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Crystal structure and Hirshfeld surface analysis of 1,3,3,4,4,5,5-heptafluoro-2-(3-[(2,3,3,4,4,5,5-heptafluorocyclopenten-1-yl)oxy]-2-{[(2,3,3,4,4,5,5-heptafluorocyclopenten-1-yl)oxy]methyl}-2-methylpropoxy)cyclopentene

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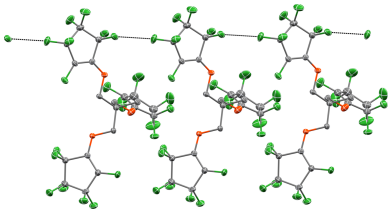
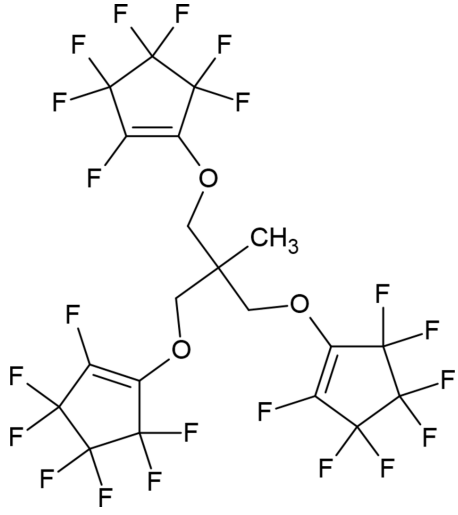
In the title compound, $C_{20}H_9F_{21}O_3$, a central sp^3-hybridized carbon atom is decorated with three heptafluoro-2-methyloxy(cyclopent-1-ene) arms and a methyl group. The primary packing is determined by C—F···F—C interactions, forming [001] chains, which are consolidated *via* weaker C—F···F—C and C—H···F—C contacts. A Hirshfeld surface analysis was conducted to aid in the visualization of these various influences on the packing: this revealed that the largest contribution to the surface contacts arises from F···F interactions (53.5%), followed by F···H/H···F (34.5%) and F···C/C···F (7.1%).

1. Chemical context

Perfluorocyclopentene (C_5F_8; PFCP) is known to be selectively reactive towards nucleophilic addition at the fluoroolefin, *via* simultaneous addition at the 1- and 5-positions or controlled to only add at the 1-position (Alvino *et al.*, 2020). In the former case, the fluorine atom in the 5-position is latently reactive and can be utilized to create more complex fluorinated molecules and materials (Lauer *et al.*, 2024). As such, the synthesis and single-crystal structure of the title compound, $C_{20}H_9F_2O_3$, is reported herein. This molecule was designed to be tri-functional, in that it contains three latently reactive fluorine atoms, which could be employed in designing more complex materials, such as a dendrimer core or for cross-linking (Abbasi *et al.*, 2014; Weerasinghe *et al.*, 2023).





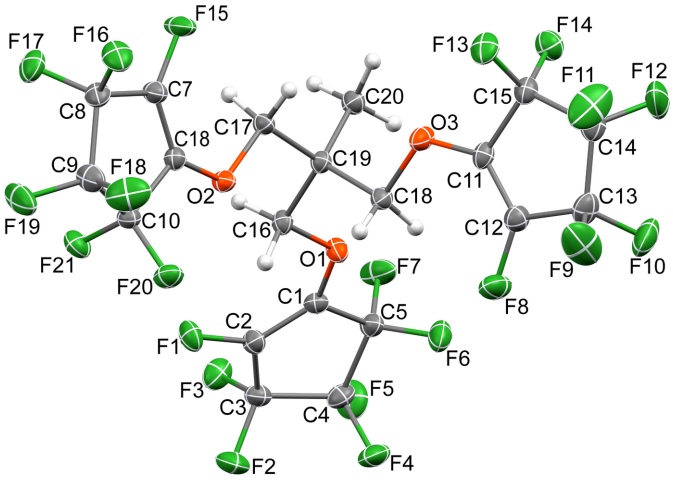


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are shown at the 50% probability level.

2. Structural commentary

The structure of the title highly fluorinated alkyl ether molecule, $C_{20}H_9F_{21}O_3$, consists of a central sp^3-hybridized carbon atom (C19) covalently bound to a methyl group (C20) and three heptafluoro-2-methyloxy(cyclopent-1-ene) arms (Fig. 1). The geometry around C19 is nearly that of an ideal tetrahedral sp^3 geometry, with an average C—C—C bond angle of 109.47°. Using a plane defined by C16, C17 and C18, the three non-methyl carbon atoms bound to the sp^3 carbon atom as reference, two of the ether oxygen atoms (O1 and O3) are oriented to the methyl side of the plane, with the third ether oxygen atom (O2) below the plane. Within the cyclopentenyl rings, the C=C double-bond lengths range from 1.328 (3) to 1.334 (3) Å. The C—C single bonds to either side of the C=C double bond are approximately 0.15 Å longer, ranging from 1.478 (3) to 1.497 (2) Å. The final two C—C single bonds in the ring are longer yet, ranging from 1.537 (3) to 1.554 (3) Å. The r.m.s. cyclopentenyl ring plane angle with respect to the plane defined by its corresponding $C_{ether}—Csp^3—C_{methyl}$ fragment range from 14.62 (15) to 40.25 (13)°.

