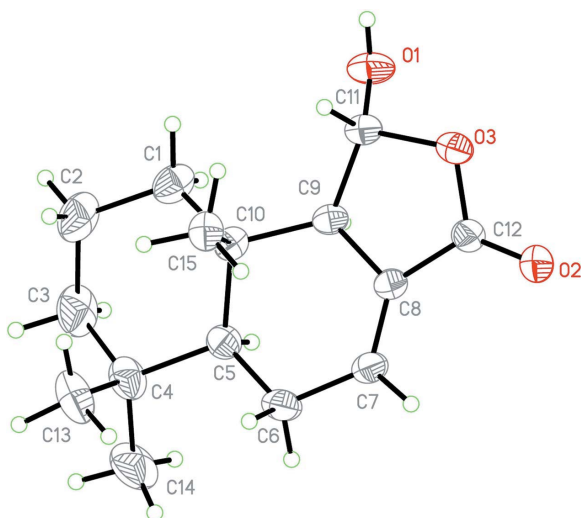


Figure 1

A view of the molecule of (I), with displacement ellipsoids drawn at the 30% probability level.

Table 1

Experimental details.

Crystal data	
Chemical formula	$\text{C}_{15}\text{H}_{22}\text{O}_3$
M_r	250.32
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	295
a, b, c (Å)	8.2892 (10), 8.3401 (7), 11.0225 (13)
β (°)	108.750 (13)
V (Å ³)	721.58 (15)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.24 × 0.18 × 0.12
Data collection	
Diffractometer	Oxford Diffraction Gemini CCD S Ultra diffractometer
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)
$T_{\text{min}}, T_{\text{max}}$	0.967, 0.988
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11012, 3411, 2519
R_{int} ($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.032 0.678
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.043, 0.097, 1.02
No. of reflections	3411
No. of parameters	170
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.15, -0.16

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *SHELXS* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2008), *XP* in *SHELXTL* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

C10) displays a half-chair conformation [$\theta = 51.6$ (3)° and $\varphi = 310.8$ (4)° = $5 \times 60 + 10.8^\circ$; $\theta = 50.8$ and $\varphi = k \times 60 + 30^\circ$ for an ideal half-chair conformation (Boeyens, 1978)] and five-membered lactone ring *C* (atoms C8/C9/C11/C12/O3) displays an envelope conformation [$\varphi = 62.9$ (8)° = $2 \times 36 - 9.1^\circ$; $\varphi = k \times 36 + 0^\circ$ for an ideal envelope conformation (Cremer & Pople, 1975)], the carbonyl group at atom C12 being conjugated with the 'outer' C7=C8 double bond. A full comparison of (I) was discussed previously (Paz Robles *et al.*, 2014), and also applies to (II), with three related literature compounds,

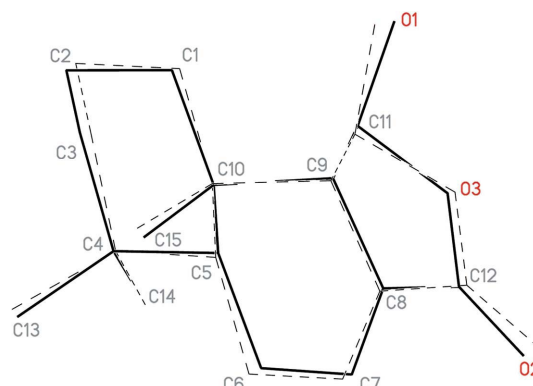
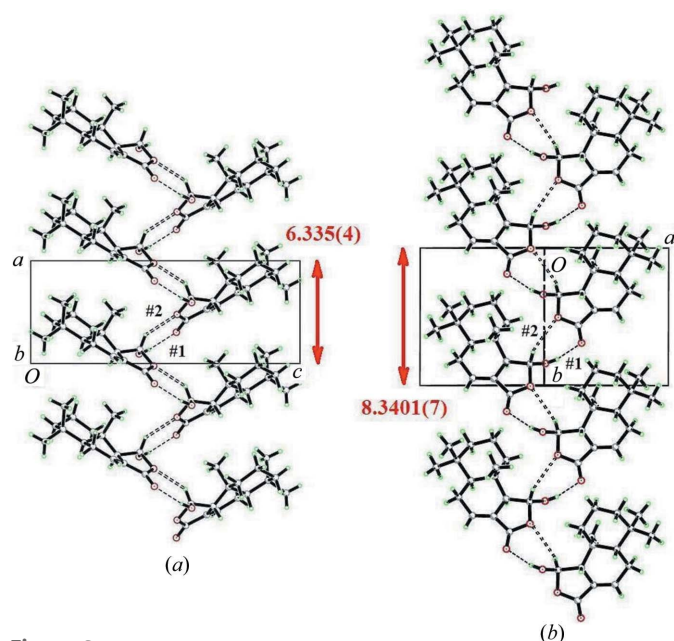


