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1-[2,4-Bis(4-fluorophenoxy)phenyl]-ethanone

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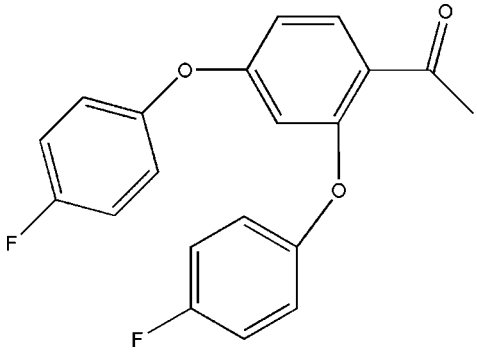
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.068; wR factor = 0.198; data-to-parameter ratio = 12.3.

The title compound, $C_{20}H_{14}F_2O_3$, has been obtained in a search for new fluorine-containing compounds with better biological activity. The two fluorophenyl rings are oriented at angles of 64.03 (2) and 64.55 (3)° to the ethanone-substituted benzene ring. The structure is stabilized by C—H···O hydrogen bonds, in addition to van der Waals forces.

Related literature

For related literatures see: Allen *et al.* (1987); Thierry & Bernard (2002); Xu *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{14}F_2O_3$
M_r = 340.31
Triclinic, $P\overline{1}$
a = 6.746 (2) Å
b = 9.573 (2) Å
c = 13.335 (3) Å
α = 100.52 (3)°
β = 98.43 (3)°
γ = 95.68 (3)°
V = 830.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.969, T_{max} = 0.981
4425 measured reflections
2798 independent reflections
2258 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.198
S = 1.11
2798 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1^{i}	0.93	2.46	3.376 (3)	167

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2280).

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Xu, L.-Z., Bi, W.-Z. & Zhai, Z.-W. (2007). *Acta Cryst.* E**63**, o3243.

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supplementary materials

Acta Cryst. (2007). E**63**, o3825 [**doi:10.1107/S1600536807040056**]

1-[2,4-Bis(4-fluorophenoxy)phenyl]ethanone

G.-N. Li, Y.-X. Jiang, Z.-W. Zhai, Z.-J. Xu and L.-Z. Xu

Comment

Recently, interest in fluorine-containing compounds is continuously growing since fluorinated organic products present unique properties that are of great interest for a variety of applications (Thierry & Bernard, 2002). The title compound (I) was synthesized as a useful intermediate for the synthesis of compounds with better biological activity. We report here the crystal structure of (I).

In (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987) and in a good agreement with those reported previously (Xu *et al.*, 2007)·The two fluorophenyl rings (C9—C14) and (C15—C20) are oriented at angles of 64.03 (2) and 64.55 (3)°, respectively, to the ethanone substituted phenyl ring (C1—C6). The structure is stabilized by hydrogen bonds of C—H···O type, in addition to van der Waals forces.

Experimental

Acetyl chloride (10 mmol) was added dropwise to a solution of 1,3-bis(4-fluorophenoxy)benzene (10 mmol), aluminium oxide (13 mmol), carbon sulfide (20 ml) and the mixture was heated under reflux for 2 h. Then the mixture was extracted with CS_2 (15 ml) and the organic layer was washed with 50% NaOH solution and water. The excess CS_2 was removed on a water vacuum pump to obtain the final product (80% yield). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Figures

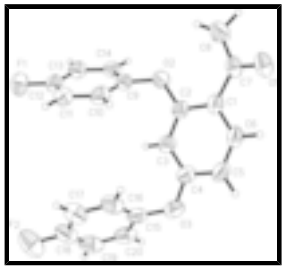

Fig. 1. View of the title compound (I), with displacement ellipsoids drawn at the 40% probability level.

Fig. 2. A packing diagram of the molecule of the title compound. Hydrogen bonds are shown as dashed lines.