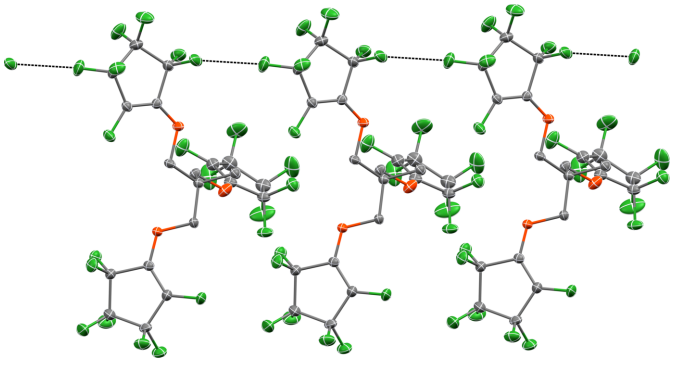


Figure 2
Part of the packing of the title compound showing chains formed by short C—F···F—C interactions, propagating along the *a*-axis direction.

Table 1
Percentage contribution of inter-atomic contacts to the Hirshfeld surface for the title compound.

Contact	Percentage contribution
F···F	53.5
F···H/H···F	34.5
F···C/C···F	7.1
F···O/O···F	3.0
H···H	2.1

3. Supramolecular features

The primary directional interaction in the extended structure occurs as a short C—F···F—C interaction between F2 and F7^{i} [symmetry code: (i) $x-1, y, z$] at 2.5983 (16) Å, compared to a van der Waals separation of about 2.94 Å. This interaction contributes to the formation of chains propagating along the *a*-axis direction (Fig. 2). The packing is consolidated in the crystallographic *c*-axis direction *via* a weak C—F···F—C interaction between F7 and F13^{ii} [symmetry code: (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$] at 2.6848 (15) Å and in the *b*-axis direction by a C—H···F hydrogen bond between C17—H17*A* and F9^{iii} [symmetry code: (iii) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$] at 2.546 (2) Å [angle = 127.61 (14)°].

Hirshfeld surface analysis was used to investigate the presence of hydrogen bonds and intermolecular interactions in the crystal structure. The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (Spackman & McKinnon, 2002) were generated by *CrystalExplorer17.5* (Turner *et al.*, 2017), using a standard surface resolution. The pale-red spots symbolize short contacts and negative d_{norm} values on the corresponding surface plots shown in Fig. 3, associated with their relative contributions to the Hirshfeld surface.

The largest contribution to the overall crystal packing in the title compound is from F···F interactions (53.3%), repre-

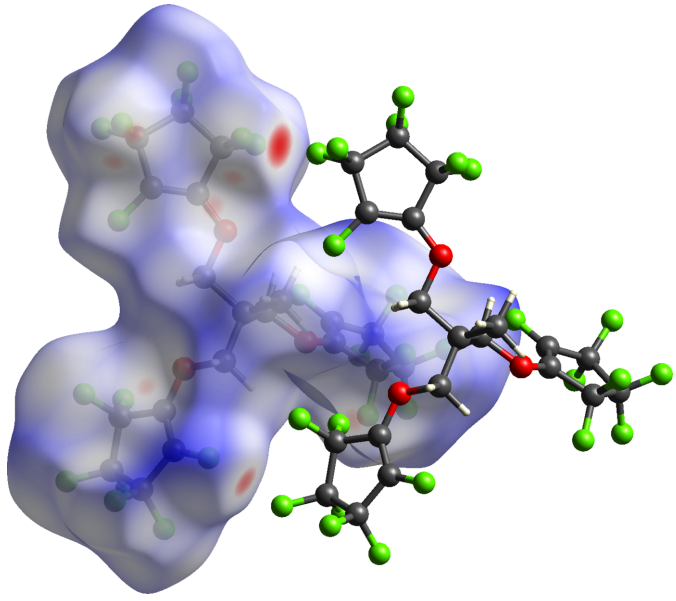


Figure 3
Map of d_{norm} onto the Hirshfeld surface for the title compound.

