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2,2′,5,5′-Tetrakis(trifluoromethyl)biphenyl

Keith B. Dillon, Natalia V. Zorina, Dmitry S. Yufit* and Judith A. K. Howard

Chemistry Department, University of Durham, South Road, Durham DH1 3LE, England

Correspondence e-mail: d.s.yufit@durham.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.053
wR factor = 0.161
Data-to-parameter ratio = 14.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{16}H_6F_{12}$, has been obtained as a by-product of the reaction between 2,5-bis(trifluoromethyl)-phenyllithium and zinc(II) chloride. The asymmetric unit contains two independent molecules with a similar almost perpendicular conformation of the biphenyl fragments.

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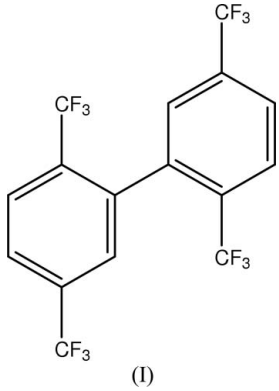
Comment

As a part of our ongoing studies into the reactions between lithiated trifluoromethyl-substituted aromatic compounds and main group halides (Batsanov *et al.*, 2001; Batsanov *et al.*, 2002; Batsanov *et al.*, 2003; Cornet *et al.*, 2003; Cornet *et al.*, 2005), we have reacted lithiated 1,4-bis(trifluoromethyl)benzene (ArLi) with zinc(II) chloride in diethyl ether solution. A few crystals were isolated from the reaction mixture and X-ray analysis proved them to be a by-product of the reaction, 2,5,2′,5′-tetrakis(trifluoromethyl)biphenyl (I), probably formed *via* a radical reaction.



(I)

The structures of the two molecules in the asymmetric unit of (I) are shown in Fig. 1, while selected bond distances and

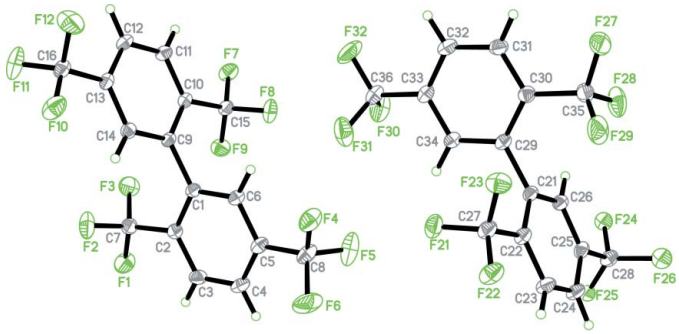


Figure 1
The two independent molecules of (I), with the minor component of the disordered F atoms omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

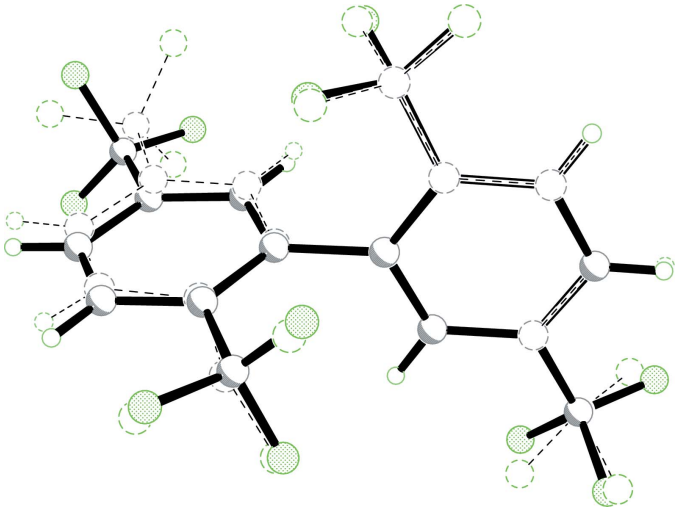


Figure 2
Least-squares fit of the two independent molecules. The minor components of the disordered F atoms are omitted for clarity.

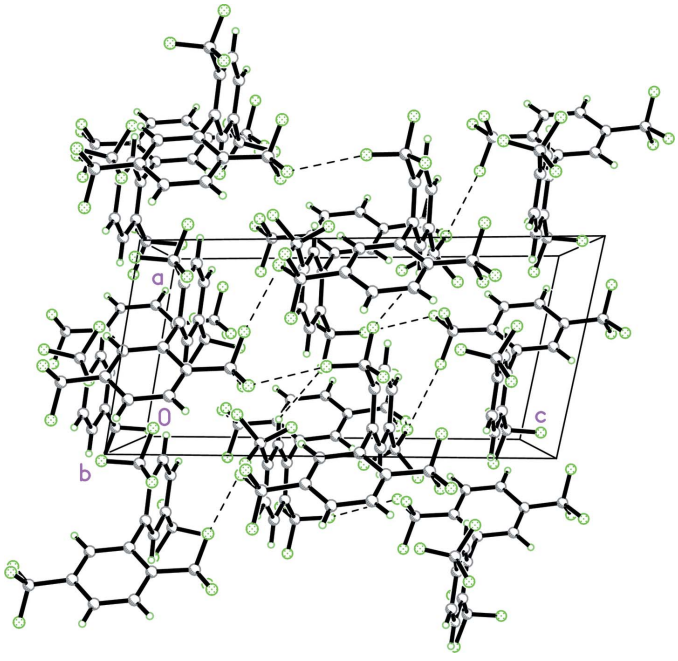


Figure 3
Packing of the molecules of (I) in the crystal structure, viewed along the *b* axis. Dashed lines correspond to short H···F and F···F intermolecular contacts.

