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(S)-2-[(S)-2,2,2-Trifluoro-1-hydroxyethyl]-1-tetralone

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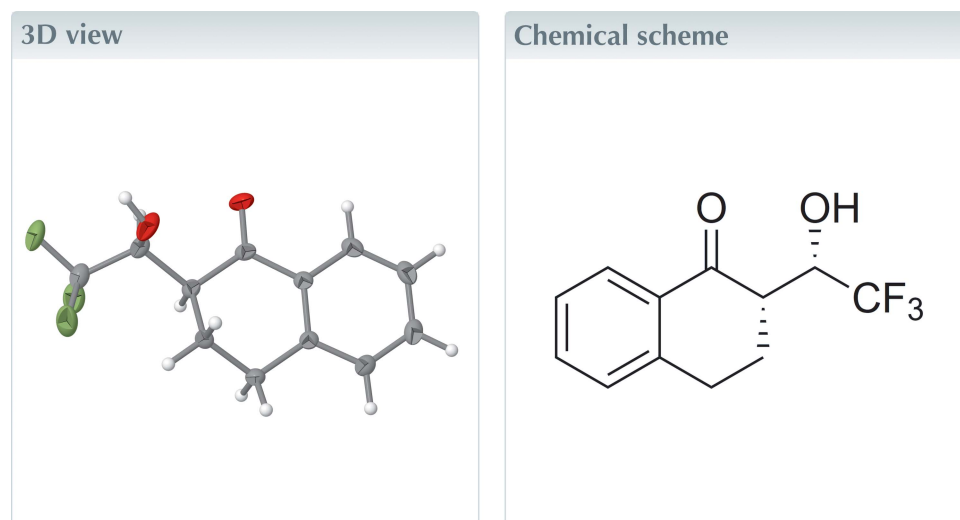
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Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure of the title compound, C₁₂H₁₁F₃O₂, was elucidated by low-temperature single-crystal X-ray diffraction. The enantiopure compound crystallizes in the Sohncke space group *P*2₁ and features one molecule in the asymmetric unit. The structure displays intermolecular O—H...O hydrogen bonding, which links the molecules into infinite chains propagating parallel to [010]. The absolute configuration was established from anomalous dispersion.



Structure description

Dynamic kinetic resolution (DKR) based on Ru^{II}-catalyzed Noyori–Ikariya asymmetric transfer hydrogenation (ATH) has proven to be a highly efficient strategy for the stereoconvergent synthesis of secondary alcohols (Cotman, 2021). The commercial availability of a wide range of Ru^{II} catalysts, comparatively mild reaction conditions, and the ability to use racemic mixtures of ketones as starting materials make this approach particularly attractive for the synthesis of β -substituted benzyl alcohols, which have been shown to be valuable building blocks for pharmaceuticals and can crystallize as homochiral single-component mechanically responsive crystals that exhibit elastic or plastic flexibility (Cotman *et al.*, 2019, 2022). When ATH of non-symmetric CF₃-substituted 1,3-diketones was attempted, it was found that two consecutive DKR–ATH reactions can occur and that diastereo- and enantiopure 1,3-diols can be obtained in a one-pot process (Cotman *et al.*, 2016). The use of milder reaction conditions enabled the preparation of mono-reduced alcohols, which include the title compound.

(S)-2-[(S)-2,2,2-trifluoro-1-hydroxyethyl]-1-tetralone crystallizes in the monoclinic space group *P*2₁ with one molecule in the asymmetric unit (Fig. 1). The cyclohexanone ring adopts a half-boat (envelope) conformation (Cremer & Pople, 1975), with atoms C1,



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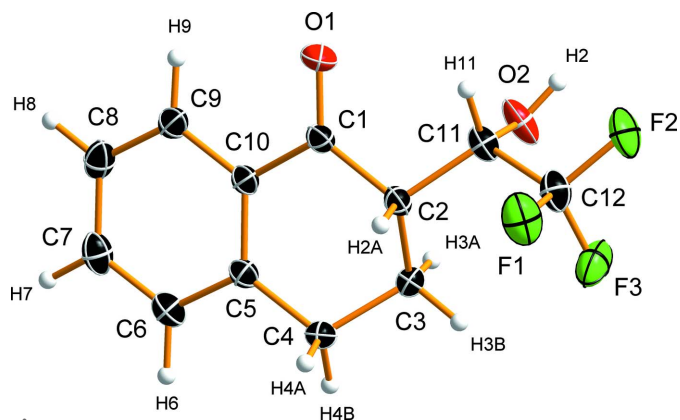


Figure 1
Molecular structure of the title compound and the atom-labeling scheme. Displacement ellipsoids are shown at the 50% probability level and hydrogen atoms are depicted as spheres of arbitrary radius.