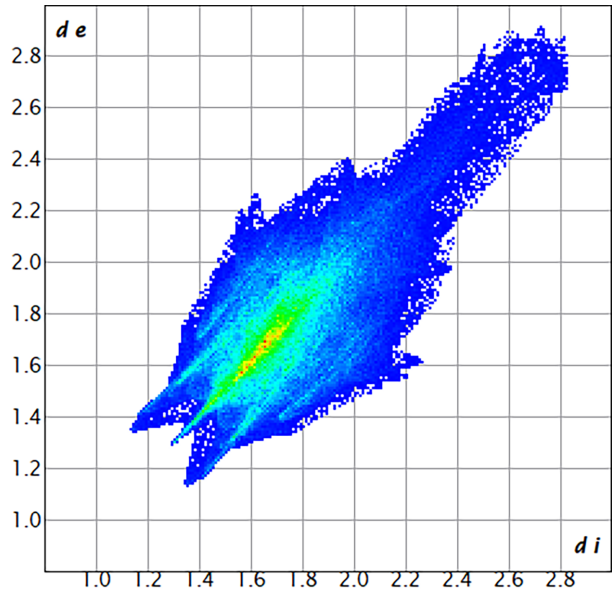


Figure 4
The overall two-dimensional fingerprint plot for the title compound.

sented as a single, central spike on the fingerprint plot at 1.30 Å < (d_i + d_e) < 1.35 Å (Fig. 4, Table 1). A significant portion of the intermolecular interactions can also be attributed to F···H/H···F interactions (34.5%), visible on the fingerprint plot as a pair of spikes at 1.15 Å < (d_i + d_e) < 1.35 Å. The remaining 12% of the interactions are attributed to F···C/C···F, F···O/O···F, and H···H contacts.

4. Database survey

A search of the November 2023 release of the Cambridge Structure Database (CSD; Groom *et al.*, 2016), with updates through September 2024, was performed using the program *ConQuest* (Bruno *et al.*, 2002). A for search the perfluorocyclopentene-ether moiety yielded one result, 4,4′-bis-[(2,3,3,4,4,5,5-heptafluorocyclopent-1-en-1-yl)oxy]biphenyl (CSD refcode GILXUW; Sharma *et al.*, 2013). This compound contains a pair of perfluorocyclopentenyl rings bound through an ether linkage to a 4,4′-bisphenol aromatic core. A short ring C═C bond is observed, flanked by two medium length C—C bonds and two long C—C bonds to complete the ring, similar to the pattern observed in the title compound. A search for the non-fluorinated analog yielded four results. While the C═C double bond is clearly observed, the remaining four C—C bonds within the ring are more similar in bond length to one another.

5. Synthesis and crystallization

The title compound was prepared by a modified literature procedure (Alvino *et al.*, 2020) using dimethylformamide (DMF) (20 ml), perfluorocyclopentene (3.0 ml, 22.4 mmol), trimethylolethane (0.81 g, 6.7 mmol), and triethylamine (2.8 ml, 20.2 mmol). The isolated compound (1.0 g) was purified using a plug of silica gel and 80 ml of a 1:3 hexane:ethyl acetate solution. All volatiles were removed under reduced pressure and the compound was obtained as a faint yellow, waxy solid (0.57 g, 57%). Crystals of the title compound, in the form of faint-yellow rectangular prisms, were obtained by slow evaporation from diethyl ether solution. ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.37 (*d*, –CH_2–, 6H, J_{HF} = 2.5 Hz), 1.25 (*s*, –CH_3, 3H); ^{19}F NMR (470 MHz, $CDCl_3$): δ −115.2 (*d*, 6F, J_{FF} = 12.7 MHz), −115.8 (*d*, 6F, J_{FF} = 10.8), −129.4 (*s*, 6F), −158.2 (*bs*, 3F); ^{13}C NMR (125 MHz, $CDCl_3$): δ 72.9 {*d*, –[(–CH_2)$_3$$CCH_3$], J_{CF} = 4.5 Hz], 41.3 [–(CH_2)$_3$$CCH_3$], 15.8 [–($CH_2$)$_3$$CCH_3$].

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_9F_{21}O_3$
M_r	696.26
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.0271 (1), 19.2243 (1), 17.7558 (1)
β (°)	97.332 (1)
V (Å^3)	2379.04 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.21
Crystal size (mm)	0.23 × 0.09 × 0.07
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix3000
Absorption correction	Gaussian [*CrysAlis PRO*; Rigaku OD, 2019)
T_{min}, T_{max}	0.681, 1.000
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	23552, 4403, 4160
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.605
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.088, 1.07
No. of reflections	4403
No. of parameters	398
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.90, −0.49

Computer programs: *CrysAlis PRO* (Rigaku OD, 2019), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The coordinates of all H atoms were freely refined.