angles are listed in Table 1. The asymmetric unit contains two crystallographically independent molecules, both of them adopting a similar perpendicular conformation of the biphenyl fragment and differing slightly in the orientation of CF_3 groups (Fig. 2). The perpendicular conformation, with an absolute value of the torsion angle around the central C–C bond close to 90°, is typical for 2,2′-substituted biphenyls [see, for example, Leser & Rabinovich (1978, and references therein) and Nieger *et al.* (1998)]. The lengths of the central C–C bonds in (I) [1.498 (2) and 1.499 (2) Å] are well within the range of the central bond lengths in substituted biphenyls (Bahl *et al.*, 1996; Shimada *et al.*, 2003). The geometrical parameters of the CF_3 groups are also entirely comparable with those described in the literature for other CF_3-substituted benzene derivatives (Lynch *et al.*, 1992; Couldwell & Penfold, 1976; Baenziger *et al.*, 1995).

The packing of the molecules of (I) in the crystal structure is determined by a number of short C–H···F and F···F interactions, which link molecules in a three-dimensional network (Fig. 3). The role of such interactions in crystal engineering has been discussed recently by Reichenbächer *et al.* (2005). The shortest contacts of each type are H34···F27($1 + x$, y, z) 2.52 (2) and F24···F32($-x$, $1 - y$, $1 - z$) 2.788 (2) Å.

Experimental

A solution of $ZnCl_2$ (3.07 g, 22.5 mmol) in diethyl ether was added *via* a cannula, with stirring, to a solution of ArLi (22.5 mmol) in diethyl ether at 195 K. ArLi was prepared *in situ* from ArH (5.3 g, 24.8 mmol) and *n*-BuLi (22.5 mmol from a 1.6 *M* solution in hexane) in diethyl ether at 195 K. The mixture was allowed to warm to room temperature, and most of the solvent was removed *in vacuo*. A liquid layer above an oily layer was produced. The liquid layer was separated, and left in a tube at room temperature to see whether crystals would form. Crystals of (I) were observed on the following day and were isolated. The title compound, (I), was also characterized by ^{19}F NMR spectroscopy, giving the expected two singlets in a 1:1 ratio at −59.2 and −63.9 p.p.m., assigned to the CF_3 groups *ortho* and *meta* to the ring junction, respectively, and by elemental analysis (Found, C, 43.7, H, 1.38%; $C_{16}H_6F_{12}$ requires C, 45.1, H, 1.42%). All manipulations of air- and/or moisture-sensitive compounds were performed either under an inert atmosphere of dry nitrogen or *in vacuo*, using standard Schlenk and cannula techniques, or in a nitrogen-filled glovebox. ^{19}F NMR spectra were recorded on a Varian Unity 300 Fourier-transform spectrometer at 282.2 MHz; chemical shifts were measured relative to external $CFCl_3$.

Crystal data

$C_{16}H_6F_{12}$
M_r = 426.21
Triclinic, $P\overline{1}$
a = 7.4296 (2) Å
b = 14.3048 (4) Å
c = 15.1315 (4) Å
α = 79.73 (1)°
β = 77.21 (1)°
γ = 76.39 (1)°
V = 1510.6 (1) Å^3
Z = 4
D_x = 1.874 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6646 reflections
θ = 2.2–31.0°
μ = 0.21 mm^{-1}
T = 120 (2) K
Block, colourless
0.36 × 0.32 × 0.24 mm

Data collection

Bruker SMART 6000 CCD diffractometer
ω scans
Absorption correction: none
14596 measured reflections
8297 independent reflections
6387 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 29.5°
$h = -10 \rightarrow 10$
$k = -19 \rightarrow 19$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.161
S = 1.05
8297 reflections
558 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2 + 0.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C9	1.498 (2)	C21—C29	1.499 (2)
C6—C1—C2	118.26 (13)	C26—C21—C22	118.54 (13)
C6—C1—C9	117.08 (13)	C26—C21—C29	117.99 (13)
C2—C1—C9	124.53 (13)	C22—C21—C29	123.17 (13)
C14—C9—C10	118.70 (13)	C34—C29—C30	118.16 (14)
C14—C9—C1	117.35 (13)	C34—C29—C21	116.95 (13)
C10—C9—C1	123.69 (13)	C30—C29—C21	124.79 (13)
C2—C1—C9—C14	85.42 (18)	C22—C21—C29—C34	−79.54 (19)

One of the CF_3 groups (F24–F26) is severely disordered and has been modelled by several sets of F atoms with partial occupancy (site-occupancy factors 0.4:0.3:0.3). These atoms were refined isotropically. H atom parameters were refined freely [C—H = 0.91 (3)–0.97 (2) Å].

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-NT* (Bruker, 1998); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

DSY is grateful to the EPSRC (UK) for financial support.