Figure 2

Superposition of structures (I) (broken lines) and (II) (full lines).


Figure 3

View of the hydrogen-bonded chains in (a) (I) and (b) (II), with the intrachain hydrogen bonds drawn as broken lines. Hashes ('#') refer to the hydrogen-bond entries in Table 2.

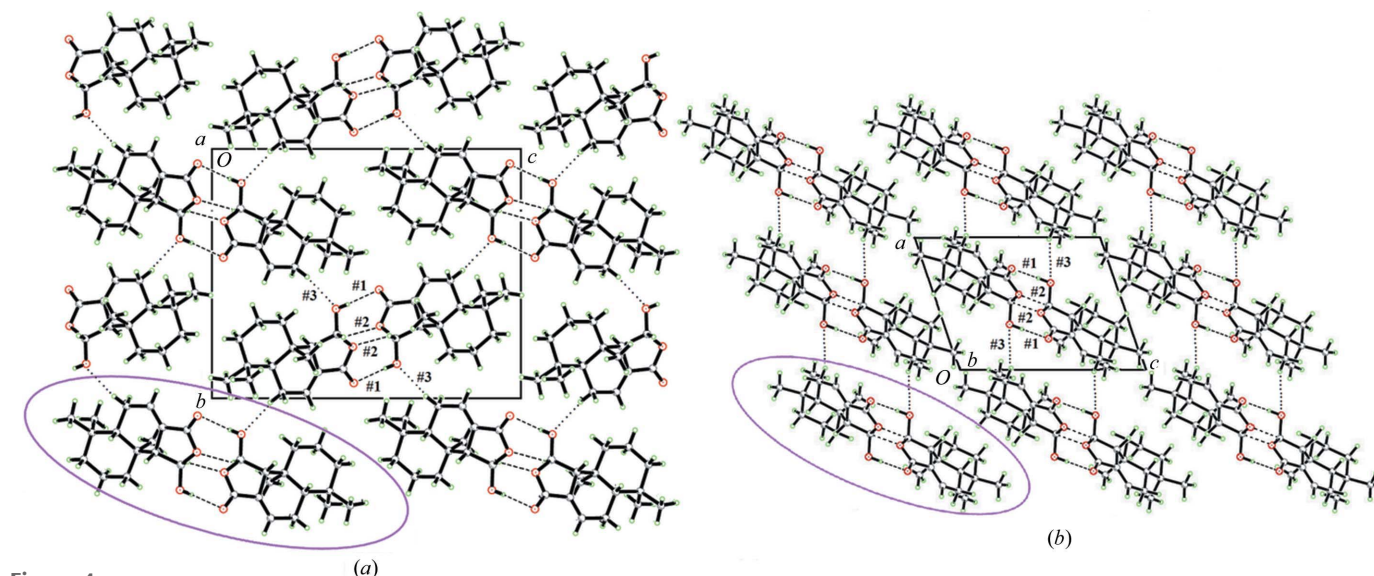
Table 2

Comparison of the hydrogen-bond geometries of (I) and (II) (Å, °).

Symmetry codes appear in the order (I),(II) and the O—H and C—H values in (I) have been normalized to match those in (II), the remaining values being recalculated accordingly.