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Crystal structure and Hirshfeld surface analysis of 1,3,3,4,4,5,5-hepta-fluoro-2-(3-[(2,3,3,4,4,5,5-heptafluorocyclopenten-1-yl)oxy]-2-{[(2,3,3,4,4,5,5-heptafluorocyclopenten-1-yl)oxy]methyl}-2-methylpropoxy)cyclopentene

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Computing details

1,3,3,4,4,5,5-Heptafluoro-2-(3-[(2,3,3,4,4,5,5-heptafluorocyclopenten-1-yl)oxy]-2-{[(2,3,3,4,4,5,5-heptafluorocyclopenten-1-yl)oxy]methyl}-2-methylpropoxy)cyclopentene

Crystal data

$C_{20}H_9F_{21}O_3$
M_r = 696.26
Monoclinic, $P2_1/c$
a = 7.0271 (1) Å
b = 19.2243 (1) Å
c = 17.7558 (1) Å
β = 97.332 (1)°
V = 2379.04 (4) Å^3
Z = 4
$F(000)$ = 1376.511
D_x = 1.944 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 18314 reflections
θ = 3.4–68.7°
μ = 2.21 mm^{-1}
T = 100 K
Needle, colourless
0.23 × 0.09 × 0.07 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
φ and ω scans
Absorption correction: gaussian [CrysAlisPro; Rigaku OD, 2019)
T_{min} = 0.681, T_{max} = 1.000
23552 measured reflections
4403 independent reflections
4160 reflections with $I \geq 2u(I)$
R_{int} = 0.020
θ_{max} = 68.9°, θ_{min} = 3.4°
h = −8→8
k = −23→21
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.088
S = 1.07
4403 reflections
398 parameters
0 restraints
13 constraints
Primary atom site location: dual
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 2.693P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.16671 (15)	0.06887 (6)	0.41851 (6)	0.0265 (3)
F2	0.05627 (16)	0.07023 (7)	0.56596 (7)	0.0360 (3)
F3	0.26356 (18)	−0.01232 (6)	0.56315 (6)	0.0303 (3)
F4	0.29905 (18)	0.15059 (7)	0.64289 (7)	0.0370 (3)
F5	0.4531 (2)	0.05472 (7)	0.67162 (7)	0.0394 (3)
F6	0.60320 (18)	0.18574 (7)	0.58931 (7)	0.0332 (3)
F7	0.69217 (16)	0.07832 (7)	0.57776 (7)	0.0364 (3)
F8	0.54974 (18)	0.40300 (6)	0.39070 (8)	0.0365 (3)
F9	0.6667 (2)	0.53068 (7)	0.32545 (11)	0.0556 (4)
F10	0.8592 (2)	0.50227 (8)	0.42497 (8)	0.0489 (4)
F11	0.9283 (3)	0.51416 (7)	0.24445 (8)	0.0562 (4)
F12	1.12533 (19)	0.48847 (7)	0.34431 (9)	0.0490 (4)
F13	0.92808 (17)	0.38965 (6)	0.20407 (6)	0.0300 (3)
F14	1.11525 (16)	0.36215 (6)	0.30559 (7)	0.0284 (3)
F15	0.53049 (15)	0.16320 (7)	0.06431 (6)	0.0321 (3)
F16	0.26253 (17)	0.22500 (7)	−0.04917 (6)	0.0322 (3)
F17	0.17650 (18)	0.11897 (6)	−0.03126 (6)	0.0321 (3)
F18	0.0027 (2)	0.27674 (7)	0.01901 (7)	0.0436 (3)
F19	−0.13285 (18)	0.17587 (9)	0.00174 (7)	0.0481 (4)
F20	−0.00523 (15)	0.25007 (6)	0.15861 (6)	0.0261 (2)
F21	−0.03121 (15)	0.13923 (6)	0.14101 (7)	0.0276 (3)
O1	0.54484 (17)	0.15167 (7)	0.43624 (7)	0.0201 (3)
O2	0.34863 (17)	0.18994 (7)	0.21007 (7)	0.0187 (3)
O3	0.7469 (2)	0.29766 (7)	0.29659 (8)	0.0249 (3)
C1	0.4486 (2)	0.12012 (9)	0.48619 (10)	0.0176 (4)
C2	0.2853 (3)	0.08400 (10)	0.48122 (10)	0.0192 (4)
C3	0.2388 (3)	0.05780 (10)	0.55538 (11)	0.0223 (4)
C4	0.3839 (3)	0.09592 (10)	0.61344 (10)	0.0237 (4)
C5	0.5398 (3)	0.12188 (10)	0.56695 (10)	0.0215 (4)
C6	0.2748 (2)	0.18792 (9)	0.13720 (10)	0.0172 (4)
C7	0.3486 (3)	0.17718 (10)	0.07275 (10)	0.0210 (4)
C8	0.2073 (3)	0.18092 (10)	0.00375 (10)	0.0226 (4)
C9	0.0244 (3)	0.20780 (12)	0.03398 (11)	0.0276 (4)
C10	0.0619 (3)	0.19687 (10)	0.12074 (10)	0.0192 (4)
C11	0.7822 (3)	0.36440 (9)	0.31298 (10)	0.0196 (4)
C12	0.7004 (3)	0.41170 (10)	0.35294 (11)	0.0234 (4)
C13	0.7921 (3)	0.48097 (10)	0.35442 (12)	0.0291 (4)
C14	0.9557 (3)	0.47250 (10)	0.30511 (12)	0.0280 (4)
C15	0.9490 (3)	0.39496 (10)	0.28019 (10)	0.0210 (4)
C16	0.4700 (2)	0.14610 (9)	0.35623 (10)	0.0178 (4)
H16a	0.4625 (2)	0.09673 (9)	0.34028 (10)	0.0213 (4)*
H16b	0.3401 (2)	0.16670 (9)	0.34662 (10)	0.0213 (4)*
C17	0.5524 (2)	0.17454 (9)	0.22766 (10)	0.0173 (4)
H17a	0.5779 (2)	0.12577 (9)	0.21408 (10)	0.0208 (4)*
H17b	0.6280 (2)	0.20554 (9)	0.19828 (10)	0.0208 (4)*