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supporting information

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S1. Comment

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S2. Experimental

A solution of $ZnCl_2$ (3.07 g, 22.5 mmol) in diethyl ether was added *via* cannula, with stirring, to a solution of ArLi (22.5 mmol) in diethyl ether at 195 K. ArLi was prepared *in situ* from ArH (5.3 g, 24.8 mmol) and n-BuLi (22.5 mmol from a 1.6 *M* solution in hexane) in diethyl ether at −78° C. The mixture was allowed to warm to room temperature, and most of the solvent was removed *in vacuo*. A liquid layer above an oily layer was produced. The liquid layer was separated, and left in a tube at room temperature to see whether crystals would form. Crystals of (I) were observed on the following day and were isolated. The title compound, (I), was also characterized by ^{19}F NMR spectroscopy, giving the expected two singlets in a 1:1 ratio at −59.2 and −63.9 p.p.m., assigned to the CF_3 groups *ortho* and *meta* to the ring junction, respectively, and by elemental analysis (Found, C, 43.7, H, 1.38%; $C_{16}H_6F_{12}$ requires C, 45.1, H, 1.42%). All manipulations of air- and/or moisture-sensitive compounds were performed either under an inert atmosphere of dry nitrogen or *in vacuo*, using standard Schlenk and cannula techniques, or in a nitrogen-filled glovebox. ^{19}F NMR spectra were recorded on a Varian Unity 300 Fourier-transform spectrometer at 282.2 MHz; chemical shifts were measured relative to external $CFCl_3$.

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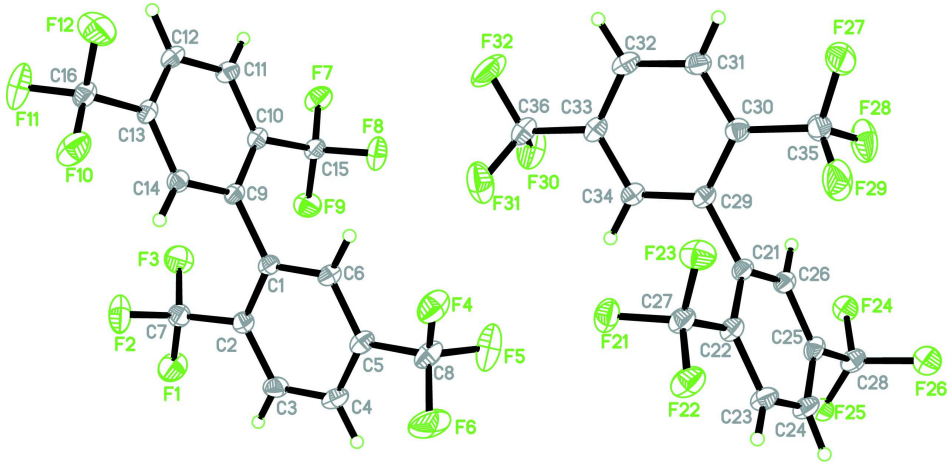
One of the CF_3-groups (F24–F26) is severely disordered and has been modelled by several sets of F-atoms with partial occupancy. These atoms were refined isotropically.



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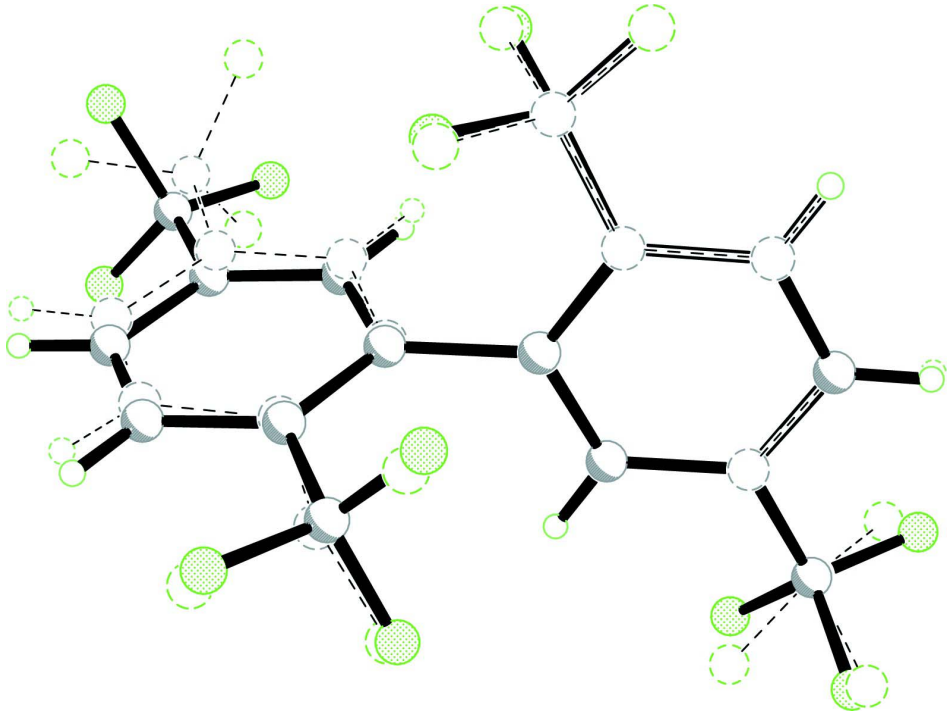

Figure 2

Overlap of the two independent molecules. Disordered F atoms are omitted for clarity.

