

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

3-Fluoro-2,4,5-triphenylfuran

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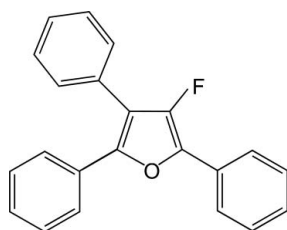
Received 8 October 2007; accepted 10 October 2007

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.045; wR factor = 0.119; data-to-parameter ratio = 13.3.

The title compound, $\text{C}_{22}\text{H}_{15}\text{FO}$, is the first example of a crystallographically characterized fully substituted fluoro-furan. Although the F atom does not appear to participate in aryl- π attractions or classical hydrogen bonding, the title compound does contain four unique intermolecular π - π stacking interactions that have an atom-to-centroid range of 3.53 (4)–3.64 (4) Å. The phenyl ring located between the F and O atoms is only 9.55 (7)° from being coplanar with the furan ring, whereas the other aromatic planes form angles of 41.71 (1) and 20.45 (1)° with the ring.

Related literature

For related literature, see: Hammond (2005); Schlosser (1998); Uneyama (2006); Allen (2002); Arimitsu & Hammond (2006); Arimitsu *et al.* (2007); Desiraju (1995); Janiak (2000); Xu & Chen (2003).



Experimental

Crystal data

$\text{C}_{22}\text{H}_{15}\text{FO}$
 $M_r = 314.34$
 Orthorhombic, *Pbca*
 $a = 7.5865$ (9) Å
 $b = 19.9375$ (15) Å
 $c = 20.4751$ (19) Å

$V = 3097.0$ (5) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 100$ (2) K
 $0.41 \times 0.38 \times 0.35$ mm

Data collection

Bruker SMART APEX
 diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 2001)
 $T_{\min} = 0.861$, $T_{\max} = 0.962$

24875 measured reflections
 3687 independent reflections
 3398 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.119$
 $S = 1.06$
 3687 reflections

277 parameters
 All H-atom parameters refined
 $\Delta\rho_{\text{max}} = 0.59$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

This research was supported by the National Science Foundation (grant to GBH: CHE-0513483). MSM thanks the Kentucky Research Challenge Trust Fund for the purchase of CCD X-ray equipment and an upgrade of our X-ray facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2071).

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supplementary materials

Acta Cryst. (2007). E63, o4337 [doi:10.1107/S1600536807049902]

3-Fluoro-2,4,5-triphenylfuran

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Comment

The furan ring system is a critical structural moiety of a variety of natural products, active pharmaceuticals, agricultural compounds, and synthetic precursors. One particularly underdeveloped area of furan chemistry is the synthesis of fluorine containing systems. This is exceptionally puzzling due to the interesting pharmacokinetic properties fluorine can instill into the parent molecule (Uneyama, 2006; Schlosser, 1998; Hammond, 2005). Recently, our group reported the facile, indium mediated synthesis of α,α -difluorohomopropargyl alcohols (Arimitsu & Hammond, 2006; Arimitsu *et al.*, 2007). The synthetic usefulness of these alcohols in heterocyclizations was demonstrated with a silver catalyzed synthesis of 3-fluoro-2,5-disubstituted furans. If an electrophile could be trapped using this methodology it could provide a critical synthetic handle at the 4-position of the fluorofurans, which in turn could provide ready access to hitherto unknown 3-fluoro-2,4,5-trisubstituted furans such as the title compound.

A search of the Cambridge crystallographic database revealed that the title compound represents the first structurally characterized fully substituted fluorofuran (Allen, 2002). The atomic labelling scheme is shown in Fig. 1 (*ORTEP-3*, Farrugia, 1997) and a partial packing diagram (Fig. 2) identifies the aromatic rings involved in the intermolecular π stacking analysis (Janiak, 2000). Neighboring five-membered furan rings are involved in two intermolecular π - π stacking interactions along the crystallographic *a* axis. The first slipped stack interaction between furan rings is 3.61 (4) Å, between C2 at (*x*, *y*, *z*) and the centroid of the five-membered ring at (*x* + 1/2, *y*, 1/2 - *z*). There is a second slipped π stack interaction of 3.64 (4) Å from C1 at (*x* + 1/2, *y*, 1/2 - *z*) to the centroid of the furan ring at (*x*, *y*, *z*). There are also two slipped π stack intermolecular interactions formed between the phenyl group containing C5—C10 (Ph1) at (*x*, *y*, *z*) with the phenyl group containing C17—C22 (Ph3) of the neighboring molecule at (*x* + 1/2, *y*, 1/2 - *z*). The intermolecular C7 (*x*, *y*, *z*) to C17—C22 centroid distance is 3.53 (4) Å. The second intermolecular interaction of 3.64 (4) Å is between C17 (*x* + 1/2, *y*, 1/2 - *z*) and the C5—C10 centroid.