C18	0.5989 (3)	0.26292 (9)	0.33273 (10)	0.0190 (4)
H18a	0.6218 (3)	0.26940 (9)	0.38846 (10)	0.0229 (4)*
H18b	0.4709 (3)	0.28201 (9)	0.31370 (10)	0.0229 (4)*
C19	0.6095 (2)	0.18591 (9)	0.31262 (10)	0.0163 (3)
C20	0.8146 (2)	0.15762 (10)	0.33228 (10)	0.0200 (4)
H20a	0.8608 (8)	0.1678 (6)	0.3856 (2)	0.0300 (6)*
H20b	0.8145 (4)	0.10719 (14)	0.3242 (7)	0.0300 (6)*
H20c	0.8992 (5)	0.1798 (5)	0.2996 (5)	0.0300 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0214 (5)	0.0330 (6)	0.0232 (6)	−0.0069 (5)	−0.0039 (4)	0.0037 (5)
F2	0.0233 (6)	0.0477 (8)	0.0402 (7)	−0.0013 (5)	0.0156 (5)	−0.0023 (6)
F3	0.0451 (7)	0.0206 (6)	0.0263 (6)	−0.0036 (5)	0.0084 (5)	0.0029 (5)
F4	0.0411 (7)	0.0335 (7)	0.0409 (7)	−0.0024 (6)	0.0230 (6)	−0.0146 (6)
F5	0.0514 (8)	0.0411 (7)	0.0236 (6)	−0.0063 (6)	−0.0031 (5)	0.0101 (5)
F6	0.0387 (7)	0.0368 (7)	0.0247 (6)	−0.0157 (5)	0.0061 (5)	−0.0092 (5)
F7	0.0242 (6)	0.0605 (9)	0.0230 (6)	0.0171 (6)	−0.0028 (5)	−0.0048 (6)
F8	0.0366 (7)	0.0267 (6)	0.0502 (8)	−0.0005 (5)	0.0211 (6)	−0.0091 (6)
F9	0.0435 (8)	0.0204 (6)	0.1018 (13)	0.0097 (6)	0.0048 (8)	0.0101 (7)
F10	0.0689 (10)	0.0416 (8)	0.0381 (8)	−0.0207 (7)	0.0138 (7)	−0.0219 (6)
F11	0.1066 (13)	0.0237 (7)	0.0411 (8)	0.0014 (8)	0.0204 (8)	0.0155 (6)
F12	0.0346 (7)	0.0389 (8)	0.0721 (10)	−0.0132 (6)	0.0020 (7)	−0.0240 (7)
F13	0.0411 (7)	0.0338 (7)	0.0151 (5)	−0.0073 (5)	0.0034 (5)	0.0020 (5)
F14	0.0254 (6)	0.0282 (6)	0.0307 (6)	0.0003 (5)	0.0002 (5)	0.0029 (5)
F15	0.0181 (5)	0.0552 (8)	0.0241 (6)	0.0040 (5)	0.0071 (4)	−0.0070 (5)
F16	0.0359 (6)	0.0416 (7)	0.0197 (6)	−0.0083 (5)	0.0063 (5)	0.0070 (5)
F17	0.0421 (7)	0.0334 (7)	0.0202 (6)	−0.0071 (5)	0.0017 (5)	−0.0064 (5)
F18	0.0531 (8)	0.0464 (8)	0.0319 (7)	0.0215 (7)	0.0074 (6)	0.0164 (6)
F19	0.0238 (6)	0.0941 (12)	0.0253 (6)	−0.0156 (7)	−0.0009 (5)	−0.0091 (7)
F20	0.0235 (5)	0.0290 (6)	0.0264 (6)	0.0072 (5)	0.0047 (4)	−0.0029 (5)
F21	0.0226 (5)	0.0294 (6)	0.0316 (6)	−0.0074 (5)	0.0064 (5)	0.0031 (5)
O1	0.0202 (6)	0.0251 (7)	0.0148 (6)	−0.0052 (5)	0.0014 (5)	0.0013 (5)
O2	0.0167 (6)	0.0251 (7)	0.0139 (6)	0.0018 (5)	0.0008 (5)	−0.0010 (5)
O3	0.0336 (7)	0.0160 (6)	0.0279 (7)	−0.0067 (6)	0.0146 (6)	−0.0047 (5)
C1	0.0179 (8)	0.0187 (8)	0.0167 (9)	0.0029 (7)	0.0036 (7)	0.0011 (7)
C2	0.0171 (8)	0.0213 (9)	0.0183 (9)	0.0011 (7)	−0.0006 (7)	0.0001 (7)
C3	0.0211 (9)	0.0226 (9)	0.0244 (10)	0.0010 (7)	0.0079 (7)	0.0003 (8)
C4	0.0306 (10)	0.0238 (10)	0.0175 (9)	0.0019 (8)	0.0064 (8)	−0.0005 (7)
C5	0.0187 (9)	0.0267 (10)	0.0187 (9)	0.0010 (7)	0.0012 (7)	−0.0036 (8)
C6	0.0184 (8)	0.0170 (8)	0.0159 (8)	−0.0009 (7)	0.0012 (7)	0.0008 (7)
C7	0.0176 (8)	0.0265 (10)	0.0194 (9)	−0.0002 (7)	0.0042 (7)	−0.0009 (7)
C8	0.0259 (9)	0.0283 (10)	0.0142 (8)	−0.0044 (8)	0.0050 (7)	0.0005 (7)
C9	0.0211 (9)	0.0411 (12)	0.0197 (10)	0.0005 (8)	−0.0009 (7)	0.0026 (8)
C10	0.0186 (9)	0.0216 (9)	0.0179 (9)	−0.0001 (7)	0.0045 (7)	−0.0004 (7)
C11	0.0266 (9)	0.0153 (9)	0.0162 (8)	−0.0025 (7)	0.0001 (7)	0.0004 (7)
C12	0.0263 (9)	0.0199 (9)	0.0244 (10)	−0.0006 (8)	0.0042 (8)	−0.0005 (8)

