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(1*S*,2*S*)-2-[(*S*)-2,2,2-Trifluoro-1-hydroxyethyl]-1-tetralol

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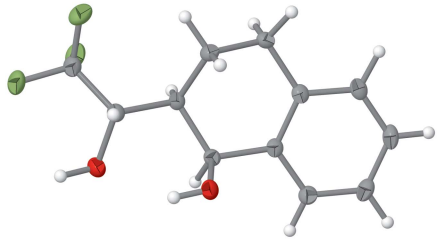
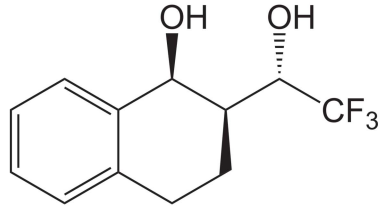
The crystal structure of the title enantiopure tetralol derivative {systematic name: (1*S*,2*S*)-2-[(*S*)-2,2,2-trifluoro-1-hydroxyethyl]-1,2,3,4-tetrahydronaphthalen-1-ol}, $C_{12}H_{13}F_3O_2$, synthesized by asymmetric transfer hydrogenation, was elucidated by low-temperature single-crystal X-ray diffraction. The enantiopure compound crystallizes in the Sohncke space group $P2_12_12_1$ with one molecule in the asymmetric unit and features intramolecular as well as intermolecular O—H···O hydrogen bonding. The absolute configuration was established from anomalous dispersion effects.

3D view



Chemical scheme



Structure description

Homochiral fluorinated alcohols, which are considered to be emerging structural motifs in medicinal chemistry (Cotman, 2021), can be obtained in high yields employing dynamic kinetic resolution (DKR) with Noyori–Ikariya asymmetric transfer hydrogenation (ATH) (Betancourt *et al.*, 2021; Cotman *et al.* 2022; Molina Betancourt *et al.*, 2022). When Ru^{II}-catalyzed DKR–ATH was applied to CF_3CO-substituted benzofused cyclic ketones, it was observed that single or double reduction occurs, yielding either diastereo- and enantiopure monoalcohols or 1,3-diols (Cotman *et al.*, 2016). The crystal structure of the mono-reduced product (*S*)-2-[(*S*)-2,2,2-trifluoro-1-hydroxyethyl]-1-tetralone has been described previously (Motaln *et al.*, 2023) and herein the crystal structure of the corresponding diol is presented.

(1*S*,2*S*)-2-[(*S*)-2,2,2-Trifluoro-1-hydroxyethyl]-1-tetralol crystallizes in the orthorhombic $P2_12_12_1$ space group with one molecule in the asymmetric unit (Fig. 1). The cyclohexanol ring adopts a half-chair conformation (Cremer & Pople, 1975), with the C2 atom located 0.251 (3) Å below and the C3 atom 0.497 (4) Å above the plane defined by atoms C1, C4, C5, and C10 (r.m.s.d. of 0.013 Å). This plane is essentially coplanar with the

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.83 (4)	2.23 (4)	2.854 (2)	133 (3)
O2—H2···O1^{i}	0.94 (4)	1.87 (4)	2.789 (2)	168 (3)

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

aromatic ring – the angle between the plane normals is 2.79 (9)° and the r.m.s. deviation of the plane defined by all coplanar atoms C1, C4–C10 is 0.025 Å. Tetralol derivatives with similar half-chair conformations have been reported, for example, 2,2,2-trifluoro-*N*-(1-hydroxy-1,2,3,4-tetrahydronaphthalen-2-yl)acetamide (CSD refcode ALUXUC; Miyazawa *et al.*, 2016), (1*S*,2*S*)-7-methoxy-2-(trifluoromethyl)-1-tetralol (YEDBOC; Cotman *et al.*, 2022), and plastically flexible (1*R*,2*S*)-2-(trifluoromethylthio)-1-tetralol (YEDCAP; Cotman *et al.*, 2022).