1-[2,4-Bis(4-fluorophenoxy)phenyl]ethanone

Crystal data

$C_{20}H_{14}F_2O_3$	$Z = 2$
$M_r = 340.31$	$F_{000} = 352$
Triclinic, $P\overline{1}$	$D_x = 1.361$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.746$ (2) Å	Cell parameters from 2755 reflections
$b = 9.573$ (2) Å	$\theta = 2.4$–24.8º
$c = 13.335$ (3) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 100.52$ (3)º	$T = 298$ (2) K
$\beta = 98.43$ (3)º	Block, colorless
$\gamma = 95.68$ (3)º	0.30 × 0.20 × 0.18 mm
$V = 830.5$ (3) Å^3	

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer	2798 independent reflections
Radiation source: Rotating Anode	2258 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
$T = 298$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 2.9$º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -8 \rightarrow 8$
$T_{min} = 0.969$, $T_{max} = 0.981$	$k = -11 \rightarrow 10$
4425 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.098P)^2 + 0.2416P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.198$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.11$	$\Delta\rho_{max} = 0.21$ e Å^{-3}

2798 reflections

228 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.22$ e Å^{-3}

Extinction correction: SHELXTL (Sheldrick, 2001), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.062 (10)

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 $F^2 > 2\text{sigma}(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.8326 (3)	0.3501 (2)	−0.04283 (15)	0.0936 (7)
F2	1.0613 (4)	0.9902 (3)	0.1086 (2)	0.1280 (10)
O1	0.1919 (3)	0.3955 (2)	0.54241 (14)	0.0695 (6)
O2	0.3463 (3)	0.3970 (2)	0.25339 (14)	0.0720 (6)
O3	0.4744 (4)	0.9133 (2)	0.34425 (18)	0.0815 (7)
C1	0.2820 (3)	0.5192 (3)	0.41566 (18)	0.0503 (6)
C2	0.3478 (4)	0.5248 (3)	0.32182 (18)	0.0515 (6)
C3	0.4082 (4)	0.6547 (3)	0.29566 (19)	0.0564 (7)
H3A	0.4445	0.6565	0.2312	0.068*
C4	0.4139 (4)	0.7808 (3)	0.3659 (2)	0.0595 (7)
C5	0.3509 (4)	0.7798 (3)	0.4596 (2)	0.0663 (8)
H5A	0.3520	0.8650	0.5063	0.080*
C6	0.2867 (4)	0.6510 (3)	0.4826 (2)	0.0605 (7)
H6A	0.2442	0.6509	0.5459	0.073*
C7	0.2111 (3)	0.3868 (3)	0.45263 (19)	0.0552 (7)
C8	0.1539 (6)	0.2446 (4)	0.3795 (3)	0.0796 (9)
H8A	0.0834	0.1786	0.4125	0.119*
H8B	0.2737	0.2079	0.3610	0.119*
H8C	0.0679	0.2563	0.3184	0.119*
C9	0.4752 (4)	0.3906 (3)	0.17958 (19)	0.0542 (7)
C10	0.6793 (5)	0.4384 (3)	0.2068 (2)	0.0611 (7)
H10A	0.7348	0.4790	0.2752	0.073*
C11	0.8014 (5)	0.4251 (3)	0.1309 (2)	0.0648 (7)
H11A	0.9391	0.4576	0.1470	0.078*
C12	0.7127 (5)	0.3626 (3)	0.0316 (2)	0.0610 (7)
C13	0.5120 (5)	0.3126 (3)	0.0045 (2)	0.0629 (7)
H13A	0.4578	0.2693	−0.0636	0.075*