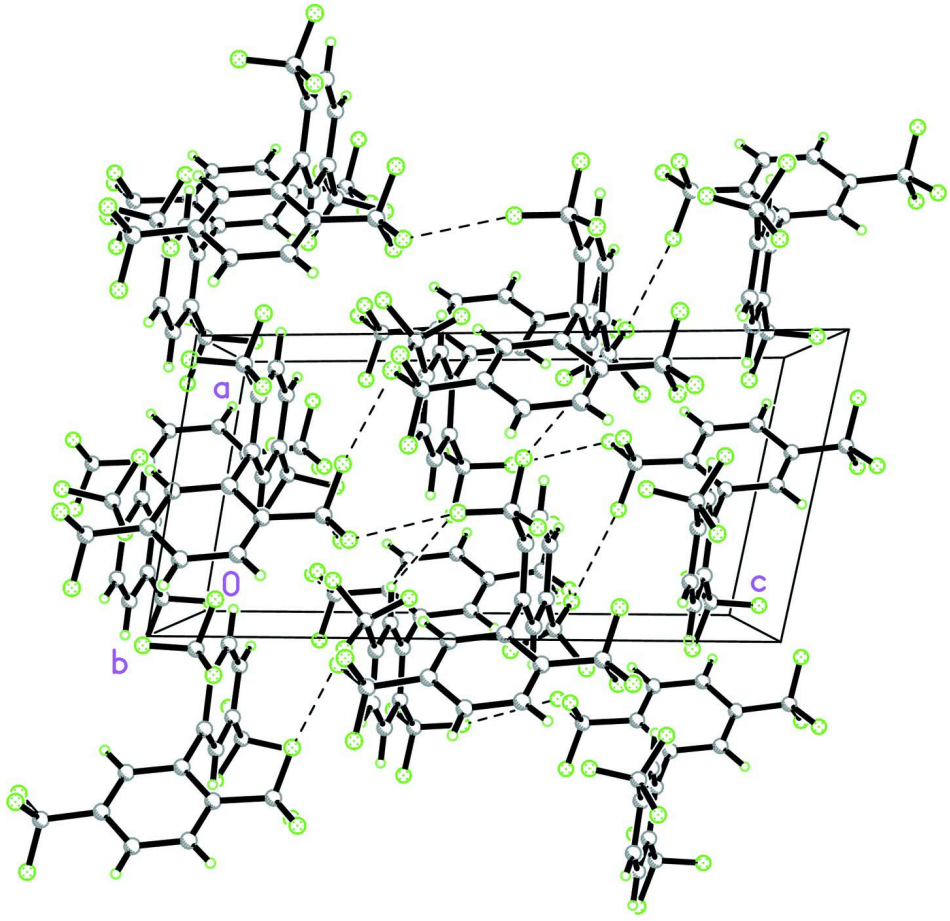

Figure 3

Packing of the molecules of (I) in the crystal, viewed along the *b* axis. Dashed lines correspond to short H···F and F···F intermolecular contacts.

2,2′,5,5′-Tetrakis(trifluoromethyl)biphenyl

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$\beta = 77.21$ (1)°
$\gamma = 76.39$ (1)°
$V = 1510.6$ (1) Å^3
$Z = 4$
$F(000) = 840$
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Cell parameters from 6646 reflections
$\theta = 2.2$–31.0°
$\mu = 0.21$ mm^{-1}
$T = 120$ K
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Graphite monochromator
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14596 measured reflections
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6387 reflections with $I > 2\sigma(I)$

R_{int} = 0.033
θ_{max} = 29.5°, θ_{min} = 1.4°
h = −10→10
k = −19→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.161
S = 1.05
8297 reflections
558 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2 + 0.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.
One of the CF3-groups is severely disordered.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
F1	1.10437 (15)	0.71425 (8)	0.07710 (9)	0.0371 (3)	
F2	0.94316 (17)	0.77359 (9)	−0.02873 (8)	0.0387 (3)	
F3	0.84579 (15)	0.81778 (8)	0.10442 (9)	0.0344 (3)	
F4	0.38913 (16)	0.43902 (8)	0.11119 (8)	0.0327 (3)	
F5	0.5047 (2)	0.38635 (9)	0.23298 (8)	0.0453 (3)	
F6	0.65920 (18)	0.34254 (8)	0.10462 (11)	0.0466 (3)	
F7	0.32362 (15)	0.86682 (7)	0.29303 (7)	0.0273 (2)	
F8	0.31604 (16)	0.72235 (8)	0.27430 (7)	0.0300 (2)	
F9	0.58185 (14)	0.76499 (8)	0.25602 (7)	0.0279 (2)	
F10	0.41727 (18)	0.85770 (8)	−0.19164 (7)	0.0348 (3)	
F11	0.4192 (2)	1.00196 (9)	−0.17434 (8)	0.0411 (3)	
F12	0.15851 (16)	0.95277 (11)	−0.14289 (8)	0.0461 (3)	
F21	0.18170 (16)	0.27611 (8)	0.22043 (7)	0.0300 (2)	
F22	0.16117 (17)	0.13289 (8)	0.20441 (7)	0.0299 (2)	
F23	−0.09013 (15)	0.23801 (8)	0.24520 (7)	0.0303 (2)	
F24	0.1072 (4)	0.13992 (18)	0.68768 (16)	0.0249 (5)*	0.50
F25	0.3588 (4)	0.0570 (3)	0.63625 (19)	0.0195 (6)*	0.40
F26	0.0686 (5)	0.0009 (2)	0.6733 (2)	0.0308 (8)*	0.40
F24A	0.0625 (4)	0.12488 (19)	0.69245 (17)	0.0306 (6)*	0.50
F25A	0.3549 (6)	0.0895 (4)	0.6347 (3)	0.0318 (11)*	0.30
F26A	0.1285 (8)	−0.0147 (3)	0.6646 (2)	0.0129 (6)*	0.30