The fluorine atom sits (dev 0.007 (1) Å) in the same plane as the furan ring, which has a mean deviation of 0.009 (1) Å. The F1—H6 non-bonded contact is 2.416 (17) Å with a F1...C6 separation of 3.0814 (17) Å and the C6—H6...F1 angle is 126.3 (4)°. The O1...H10 non-bonded contact is 2.491 (17) Å with a O1...C10 separation of 2.8250 (16) Å and the C10—H10...O1 angle is 99.0 (4)°. Neither is representative of a classical intramolecular hydrogen bond (Desiraju, 1995). It is however noteworthy that the C5—C10 phenyl plane (dev 0.001 (1) Å), located between F1 and O1, is only 9.55 (7)° from being coplanar with the furan ring, whereas the C11—C16 (dev 0.008 (1) Å) and the C17—C22 (dev 0.004 (1) Å) aromatic planes form angles of 41.71° and 20.45°, respectively, with the five-membered furan ring. The *x*-ray structure of the related complex 3-fluoro-2-(4-methoxyphenyl)-5-phenylfuran previously reported (Xu & Chen, 2003; CSD refcode HACYUG) contains two aromatic substituents and shows similar π stacking interactions to the title compound. Interestingly, the methoxyphenyl group located at position 2 of the furan ring in this compound is also nearly coplanar (angle of 1.99°) with the furan plane. The fact that the only two crystal structures known for fluorofurans both show this coplanarity may suggest the possibility of an F...H interaction, but this needs to be proven with more structurally related analogues.

Experimental

To a microwave vial were added Pd(PPh₃)₄ (23.1 mg, 0.02 mmol), benzene boronic acid (97.5 mg, 0.8 mmol), 3-fluoro-4-iodo-2,5-diphenyl-furan (74.4 mg, 0.2 mmol) in 4.0 ml of toluene, 0.4 ml EtOH, and 0.4 ml of aq. 2M Na₂CO₃. The vial was capped and purged with argon before microwave irradiation (388 K, 30 min). Column chromatography (neat hexane/silica) yielded the title compound (63.0 mg, 98%). Crystals for X-ray analysis were obtained upon slow evaporation of a hexane solution of the title compound at room temperature.

Refinement

Phenyl hydrogen atoms were located from difference maps and refined isotropically. C—H Bond distances range from 0.958 (17) Å to 1.01 (2) Å with an average of 0.977 (19) Å. The highest peak, 0.59 e/Å³, and deepest trough, -0.24 e/Å³, are located 1.53 Å from O1 and 0.46 Å from F1, respectively.

Figures

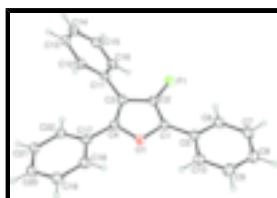


Fig. 1. ORTEP-3 (Farrugia, 1997) drawing of the title compound with atom labels showing 50% probability displacement ellipsoids for non-H atoms.



Fig. 2. Packing diagram illustrating centroid-to-centroid contacts of the furan and phenyl rings involved in π stacking interactions.

3-Fluoro-2,4,5-triphenylfuran

Crystal data

C₂₂H₁₅FO

$M_r = 314.34$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 7.5865$ (9) Å

$b = 19.9375$ (15) Å

$c = 20.4751$ (19) Å

$V = 3097.0$ (5) Å³

$Z = 8$

$F_{000} = 1312$

$D_x = 1.348$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 8241 reflections

