IUCrData

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2,2,3,3,4,4,5,5-Octafluorohexane-1,6-diol. Corrigendum

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In the paper by Feightner *et al.* [*IUCrData* (2020), **5**, x200445], there was an error in the name of the title compound.

The name of the title compound in the paper by Feightner *et al.* (2020) is incorrect and should be '2,2,4,4,5,5,7,7-octafluoro-3,6-dioxaoctane-1,8-diol'. The scheme and chemical data within the article are correct.

References

Feightner, K., Powell, D. R. & Burba, C. M. (2020). *IUCrData*, **5**, x200445.

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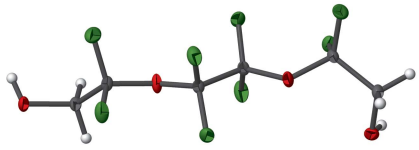
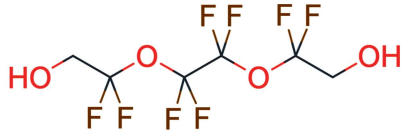
Structural data: full structural data are available from iucrdata.iucr.org

In the crystal of the title compound, $C_6H_6F_8O_4$, O—H···O hydrogen bonds involving the hydroxy groups connect the molecules, forming a two-dimensional network parallel to (100). These hydrogen-bonding interactions appear to drive the O—C—C—O torsion angles into a *gauche–trans–trans* series of conformations along the backbone of the molecule.

3D view



Chemical scheme



Structure description

Ionic liquids have attracted considerable interest as solvents for a variety of applications. 'Solvate' ionic liquids (SILs) are a new class of ionic liquids that consist of equimolar mixtures of inorganic salts and molecular solvents capable of chelating the cations of the salt (Ueno *et al.*, 2012, 2015; Mandai *et al.*, 2014, 2015). Most research on SILs focus on methyl-capped ethylene oxide molecular solvents, which are collectively known as 'glymes'. Structural variation of the chelating compound will undoubtedly influence cation–solvent interactions and provide alternative means for tuning SIL properties (Saito *et al.*, 2016). Our lab has pursued this line of research by examining partially fluorinated molecular solvents for SIL applications. During our experiments, we isolated and determined the structure of the title compound, a partially fluorinated derivative of triethylene glycol. The molecular structure of the title compound is shown in Fig. 1. In the crystal, O—H···O hydrogen bonds involving the terminal hydroxyl groups (see Table 1) connect the molecules, forming a two-dimensional network parallel to (100) (Fig. 2). In addition, a weak intermolecular C—H···F hydrogen bond is observed within this network. These hydrogen-bonding interactions appear to drive the O—C—C—O torsion angles into a *gauche–trans–trans* series of conformations along the backbone of the molecule: O1—C1—C2—O2 = 66.3 (2), O2—C3—C4—O2 = −168.91 (15), and O3—C5—C6—O4 = −177.92 (15)°. By way of comparison, the O—C—C—O torsion angles

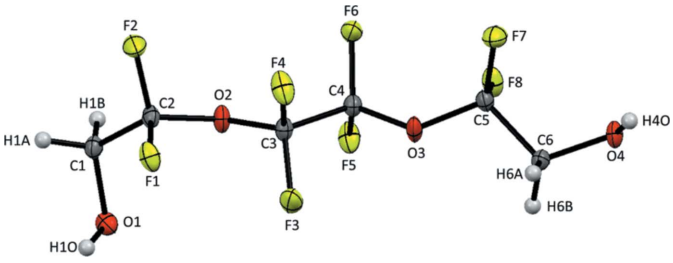


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are shown at 50% probability level.

are *gauche* in monoglyme (Yoshihiro *et al.*, 1996) and longer chain glymes (Johansson *et al.*, 2010; Hyun *et al.*, 2001; Tadokoro, 1964).

Synthesis and crystallization

2,2,3,3,4,4,5,5-Octafluoro-1,6-hexanediol (1.94 mmol) was added to a 1:1 molar ratio mixture of lithium bis(trifluoromethanesulfonyl)imide (2.3 mmol) and 2,2′-[ethane-1,2-diylbis(oxy)]di(ethan-1-ol) (commonly known as triethylene glycol; 2.3 mmol). The resulting mixture was stirred at 353 K for 6 h to produce a homogenous, viscous solution. Colorless, plate-shaped single crystals formed from the solution upon standing over a period of days.