F25B	0.3470 (6)	0.0249 (3)	0.6370 (3)	0.0302 (10)*	0.30
F26B	0.1969 (8)	−0.0233 (3)	0.6535 (3)	0.0382 (12)*	0.30
F27	−0.60254 (15)	0.31200 (9)	0.44845 (10)	0.0448 (3)	
F28	−0.41380 (18)	0.24118 (10)	0.53853 (8)	0.0432 (3)	
F29	−0.36502 (19)	0.20147 (9)	0.40477 (10)	0.0449 (3)	
F30	0.10254 (19)	0.58030 (9)	0.40298 (8)	0.0412 (3)	
F31	0.16418 (19)	0.55415 (9)	0.26486 (9)	0.0450 (3)	
F32	−0.07548 (19)	0.66232 (8)	0.31026 (12)	0.0532 (4)	
C1	0.6279 (2)	0.67624 (10)	0.09371 (10)	0.0161 (3)	
C2	0.8238 (2)	0.65870 (11)	0.08771 (10)	0.0183 (3)	
C3	0.9269 (2)	0.56457 (12)	0.10235 (11)	0.0216 (3)	
C4	0.8380 (2)	0.48609 (12)	0.12217 (11)	0.0225 (3)	
C5	0.6450 (2)	0.50273 (11)	0.12671 (10)	0.0195 (3)	
C6	0.5400 (2)	0.59670 (11)	0.11386 (10)	0.0176 (3)	
C7	0.9284 (2)	0.74106 (12)	0.06075 (11)	0.0226 (3)	
C8	0.5487 (2)	0.41801 (12)	0.14445 (12)	0.0248 (3)	
C9	0.5066 (2)	0.77423 (10)	0.07366 (10)	0.0156 (3)	
C10	0.3977 (2)	0.82988 (10)	0.14128 (10)	0.0163 (3)	
C11	0.2750 (2)	0.91651 (11)	0.11829 (11)	0.0196 (3)	
C12	0.2583 (2)	0.94814 (11)	0.02764 (11)	0.0198 (3)	
C13	0.3652 (2)	0.89272 (11)	−0.03962 (10)	0.0173 (3)	
C14	0.4896 (2)	0.80703 (11)	−0.01743 (10)	0.0171 (3)	
C15	0.4058 (2)	0.79644 (11)	0.24083 (10)	0.0188 (3)	
C16	0.3403 (2)	0.92585 (12)	−0.13717 (11)	0.0208 (3)	
C21	0.0055 (2)	0.22761 (10)	0.42391 (10)	0.0165 (3)	
C22	0.1031 (2)	0.16977 (11)	0.35574 (10)	0.0187 (3)	
C23	0.2186 (2)	0.08049 (12)	0.37777 (11)	0.0225 (3)	
C24	0.2397 (2)	0.04787 (12)	0.46767 (11)	0.0226 (3)	
C25	0.1442 (2)	0.10517 (11)	0.53520 (10)	0.0185 (3)	
C26	0.0276 (2)	0.19384 (11)	0.51427 (10)	0.0178 (3)	
C27	0.0878 (2)	0.20360 (11)	0.25687 (11)	0.0217 (3)	
C28	0.1760 (2)	0.07114 (12)	0.63168 (11)	0.0220 (3)	
C29	−0.1060 (2)	0.32824 (11)	0.40372 (10)	0.0170 (3)	
C30	−0.3034 (2)	0.35338 (11)	0.41677 (10)	0.0187 (3)	
C31	−0.3950 (2)	0.44957 (12)	0.40006 (11)	0.0219 (3)	
C32	−0.2927 (2)	0.52315 (12)	0.37192 (11)	0.0229 (3)	
C33	−0.0974 (2)	0.49846 (11)	0.36024 (10)	0.0197 (3)	
C34	−0.0051 (2)	0.40239 (11)	0.37479 (10)	0.0185 (3)	
C35	−0.4206 (2)	0.27667 (12)	0.45118 (12)	0.0242 (3)	
C36	0.0198 (2)	0.57498 (12)	0.33458 (12)	0.0244 (3)	
H3	1.055 (3)	0.5554 (16)	0.0990 (15)	0.027 (5)*	
H4	0.906 (3)	0.4240 (17)	0.1318 (15)	0.031 (6)*	
H6	0.409 (3)	0.6068 (15)	0.1194 (14)	0.022 (5)*	
H11	0.206 (3)	0.9520 (16)	0.1636 (16)	0.028 (5)*	
H12	0.175 (3)	1.0073 (16)	0.0137 (14)	0.022 (5)*	
H14	0.562 (3)	0.7703 (15)	−0.0652 (15)	0.024 (5)*	
H23	0.279 (4)	0.0440 (19)	0.3322 (18)	0.043 (7)*	
H24	0.322 (3)	−0.0114 (17)	0.4790 (15)	0.028 (5)*	