C13	0.0358 (11)	0.0162 (9)	0.0342 (11)	0.0024 (8)	0.0009 (9)	−0.0031 (8)
C14	0.0366 (11)	0.0192 (10)	0.0274 (10)	−0.0065 (8)	0.0015 (8)	0.0037 (8)
C15	0.0271 (9)	0.0193 (9)	0.0162 (9)	−0.0022 (7)	0.0012 (7)	0.0022 (7)
C16	0.0191 (8)	0.0196 (9)	0.0139 (8)	−0.0026 (7)	−0.0009 (7)	0.0004 (7)
C17	0.0146 (8)	0.0201 (9)	0.0171 (8)	0.0011 (7)	0.0013 (6)	−0.0011 (7)
C18	0.0212 (9)	0.0170 (9)	0.0198 (9)	−0.0035 (7)	0.0061 (7)	−0.0012 (7)
C19	0.0176 (8)	0.0161 (9)	0.0151 (8)	−0.0007 (7)	0.0015 (6)	−0.0002 (7)
C20	0.0184 (8)	0.0215 (9)	0.0195 (9)	0.0009 (7)	0.0004 (7)	−0.0003 (7)

Geometric parameters (Å, º)

F1—C2	1.335 (2)	C1—C5	1.495 (2)
F2—C3	1.341 (2)	C2—C3	1.485 (3)
F3—C3	1.364 (2)	C3—C4	1.540 (3)
F4—C4	1.347 (2)	C4—C5	1.536 (3)
F5—C4	1.343 (2)	C6—C7	1.331 (3)
F6—C5	1.349 (2)	C6—C10	1.497 (2)
F7—C5	1.354 (2)	C7—C8	1.477 (3)
F8—C12	1.334 (2)	C8—C9	1.543 (3)
F9—C13	1.356 (2)	C9—C10	1.544 (3)
F10—C13	1.345 (3)	C11—C12	1.328 (3)
F11—C14	1.336 (2)	C11—C15	1.494 (3)
F12—C14	1.337 (2)	C12—C13	1.478 (3)
F13—C15	1.345 (2)	C13—C14	1.540 (3)
F14—C15	1.354 (2)	C14—C15	1.554 (3)
F15—C7	1.333 (2)	C16—H16a	0.9900
F16—C8	1.358 (2)	C16—H16b	0.9900
F17—C8	1.348 (2)	C16—C19	1.530 (2)
F18—C9	1.357 (3)	C17—H17a	0.9900
F19—C9	1.328 (2)	C17—H17b	0.9900
F20—C10	1.342 (2)	C17—C19	1.527 (2)
F21—C10	1.359 (2)	C18—H18a	0.9900
O1—C1	1.329 (2)	C18—H18b	0.9900
O1—C16	1.454 (2)	C18—C19	1.527 (2)
O2—C6	1.332 (2)	C19—C20	1.538 (2)
O2—C17	1.457 (2)	C20—H20a	0.9800
O3—C11	1.332 (2)	C20—H20b	0.9800
O3—C18	1.453 (2)	C20—H20c	0.9800
C1—C2	1.334 (3)		

