Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (2*E*,6*E*)-2,6-Bis(2,5-difluorobenzylidene)-cyclohexanone

**Chengxi Jiang,[a,b] Zhiguo Feng,[b] Bo Song,[b] Xiaoxia Li[b] and Xiaokun Li[a]***

[a]Ministry of Education, Engineering Research Center of Bioreactor and Pharmaceutical Development, Jilin Agricultural University, Changchun 130118, People's Republic of China, and [b]School of Pharmacy, Wenzhou Medical College, Wenzhou, Zhejiang Province 325035, People's Republic of China
Correspondence e-mail: proflxk@163.com

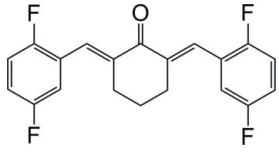
Received 24 March 2010; accepted 26 March 2010

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.056; $wR$ factor = 0.156; data-to-parameter ratio = 15.1.

In the title compound, $C_{20}H_{14}F_4O$, a derivative of curcumin, the dihedral angle between the two aromatic rings is 27.19 (13)°. The C=C double bonds have an *E* configuration.

## Related literature

For background and related structures, see: Liang *et al.* (2007*a*,*b*, 2009); Zhao *et al.* (2009, 2010*a*,*b*).




## Experimental

### Crystal data

$C_{20}H_{14}F_4O$
$M_r$ = 346.31
Monoclinic, $P2_1/c$
$a$ = 15.824 (2) Å
$b$ = 6.3128 (8) Å
$c$ = 17.097 (2) Å
$\beta$ = 111.756 (3)°
$V$ = 1586.2 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 293 K
0.43 × 0.35 × 0.27 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min}$ = 0.490, $T_{max}$ = 1.000
8935 measured reflections
3425 independent reflections
2018 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.156
$S$ = 0.93
3425 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −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, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We acknowledge the X-ray crystallographic service at the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2751).

## References

Bruker (2002). *SMART, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Liang, G., Shao, L. L., Wang, Y., Zhao, C. G., Chu, Y. H., Xiao, J., Zhao, Y., Li, X. K. & Yang, S. L. (2009). *Bioorg. Med. Chem.* **17**, 2623–2631.
Liang, G., Tian, J.-L., Zhao, C.-G. & Li, X.-K. (2007*a*). *Acta Cryst.* E**63**, o3630.
Liang, G., Yang, S.-L., Wang, X.-H., Li, Y.-R. & Li, X.-K. (2007*b*). *Acta Cryst.* E**63**, o4118.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhao, C. G., Yang, J., Huang, Y., Liang, G. & Li, X. K. (2009). *Z. Kristallogr. New Cryst. Struct.* **224**, 337–338.
Zhao, C. G., Yang, J., Liang, D. L., Tang, Q. Q., Zhang, Y., Liang, G. & Li, X. K. (2010*a*). *Chin. J . Org. Chem.* **30**, 289–294.
Zhao, C. G., Yang, J., Wang, Y., Liang, D. L., Yang, X. Y., Wu, J. Z., Wu, X. P., Yang, S. L., Li, X. K. & Liang, G. (2010*b*). *Bioorg. Med. Chem.* doi: 10.1016/j.bmc.2010.03.001.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o1009 [ **doi:10.1107/S1600536810011499** ]

# (2*E*,6*E*)-2,6-Bis(2,5-difluorobenzylidene)cyclohexanone

**C. Jiang, Z. Feng, B. Song, X. Li and X. Li**

## Comment

The title compound, (2E,6E)-2,6-bis(2,5-difluorobenzylidene)cyclohexanone (I), is one of mono-carbonyl analogues of curcumin designed and synthesized by our group. The need for curcumin-like compounds with improved bioavailability characteristics has led to the chemical synthesis of a series of analogues, using curcumin as the primary structure. In our previous study, a series of fluorine-containing, mono-carbonyl analogues of curcumin were designed and synthesized by the deletion of β-diketone moiety, and their bioactivities were evaluated (Liang *et al.*, 2009; Zhao *et al.*, 2010a,b). Among those compounds, the cyclohexanone-containing analogues exhibited better anti-tumor properties and a wider anti-tumor spectrum than acetone- and cyclopentanone-containing analogues. Therefore, the structure of one of cyclohexanone-containing compounds (I), was further determined and analyzed using single-crystal X-ray diffraction. Accumulation of detailed structural and pharmacological data facilitated the explanation of the observed structure–activity relationships and modeling of new compounds with potential biological activity.