H26	−0.036 (3)	0.2320 (16)	0.5626 (15)	0.026 (5)*
H31	−0.526 (3)	0.4667 (18)	0.4048 (16)	0.038 (6)*
H32	−0.353 (3)	0.5905 (16)	0.3605 (15)	0.029 (5)*
H34	0.130 (3)	0.3863 (15)	0.3643 (14)	0.026 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0197 (5)	0.0337 (6)	0.0579 (8)	−0.0088 (4)	−0.0152 (5)	0.0081 (5)
F2	0.0429 (7)	0.0452 (7)	0.0281 (6)	−0.0215 (5)	−0.0069 (5)	0.0122 (5)
F3	0.0295 (5)	0.0239 (5)	0.0513 (7)	−0.0118 (4)	−0.0003 (5)	−0.0094 (5)
F4	0.0339 (6)	0.0240 (5)	0.0461 (7)	−0.0102 (4)	−0.0203 (5)	0.0015 (5)
F5	0.0717 (9)	0.0406 (7)	0.0332 (6)	−0.0345 (6)	−0.0187 (6)	0.0115 (5)
F6	0.0427 (7)	0.0207 (5)	0.0806 (10)	−0.0021 (5)	−0.0129 (6)	−0.0214 (6)
F7	0.0386 (6)	0.0212 (5)	0.0201 (5)	0.0013 (4)	−0.0068 (4)	−0.0061 (4)
F8	0.0426 (6)	0.0250 (5)	0.0241 (5)	−0.0175 (4)	−0.0034 (4)	0.0031 (4)
F9	0.0241 (5)	0.0358 (6)	0.0214 (5)	0.0010 (4)	−0.0094 (4)	−0.0007 (4)
F10	0.0542 (7)	0.0265 (5)	0.0228 (5)	0.0008 (5)	−0.0143 (5)	−0.0044 (4)
F11	0.0718 (9)	0.0316 (6)	0.0268 (6)	−0.0280 (6)	−0.0160 (5)	0.0099 (5)
F12	0.0239 (5)	0.0807 (10)	0.0277 (6)	0.0012 (6)	−0.0124 (4)	0.0022 (6)
F21	0.0415 (6)	0.0235 (5)	0.0228 (5)	−0.0100 (4)	−0.0018 (4)	0.0021 (4)
F22	0.0452 (6)	0.0219 (5)	0.0207 (5)	0.0000 (4)	−0.0071 (4)	−0.0061 (4)
F23	0.0291 (5)	0.0365 (6)	0.0229 (5)	0.0021 (4)	−0.0109 (4)	−0.0023 (4)
F27	0.0215 (5)	0.0410 (7)	0.0691 (9)	−0.0108 (5)	−0.0163 (5)	0.0154 (6)
F28	0.0437 (7)	0.0565 (8)	0.0303 (6)	−0.0255 (6)	−0.0123 (5)	0.0188 (5)
F29	0.0476 (7)	0.0343 (6)	0.0562 (8)	−0.0237 (5)	0.0070 (6)	−0.0153 (6)
F30	0.0596 (8)	0.0418 (7)	0.0346 (6)	−0.0287 (6)	−0.0208 (6)	0.0020 (5)
F31	0.0546 (8)	0.0417 (7)	0.0410 (7)	−0.0287 (6)	0.0110 (6)	−0.0114 (5)
F32	0.0459 (7)	0.0172 (5)	0.0966 (12)	−0.0076 (5)	−0.0286 (7)	0.0129 (6)
C1	0.0174 (6)	0.0141 (6)	0.0162 (6)	−0.0013 (5)	−0.0041 (5)	−0.0015 (5)
C2	0.0176 (6)	0.0179 (7)	0.0187 (7)	−0.0027 (5)	−0.0038 (5)	−0.0010 (5)
C3	0.0171 (7)	0.0216 (7)	0.0243 (7)	0.0009 (6)	−0.0057 (6)	−0.0023 (6)
C4	0.0249 (7)	0.0154 (7)	0.0251 (8)	0.0030 (6)	−0.0080 (6)	−0.0026 (6)
C5	0.0248 (7)	0.0144 (7)	0.0203 (7)	−0.0027 (5)	−0.0081 (6)	−0.0023 (5)
C6	0.0182 (6)	0.0145 (7)	0.0201 (7)	−0.0013 (5)	−0.0064 (5)	−0.0015 (5)
C7	0.0171 (7)	0.0227 (8)	0.0269 (8)	−0.0050 (6)	−0.0047 (6)	0.0020 (6)
C8	0.0325 (8)	0.0154 (7)	0.0295 (8)	−0.0040 (6)	−0.0138 (7)	−0.0020 (6)
C9	0.0158 (6)	0.0132 (6)	0.0182 (7)	−0.0035 (5)	−0.0054 (5)	0.0003 (5)
C10	0.0179 (6)	0.0146 (6)	0.0170 (6)	−0.0039 (5)	−0.0050 (5)	−0.0005 (5)
C11	0.0214 (7)	0.0156 (7)	0.0211 (7)	−0.0010 (5)	−0.0052 (5)	−0.0031 (6)
C12	0.0220 (7)	0.0134 (7)	0.0234 (7)	−0.0012 (5)	−0.0083 (6)	0.0007 (5)
C13	0.0191 (6)	0.0156 (7)	0.0180 (7)	−0.0056 (5)	−0.0065 (5)	0.0021 (5)
C14	0.0175 (6)	0.0162 (7)	0.0181 (7)	−0.0037 (5)	−0.0049 (5)	−0.0015 (5)
C15	0.0217 (7)	0.0159 (7)	0.0182 (7)	−0.0029 (5)	−0.0044 (5)	−0.0011 (5)
C16	0.0226 (7)	0.0193 (7)	0.0205 (7)	−0.0040 (6)	−0.0077 (6)	0.0017 (6)
C21	0.0168 (6)	0.0133 (6)	0.0193 (7)	−0.0024 (5)	−0.0055 (5)	0.0002 (5)
C22	0.0229 (7)	0.0150 (7)	0.0179 (7)	−0.0027 (5)	−0.0055 (5)	−0.0006 (5)
C23	0.0277 (8)	0.0159 (7)	0.0218 (7)	0.0012 (6)	−0.0047 (6)	−0.0039 (6)