No.	D—H...A	D—H		H...A		D...A		D—H...A	
		(I)	(II)	(I)	(II)	(I)	(II)	(I)	(II)
#1	O1—H1O...O2 ^{i,iii}	0.81	0.81 (3)	2.05	1.96 (3)	2.85	2.758 (3)	171	167 (3)
#2	C11—H11...O3 ^{i,iii}	0.98	0.98	2.40	2.62	3.19	3.40	137	137
#3	C6—H6B...O1 ^{ii,iv}	0.97	0.97	2.67	2.69	3.63	3.39	172	130

Symmetry codes for (I): (i) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; for (II): (iii) $-x + 1, y - \frac{1}{2}, -z + 1$; (iv) $x + 1, y, z$.


Figure 4

Packing views of (a) (I) and (b) (II), drawn along the chain directions, showing (encircled) in projection and in broken lines the intra/interchain hydrogen bonds. Hashes ('#') refer to the hydrogen-bond entries in Table 2.

namely drimenin [Cambridge Structural Database (CSD; Version 5.34; Groom & Allen, 2014) refcode DIWSEI (Brito, López-Rodríguez *et al.*, 2008)], cinnamolide (CSD refcode UTONUN; Brito, Cardenas *et al.*, 2008) and 3-hydroxy-7-drimen-12,11-olide hemihydrate (CSD refcode UCOKUT; Zhang *et al.*, 2006).

It is in the supramolecular structure where the most interesting features setting the structures of (I) and (II) apart can be found. To begin with, the same intramolecular interactions appear in both, and are compared in Table 2. The most significant involves the strong hydrogen bond (entry #1 in Table 2) that defines chains threaded along a 2_1 axis, *i.e.* running along [100] in (I) and along [010] in (II). In these chains, individual component molecules are stacked in a head-to-head fashion with rather short C(6) sequences (Bernstein *et al.*, 1995). There are, however, significant differences: in the case of (I), there is an extra C—H...O hydrogen bond completing the chain linkage (entry #2 in Table 2), an interaction which in (II) is weakened and insignificant. As a result, there is a lengthening of pitch accompanied with a shortening of the chain width (Fig. 3).

Inspection of Fig. 4, which presents a projection of the structures along the chain directions, discloses another

difference: in the case of (I) (space group $P2_12_12_1$), the chains are disposed along b and c in a ‘criss-cross’ fashion, following the scheme forced by the 2_1 axis running along [010] and [001], resulting in more efficient packing evidenced by the slight reduction of the Kitaigorodskii packing index from 64.7 for (I) to 63.2 for (II) (calculated using *PLATON*; Spek, 2009).

Both structures are comparable with respect to the few interactions significantly stronger than the background dispersive forces. The shortest interchain C—H...O contacts are described in Table 2 (entry #3) and represented by dotted lines in Fig. 4. These extremely weak interactions influence the parallel chains to form higher dimensional superstructures, *viz.* a three-dimensional lattice in (I) and two-dimensional sheets parallel to (001) in (II) (Fig. 4).

Finally, it is worth making a few remarks regarding the pertinence of the term ‘one-dimensional isostructurality’, as applied to (I) and (II). Albeit of general use, the concept of ‘isostructurality’ appears as a rather vague one. According to the IUCr online dictionary of crystallography the term applies to: (a) ‘... crystals with the same structure, but not necessarily the same cell dimensions ...’ and (b) ‘... with a ‘comparable’ variability in the atomic coordinates to that of the cell dimensions ...’. This leaves open the main issue of how much difference is allowed between structures that are considered to be isostructural.

At the other extreme, as discussed by Coles *et al.* (2014), the concepts of polymorphism, wherein the same molecules crystallize in different structures, and of isostructurality, wherein there is emphasis on structural similarity, are opposed to each other and therefore it is unlikely that an isostructural polymorph could exist.

Fabian & Kalman (1999, 2004) showed that although isostructurality is traditionally considered as a three-dimensional consequence involving whole molecules, it is acceptable to broaden the concept to include two-dimensional structures with similar layers and one-dimensional structures with similar rows or strips. Furthermore, in their 2004 paper, they presented a frequency analysis of isostructurality and distribution per dimensionality as follows: 44% (zero-dimensional), 17% (one-dimensional), 13% (two-dimensional) and 26% (three-dimensional).