In this paper, we report the molecular and crystal structures of fluorine-containing, mono-carbonyl analogues of curcumin, (I). The molecule (I), consists of three ring systems, i.e., one cyclohexanone ring and two aryl rings. The central cyclohexanone ring has a distorted chair conformation, and molecular structures have an *E*-configuration towards the central olefinic bonds, exhibiting a butterfly-shaped geometry. The dihedral angle between the two terminal phenyl rings is 27.19 (13)°, and the two phenyl rings are twisted out of the plane of the central cyclohexanone on the two sides, respectively. Among these derivatives, some of them were reported of their crystal structures (Liang *et al.*, 2007a,b; Zhao *et al.*, 2009; Zhao *et al.*, 2010a,b).

## Experimental

Cyclohexanone (7.5 mmol) was dissolved in ethanol (5 ml) and crushed KOH (15 mmol) was added. The flask was immersed in a bath of crushed ice and a solution of 2,5-difluorobenzaldehyde (15 mmol) in ethanol (5 mmol) was added. The reaction mixture was stirred at 300 K and completion of the reaction was monitored by thin-layer chromatography. Ice-cold water was added to the reaction mixture after 48 h and the yellow solid that separated was filtered off, washed with water and cold ethanol, dried and purified by column chromatography on silica gel (yield: 45.3%). Single crystals of the title compound were grown in a $CH_2Cl_2$/$CH_3OH$ mixture (5:2 *v*/*v*) by slow evaporation (mp 132-135.4 K).

## Refinement

The H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

## Figures

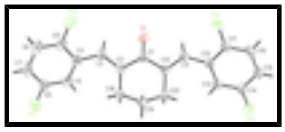


Fig. 1. The molecular structure of the title compound, showing 30% displacement ellipsoids for the non-hydrogen atoms. Hydrogen atoms are drawn as spheres of arbitrary radius.

## (2*E*,6*E*)-2,6-Bis(2,5-difluorobenzylidene)cyclohexanone

### *Crystal data*

| | |
|---|---|
| $C_{20}H_{14}F_4O$ | $F(000) = 712$ |
| $M_r = 346.31$ | $D_x = 1.450$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 15.824$ (2) Å | Cell parameters from 1858 reflections |
| $b = 6.3128$ (8) Å | $\theta = 2.4$–$22.3°$ |
| $c = 17.097$ (2) Å | $\mu = 0.12$ mm$^{-1}$ |
| $\beta = 111.756$ (3)° | $T = 293$ K |
| $V = 1586.2$ (3) Å$^3$ | Prismatic, colorless |
| $Z = 4$ | 0.43 × 0.35 × 0.27 mm |

### *Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3425 independent reflections |
| Radiation source: fine-focus sealed tube | 2018 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.049$ |
| phi and ω scans | $\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | $h = -15\rightarrow20$ |
| $T_{min} = 0.490$, $T_{max} = 1.000$ | $k = -7\rightarrow8$ |
| 8935 measured reflections | $l = -21\rightarrow18$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | H-atom parameters constrained |
| $wR(F^2) = 0.156$ | $w = 1/[\sigma^2(F_o^2) + (0.082P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.93$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3425 reflections | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| 227 parameters | $\Delta\rho_{min} = -0.24$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.015 (2)