$\theta = 2.3$ – 28.1°

$\mu = 0.09$ mm⁻¹

$T = 100$ (2) K

Prism, colorless

$0.41 \times 0.38 \times 0.35$ mm

Data collection

Bruker SMART APEX diffractometer	3687 independent reflections
Radiation source: fine-focus sealed tube	3398 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.021$
$T = 100(2)$ K	$\theta_{\text{max}} = 28.1^\circ$
ω scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$h = -10 \rightarrow 9$
$T_{\text{min}} = 0.861$, $T_{\text{max}} = 0.962$	$k = -26 \rightarrow 26$
24875 measured reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	All H-atom parameters refined
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 1.6834P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3687 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
277 parameters	$\Delta\rho_{\text{max}} = 0.59 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

Experimental. Data were collected with a Bruker *SMART APEX* CCD-based diffractometer using ω -scans of width 0.3° and 30 s duration at a crystal-to-detector distance of 4.908 cm. Intensity decay over the course of the data collection was evaluated by recollecting the first 50 frames of data at the end of the experiment. No significant decay was noted.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.24250 (12)	0.14903 (4)	0.30129 (4)	0.0193 (2)
F1	0.36667 (12)	0.26745 (4)	0.18364 (4)	0.0268 (2)
C1	0.26352 (17)	0.16753 (6)	0.23730 (6)	0.0188 (3)
C2	0.32872 (17)	0.23095 (6)	0.23764 (6)	0.0195 (3)
C3	0.34605 (16)	0.25496 (6)	0.30272 (6)	0.0194 (3)
C4	0.29465 (15)	0.20144 (6)	0.34049 (6)	0.0184 (3)
C5	0.20939 (16)	0.12118 (6)	0.18630 (6)	0.0195 (3)
C6	0.2446 (2)	0.13500 (7)	0.12062 (7)	0.0260 (3)
H6	0.308 (2)	0.1752 (9)	0.1103 (8)	0.027 (4)*
C7	0.1890 (2)	0.09044 (8)	0.07241 (7)	0.0304 (3)
H7	0.215 (2)	0.1031 (9)	0.0283 (10)	0.037 (5)*