For (I) and (II), the hydrogen-bonded chain threaded by a 2_1 axis is a topological leitmotif common to both polymorphs satisfying the first requirement of isostructurality. Clearly,

both chains differ in their chain pitch, in agreement with the $a(\text{I})/b(\text{II})$ cell-dimension ratio, thereby satisfying the second requirement as well. Therefore, it is appropriate to describe the (I)/(II) phase pair as a borderline case of one-dimensional isostructural polymorphism.

Acknowledgements

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2013* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

(1*R*,5*aS*,9*aS*,9*bR*)-1-Hydroxy-6,6,9*a*-\ trimethyldodecahydronaphtho[1,2-*c*]furan-3-one

Crystal data

$C_{15}H_{22}O_3$	$F(000) = 272$
$M_r = 250.32$	$D_x = 1.152 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.2892 (10) \text{ \AA}$	Cell parameters from 3400 reflections
$b = 8.3401 (7) \text{ \AA}$	$\theta = 3.9\text{--}25.4^\circ$
$c = 11.0225 (13) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 108.750 (13)^\circ$	$T = 295 \text{ K}$
$V = 721.58 (15) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.24 \times 0.18 \times 0.12 \text{ mm}$

Data collection

Oxford Diffraction Gemini CCD S Ultra diffractometer	3411 independent reflections
ω scans, thick slices	2519 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)	$R_{\text{int}} = 0.032$
$T_{\text{min}} = 0.967$, $T_{\text{max}} = 0.988$	$\theta_{\text{max}} = 28.8^\circ$, $\theta_{\text{min}} = 3.9^\circ$
11012 measured reflections	$h = -11 \rightarrow 11$
	$k = -11 \rightarrow 11$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.0646P]$
$wR(F^2) = 0.097$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3411 reflections	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
170 parameters	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$
1 restraint	

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.

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	0.3432 (2)	0.3387 (3)	0.3519 (2)	0.0627 (5)
H1O	0.308 (4)	0.309 (4)	0.409 (3)	0.073 (10)*
O2	0.7646 (2)	0.6896 (2)	0.46443 (18)	0.0591 (5)
O3	0.5689 (2)	0.5045 (2)	0.45756 (17)	0.0553 (5)
C1	0.5275 (4)	0.0419 (3)	0.2243 (3)	0.0612 (7)
H1A	0.4799	0.0129	0.2909	0.073*
H1B	0.4386	0.0943	0.1562	0.073*
C2	0.5820 (5)	-0.1096 (4)	0.1718 (3)	0.0824 (10)
H2A	0.6639	-0.1675	0.2408	0.099*
H2B	0.4838	-0.1783	0.1357	0.099*
C3	0.6610 (5)	-0.0691 (4)	0.0695 (3)	0.0839 (10)
H3A	0.5760	-0.0165	-0.0010	0.101*
H3B	0.6932	-0.1679	0.0371	0.101*
C4	0.8176 (4)	0.0393 (3)	0.1162 (3)	0.0650 (8)
C5	0.7668 (3)	0.1913 (3)	0.1786 (2)	0.0468 (6)
H5	0.6822	0.2465	0.1078	0.056*
C6	0.9134 (3)	0.3110 (3)	0.2271 (3)	0.0609 (7)
H6A	1.0134	0.2543	0.2801	0.073*
H6B	0.9401	0.3543	0.1541	0.073*
C7	0.8772 (3)	0.4465 (3)	0.3024 (2)	0.0514 (6)
H7	0.9555	0.5297	0.3282	0.062*
C8	0.7363 (3)	0.4511 (3)	0.3333 (2)	0.0423 (5)
C9	0.6015 (3)	0.3248 (3)	0.2981 (2)	0.0397 (5)
H9	0.5178	0.3558	0.2162	0.048*
C10	0.6744 (3)	0.1602 (3)	0.2793 (2)	0.0425 (5)
C11	0.5168 (3)	0.3423 (3)	0.4014 (2)	0.0457 (6)
H11	0.5577	0.2592	0.4670	0.055*
C12	0.6971 (3)	0.5629 (3)	0.4220 (2)	0.0467 (6)
C13	0.9684 (5)	-0.0556 (4)	0.2049 (3)	0.0888 (11)
H13A	0.9368	-0.1005	0.2743	0.133*
H13B	1.0641	0.0148	0.2386	0.133*
H13C	0.9986	-0.1403	0.1573	0.133*
C14	0.8664 (5)	0.0924 (5)	-0.0011 (3)	0.0933 (11)
H14A	0.8705	0.0004	-0.0524	0.140*
H14B	0.9762	0.1431	0.0270	0.140*
H14C	0.7830	0.1667	-0.0512	0.140*
C15	0.7933 (3)	0.0989 (3)	0.4082 (2)	0.0506 (6)
H15A	0.7319	0.0925	0.4685	0.076*
H15B	0.8876	0.1713	0.4399	0.076*