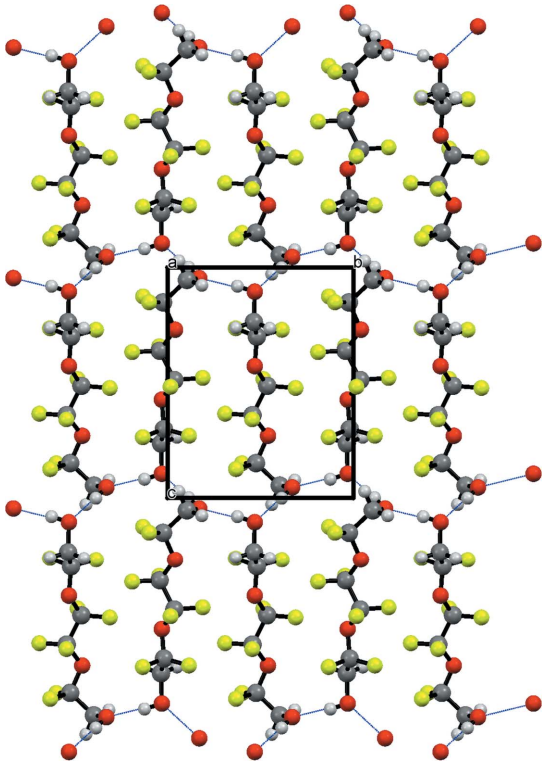


Figure 2
Part of the crystal structure with hydrogen bonds shown as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O4^{i}	0.84 (4)	1.87 (4)	2.705 (2)	172 (3)
O4—H4O···O1^{ii}	0.85 (4)	1.82 (4)	2.661 (2)	173 (3)
C6—H6B···F4^{iii}	0.99	2.52	3.416 (2)	151

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_6F_8O_4$
M_r	294.11
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	5.3009 (8), 8.6250 (12), 10.6976 (14)
β (°)	91.146 (5)
V (Å^3)	489.00 (12)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.25
Crystal size (mm)	0.49 × 0.49 × 0.05
Data collection	
Diffractometer	Bruker Photon II CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.543, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14748, 2985, 2896
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.100, 1.00
No. of reflections	2985
No. of parameters	170
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.40

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

Refinement

Crystal data, data collection methods, and structural refinement details are provided in Table 2. The absolute structure of the title compound could not be established in the refinement reported here.

Acknowledgements

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full crystallographic data

IUCrData (2020). **5**, x200445 [https://doi.org/10.1107/S2414314620004459]

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2,2,3,3,4,4,5,5-Octafluorohexane-1,6-diol

Crystal data

$C_6H_6F_8O_4$
M_r = 294.11
Monoclinic, $P2_1$
a = 5.3009 (8) Å
b = 8.6250 (12) Å
c = 10.6976 (14) Å
β = 91.146 (5)°
V = 489.00 (12) Å^3
Z = 2
$F(000)$ = 292
D_x = 1.997 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9936 reflections
θ = 3.0–30.5°
μ = 0.25 mm^{-1}
T = 100 K
Plate, colourless
0.49 × 0.49 × 0.05 mm

Data collection

Bruker Photon II CMOS diffractometer
Radiation source: microfocus sealed tube
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.543, T_{max} = 0.746
14748 measured reflections
2985 independent reflections
2896 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 30.5°, θ_{min} = 3.0°
h = −7→7
k = −12→12
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.100
S = 1.00
2985 reflections
170 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 0.078P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.5 (6)

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.