C16—O1—C1	117.84 (13)	C15—C11—C12	110.70 (16)
C17—O2—C6	116.93 (13)	C11—C12—F8	127.44 (17)
C18—O3—C11	118.06 (14)	C13—C12—F8	118.43 (17)
C2—C1—O1	134.45 (17)	C13—C12—C11	114.13 (17)
C5—C1—O1	115.95 (15)	F10—C13—F9	105.80 (17)
C5—C1—C2	109.57 (16)	C12—C13—F9	111.57 (17)
C1—C2—F1	127.48 (17)	C12—C13—F10	113.02 (18)
C3—C2—F1	118.77 (15)	C14—C13—F9	110.79 (18)

C3—C2—C1	113.75 (16)	C14—C13—F10	111.31 (17)
F3—C3—F2	105.90 (15)	C14—C13—C12	104.47 (16)
C2—C3—F2	112.73 (16)	F12—C14—F11	108.02 (17)
C2—C3—F3	112.67 (15)	C13—C14—F11	110.69 (18)
C4—C3—F2	112.63 (15)	C13—C14—F12	111.12 (17)
C4—C3—F3	109.73 (15)	C15—C14—F11	110.45 (16)
C4—C3—C2	103.32 (15)	C15—C14—F12	111.18 (17)
F5—C4—F4	107.25 (15)	C15—C14—C13	105.40 (15)
C3—C4—F4	110.08 (16)	F14—C15—F13	106.17 (15)
C3—C4—F5	112.23 (16)	C11—C15—F13	111.80 (15)
C5—C4—F4	109.66 (16)	C11—C15—F14	111.93 (15)
C5—C4—F5	113.06 (16)	C14—C15—F13	110.77 (15)
C5—C4—C3	104.57 (14)	C14—C15—F14	111.00 (15)
F7—C5—F6	107.20 (15)	C14—C15—C11	105.26 (15)
C1—C5—F6	112.84 (16)	H16a—C16—O1	110.45 (9)
C1—C5—F7	110.89 (15)	H16b—C16—O1	110.45 (9)
C4—C5—F6	111.66 (15)	H16b—C16—H16a	108.6
C4—C5—F7	109.16 (16)	C19—C16—O1	106.40 (13)
C4—C5—C1	105.08 (14)	C19—C16—H16a	110.45 (9)
C7—C6—O2	133.91 (17)	C19—C16—H16b	110.45 (9)
C10—C6—O2	116.23 (15)	H17a—C17—O2	110.09 (9)
C10—C6—C7	109.82 (16)	H17b—C17—O2	110.09 (9)
C6—C7—F15	127.73 (17)	H17b—C17—H17a	108.4
C8—C7—F15	117.98 (15)	C19—C17—O2	108.07 (13)
C8—C7—C6	114.29 (16)	C19—C17—H17a	110.09 (9)
F17—C8—F16	105.98 (14)	C19—C17—H17b	110.09 (9)
C7—C8—F16	112.53 (16)	H18a—C18—O3	110.44 (9)
C7—C8—F17	113.01 (16)	H18b—C18—O3	110.44 (9)
C9—C8—F16	110.84 (16)	H18b—C18—H18a	108.6
C9—C8—F17	111.36 (16)	C19—C18—O3	106.45 (14)
C9—C8—C7	103.24 (15)	C19—C18—H18a	110.44 (9)
F19—C9—F18	107.48 (17)	C19—C18—H18b	110.44 (9)
C8—C9—F18	109.68 (16)	C17—C19—C16	108.89 (14)
C8—C9—F19	112.29 (17)	C18—C19—C16	108.24 (14)
C10—C9—F18	109.21 (16)	C18—C19—C17	110.82 (14)
C10—C9—F19	113.19 (16)	C20—C19—C16	110.53 (14)
C10—C9—C8	104.95 (15)	C20—C19—C17	107.11 (14)
F21—C10—F20	106.06 (14)	C20—C19—C18	111.24 (14)
C6—C10—F20	113.34 (15)	H20a—C20—C19	109.5
C6—C10—F21	110.95 (15)	H20b—C20—C19	109.5
C9—C10—F20	111.73 (15)	H20b—C20—H20a	109.5
C9—C10—F21	110.42 (15)	H20c—C20—C19	109.5
C9—C10—C6	104.44 (14)	H20c—C20—H20a	109.5
C12—C11—O3	134.00 (18)	H20c—C20—H20b	109.5
C15—C11—O3	115.30 (16)		

F1—C2—C1—O1	0.3 (3)	F14—C15—C14—C13	−119.26 (16)
F1—C2—C1—C5	−177.52 (19)	F15—C7—C6—O2	1.5 (3)