supplementary materials

C8	0.0992 (2)	0.03254 (8)	0.08894 (7)	0.0303 (3)
H8	0.060 (3)	0.0013 (10)	0.0532 (9)	0.045 (5)*
C9	0.0633 (2)	0.01869 (7)	0.15384 (7)	0.0292 (3)
H9	-0.003 (3)	-0.0234 (10)	0.1652 (9)	0.038 (5)*
C10	0.11767 (18)	0.06254 (7)	0.20227 (7)	0.0243 (3)
H10	0.091 (2)	0.0522 (8)	0.2489 (9)	0.030 (4)*
C11	0.39500 (16)	0.32426 (6)	0.32030 (6)	0.0191 (3)
C12	0.30502 (17)	0.36018 (6)	0.36857 (6)	0.0209 (3)
H12	0.210 (2)	0.3385 (8)	0.3916 (8)	0.025 (4)*
C13	0.35095 (18)	0.42630 (7)	0.38218 (6)	0.0237 (3)
H13	0.288 (2)	0.4511 (9)	0.4165 (9)	0.033 (5)*
C14	0.48662 (19)	0.45735 (7)	0.34824 (7)	0.0256 (3)
H14	0.519 (2)	0.5038 (9)	0.3574 (8)	0.029 (4)*
C15	0.57389 (19)	0.42260 (7)	0.29931 (7)	0.0256 (3)
H15	0.666 (2)	0.4434 (9)	0.2744 (9)	0.033 (5)*
C16	0.52771 (18)	0.35688 (7)	0.28521 (6)	0.0227 (3)
H16	0.588 (2)	0.3326 (8)	0.2512 (8)	0.023 (4)*
C17	0.29370 (16)	0.18711 (6)	0.41057 (6)	0.0186 (3)
C18	0.19434 (18)	0.13319 (7)	0.43419 (7)	0.0233 (3)
H18	0.118 (2)	0.1069 (8)	0.4032 (9)	0.029 (4)*
C19	0.1970 (2)	0.11738 (7)	0.50027 (7)	0.0277 (3)
H19	0.126 (2)	0.0805 (9)	0.5154 (9)	0.034 (5)*
C20	0.2979 (2)	0.15475 (7)	0.54358 (7)	0.0276 (3)
H20	0.297 (2)	0.1453 (9)	0.5882 (9)	0.030 (4)*
C21	0.39791 (19)	0.20809 (7)	0.52025 (6)	0.0248 (3)
H21	0.470 (2)	0.2344 (8)	0.5490 (8)	0.026 (4)*
C22	0.39726 (17)	0.22406 (6)	0.45427 (6)	0.0210 (3)
H22	0.474 (2)	0.2595 (8)	0.4383 (8)	0.024 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0223 (4)	0.0194 (4)	0.0161 (4)	0.0000 (3)	-0.0005 (3)	-0.0001 (3)
F1	0.0369 (5)	0.0251 (4)	0.0184 (4)	-0.0011 (3)	0.0038 (3)	0.0047 (3)
C1	0.0195 (6)	0.0210 (6)	0.0160 (6)	0.0033 (5)	0.0010 (4)	0.0013 (4)
C2	0.0220 (6)	0.0194 (6)	0.0170 (6)	0.0029 (5)	0.0006 (5)	0.0018 (4)
C3	0.0183 (5)	0.0209 (6)	0.0191 (6)	0.0030 (5)	-0.0001 (4)	0.0004 (4)
C4	0.0178 (6)	0.0181 (6)	0.0194 (6)	0.0014 (4)	-0.0015 (4)	-0.0027 (4)
C5	0.0194 (6)	0.0214 (6)	0.0177 (6)	0.0050 (5)	-0.0012 (4)	-0.0011 (4)
C6	0.0307 (7)	0.0277 (7)	0.0195 (6)	0.0050 (6)	0.0016 (5)	0.0019 (5)
C7	0.0369 (8)	0.0371 (8)	0.0173 (6)	0.0111 (6)	-0.0014 (6)	-0.0011 (5)
C8	0.0319 (7)	0.0317 (7)	0.0273 (7)	0.0068 (6)	-0.0091 (6)	-0.0077 (6)
C9	0.0293 (7)	0.0271 (7)	0.0311 (7)	-0.0010 (6)	-0.0049 (6)	-0.0040 (6)
C10	0.0248 (6)	0.0245 (6)	0.0235 (6)	0.0007 (5)	-0.0011 (5)	-0.0013 (5)
C11	0.0204 (6)	0.0182 (6)	0.0186 (6)	0.0024 (5)	-0.0032 (4)	0.0022 (4)
C12	0.0223 (6)	0.0221 (6)	0.0182 (6)	0.0015 (5)	-0.0006 (5)	0.0019 (5)
C13	0.0292 (7)	0.0226 (6)	0.0193 (6)	0.0052 (5)	-0.0042 (5)	-0.0009 (5)
C14	0.0326 (7)	0.0186 (6)	0.0255 (6)	-0.0001 (5)	-0.0081 (5)	0.0025 (5)

C15	0.0259 (6)	0.0236 (6)	0.0273 (7)	-0.0022 (5)	-0.0017 (5)	0.0060 (5)
C16	0.0229 (6)	0.0230 (6)	0.0221 (6)	0.0028 (5)	0.0008 (5)	0.0023 (5)
C17	0.0182 (6)	0.0183 (6)	0.0195 (6)	0.0030 (4)	0.0005 (4)	0.0009 (4)
C18	0.0242 (6)	0.0220 (6)	0.0236 (6)	-0.0014 (5)	0.0010 (5)	0.0009 (5)
C19	0.0318 (7)	0.0256 (7)	0.0258 (7)	-0.0016 (6)	0.0062 (6)	0.0050 (5)
C20	0.0374 (8)	0.0273 (7)	0.0180 (6)	0.0075 (6)	0.0037 (5)	0.0021 (5)
C21	0.0305 (7)	0.0232 (6)	0.0207 (6)	0.0051 (5)	-0.0032 (5)	-0.0031 (5)
C22	0.0225 (6)	0.0190 (6)	0.0215 (6)	0.0009 (5)	-0.0010 (5)	0.0005 (5)

Geometric parameters (Å, °)