C2, C4, C5, and C10 being essentially coplanar (r.m.s.d. of 0.007 Å), whereas the C3 atom is located 0.683 (2) Å below this plane. Moreover, the atoms of the planar part of the cyclohexanone ring are essentially coplanar with the aromatic ring. The dihedral angle between the planes (plane normals) is 2.01 (6)° and the r.m.s.d. of the plane defined by atoms C1, C2, C4–C10 is 0.019 Å. A similar half-boat conformation was previously observed in the structure of (±)-1-tetralone-3-carboxylic acid (CSD refcode QIJGAR), whereas the related (±)-1-tetralone-2-acetic acid (QIJGEV) exhibits a half-chair conformation (Barcon *et al.*, 2001).

In the crystal structure of the title compound, intermolecular O–H···O hydrogen bonds with an O···O distance of 2.7548 (16) Å (Table 1), involving hydroxyl and carbonyl groups of the adjacent molecules related by the 2_1 screw axis, link the molecules into infinite zigzag chains propagating parallel to [010] (Figs. 2, 3). The graph-set motif of the chains is C(6) (Etter *et al.*, 1990).

Synthesis and crystallization

The title compound was prepared from 2-trifluoroacetyl-1-tetralone (242 mg, 1.0 mmol) added to a HCO₂H/Et₃N 5:2

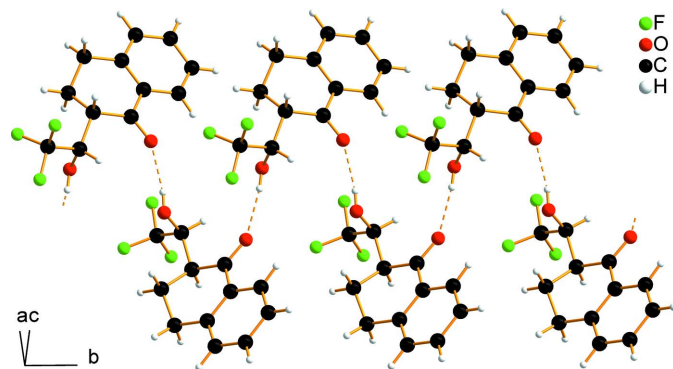


Figure 2
Intermolecular O–H···O=C hydrogen bonds connect the molecules into infinite zigzag chains running parallel to [010].