C14	0.3894 (4)	0.3270 (3)	0.07976 (19)	0.0572 (7)
H14A	0.2519	0.2943	0.0629	0.069*
C15	0.6225 (5)	0.9241 (3)	0.2822 (2)	0.0650 (8)
C16	0.7975 (5)	0.8591 (3)	0.2959 (2)	0.0708 (8)
H16A	0.8162	0.8025	0.3454	0.085*
C17	0.9435 (5)	0.8794 (4)	0.2352 (3)	0.0788 (9)
H17A	1.0593	0.8342	0.2414	0.095*
C18	0.9138 (6)	0.9673 (4)	0.1659 (3)	0.0812 (10)
C19	0.7423 (6)	1.0335 (3)	0.1517 (3)	0.0858 (11)
H19A	0.7262	1.0919	0.1033	0.103*
C20	0.5954 (6)	1.0112 (3)	0.2107 (3)	0.0770 (9)
H20A	0.4784	1.0547	0.2025	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1111 (15)	0.1002 (14)	0.0762 (12)	0.0141 (12)	0.0497 (11)	0.0073 (10)
F2	0.126 (2)	0.146 (2)	0.1240 (19)	−0.0163 (17)	0.0406 (16)	0.0590 (17)
O1	0.0619 (12)	0.0960 (15)	0.0501 (11)	−0.0013 (10)	0.0122 (9)	0.0167 (10)
O2	0.1009 (15)	0.0544 (11)	0.0554 (11)	−0.0125 (10)	0.0350 (11)	−0.0076 (9)
O3	0.1117 (18)	0.0508 (11)	0.0873 (15)	0.0160 (11)	0.0374 (13)	0.0076 (10)
C1	0.0400 (12)	0.0630 (15)	0.0437 (13)	0.0040 (11)	0.0045 (9)	0.0029 (11)
C2	0.0526 (13)	0.0534 (14)	0.0437 (13)	0.0027 (11)	0.0074 (10)	0.0003 (10)
C3	0.0668 (16)	0.0562 (15)	0.0453 (13)	0.0082 (12)	0.0114 (11)	0.0061 (11)
C4	0.0660 (16)	0.0512 (14)	0.0591 (16)	0.0091 (12)	0.0098 (12)	0.0050 (12)
C5	0.0694 (17)	0.0626 (17)	0.0623 (17)	0.0104 (14)	0.0189 (14)	−0.0069 (13)
C6	0.0534 (15)	0.0759 (18)	0.0490 (14)	0.0067 (13)	0.0156 (11)	−0.0006 (13)
C7	0.0398 (12)	0.0766 (17)	0.0469 (14)	−0.0005 (12)	0.0065 (10)	0.0115 (12)
C8	0.092 (2)	0.0726 (19)	0.0683 (18)	−0.0170 (17)	0.0211 (16)	0.0073 (15)
C9	0.0776 (18)	0.0418 (12)	0.0442 (13)	0.0043 (12)	0.0200 (12)	0.0052 (10)
C10	0.0772 (18)	0.0581 (15)	0.0436 (13)	0.0074 (14)	0.0055 (12)	0.0030 (11)
C11	0.0667 (17)	0.0605 (16)	0.0672 (17)	0.0096 (13)	0.0137 (14)	0.0099 (13)
C12	0.084 (2)	0.0541 (15)	0.0503 (15)	0.0157 (14)	0.0269 (14)	0.0090 (12)
C13	0.090 (2)	0.0548 (15)	0.0398 (13)	0.0043 (14)	0.0112 (13)	0.0005 (11)
C14	0.0724 (17)	0.0460 (13)	0.0495 (14)	0.0006 (12)	0.0097 (12)	0.0045 (11)
C15	0.089 (2)	0.0406 (13)	0.0598 (16)	−0.0016 (14)	0.0094 (14)	0.0027 (12)
C16	0.087 (2)	0.0630 (17)	0.0603 (17)	−0.0003 (16)	0.0029 (15)	0.0208 (13)
C17	0.0735 (19)	0.079 (2)	0.083 (2)	−0.0035 (16)	0.0030 (16)	0.0288 (17)
C18	0.094 (2)	0.073 (2)	0.072 (2)	−0.0183 (19)	0.0111 (17)	0.0231 (16)
C19	0.120 (3)	0.0581 (18)	0.077 (2)	−0.0054 (19)	0.004 (2)	0.0274 (16)
C20	0.101 (2)	0.0448 (15)	0.083 (2)	0.0085 (15)	0.0073 (18)	0.0136 (14)

Geometric parameters (Å, °)

F1—C12	1.365 (3)	C9—C14	1.373 (4)
F2—C18	1.366 (4)	C9—C10	1.380 (4)
O1—C7	1.212 (3)	C10—C11	1.392 (4)
O2—C2	1.384 (3)	C10—H10A	0.9300
O2—C9	1.403 (3)	C11—C12	1.370 (4)