C24	0.0250 (7)	0.0150 (7)	0.0250 (8)	0.0014 (6)	−0.0079 (6)	0.0010 (6)
C25	0.0209 (7)	0.0163 (7)	0.0185 (7)	−0.0044 (5)	−0.0071 (5)	0.0024 (5)
C26	0.0184 (6)	0.0159 (7)	0.0190 (7)	−0.0029 (5)	−0.0049 (5)	−0.0011 (5)
C27	0.0275 (8)	0.0174 (7)	0.0185 (7)	−0.0008 (6)	−0.0055 (6)	−0.0013 (6)
C28	0.0257 (7)	0.0187 (7)	0.0211 (7)	−0.0014 (6)	−0.0091 (6)	0.0007 (6)
C29	0.0206 (7)	0.0143 (6)	0.0160 (6)	−0.0017 (5)	−0.0057 (5)	−0.0010 (5)
C30	0.0199 (7)	0.0187 (7)	0.0171 (6)	−0.0026 (5)	−0.0051 (5)	−0.0010 (5)
C31	0.0201 (7)	0.0204 (7)	0.0223 (7)	0.0014 (6)	−0.0049 (6)	−0.0016 (6)
C32	0.0275 (8)	0.0160 (7)	0.0233 (7)	0.0015 (6)	−0.0074 (6)	−0.0024 (6)
C33	0.0259 (7)	0.0146 (7)	0.0191 (7)	−0.0037 (6)	−0.0067 (6)	−0.0013 (5)
C34	0.0205 (7)	0.0158 (7)	0.0193 (7)	−0.0022 (5)	−0.0064 (5)	−0.0013 (5)
C35	0.0197 (7)	0.0252 (8)	0.0258 (8)	−0.0052 (6)	−0.0057 (6)	0.0039 (6)
C36	0.0320 (8)	0.0163 (7)	0.0266 (8)	−0.0057 (6)	−0.0107 (6)	0.0004 (6)

Geometric parameters (Å, º)

F1—C7	1.3382 (18)	C5—C6	1.391 (2)
F2—C7	1.340 (2)	C5—C8	1.503 (2)
F3—C7	1.334 (2)	C6—H6	0.93 (2)
F4—C8	1.3385 (19)	C9—C14	1.398 (2)
F5—C8	1.329 (2)	C9—C10	1.399 (2)
F6—C8	1.341 (2)	C10—C11	1.394 (2)
F7—C15	1.3383 (18)	C10—C15	1.507 (2)
F8—C15	1.3476 (17)	C11—C12	1.389 (2)
F9—C15	1.3363 (18)	C11—H11	0.92 (2)
F10—C16	1.3312 (19)	C12—C13	1.389 (2)
F11—C16	1.3344 (19)	C12—H12	0.95 (2)
F12—C16	1.3324 (19)	C13—C14	1.388 (2)
F21—C27	1.3538 (19)	C13—C16	1.506 (2)
F22—C27	1.3363 (18)	C14—H14	0.96 (2)
F23—C27	1.3370 (19)	C21—C26	1.399 (2)
F24—C28	1.348 (3)	C21—C22	1.402 (2)
F25—C28	1.341 (3)	C21—C29	1.499 (2)
F26—C28	1.404 (4)	C22—C23	1.392 (2)
F24A—C28	1.323 (3)	C22—C27	1.509 (2)
F25A—C28	1.426 (5)	C23—C24	1.388 (2)
F26A—C28	1.337 (4)	C23—H23	0.91 (3)
F25B—C28	1.300 (4)	C24—C25	1.387 (2)
F26B—C28	1.312 (5)	C24—H24	0.94 (2)
F27—C35	1.3341 (19)	C25—C26	1.386 (2)
F28—C35	1.336 (2)	C25—C28	1.506 (2)
F29—C35	1.324 (2)	C26—H26	0.96 (2)
F30—C36	1.337 (2)	C29—C34	1.393 (2)
F31—C36	1.347 (2)	C29—C30	1.403 (2)
F32—C36	1.316 (2)	C30—C31	1.390 (2)
C1—C6	1.397 (2)	C30—C35	1.510 (2)
C1—C2	1.403 (2)	C31—C32	1.393 (2)
C1—C9	1.498 (2)	C31—H31	0.94 (2)

C2—C3	1.390 (2)	C32—C33	1.389 (2)
C2—C7	1.509 (2)	C32—H32	0.97 (2)
C3—C4	1.389 (2)	C33—C34	1.387 (2)
C3—H3	0.92 (2)	C33—C36	1.502 (2)
C4—C5	1.385 (2)	C34—H34	0.96 (2)
C4—H4	0.92 (2)		