H15C 0.8350 -0.0055 0.3968 0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0392 (10)	0.0867 (14)	0.0655 (12)	-0.0038 (9)	0.0214 (9)	0.0109 (11)
O2	0.0632 (12)	0.0465 (10)	0.0743 (12)	-0.0044 (9)	0.0315 (10)	-0.0102 (10)
O3	0.0548 (10)	0.0582 (10)	0.0636 (11)	-0.0037 (8)	0.0337 (9)	-0.0075 (9)
C1	0.0668 (17)	0.0648 (18)	0.0476 (13)	-0.0229 (14)	0.0124 (12)	-0.0067 (13)
C2	0.109 (3)	0.0650 (19)	0.0684 (19)	-0.0350 (18)	0.0211 (19)	-0.0268 (16)
C3	0.116 (3)	0.073 (2)	0.0601 (18)	-0.011 (2)	0.0242 (19)	-0.0281 (16)
C4	0.082 (2)	0.0631 (18)	0.0529 (15)	0.0051 (15)	0.0252 (15)	-0.0128 (14)
C5	0.0521 (14)	0.0506 (14)	0.0389 (12)	-0.0007 (12)	0.0166 (10)	-0.0026 (11)
C6	0.0585 (16)	0.0675 (17)	0.0694 (17)	-0.0092 (14)	0.0384 (14)	-0.0122 (15)
C7	0.0540 (15)	0.0499 (14)	0.0571 (14)	-0.0124 (12)	0.0274 (12)	-0.0041 (12)
C8	0.0460 (13)	0.0422 (12)	0.0418 (12)	-0.0017 (11)	0.0187 (10)	0.0038 (10)
C9	0.0371 (11)	0.0480 (13)	0.0329 (11)	-0.0022 (10)	0.0099 (9)	0.0051 (10)
C10	0.0450 (13)	0.0446 (13)	0.0350 (11)	-0.0066 (10)	0.0088 (10)	-0.0011 (10)
C11	0.0397 (13)	0.0534 (15)	0.0457 (12)	-0.0018 (11)	0.0160 (10)	0.0056 (12)
C12	0.0469 (14)	0.0450 (14)	0.0515 (13)	0.0041 (11)	0.0203 (11)	0.0042 (12)
C13	0.107 (3)	0.075 (2)	0.087 (2)	0.027 (2)	0.035 (2)	-0.0165 (19)
C14	0.123 (3)	0.104 (3)	0.070 (2)	0.012 (2)	0.055 (2)	-0.016 (2)
C15	0.0584 (15)	0.0479 (14)	0.0418 (13)	0.0033 (11)	0.0108 (11)	0.0013 (11)

Geometric parameters (Å, °)