Refinement. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.7033 (3)	0.36867 (16)	0.87486 (11)	0.0193 (3)
F2	1.1035 (3)	0.40107 (18)	0.84955 (14)	0.0238 (3)
F3	0.4638 (2)	0.4558 (2)	0.65888 (13)	0.0241 (3)
F4	0.7907 (3)	0.31004 (16)	0.63351 (13)	0.0232 (3)
F5	0.7219 (3)	0.68928 (15)	0.52189 (12)	0.0214 (3)
F6	1.0050 (2)	0.51638 (17)	0.48334 (12)	0.0192 (3)
F7	0.7953 (2)	0.36716 (19)	0.26323 (13)	0.0225 (3)
F8	0.7493 (3)	0.61560 (17)	0.26968 (12)	0.0204 (3)
O1	0.6422 (3)	0.67095 (18)	0.95429 (14)	0.0166 (3)
H1O	0.556 (6)	0.614 (5)	1.001 (3)	0.020*
O2	0.8372 (3)	0.54080 (17)	0.73056 (13)	0.0155 (3)
O3	0.5994 (3)	0.46959 (19)	0.42741 (13)	0.0167 (3)
O4	0.4017 (3)	0.46960 (18)	0.10482 (13)	0.0155 (3)
H4O	0.395 (6)	0.376 (5)	0.081 (3)	0.019*
C1	0.8841 (4)	0.6040 (2)	0.94631 (18)	0.0155 (3)
H1A	0.935916	0.560859	1.028644	0.019*
H1B	1.007975	0.684471	0.923235	0.019*
C2	0.8810 (3)	0.4762 (2)	0.84895 (17)	0.0144 (3)
C3	0.7124 (3)	0.4577 (2)	0.63955 (17)	0.0137 (3)
C4	0.7627 (3)	0.5366 (2)	0.51257 (17)	0.0130 (3)
C5	0.6362 (3)	0.4807 (2)	0.29963 (17)	0.0133 (3)
C6	0.3799 (3)	0.4651 (2)	0.23611 (17)	0.0138 (3)
H6A	0.301564	0.365806	0.260933	0.017*
H6B	0.269087	0.550509	0.263425	0.017*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0299 (6)	0.0142 (5)	0.0140 (6)	−0.0041 (5)	0.0021 (5)	0.0020 (4)
F2	0.0236 (6)	0.0300 (7)	0.0180 (6)	0.0135 (5)	−0.0003 (5)	0.0004 (5)
F3	0.0166 (5)	0.0397 (8)	0.0161 (5)	−0.0061 (6)	0.0016 (4)	0.0022 (6)
F4	0.0426 (8)	0.0115 (5)	0.0154 (6)	0.0009 (5)	−0.0001 (5)	0.0005 (4)
F5	0.0357 (7)	0.0126 (6)	0.0158 (6)	0.0026 (5)	−0.0025 (5)	0.0015 (5)
F6	0.0138 (5)	0.0295 (7)	0.0145 (5)	−0.0016 (4)	0.0008 (4)	0.0025 (5)
F7	0.0183 (5)	0.0271 (7)	0.0221 (6)	0.0067 (5)	−0.0018 (5)	−0.0056 (6)
F8	0.0256 (6)	0.0218 (6)	0.0139 (5)	−0.0114 (5)	−0.0010 (4)	0.0020 (5)
O1	0.0205 (6)	0.0135 (6)	0.0157 (6)	0.0030 (5)	0.0022 (5)	0.0021 (5)
O2	0.0229 (6)	0.0139 (6)	0.0095 (6)	−0.0027 (5)	−0.0031 (5)	0.0014 (5)
O3	0.0181 (6)	0.0235 (7)	0.0085 (5)	−0.0073 (6)	−0.0021 (4)	0.0004 (6)
O4	0.0224 (6)	0.0143 (6)	0.0097 (6)	−0.0018 (5)	−0.0029 (5)	−0.0011 (5)
C1	0.0178 (8)	0.0169 (8)	0.0116 (7)	0.0003 (6)	−0.0025 (6)	−0.0014 (6)
C2	0.0180 (7)	0.0147 (8)	0.0105 (7)	0.0019 (7)	−0.0017 (6)	0.0021 (6)
C3	0.0169 (7)	0.0132 (8)	0.0111 (7)	−0.0024 (6)	−0.0010 (6)	0.0011 (6)
C4	0.0149 (7)	0.0134 (8)	0.0108 (7)	−0.0009 (6)	−0.0008 (6)	0.0005 (6)
C5	0.0149 (7)	0.0151 (8)	0.0101 (7)	−0.0025 (6)	0.0004 (6)	−0.0007 (6)

C6	0.0136 (6)	0.0163 (8)	0.0116 (7)	−0.0007 (7)	−0.0015 (5)	−0.0010 (6)