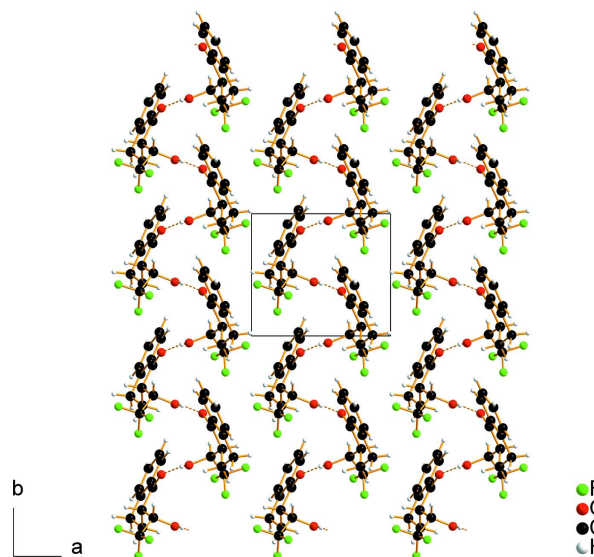
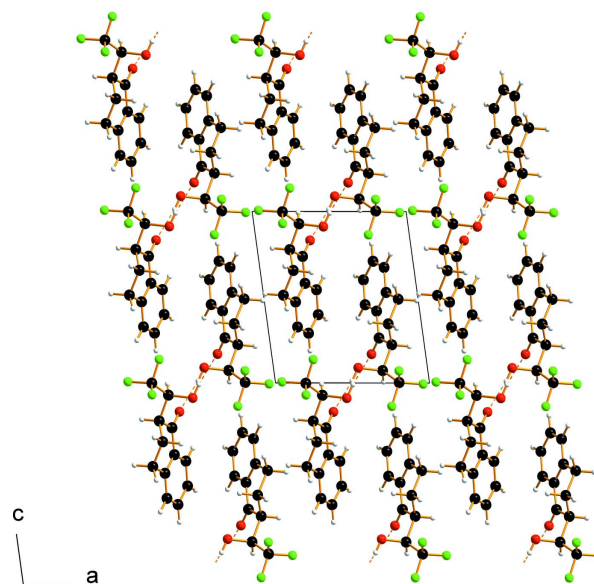
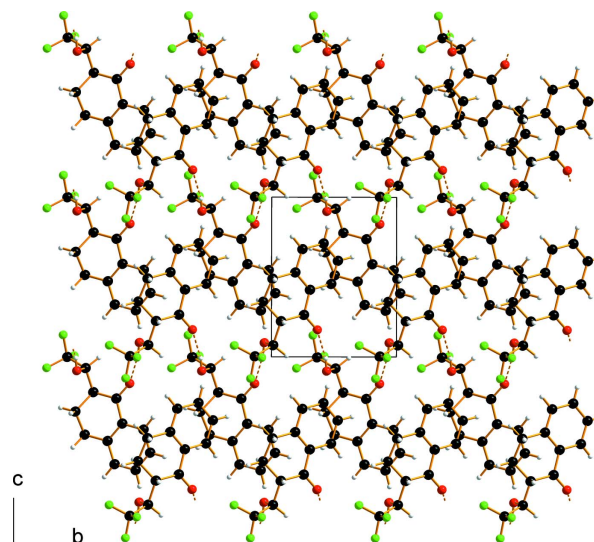


Figure 3
Packing diagrams of the title compound viewed along [100] (top), [010] (middle), and [001] (bottom).

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2\cdots O1^i$	0.79 (3)	1.97 (3)	2.7548 (16)	168 (3)

Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + 2$.

(0.5 ml) solution containing the active (*S,S*)-diphenylethylenediamine-based Ru^{II} catalyst with an S:C ratio of 2000:1 (Cotman *et al.*, 2016). Upon addition of the co-solvent chlorobenzene (1 ml), the mixture was warmed to 40 °C and stirred for 23 h, while being continuously flushed with N₂. The resulting mixture was partitioned between EtOAc (10 ml) and H₂O (5 ml), with the organic layer later washed with H₂O (5 ml) and brine (5 ml), filtered through a bed of silica gel/Na₂SO₄, and concentrated. The procedure resulted in the formation of a crude white product (239 mg, 98% yield), containing the title compound (d.r. = 89:11, 72% ee) and 2.5% of the corresponding diol. After purification by flash chromatography (hexane/EtOAc gradient 9:1 to 7:1), the diastereomerically pure monoalcohol was isolated (157 mg, 64% yield). The enantiomeric excess was upgraded to >99% by crystallization from cyclohexane (109 mg, 45% yield). Crystals suitable for single-crystal X-ray diffraction analysis were grown from a chloroform solution. A suitable crystal was selected under a polarizing microscope and mounted on a MiTeGen Dual Thickness MicroLoop LD using Baysilone-Paste (Bayer-Silicone, mittelviskos).

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. The positions of the hydrogen atoms were freely refined, including their isotropic displacement parameter U (Cooper *et al.*, 2010). The absolute configuration was established as *S,S* for C2 and C11, respectively, based on the anomalous dispersion effects [Flack x = -0.07 (3); Hooft y = -0.04 (2); Parsons *et al.*, 2013; Hooft *et al.*, 2008].

Funding information

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₁₁ F ₃ O ₂
M_r	244.21
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	8.23147 (11), 7.16385 (9), 9.24494 (14)
β (°)	97.8459 (13)
V (Å ³)	540.06 (1)
Z	2
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	1.18
Crystal size (mm)	0.16 × 0.10 × 0.07
Data collection	
Diffractometer	XtaLAB Synergy-S, Dualflex, Eiger2 R CdTe 1M
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Rigaku OD, 2022)
T_{\min}, T_{\max}	0.832, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13577, 2210, 2186
R_{int}	0.025
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.022, 0.056, 1.06
No. of reflections	2210
No. of parameters	198
No. of restraints	1
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.14, -0.14
Absolute structure	Flack x determined using 976 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.07 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SUPERFLIP* (Palatinus & Chapuis, 2007; Palatinus & van der Lee, 2008; Palatinus *et al.*, 2012), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *DIAMOND* (Brandenburg, 2005), and *publCIF* (Westrip, 2010).