O3—C4	1.388 (3)	C11—H11A	0.9300
O3—C15	1.395 (4)	C12—C13	1.363 (4)
C1—C2	1.396 (3)	C13—C14	1.387 (4)
C1—C6	1.401 (4)	C13—H13A	0.9300
C1—C7	1.502 (4)	C14—H14A	0.9300
C2—C3	1.391 (4)	C15—C20	1.381 (4)
C3—C4	1.380 (4)	C15—C16	1.392 (5)
C3—H3A	0.9300	C16—C17	1.385 (4)
C4—C5	1.379 (4)	C16—H16A	0.9300
C5—C6	1.369 (4)	C17—C18	1.365 (5)
C5—H5A	0.9300	C17—H17A	0.9300
C6—H6A	0.9300	C18—C19	1.378 (5)
C7—C8	1.501 (4)	C19—C20	1.376 (5)
C8—H8A	0.9600	C19—H19A	0.9300
C8—H8B	0.9600	C20—H20A	0.9300
C8—H8C	0.9600		
C2—O2—C9	119.45 (19)	C9—C10—H10A	120.3
C4—O3—C15	118.9 (2)	C11—C10—H10A	120.3
C2—C1—C6	116.3 (2)	C12—C11—C10	118.0 (3)
C2—C1—C7	126.7 (2)	C12—C11—H11A	121.0
C6—C1—C7	117.0 (2)	C10—C11—H11A	121.0
O2—C2—C3	120.4 (2)	C13—C12—F1	119.1 (2)
O2—C2—C1	118.2 (2)	C13—C12—C11	123.0 (3)
C3—C2—C1	121.4 (2)	F1—C12—C11	117.9 (3)
C4—C3—C2	119.6 (2)	C12—C13—C14	119.2 (2)
C4—C3—H3A	120.2	C12—C13—H13A	120.4
C2—C3—H3A	120.2	C14—C13—H13A	120.4
C5—C4—C3	120.7 (3)	C9—C14—C13	118.7 (3)
C5—C4—O3	117.2 (2)	C9—C14—H14A	120.7
C3—C4—O3	122.0 (2)	C13—C14—H14A	120.7
C6—C5—C4	118.7 (2)	C20—C15—C16	120.8 (3)
C6—C5—H5A	120.6	C20—C15—O3	117.0 (3)
C4—C5—H5A	120.6	C16—C15—O3	122.1 (3)
C5—C6—C1	123.3 (2)	C17—C16—C15	119.4 (3)
C5—C6—H6A	118.4	C17—C16—H16A	120.3
C1—C6—H6A	118.4	C15—C16—H16A	120.3
O1—C7—C8	119.0 (3)	C18—C17—C16	118.5 (3)
O1—C7—C1	119.5 (2)	C18—C17—H17A	120.7
C8—C7—C1	121.4 (2)	C16—C17—H17A	120.7
C7—C8—H8A	109.5	C17—C18—F2	118.1 (4)
C7—C8—H8B	109.5	C17—C18—C19	122.9 (3)
H8A—C8—H8B	109.5	F2—C18—C19	119.0 (3)
C7—C8—H8C	109.5	C20—C19—C18	118.6 (3)
H8A—C8—H8C	109.5	C20—C19—H19A	120.7
H8B—C8—H8C	109.5	C18—C19—H19A	120.7
C14—C9—C10	121.8 (2)	C19—C20—C15	119.7 (3)
C14—C9—O2	116.4 (2)	C19—C20—H20A	120.1
C10—C9—O2	121.8 (2)	C15—C20—H20A	120.1
C9—C10—C11	119.3 (2)		

C9—O2—C2—C3	25.4 (4)	C14—C9—C10—C11	1.6 (4)
C9—O2—C2—C1	−156.4 (2)	O2—C9—C10—C11	177.9 (2)
C6—C1—C2—O2	179.8 (2)	C9—C10—C11—C12	−0.9 (4)
C7—C1—C2—O2	1.1 (4)	C10—C11—C12—C13	−0.4 (4)
C6—C1—C2—C3	−2.0 (4)	C10—C11—C12—F1	179.8 (2)
C7—C1—C2—C3	179.3 (2)	F1—C12—C13—C14	−179.1 (2)
O2—C2—C3—C4	−178.3 (2)	C11—C12—C13—C14	1.1 (4)
C1—C2—C3—C4	3.5 (4)	C10—C9—C14—C13	−0.9 (4)
C2—C3—C4—C5	−3.2 (4)	O2—C9—C14—C13	−177.4 (2)
C2—C3—C4—O3	179.5 (3)	C12—C13—C14—C9	−0.4 (4)
C15—O3—C4—C5	149.4 (3)	C4—O3—C15—C20	139.8 (3)
C15—O3—C4—C3	−33.2 (4)	C4—O3—C15—C16	−44.8 (4)
C3—C4—C5—C6	1.4 (4)	C20—C15—C16—C17	−1.7 (4)
O3—C4—C5—C6	178.9 (3)	O3—C15—C16—C17	−176.9 (3)
C4—C5—C6—C1	0.1 (4)	C15—C16—C17—C18	2.3 (5)
C2—C1—C6—C5	0.2 (4)	C16—C17—C18—F2	178.0 (3)
C7—C1—C6—C5	179.0 (3)	C16—C17—C18—C19	−1.9 (5)
C2—C1—C7—O1	167.1 (2)	C17—C18—C19—C20	0.7 (5)
C6—C1—C7—O1	−11.5 (4)	F2—C18—C19—C20	−179.2 (3)
C2—C1—C7—C8	−15.8 (4)	C18—C19—C20—C15	0.0 (5)
C6—C1—C7—C8	165.5 (3)	C16—C15—C20—C19	0.5 (4)
C2—O2—C9—C14	−132.5 (3)	O3—C15—C20—C19	175.9 (3)
C2—O2—C9—C10	51.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10A···O1^{i}	0.93	2.46	3.376 (3)	167