*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**. 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 | 0.40753 (15) | 0.4774 (3) | 1.14644 (10) | 0.1192 (7) |
| F2 | 0.42662 (12) | 1.2350 (2) | 1.00801 (10) | 0.0934 (5) |
| F3 | 0.00929 (10) | 0.5237 (2) | 0.36811 (8) | 0.0809 (5) |
| F4 | 0.16575 (11) | 1.2677 (2) | 0.49902 (9) | 0.0839 (5) |
| O1 | 0.17234 (12) | 1.1232 (3) | 0.76698 (9) | 0.0796 (6) |
| C1 | 0.20606 (14) | 0.9520 (4) | 0.76181 (12) | 0.0520 (6) |
| C2 | 0.26784 (13) | 0.8418 (3) | 0.83949 (12) | 0.0466 (5) |
| C3 | 0.29758 (14) | 0.9609 (4) | 0.90938 (13) | 0.0556 (6) |
| H3 | 0.2766 | 1.0999 | 0.9033 | 0.067* |
| C4 | 0.35876 (14) | 0.9001 (4) | 0.99398 (12) | 0.0528 (6) |
| C5 | 0.35519 (16) | 0.7068 (4) | 1.03101 (14) | 0.0633 (6) |
| H5 | 0.3125 | 0.6053 | 1.0019 | 0.076* |
| C6 | 0.4149 (2) | 0.6673 (5) | 1.11059 (15) | 0.0760 (8) |
| C7 | 0.47922 (18) | 0.8090 (6) | 1.15698 (15) | 0.0836 (9) |
| H7 | 0.5196 | 0.7755 | 1.2108 | 0.100* |
| C8 | 0.48225 (18) | 1.0026 (5) | 1.12152 (16) | 0.0794 (8) |
| H8 | 0.5247 | 1.1039 | 1.1512 | 0.095* |
| C9 | 0.42230 (17) | 1.0439 (4) | 1.04241 (14) | 0.0654 (7) |
| C10 | 0.18662 (13) | 0.8503 (3) | 0.67808 (12) | 0.0466 (5) |
| C11 | 0.14905 (14) | 0.9764 (3) | 0.61179 (13) | 0.0517 (6) |
| H11 | 0.1403 | 1.1160 | 0.6244 | 0.062* |
| C12 | 0.11951 (13) | 0.9273 (3) | 0.52187 (12) | 0.0470 (5) |
| C13 | 0.07950 (14) | 0.7364 (3) | 0.48623 (12) | 0.0503 (5) |
| H13 | 0.0731 | 0.6275 | 0.5202 | 0.060* |
| C14 | 0.04988 (14) | 0.7102 (4) | 0.40128 (13) | 0.0556 (6) |
| C15 | 0.05733 (15) | 0.8634 (4) | 0.34722 (14) | 0.0614 (7) |
| H15 | 0.0367 | 0.8396 | 0.2895 | 0.074* |
| C16 | 0.09649 (17) | 1.0538 (4) | 0.38151 (14) | 0.0629 (7) |
| H16 | 0.1025 | 1.1624 | 0.3472 | 0.076* |
| C17 | 0.12608 (15) | 1.0796 (3) | 0.46646 (14) | 0.0562 (6) |
| C18 | 0.29633 (15) | 0.6182 (3) | 0.83255 (12) | 0.0528 (6) |