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full crystallographic data

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(S)-2-[(S)-2,2,2-Trifluoro-1-hydroxyethyl]-1-tetralone

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(S)-2-[(S)-2,2,2-Trifluoro-1-hydroxyethyl]-1-tetralone*Crystal data*

$C_{12}H_{11}F_3O_2$

$M_r = 244.21$

Monoclinic, $P2_1$

$a = 8.23147$ (11) Å

$b = 7.16385$ (9) Å

$c = 9.24494$ (14) Å

$\beta = 97.8459$ (13)°

$V = 540.06$ (1) Å³

$Z = 2$

$F(000) = 252$

$D_x = 1.502$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 11151 reflections

$\theta = 4.8$ – 75.9 °

$\mu = 1.18$ mm⁻¹

$T = 100$ K

Irregular, colourless

$0.16 \times 0.10 \times 0.07$ mm

Data collection

XtaLAB Synergy-S, Dualflex, Eiger2 R CdTe

1M

diffractometer

Radiation source: micro-focus sealed X-ray

tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 13.3333 pixels mm⁻¹

ω scans

Absorption correction: gaussian

(CrysAlisPro; Rigaku OD, 2022)

$T_{\min} = 0.832$, $T_{\max} = 1.000$

13577 measured reflections

2210 independent reflections

2186 reflections with $I > 2\sigma(I)$

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

$\theta_{\max} = 76.0$ °, $\theta_{\min} = 4.8$ °

$h = -10$ → 10

$k = -9$ → 8

$l = -11$ → 11

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.056$

$S = 1.06$

2210 reflections

198 parameters

1 restraint

Primary atom site location: iterative

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0312P)^2 + 0.0761P]$

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

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

$\Delta\rho_{\max} = 0.14$ e Å⁻³

$\Delta\rho_{\min} = -0.14$ e Å⁻³

Absolute structure: Flack x determined using

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

Absolute structure parameter: -0.07 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. Standard uncertainties involving l.s. planes were estimated using ShelXL matrix (within Olex2). 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
F2	0.26550 (14)	0.33275 (16)	1.13591 (11)	0.0382 (3)
F1	0.04271 (12)	0.42167 (17)	1.00572 (12)	0.0399 (3)
F3	0.18733 (16)	0.20130 (15)	0.92934 (12)	0.0410 (3)
O1	0.35100 (16)	0.86561 (17)	0.83139 (13)	0.0334 (3)
O2	0.44946 (14)	0.4422 (2)	0.91134 (13)	0.0332 (3)
C10	0.27986 (17)	0.8069 (2)	0.58052 (17)	0.0193 (3)