O1—C1	1.3704 (14)	C11—C12	1.3984 (17)
O1—C4	1.3758 (15)	C12—C13	1.3916 (18)
F1—C2	1.3546 (14)	C12—H12	0.966 (17)
C1—C2	1.3578 (18)	C13—C14	1.388 (2)
C1—C5	1.4537 (17)	C13—H13	0.984 (18)
C2—C3	1.4219 (17)	C14—C15	1.386 (2)
C3—C4	1.3743 (18)	C14—H14	0.977 (17)
C3—C11	1.4753 (17)	C15—C16	1.3866 (19)
C4—C17	1.4631 (17)	C15—H15	0.959 (19)
C5—C6	1.3984 (18)	C16—H16	0.964 (17)
C5—C10	1.3993 (19)	C17—C18	1.3993 (18)
C6—C7	1.394 (2)	C17—C22	1.4002 (18)
C6—H6	0.958 (17)	C18—C19	1.3892 (19)
C7—C8	1.383 (2)	C18—H18	1.005 (18)
C7—H7	0.959 (19)	C19—C20	1.388 (2)
C8—C9	1.384 (2)	C19—H19	0.965 (18)
C8—H8	1.01 (2)	C20—C21	1.391 (2)
C9—C10	1.3849 (19)	C20—H20	0.932 (18)
C9—H9	1.004 (19)	C21—C22	1.3879 (18)
C10—H10	0.999 (18)	C21—H21	0.961 (17)
C11—C16	1.3976 (18)	C22—H22	0.973 (17)
C1—O1—C4	108.65 (10)	C13—C12—C11	120.29 (12)
C2—C1—O1	106.75 (10)	C13—C12—H12	121.0 (10)
C2—C1—C5	134.32 (11)	C11—C12—H12	118.7 (10)
O1—C1—C5	118.87 (11)	C14—C13—C12	120.53 (12)
F1—C2—C1	124.99 (11)	C14—C13—H13	119.6 (10)
F1—C2—C3	124.36 (11)	C12—C13—H13	119.8 (10)
C1—C2—C3	110.61 (11)	C15—C14—C13	119.55 (12)
C4—C3—C2	103.87 (11)	C15—C14—H14	119.5 (10)
C4—C3—C11	131.39 (12)	C13—C14—H14	120.9 (10)
C2—C3—C11	124.56 (11)	C14—C15—C16	120.13 (13)
C3—C4—O1	110.06 (11)	C14—C15—H15	121.0 (11)
C3—C4—C17	134.83 (12)	C16—C15—H15	118.8 (11)
O1—C4—C17	114.99 (10)	C15—C16—C11	120.98 (13)
C6—C5—C10	118.98 (12)	C15—C16—H16	120.3 (10)
C6—C5—C1	120.76 (12)	C11—C16—H16	118.8 (9)
C10—C5—C1	120.25 (11)	C18—C17—C22	119.05 (12)
C7—C6—C5	119.84 (14)	C18—C17—C4	119.45 (11)