In the crystal of the title compound, intramolecular and intermolecular O—H···O hydrogen bonds with O···O distances of 2.854 (2) and 2.789 (2) Å, respectively, link adjacent molecules related by the 2_1 screw axis, into chains parallel to [010] (Table 1 and Figs. 2 and 3). The graph-set motifs of the hydrogen bonds are *S*(6) and *C*(6) (Etter *et al.*, 1990).

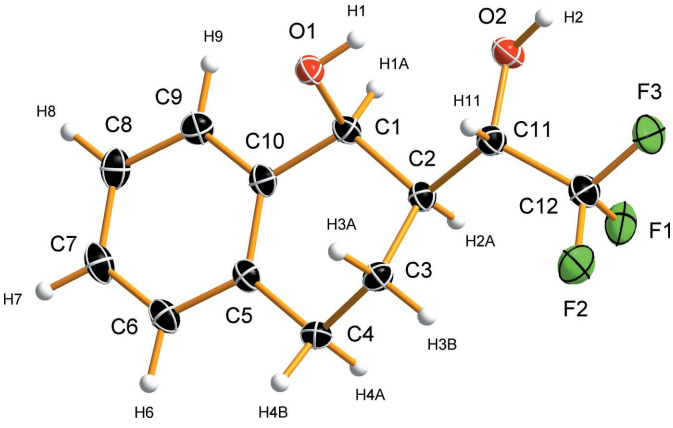


Figure 1
Molecular structure of (1*S*,2*S*)-2-[(*S*)-2,2,2-trifluoro-1-hydroxyethyl]-1-tetralol showing the atom-labeling scheme. Thermal displacement ellipsoids are drawn at the 50% probability level and the hydrogen atoms are shown as spheres of arbitrary radius.

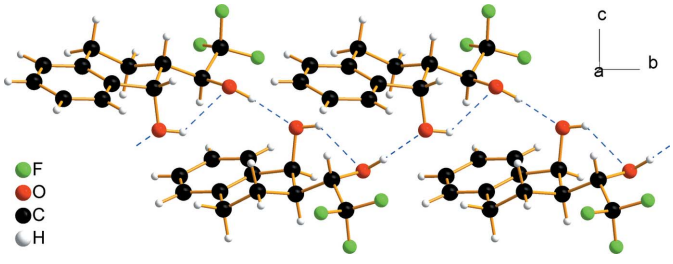


Figure 2
Helical hydrogen-bonded chain extending parallel to [010] that involves intermolecular and intramolecular O—H···O hydrogen bonds, which are indicated by blue dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{13}F_3O_2$
M_r	246.22
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, b, c (Å)	7.75558 (10), 9.02843 (10), 15.5656 (2)
V (Å^3)	1089.92 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.17
Crystal size (mm)	0.08 × 0.07 × 0.06
Data collection	
Diffractometer	XtaLAB Synergy-S, Dualflex, Eiger2 R CdTe 1M
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.886, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38720, 2273, 2255
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.073, 1.06
No. of reflections	2273
No. of parameters	207
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.17
Absolute structure	Flack x determined using 929 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.06 (5)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *OLEX2.solve* (Dolomanov *et al.*, 2009), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009), *DIAMOND* (Brandenburg, 2005) and *publCIF* (Westrip, 2010).

Synthesis and crystallization

The title compound was prepared from 2-trifluoroacetyl-1-tetralone (100 mg, 0.412 mmol) added to a HCO_2H/Et_3N 3:2 (0.21 ml) solution containing the active (*S*,*S*)-diphenylethyl-