C1	0.28808 (18)	0.7590 (2)	0.73748 (16)	0.0213 (3)
C5	0.20219 (17)	0.6892 (2)	0.47174 (16)	0.0189 (3)
C2	0.21111 (17)	0.5750 (2)	0.77698 (16)	0.0201 (3)
C9	0.34870 (17)	0.9768 (2)	0.54318 (18)	0.0239 (3)
C6	0.19256 (18)	0.7460 (2)	0.32605 (17)	0.0240 (3)
C12	0.1966 (2)	0.3660 (2)	0.99739 (17)	0.0276 (3)
C3	0.21572 (18)	0.4307 (2)	0.65536 (16)	0.0209 (3)
C11	0.29360 (18)	0.5124 (2)	0.92764 (16)	0.0239 (3)
C8	0.33780 (18)	1.0304 (2)	0.3984 (2)	0.0279 (3)
C4	0.12924 (17)	0.5066 (2)	0.51106 (16)	0.0219 (3)
C7	0.25885 (19)	0.9149 (3)	0.28981 (18)	0.0277 (3)
H2A	0.099 (2)	0.599 (3)	0.786 (2)	0.020 (4)*
H3A	0.332 (2)	0.396 (3)	0.6443 (19)	0.019 (4)*
H4B	0.140 (2)	0.413 (3)	0.432 (2)	0.024 (4)*
H11	0.298 (2)	0.619 (3)	0.993 (2)	0.024 (5)*
H9	0.406 (2)	1.054 (3)	0.620 (2)	0.028 (5)*
H4A	0.010 (2)	0.524 (3)	0.519 (2)	0.020 (4)*
H3B	0.165 (2)	0.314 (3)	0.680 (2)	0.030 (5)*
H6	0.138 (2)	0.665 (3)	0.247 (2)	0.026 (5)*
H7	0.253 (2)	0.948 (3)	0.188 (2)	0.034 (5)*
H8	0.385 (3)	1.146 (3)	0.374 (2)	0.033 (5)*
H2	0.501 (3)	0.433 (4)	0.990 (3)	0.051 (7)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F2	0.0466 (6)	0.0452 (6)	0.0231 (5)	0.0074 (5)	0.0064 (4)	0.0138 (4)
F1	0.0298 (5)	0.0523 (7)	0.0399 (6)	0.0069 (5)	0.0137 (4)	0.0133 (5)
F3	0.0648 (7)	0.0252 (5)	0.0356 (6)	-0.0015 (5)	0.0162 (5)	0.0049 (4)
O1	0.0438 (7)	0.0273 (6)	0.0248 (5)	-0.0048 (5)	-0.0104 (5)	-0.0034 (5)
O2	0.0229 (5)	0.0555 (8)	0.0204 (5)	0.0102 (5)	0.0001 (4)	0.0107 (5)
C10	0.0154 (6)	0.0193 (7)	0.0221 (7)	0.0025 (5)	-0.0008 (5)	0.0012 (5)
C1	0.0201 (6)	0.0207 (7)	0.0212 (7)	0.0022 (5)	-0.0039 (5)	-0.0006 (6)
C5	0.0156 (6)	0.0211 (7)	0.0197 (7)	0.0016 (5)	0.0011 (5)	0.0002 (5)
C2	0.0189 (7)	0.0222 (7)	0.0184 (7)	0.0012 (6)	-0.0007 (5)	0.0025 (6)
C9	0.0179 (6)	0.0201 (7)	0.0322 (8)	0.0009 (5)	-0.0017 (6)	0.0021 (6)
C6	0.0219 (7)	0.0296 (8)	0.0206 (7)	0.0026 (6)	0.0028 (5)	0.0005 (6)
C12	0.0304 (8)	0.0305 (9)	0.0226 (7)	0.0066 (6)	0.0064 (6)	0.0045 (6)
C3	0.0232 (7)	0.0173 (6)	0.0216 (7)	-0.0021 (6)	0.0009 (5)	0.0017 (6)

C11	0.0236 (7)	0.0290 (8)	0.0186 (7)	0.0038 (6)	0.0012 (5)	0.0032 (6)
C8	0.0202 (6)	0.0260 (8)	0.0377 (9)	-0.0009 (6)	0.0041 (6)	0.0093 (7)
C4	0.0233 (7)	0.0211 (7)	0.0200 (7)	-0.0037 (6)	-0.0011 (5)	-0.0009 (6)
C7	0.0244 (7)	0.0339 (8)	0.0257 (8)	0.0048 (7)	0.0072 (6)	0.0086 (7)

Geometric parameters (Å, °)