supplementary materials

C7—C6—H6	121.9 (10)	C22—C17—C4	121.41 (11)
C5—C6—H6	118.2 (10)	C19—C18—C17	120.20 (13)
C8—C7—C6	120.54 (13)	C19—C18—H18	120.3 (10)
C8—C7—H7	123.5 (11)	C17—C18—H18	119.5 (10)
C6—C7—H7	115.9 (11)	C20—C19—C18	120.55 (13)
C7—C8—C9	119.90 (13)	C20—C19—H19	120.9 (11)
C7—C8—H8	118.9 (11)	C18—C19—H19	118.5 (11)
C9—C8—H8	121.2 (11)	C19—C20—C21	119.46 (13)
C10—C9—C8	120.18 (14)	C19—C20—H20	120.9 (11)
C10—C9—H9	120.7 (11)	C21—C20—H20	119.6 (11)
C8—C9—H9	119.1 (11)	C22—C21—C20	120.50 (13)
C9—C10—C5	120.55 (13)	C22—C21—H21	118.2 (10)
C9—C10—H10	119.6 (10)	C20—C21—H21	121.3 (10)
C5—C10—H10	119.9 (10)	C21—C22—C17	120.22 (12)
C16—C11—C12	118.47 (12)	C21—C22—H22	119.5 (9)
C16—C11—C3	119.46 (11)	C17—C22—H22	120.2 (9)
C12—C11—C3	121.96 (11)		
C4—O1—C1—C2	0.17 (13)	C6—C5—C10—C9	0.3 (2)
C4—O1—C1—C5	-177.28 (10)	C1—C5—C10—C9	178.98 (12)
O1—C1—C2—F1	-179.54 (11)	C4—C3—C11—C16	144.23 (14)
C5—C1—C2—F1	-2.7 (2)	C2—C3—C11—C16	-41.45 (18)
O1—C1—C2—C3	-1.62 (15)	C4—C3—C11—C12	-39.9 (2)
C5—C1—C2—C3	175.24 (13)	C2—C3—C11—C12	134.45 (13)
F1—C2—C3—C4	-179.66 (11)	C16—C11—C12—C13	-1.74 (18)
C1—C2—C3—C4	2.40 (14)	C3—C11—C12—C13	-177.69 (11)
F1—C2—C3—C11	4.7 (2)	C11—C12—C13—C14	-0.17 (19)
C1—C2—C3—C11	-173.21 (12)	C12—C13—C14—C15	1.6 (2)
C2—C3—C4—O1	-2.26 (13)	C13—C14—C15—C16	-1.1 (2)
C11—C3—C4—O1	172.92 (12)	C14—C15—C16—C11	-0.9 (2)
C2—C3—C4—C17	173.25 (13)	C12—C11—C16—C15	2.27 (19)
C11—C3—C4—C17	-11.6 (2)	C3—C11—C16—C15	178.31 (12)
C1—O1—C4—C3	1.40 (13)	C3—C4—C17—C18	165.26 (14)
C1—O1—C4—C17	-175.10 (10)	O1—C4—C17—C18	-19.39 (16)
C2—C1—C5—C6	10.0 (2)	C3—C4—C17—C22	-18.1 (2)
O1—C1—C5—C6	-173.47 (12)	O1—C4—C17—C22	157.30 (11)
C2—C1—C5—C10	-168.72 (14)	C22—C17—C18—C19	0.91 (19)
O1—C1—C5—C10	7.86 (18)	C4—C17—C18—C19	177.67 (12)
C10—C5—C6—C7	-0.2 (2)	C17—C18—C19—C20	0.0 (2)
C1—C5—C6—C7	-178.92 (12)	C18—C19—C20—C21	-0.5 (2)
C5—C6—C7—C8	0.0 (2)	C19—C20—C21—C22	0.0 (2)
C6—C7—C8—C9	0.3 (2)	C20—C21—C22—C17	0.9 (2)
C7—C8—C9—C10	-0.2 (2)	C18—C17—C22—C21	-1.35 (19)
C8—C9—C10—C5	-0.1 (2)	C4—C17—C22—C21	-178.05 (12)

Fig. 1

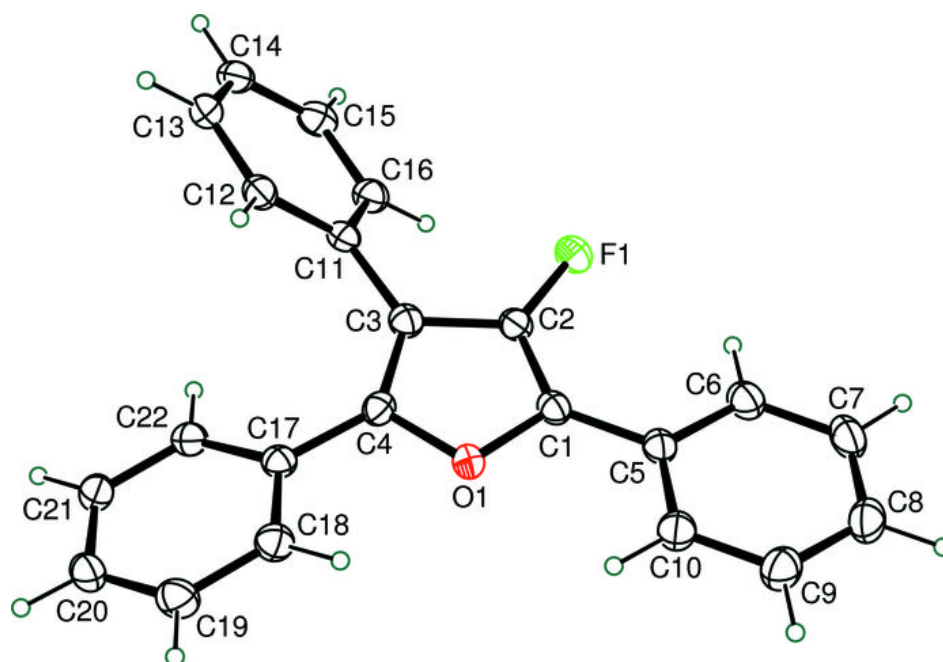


Fig. 2