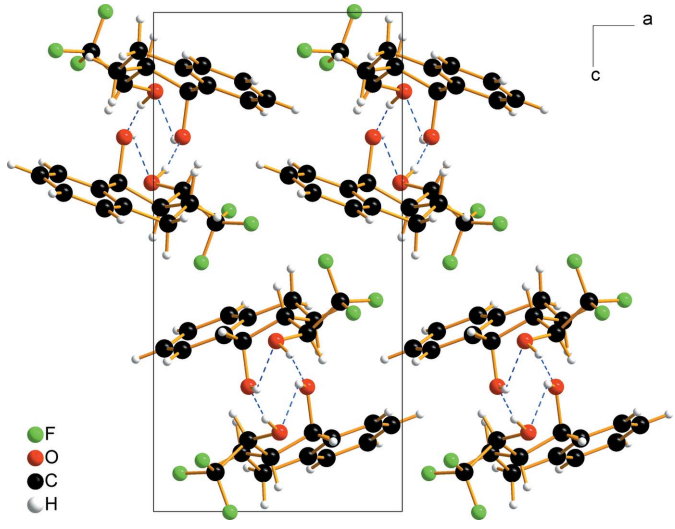


Figure 3
Molecular packing of the title compound viewed along [010]. The helical hydrogen-bonded chains are shown by blue dashed lines.

enediamine-based Ru^{II} catalyst with an S/C ratio of 1000:1 (Cotman *et al.*, 2016). Upon addition of the co-solvent chlorobenzene (0.55 ml), the mixture was warmed to 60 °C and stirred for 24 h, while being continuously flushed with N_2. The resulting mixture was partitioned between EtOAc (10 ml) and H_2O (5 ml), with the organic layer later washed with H_2O (5 ml) and brine (5 ml), filtered through a bed of silica gel/Na_2SO_4, and concentrated. The crude product was recrystallized from a 5:1 mixture of petroleum ether and diethyl ether affording colorless prisms (37 mg; 36% yield; diastereomeric ratio 97:3:0:0; enantiomeric excess >99.9%). A suitable crystal was selected under a polarizing microscope and attached to a MiTeGen Dual Thickness MicroLoop using Baysilone-Paste (Bayer-Silicone, mittelviskos) as the adhesive.

Refinement

The crystal data, data collection, and structure refinement details are summarized in Table 2. The positions of the hydrogen atoms and their isotropic displacement parameter *U* were freely refined (Cooper *et al.*, 2010). The absolute configuration was established as *S*,*S*,*S* for C1, C2, and C11, respectively, based on anomalous dispersion effects [Flack x = 0.06 (5); Hooft y = 0.07 (3)] (Parsons *et al.*, 2013; Hooft *et al.*, 2008).

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References

Betancourt, R. M., Phansavath, P. & Ratovelomanana-Vidal, V. (2021). *J. Org. Chem.* **86**, 12054–12063.
Brandenburg, K. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Cooper, R. I., Thompson, A. L. & Watkin, D. J. (2010). *J. Appl. Cryst.* **43**, 1100–1107.
Cotman, A. E. (2021). *Chem. Eur. J.* **27**, 39–53.
Cotman, A. E., Cahard, D. & Mohar, B. (2016). *Angew. Chem. Int. Ed.* **55**, 5294–5298.
Cotman, A. E., Dub, P. A., Sterle, M., Lozinšek, M., Dernovšek, J., Zajec, Ž., Zega, A., Tomašič, T. & Cahard, D. (2022). *ACS Org. Inorg. Au*, **2**, 396–404.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Hooft, R. W. W., Straver, L. H. & Spek, A. L. (2008). *J. Appl. Cryst.* **41**, 96–103.
Miyazawa, K., Koike, T. & Akita, M. (2016). *Tetrahedron*, **72**, 7813–7820.
Molina Betancourt, R., Bacheley, L., Karapetyan, A., Guillamot, G., Phansavath, P. & Ratovelomanana–Vidal, V. (2022). *ChemCatChem*, **14**, e202200595.
Motaln, K., Cotman, A. E. & Lozinšek, M. (2023). *IUCrData*, **8**, x221209.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Rigaku OD (2022). *CrysAlis PRO*. Rigaku Corporation, Wrocław, Poland.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2023). **8**, x230217 [https://doi.org/10.1107/S2414314623002171]