F2—C12	1.3490 (18)	C9—C8	1.383 (2)
F1—C12	1.3405 (19)	C9—H9	0.97 (2)
F3—C12	1.335 (2)	C6—C7	1.387 (2)
O1—C1	1.2176 (19)	C6—H6	0.99 (2)
O2—C11	1.4053 (18)	C12—C11	1.514 (2)
O2—H2	0.79 (3)	C3—C4	1.5241 (19)
C10—C1	1.484 (2)	C3—H3A	1.006 (18)
C10—C5	1.398 (2)	C3—H3B	0.97 (2)
C10—C9	1.405 (2)	C11—H11	0.98 (2)
C1—C2	1.528 (2)	C8—C7	1.392 (3)
C5—C6	1.399 (2)	C8—H8	0.95 (2)
C5—C4	1.505 (2)	C4—H4B	1.00 (2)
C2—C3	1.531 (2)	C4—H4A	1.005 (19)
C2—C11	1.531 (2)	C7—H7	0.96 (2)
C2—H2A	0.956 (19)		
C11—O2—H2	108 (2)	F3—C12—F1	107.23 (14)
C5—C10—C1	121.31 (13)	F3—C12—C11	114.29 (13)
C5—C10—C9	120.36 (14)	C2—C3—H3A	111.1 (11)
C9—C10—C1	118.31 (13)	C2—C3—H3B	110.7 (12)
O1—C1—C10	120.71 (15)	C4—C3—C2	110.27 (12)
O1—C1—C2	121.37 (14)	C4—C3—H3A	109.6 (10)
C10—C1—C2	117.90 (12)	C4—C3—H3B	110.3 (12)
C10—C5—C6	118.53 (14)	H3A—C3—H3B	104.7 (16)
C10—C5—C4	120.58 (12)	O2—C11—C2	107.78 (12)
C6—C5—C4	120.89 (13)	O2—C11—C12	109.84 (13)
C1—C2—C3	110.74 (12)	O2—C11—H11	113.2 (12)
C1—C2—C11	108.84 (12)	C2—C11—H11	108.1 (12)
C1—C2—H2A	107.6 (12)	C12—C11—C2	113.33 (12)
C3—C2—H2A	107.9 (11)	C12—C11—H11	104.8 (12)
C11—C2—C3	114.71 (12)	C9—C8—C7	119.65 (15)
C11—C2—H2A	106.8 (11)	C9—C8—H8	119.7 (13)
C10—C9—H9	118.9 (12)	C7—C8—H8	120.7 (13)
C8—C9—C10	120.21 (14)	C5—C4—C3	111.57 (12)
C8—C9—H9	120.8 (12)	C5—C4—H4B	109.4 (11)
C5—C6—H6	120.1 (12)	C5—C4—H4A	109.5 (11)
C7—C6—C5	120.92 (15)	C3—C4—H4B	108.6 (11)
C7—C6—H6	118.9 (12)	C3—C4—H4A	109.1 (11)
F2—C12—C11	110.43 (13)	H4B—C4—H4A	108.5 (15)
F1—C12—F2	106.02 (12)	C6—C7—C8	120.31 (15)
F1—C12—C11	112.07 (13)	C6—C7—H7	118.7 (13)

F3—C12—F2	106.31 (13)	C8—C7—H7	120.9 (13)
F2—C12—C11—O2	66.50 (16)	C1—C2—C11—O2	-75.25 (16)
F2—C12—C11—C2	-172.89 (13)	C1—C2—C11—C12	162.99 (13)
F1—C12—C11—O2	-175.54 (13)	C5—C10—C1—O1	-177.41 (14)
F1—C12—C11—C2	-54.93 (18)	C5—C10—C1—C2	0.9 (2)
F3—C12—C11—O2	-53.29 (17)	C5—C10—C9—C8	1.0 (2)
F3—C12—C11—C2	67.31 (18)	C5—C6—C7—C8	0.6 (2)
O1—C1—C2—C3	-153.04 (14)	C2—C3—C4—C5	56.14 (16)
O1—C1—C2—C11	-26.05 (19)	C9—C10—C1—O1	1.0 (2)
C10—C1—C2—C3	28.63 (17)	C9—C10—C1—C2	179.31 (12)
C10—C1—C2—C11	155.61 (13)	C9—C10—C5—C6	-1.0 (2)
C10—C5—C6—C7	0.2 (2)	C9—C10—C5—C4	179.61 (13)
C10—C5—C4—C3	-26.80 (19)	C9—C8—C7—C6	-0.5 (2)
C10—C9—C8—C7	-0.3 (2)	C6—C5—C4—C3	153.81 (14)
C1—C10—C5—C6	177.35 (14)	C3—C2—C11—O2	49.43 (17)
C1—C10—C5—C4	-2.1 (2)	C3—C2—C11—C12	-72.34 (16)
C1—C10—C9—C8	-177.34 (14)	C11—C2—C3—C4	179.52 (12)
C1—C2—C3—C4	-56.81 (15)	C4—C5—C6—C7	179.58 (13)

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O2—H2...O1 ⁱ	0.79 (3)	1.97 (3)	2.7548 (16)	168 (3)

Symmetry code: (i) $-x+1, y-1/2, -z+2$.