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

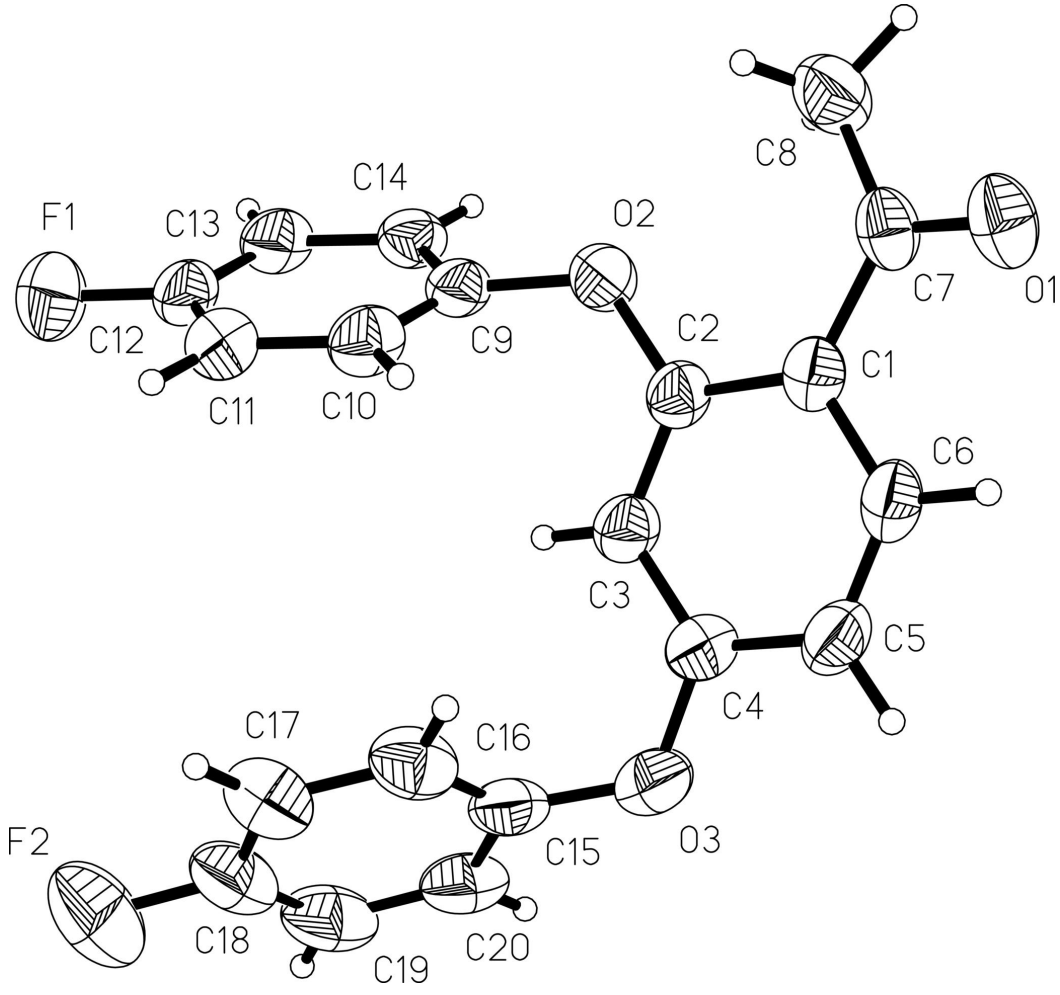
C8
C14
F1
C13
O2
C7
O1
C12
C9
C2
C1
C11
C10
C6
C3
C5
C4
C17
C16
F2
C15
O3
C18
C20
C19

Fig. 2