O1—C11	1.365 (3)	C6—C7	1.489 (3)
O1—H1O	0.81 (3)	C6—H6A	0.9700
O2—C12	1.217 (3)	C6—H6B	0.9700
O3—C12	1.337 (3)	C7—C8	1.318 (3)
O3—C11	1.493 (3)	C7—H7	0.9300
C1—C2	1.518 (4)	C8—C12	1.461 (3)
C1—C10	1.533 (3)	C8—C9	1.493 (3)
C1—H1A	0.9700	C9—C11	1.525 (3)
C1—H1B	0.9700	C9—C10	1.540 (3)
C2—C3	1.512 (5)	C9—H9	0.9800
C2—H2A	0.9700	C10—C15	1.533 (3)
C2—H2B	0.9700	C11—H11	0.9800
C3—C4	1.529 (4)	C13—H13A	0.9600
C3—H3A	0.9700	C13—H13B	0.9600
C3—H3B	0.9700	C13—H13C	0.9600
C4—C13	1.536 (5)	C14—H14A	0.9600
C4—C14	1.539 (4)	C14—H14B	0.9600
C4—C5	1.563 (4)	C14—H14C	0.9600
C5—C6	1.531 (3)	C15—H15A	0.9600
C5—C10	1.560 (3)	C15—H15B	0.9600
C5—H5	0.9800	C15—H15C	0.9600

C11—O1—H1O	107 (2)	C7—C8—C9	124.3 (2)
C12—O3—C11	111.10 (18)	C12—C8—C9	108.38 (19)
C2—C1—C10	113.0 (2)	C8—C9—C11	102.97 (18)
C2—C1—H1A	109.0	C8—C9—C10	111.75 (17)
C10—C1—H1A	109.0	C11—C9—C10	118.68 (18)
C2—C1—H1B	109.0	C8—C9—H9	107.6
C10—C1—H1B	109.0	C11—C9—H9	107.6
H1A—C1—H1B	107.8	C10—C9—H9	107.6
C3—C2—C1	110.6 (3)	C1—C10—C15	110.2 (2)
C3—C2—H2A	109.5	C1—C10—C9	109.34 (19)
C1—C2—H2A	109.5	C15—C10—C9	109.63 (18)
C3—C2—H2B	109.5	C1—C10—C5	109.53 (19)
C1—C2—H2B	109.5	C15—C10—C5	113.5 (2)
H2A—C2—H2B	108.1	C9—C10—C5	104.54 (17)
C2—C3—C4	113.9 (2)	O1—C11—O3	108.23 (19)
C2—C3—H3A	108.8	O1—C11—C9	112.26 (19)
C4—C3—H3A	108.8	O3—C11—C9	104.75 (18)
C2—C3—H3B	108.8	O1—C11—H11	110.5
C4—C3—H3B	108.8	O3—C11—H11	110.5
H3A—C3—H3B	107.7	C9—C11—H11	110.5
C3—C4—C13	109.8 (3)	O2—C12—O3	121.0 (2)
C3—C4—C14	108.1 (3)	O2—C12—C8	129.6 (2)
C13—C4—C14	107.6 (3)	O3—C12—C8	109.4 (2)
C3—C4—C5	107.9 (2)	C4—C13—H13A	109.5
C13—C4—C5	114.7 (2)	C4—C13—H13B	109.5
C14—C4—C5	108.5 (3)	H13A—C13—H13B	109.5
C6—C5—C10	112.09 (18)	C4—C13—H13C	109.5
C6—C5—C4	112.8 (2)	H13A—C13—H13C	109.5
C10—C5—C4	116.2 (2)	H13B—C13—H13C	109.5
C6—C5—H5	104.8	C4—C14—H14A	109.5
C10—C5—H5	104.8	C4—C14—H14B	109.5
C4—C5—H5	104.8	H14A—C14—H14B	109.5
C7—C6—C5	114.2 (2)	C4—C14—H14C	109.5
C7—C6—H6A	108.7	H14A—C14—H14C	109.5
C5—C6—H6A	108.7	H14B—C14—H14C	109.5
C7—C6—H6B	108.7	C10—C15—H15A	109.5
C5—C6—H6B	108.7	C10—C15—H15B	109.5
H6A—C6—H6B	107.6	H15A—C15—H15B	109.5
C8—C7—C6	121.4 (2)	C10—C15—H15C	109.5
C8—C7—H7	119.3	H15A—C15—H15C	109.5
C6—C7—H7	119.3	H15B—C15—H15C	109.5
C7—C8—C12	126.7 (2)		