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(1*S*,2*S*)-2-[(*S*)-2,2,2-Trifluoro-1-hydroxyethyl]-1,2,3,4-tetrahydronaphthalen-1-ol

Crystal data

$C_{12}H_{13}F_3O_2$
M_r = 246.22
Orthorhombic, $P2_12_12_1$
a = 7.75558 (10) Å
b = 9.02843 (10) Å
c = 15.5656 (2) Å
V = 1089.92 (2) Å^3
Z = 4
F(000) = 512
D_x = 1.501 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 29238 reflections
θ = 2.9–75.7°
μ = 1.17 mm^{-1}
T = 100 K
Cube, colourless
0.08 × 0.07 × 0.06 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} = 0.886, T_{max} = 1.000
38720 measured reflections
2273 independent reflections
2255 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 76.1°, θ_{min} = 5.7°
h = −9→8
k = −11→11
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
S = 1.06
2273 reflections
207 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 0.4546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL-2019/2 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0016 (4)
Absolute structure: Flack x determined using 929 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.06 (5)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F3	0.80337 (19)	0.85568 (15)	0.60230 (9)	0.0345 (3)
F1	0.69235 (19)	0.72956 (16)	0.49867 (9)	0.0322 (3)
O2	0.49295 (19)	0.76829 (16)	0.65842 (10)	0.0237 (3)
F2	0.89287 (17)	0.63500 (16)	0.57649 (10)	0.0355 (4)
O1	0.38269 (19)	0.51110 (16)	0.74976 (9)	0.0198 (3)
C5	0.3786 (3)	0.2240 (2)	0.61093 (12)	0.0179 (4)
C1	0.3588 (2)	0.4939 (2)	0.65812 (12)	0.0171 (4)
C10	0.2838 (3)	0.3406 (2)	0.64639 (12)	0.0178 (4)
C12	0.7506 (3)	0.7194 (2)	0.57933 (14)	0.0248 (5)
C4	0.5590 (3)	0.2478 (2)	0.57692 (13)	0.0203 (4)
C11	0.6192 (3)	0.6587 (2)	0.64276 (13)	0.0201 (4)
C9	0.1166 (3)	0.3148 (2)	0.67633 (14)	0.0211 (4)
C8	0.0440 (3)	0.1739 (3)	0.67329 (14)	0.0243 (4)
C3	0.6458 (3)	0.3820 (2)	0.61755 (13)	0.0196 (4)
C7	0.1391 (3)	0.0578 (2)	0.63868 (14)	0.0239 (4)
C2	0.5296 (2)	0.5175 (2)	0.60927 (13)	0.0178 (4)
C6	0.3043 (3)	0.0827 (2)	0.60742 (13)	0.0212 (4)
H11	0.680 (4)	0.646 (3)	0.6961 (16)	0.025 (7)*
H6	0.369 (3)	−0.005 (3)	0.5850 (16)	0.024 (6)*
H9	0.055 (4)	0.395 (3)	0.6995 (17)	0.028 (7)*
H8	−0.071 (4)	0.156 (3)	0.6950 (17)	0.031 (7)*
H3A	0.666 (3)	0.359 (3)	0.6794 (16)	0.023 (6)*
H1A	0.277 (3)	0.570 (3)	0.6402 (15)	0.015 (5)*
H4A	0.553 (4)	0.266 (3)	0.5136 (17)	0.029 (7)*
H2A	0.498 (3)	0.534 (3)	0.5494 (16)	0.022 (6)*
H4B	0.623 (3)	0.155 (3)	0.5878 (17)	0.029 (7)*
H7	0.094 (4)	−0.037 (3)	0.6371 (18)	0.031 (7)*
H3B	0.757 (3)	0.401 (3)	0.5896 (17)	0.024 (6)*
H1	0.415 (4)	0.598 (4)	0.755 (2)	0.053 (10)*
H2	0.549 (5)	0.848 (4)	0.685 (2)	0.059 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F3	0.0359 (7)	0.0259 (7)	0.0418 (7)	−0.0144 (6)	0.0096 (6)	−0.0073 (6)
F1	0.0371 (7)	0.0326 (7)	0.0271 (6)	−0.0095 (6)	0.0025 (6)	0.0059 (5)
O2	0.0221 (7)	0.0175 (7)	0.0314 (8)	0.0003 (6)	0.0003 (6)	−0.0025 (6)
F2	0.0200 (6)	0.0358 (8)	0.0507 (8)	−0.0024 (6)	0.0095 (6)	0.0009 (6)
O1	0.0238 (7)	0.0168 (7)	0.0189 (7)	−0.0023 (6)	0.0006 (6)	−0.0005 (6)