Geometric parameters (Å, º)

F1—C2	1.354 (2)	O3—C4	1.372 (2)
F2—C2	1.345 (2)	O3—C5	1.388 (2)
F3—C3	1.338 (2)	O4—C6	1.412 (2)
F4—C3	1.342 (2)	O4—H4O	0.85 (4)
F5—C4	1.338 (2)	C1—C2	1.517 (3)
F6—C4	1.339 (2)	C1—H1A	0.9900
F7—C5	1.354 (2)	C1—H1B	0.9900
F8—C5	1.351 (2)	C3—C4	1.547 (3)
O1—C1	1.410 (2)	C5—C6	1.513 (2)
O1—H1O	0.84 (4)	C6—H6A	0.9900
O2—C3	1.368 (2)	C6—H6B	0.9900
O2—C2	1.399 (2)		
C1—O1—H1O	108 (2)	F4—C3—C4	108.44 (15)
C3—O2—C2	120.31 (16)	O2—C3—C4	107.76 (16)
C4—O3—C5	121.70 (15)	F5—C4—F6	107.64 (16)
C6—O4—H4O	106 (2)	F5—C4—O3	111.28 (16)
O1—C1—C2	109.99 (15)	F6—C4—O3	112.68 (16)
O1—C1—H1A	109.7	F5—C4—C3	109.64 (16)
C2—C1—H1A	109.7	F6—C4—C3	109.31 (15)
O1—C1—H1B	109.7	O3—C4—C3	106.26 (15)
C2—C1—H1B	109.7	F8—C5—F7	105.85 (15)
H1A—C1—H1B	108.2	F8—C5—O3	111.40 (15)
F2—C2—F1	106.43 (17)	F7—C5—O3	109.52 (16)
F2—C2—O2	109.02 (16)	F8—C5—C6	111.64 (16)
F1—C2—O2	110.76 (15)	F7—C5—C6	111.42 (16)
F2—C2—C1	110.45 (15)	O3—C5—C6	107.05 (14)
F1—C2—C1	110.80 (16)	O4—C6—C5	110.69 (14)
O2—C2—C1	109.34 (16)	O4—C6—H6A	109.5
F3—C3—F4	107.59 (17)	C5—C6—H6A	109.5
F3—C3—O2	111.10 (16)	O4—C6—H6B	109.5
F4—C3—O2	112.68 (16)	C5—C6—H6B	109.5
F3—C3—C4	109.20 (15)	H6A—C6—H6B	108.1
C3—O2—C2—F2	89.9 (2)	O2—C3—C4—F5	−48.5 (2)
C3—O2—C2—F1	−26.9 (2)	F3—C3—C4—F6	−169.97 (16)
C3—O2—C2—C1	−149.29 (17)	F4—C3—C4—F6	−53.01 (19)
O1—C1—C2—F2	−173.74 (16)	O2—C3—C4—F6	69.23 (19)
O1—C1—C2—F1	−56.1 (2)	F3—C3—C4—O3	−48.1 (2)
O1—C1—C2—O2	66.3 (2)	F4—C3—C4—O3	68.84 (19)
C2—O2—C3—F3	77.1 (2)	O2—C3—C4—O3	−168.91 (15)
C2—O2—C3—F4	−43.8 (2)	C4—O3—C5—F8	−31.6 (2)
C2—O2—C3—C4	−163.34 (16)	C4—O3—C5—F7	85.1 (2)
C5—O3—C4—F5	78.4 (2)	C4—O3—C5—C6	−153.95 (17)

C5—O3—C4—F6	−42.6 (2)	F8—C5—C6—O4	59.9 (2)
C5—O3—C4—C3	−162.26 (17)	F7—C5—C6—O4	−58.2 (2)
F3—C3—C4—F5	72.2 (2)	O3—C5—C6—O4	−177.92 (15)
F4—C3—C4—F5	−170.79 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O4^{i}	0.84 (4)	1.87 (4)	2.705 (2)	172 (3)
O4—H4*O*···O1^{ii}	0.85 (4)	1.82 (4)	2.661 (2)	173 (3)
C6—H6*B*···F4^{iii}	0.99	2.52	3.416 (2)	151

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