F1—C2—C3—F2	−48.42 (18)	F15—C7—C6—C10	−176.0 (2)
F1—C2—C3—F3	71.38 (17)	F15—C7—C8—F16	−52.69 (18)
F1—C2—C3—C4	−170.27 (17)	F15—C7—C8—F17	67.32 (18)
F2—C3—C2—C1	132.64 (16)	F15—C7—C8—C9	−172.25 (19)
F2—C3—C4—F4	−21.91 (17)	F16—C8—C7—C6	127.91 (17)
F2—C3—C4—F5	97.46 (16)	F16—C8—C9—F18	−19.40 (16)
F2—C3—C4—C5	−139.63 (16)	F16—C8—C9—F19	100.03 (16)
F3—C3—C2—C1	−107.57 (17)	F16—C8—C9—C10	−136.61 (16)
F3—C3—C4—F4	−139.60 (14)	F17—C8—C7—C6	−112.08 (16)
F3—C3—C4—F5	−20.24 (16)	F17—C8—C9—F18	−137.13 (15)
F3—C3—C4—C5	102.68 (15)	F17—C8—C9—F19	−17.70 (17)
F4—C4—C3—C2	100.02 (16)	F17—C8—C9—C10	105.67 (16)
F4—C4—C5—F6	23.43 (17)	F18—C9—C8—C7	101.32 (16)
F4—C4—C5—F7	141.78 (15)	F18—C9—C10—F20	23.24 (17)
F4—C4—C5—C1	−99.23 (16)	F18—C9—C10—F21	141.03 (15)
F5—C4—C3—C2	−140.61 (16)	F18—C9—C10—C6	−99.64 (16)
F5—C4—C5—F6	−96.19 (16)	F19—C9—C8—C7	−139.25 (18)
F5—C4—C5—F7	22.16 (17)	F19—C9—C10—F20	−96.44 (18)
F5—C4—C5—C1	141.15 (16)	F19—C9—C10—F21	21.34 (19)
F6—C5—C1—O1	46.89 (17)	F19—C9—C10—C6	140.67 (18)
F6—C5—C1—C2	−134.85 (16)	F20—C10—C6—O2	46.61 (17)
F6—C5—C4—C3	141.43 (16)	F20—C10—C6—C7	−135.38 (16)
F7—C5—C1—O1	−73.39 (17)	F20—C10—C9—C8	140.77 (16)
F7—C5—C1—C2	104.87 (17)	F21—C10—C6—O2	−72.58 (15)
F7—C5—C4—C3	−100.21 (15)	F21—C10—C6—C7	105.42 (16)
F8—C12—C11—O3	0.8 (3)	F21—C10—C9—C8	−101.44 (16)
F8—C12—C11—C15	−179.4 (2)	O1—C1—C2—C3	179.1 (2)
F8—C12—C13—F9	−59.5 (2)	O1—C1—C5—C4	168.79 (17)
F8—C12—C13—F10	59.58 (19)	O1—C16—C19—C17	173.11 (13)
F8—C12—C13—C14	−179.26 (19)	O1—C16—C19—C18	−66.34 (15)
F9—C13—C12—C11	120.75 (19)	O1—C16—C19—C20	55.72 (15)
F9—C13—C14—F11	−2.68 (19)	O2—C6—C7—C8	−179.2 (2)
F9—C13—C14—F12	117.35 (17)	O2—C6—C10—C9	168.45 (17)
F9—C13—C14—C15	−122.11 (17)	O2—C17—C19—C16	50.98 (15)
F10—C13—C12—C11	−120.16 (18)	O2—C17—C19—C18	−67.96 (15)
F10—C13—C14—F11	−120.11 (17)	O2—C17—C19—C20	170.53 (14)
F10—C13—C14—F12	−0.08 (18)	O3—C11—C12—C13	−179.5 (2)
F10—C13—C14—C15	120.46 (17)	O3—C11—C15—C14	178.33 (17)
F11—C14—C13—C12	117.60 (18)	O3—C18—C19—C16	174.23 (13)
F11—C14—C15—F13	3.45 (19)	O3—C18—C19—C17	−66.43 (15)
F11—C14—C15—F14	121.15 (17)	O3—C18—C19—C20	52.62 (15)
F11—C14—C15—C11	−117.56 (18)	C1—C2—C3—C4	10.78 (17)
F12—C14—C13—C12	−122.37 (17)	C1—C5—C4—C3	18.77 (16)
F12—C14—C15—F13	−116.45 (17)	C2—C3—C4—C5	−17.70 (15)
F12—C14—C15—F14	1.24 (18)	C6—C7—C8—C9	8.35 (19)
F12—C14—C15—C11	122.54 (17)	C6—C10—C9—C8	17.88 (15)
F13—C15—C11—O3	58.00 (17)	C7—C8—C9—C10	−15.89 (16)
F13—C15—C11—C12	−121.86 (17)	C11—C12—C13—C14	1.00 (19)

F13—C15—C14—C13	123.05 (16)	C11—C15—C14—C13	2.03 (16)
F14—C15—C11—O3	−60.98 (16)	C12—C13—C14—C15	−1.83 (17)
F14—C15—C11—C12	119.16 (16)		