C5	0.0196 (9)	0.0172 (9)	0.0170 (8)	0.0007 (8)	−0.0039 (8)	0.0016 (7)
C1	0.0167 (9)	0.0158 (8)	0.0187 (9)	0.0013 (8)	−0.0009 (7)	−0.0002 (7)
C10	0.0180 (9)	0.0169 (9)	0.0184 (8)	0.0001 (8)	−0.0029 (7)	0.0025 (7)
C12	0.0261 (11)	0.0212 (10)	0.0273 (10)	−0.0053 (8)	0.0028 (8)	−0.0042 (8)
C4	0.0203 (10)	0.0178 (9)	0.0230 (10)	0.0025 (7)	0.0034 (8)	−0.0008 (8)
C11	0.0192 (9)	0.0181 (9)	0.0230 (9)	−0.0007 (8)	0.0010 (8)	−0.0015 (8)
C9	0.0178 (9)	0.0218 (10)	0.0236 (9)	0.0006 (8)	−0.0016 (8)	0.0010 (8)
C8	0.0186 (10)	0.0270 (10)	0.0273 (10)	−0.0064 (8)	−0.0037 (8)	0.0050 (9)
C3	0.0155 (8)	0.0211 (9)	0.0222 (9)	0.0006 (7)	0.0017 (8)	−0.0002 (8)
C7	0.0262 (11)	0.0189 (10)	0.0267 (10)	−0.0067 (8)	−0.0090 (9)	0.0023 (8)
C2	0.0180 (9)	0.0163 (8)	0.0192 (9)	−0.0014 (7)	0.0001 (8)	−0.0005 (7)
C6	0.0258 (10)	0.0169 (9)	0.0207 (9)	−0.0003 (8)	−0.0053 (8)	0.0010 (8)

Geometric parameters (Å, º)

F3—C12	1.345 (2)	C4—H4A	1.00 (3)
F1—C12	1.338 (3)	C4—H4B	0.99 (3)
O2—C11	1.413 (2)	C11—C2	1.542 (3)
O2—H2	0.94 (4)	C11—H11	0.96 (3)
F2—C12	1.342 (3)	C9—C8	1.392 (3)
O1—C1	1.447 (2)	C9—H9	0.94 (3)
O1—H1	0.83 (4)	C8—C7	1.390 (3)
C5—C10	1.398 (3)	C8—H8	0.96 (3)
C5—C4	1.511 (3)	C3—C2	1.525 (3)
C5—C6	1.401 (3)	C3—H3A	1.00 (3)
C1—C10	1.512 (3)	C3—H3B	0.98 (3)
C1—C2	1.542 (3)	C7—C6	1.389 (3)
C1—H1A	0.98 (2)	C7—H7	0.93 (3)
C10—C9	1.397 (3)	C2—H2A	0.98 (3)
C12—C11	1.522 (3)	C6—H6	1.00 (3)
C4—C3	1.524 (3)		
C11—O2—H2	107 (2)	O2—C11—H11	106.0 (16)
C1—O1—H1	103 (2)	C12—C11—C2	112.35 (17)
C10—C5—C4	121.21 (17)	C12—C11—H11	105.9 (16)
C10—C5—C6	119.02 (18)	C2—C11—H11	114.5 (17)
C6—C5—C4	119.76 (18)	C10—C9—H9	117.8 (17)
O1—C1—C10	105.47 (15)	C8—C9—C10	121.10 (19)
O1—C1—C2	111.18 (15)	C8—C9—H9	121.1 (17)
O1—C1—H1A	106.8 (14)	C9—C8—H8	120.9 (17)
C10—C1—C2	113.45 (16)	C7—C8—C9	119.2 (2)
C10—C1—H1A	111.3 (14)	C7—C8—H8	119.9 (17)
C2—C1—H1A	108.5 (14)	C4—C3—C2	110.02 (16)
C5—C10—C1	122.30 (17)	C4—C3—H3A	107.8 (16)
C9—C10—C5	119.60 (18)	C4—C3—H3B	110.2 (15)
C9—C10—C1	118.03 (17)	C2—C3—H3A	110.1 (15)
F3—C12—C11	111.16 (18)	C2—C3—H3B	109.8 (15)
F1—C12—F3	106.85 (18)	H3A—C3—H3B	109 (2)