C6—C1—C2	118.26 (13)	C26—C21—C22	118.54 (13)
C6—C1—C9	117.08 (13)	C26—C21—C29	117.99 (13)
C2—C1—C9	124.53 (13)	C22—C21—C29	123.17 (13)
C3—C2—C1	120.65 (14)	C23—C22—C21	120.60 (14)
C3—C2—C7	118.52 (13)	C23—C22—C27	118.60 (14)
C1—C2—C7	120.76 (13)	C21—C22—C27	120.79 (13)
C4—C3—C2	120.54 (14)	C24—C23—C22	120.31 (15)
C4—C3—H3	120.8 (14)	C24—C23—H23	121.0 (17)
C2—C3—H3	118.7 (14)	C22—C23—H23	118.7 (17)
C5—C4—C3	119.14 (14)	C25—C24—C23	119.23 (14)
C5—C4—H4	120.5 (14)	C25—C24—H24	123.4 (14)
C3—C4—H4	120.4 (14)	C23—C24—H24	117.4 (14)
C4—C5—C6	120.79 (14)	C26—C25—C24	121.02 (14)
C4—C5—C8	119.50 (14)	C26—C25—C28	120.31 (14)
C6—C5—C8	119.71 (14)	C24—C25—C28	118.63 (14)
C5—C6—C1	120.61 (14)	C25—C26—C21	120.29 (14)
C5—C6—H6	119.8 (13)	C25—C26—H26	119.0 (13)
C1—C6—H6	119.6 (13)	C21—C26—H26	120.7 (13)
F3—C7—F1	106.47 (14)	F22—C27—F23	107.16 (13)
F3—C7—F2	106.25 (14)	F22—C27—F21	106.08 (13)
F1—C7—F2	106.52 (13)	F23—C27—F21	106.14 (13)
F3—C7—C2	113.56 (13)	F22—C27—C22	112.33 (13)
F1—C7—C2	112.10 (13)	F23—C27—C22	112.89 (13)
F2—C7—C2	111.47 (14)	F21—C27—C22	111.78 (13)
F5—C8—F4	107.07 (15)	F25—C28—F24	98.5 (2)
F5—C8—F6	106.75 (15)	F25—C28—F26	121.3 (3)
F4—C8—F6	106.30 (13)	F24—C28—F26	101.4 (2)
F5—C8—C5	112.65 (13)	F25—C28—C25	111.41 (17)
F4—C8—C5	112.47 (13)	F24—C28—C25	113.58 (16)
F6—C8—C5	111.21 (14)	F26—C28—C25	109.75 (17)
C14—C9—C10	118.70 (13)	C34—C29—C30	118.16 (14)
C14—C9—C1	117.35 (13)	C34—C29—C21	116.95 (13)
C10—C9—C1	123.69 (13)	C30—C29—C21	124.79 (13)
C11—C10—C9	120.67 (13)	C31—C30—C29	120.69 (14)
C11—C10—C15	118.36 (13)	C31—C30—C35	118.70 (14)
C9—C10—C15	120.95 (13)	C29—C30—C35	120.60 (14)
C12—C11—C10	120.17 (14)	C30—C31—C32	120.62 (14)
C12—C11—H11	120.6 (14)	C30—C31—H31	121.3 (15)
C10—C11—H11	119.2 (14)	C32—C31—H31	118.0 (15)
C11—C12—C13	119.32 (14)	C33—C32—C31	118.72 (14)
C11—C12—H12	118.6 (13)	C33—C32—H32	119.2 (13)

C13—C12—H12	122.0 (13)	C31—C32—H32	122.1 (13)
C14—C13—C12	120.86 (14)	C34—C33—C32	120.89 (14)
C14—C13—C16	120.34 (14)	C34—C33—C36	117.95 (14)
C12—C13—C16	118.78 (14)	C32—C33—C36	121.13 (14)
C13—C14—C9	120.27 (14)	C33—C34—C29	120.91 (14)
C13—C14—H14	119.2 (13)	C33—C34—H34	119.9 (13)
C9—C14—H14	120.6 (13)	C29—C34—H34	119.2 (13)
F9—C15—F7	106.89 (12)	F29—C35—F27	107.48 (15)
F9—C15—F8	106.32 (13)	F29—C35—F28	106.43 (15)
F7—C15—F8	106.40 (12)	F27—C35—F28	105.79 (14)
F9—C15—C10	112.97 (12)	F29—C35—C30	113.27 (13)
F7—C15—C10	112.27 (12)	F27—C35—C30	111.97 (14)
F8—C15—C10	111.56 (12)	F28—C35—C30	111.44 (14)
F12—C16—F10	107.07 (14)	F32—C36—F30	107.86 (15)
F12—C16—F11	106.83 (14)	F32—C36—F31	106.93 (15)
F10—C16—F11	106.05 (13)	F30—C36—F31	104.34 (15)
F12—C16—C13	111.31 (13)	F32—C36—C33	113.86 (14)
F10—C16—C13	113.17 (13)	F30—C36—C33	111.46 (14)
F11—C16—C13	112.01 (13)	F31—C36—C33	111.83 (13)
C2—C1—C9—C14	85.42 (18)	C22—C21—C29—C34	−79.54 (19)