F1—C12—F2	106.60 (18)	C8—C7—H7	120.7 (17)
F1—C12—C11	114.03 (18)	C6—C7—C8	120.20 (19)
F2—C12—F3	106.17 (17)	C6—C7—H7	119.1 (17)
F2—C12—C11	111.57 (18)	C1—C2—C11	109.55 (16)
C5—C4—C3	112.12 (16)	C1—C2—H2A	105.9 (15)
C5—C4—H4A	109.0 (16)	C11—C2—H2A	108.1 (15)
C5—C4—H4B	106.6 (16)	C3—C2—C1	110.76 (16)
C3—C4—H4A	107.5 (16)	C3—C2—C11	111.62 (16)
C3—C4—H4B	112.4 (16)	C3—C2—H2A	110.7 (15)
H4A—C4—H4B	109 (2)	C5—C6—H6	121.9 (14)
O2—C11—C12	108.89 (16)	C7—C6—C5	120.86 (19)
O2—C11—C2	108.96 (16)	C7—C6—H6	117.2 (14)
F3—C12—C11—O2	47.8 (2)	C10—C1—C2—C11	−165.55 (16)
F3—C12—C11—C2	168.61 (17)	C10—C1—C2—C3	−42.0 (2)
F1—C12—C11—O2	−73.1 (2)	C10—C9—C8—C7	−0.9 (3)
F1—C12—C11—C2	47.8 (2)	C12—C11—C2—C1	−159.85 (17)
O2—C11—C2—C1	−39.1 (2)	C12—C11—C2—C3	77.1 (2)
O2—C11—C2—C3	−162.14 (16)	C4—C5—C10—C1	−4.0 (3)
F2—C12—C11—O2	166.11 (16)	C4—C5—C10—C9	179.31 (17)
F2—C12—C11—C2	−73.1 (2)	C4—C5—C6—C7	179.64 (17)
O1—C1—C10—C5	−108.6 (2)	C4—C3—C2—C1	62.5 (2)
O1—C1—C10—C9	68.1 (2)	C4—C3—C2—C11	−175.18 (16)
O1—C1—C2—C11	−46.9 (2)	C9—C8—C7—C6	−0.1 (3)
O1—C1—C2—C3	76.7 (2)	C8—C7—C6—C5	0.7 (3)
C5—C10—C9—C8	1.5 (3)	C2—C1—C10—C5	13.3 (3)
C5—C4—C3—C2	−52.3 (2)	C2—C1—C10—C9	−169.99 (17)
C1—C10—C9—C8	−175.33 (19)	C6—C5—C10—C1	175.72 (17)
C10—C5—C4—C3	23.6 (3)	C6—C5—C10—C9	−1.0 (3)
C10—C5—C6—C7	−0.1 (3)	C6—C5—C4—C3	−156.10 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.83 (4)	2.23 (4)	2.854 (2)	133 (3)
O2—H2···O1^{i}	0.94 (4)	1.87 (4)	2.789 (2)	168 (3)

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+3/2.