| | | | | |
|---|---|---|---|---|
| H18A | 0.2525 | 0.5215 | 0.8405 | 0.063* |
| H18B | 0.3549 | 0.5916 | 0.8769 | 0.063* |
| C19 | 0.30317 (15) | 0.5754 (4) | 0.74764 (12) | 0.0541 (6) |
| H19A | 0.3514 | 0.6616 | 0.7421 | 0.065* |
| H19B | 0.3188 | 0.4279 | 0.7446 | 0.065* |
| C20 | 0.21500 (14) | 0.6242 (3) | 0.67610 (12) | 0.0523 (6) |
| H20A | 0.2220 | 0.5968 | 0.6230 | 0.063* |
| H20B | 0.1677 | 0.5313 | 0.6796 | 0.063* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.193 (2) | 0.0997 (14) | 0.0587 (9) | 0.0260 (13) | 0.0392 (11) | 0.0185 (9) |
| F2 | 0.1281 (14) | 0.0767 (12) | 0.0776 (10) | −0.0307 (10) | 0.0406 (10) | −0.0231 (8) |
| F3 | 0.0950 (11) | 0.0712 (10) | 0.0577 (8) | −0.0144 (8) | 0.0066 (7) | −0.0117 (7) |
| F4 | 0.1145 (12) | 0.0498 (9) | 0.0738 (9) | −0.0116 (8) | 0.0189 (9) | 0.0087 (7) |
| O1 | 0.1081 (14) | 0.0625 (12) | 0.0539 (10) | 0.0340 (10) | 0.0133 (9) | −0.0087 (8) |
| C1 | 0.0591 (13) | 0.0470 (14) | 0.0464 (12) | 0.0073 (11) | 0.0155 (10) | −0.0066 (10) |
| C2 | 0.0484 (12) | 0.0478 (13) | 0.0427 (11) | −0.0004 (9) | 0.0159 (9) | −0.0013 (9) |
| C3 | 0.0606 (14) | 0.0549 (14) | 0.0478 (12) | 0.0038 (11) | 0.0159 (11) | −0.0042 (10) |
| C4 | 0.0539 (12) | 0.0624 (15) | 0.0421 (11) | 0.0039 (11) | 0.0179 (10) | −0.0090 (10) |
| C5 | 0.0741 (16) | 0.0689 (17) | 0.0456 (12) | −0.0015 (13) | 0.0206 (12) | −0.0073 (11) |
| C6 | 0.104 (2) | 0.082 (2) | 0.0416 (13) | 0.0253 (16) | 0.0262 (14) | 0.0058 (13) |
| C7 | 0.0701 (17) | 0.126 (3) | 0.0422 (14) | 0.0292 (18) | 0.0062 (13) | −0.0182 (16) |
| C8 | 0.0680 (17) | 0.109 (2) | 0.0561 (16) | −0.0100 (16) | 0.0176 (14) | −0.0303 (16) |
| C9 | 0.0707 (16) | 0.0769 (19) | 0.0497 (14) | −0.0028 (14) | 0.0235 (13) | −0.0184 (13) |
| C10 | 0.0472 (11) | 0.0444 (13) | 0.0433 (11) | 0.0023 (9) | 0.0113 (9) | −0.0041 (9) |
| C11 | 0.0588 (13) | 0.0431 (13) | 0.0483 (12) | 0.0081 (10) | 0.0143 (10) | −0.0010 (9) |
| C12 | 0.0463 (11) | 0.0458 (13) | 0.0454 (11) | 0.0090 (9) | 0.0128 (9) | 0.0046 (9) |
| C13 | 0.0536 (12) | 0.0474 (13) | 0.0445 (12) | 0.0013 (10) | 0.0118 (10) | 0.0054 (9) |
| C14 | 0.0550 (13) | 0.0537 (15) | 0.0494 (13) | 0.0027 (11) | 0.0092 (10) | −0.0019 (11) |
| C15 | 0.0648 (15) | 0.0728 (18) | 0.0429 (12) | 0.0142 (13) | 0.0157 (11) | 0.0048 (12) |
| C16 | 0.0729 (15) | 0.0599 (16) | 0.0547 (14) | 0.0092 (13) | 0.0221 (12) | 0.0188 (12) |
| C17 | 0.0619 (14) | 0.0417 (14) | 0.0577 (14) | 0.0045 (11) | 0.0137 (11) | 0.0063 (11) |
| C18 | 0.0606 (13) | 0.0513 (14) | 0.0437 (11) | 0.0047 (11) | 0.0161 (10) | 0.0013 (10) |
| C19 | 0.0617 (13) | 0.0494 (14) | 0.0476 (12) | 0.0110 (11) | 0.0159 (10) | −0.0016 (10) |
| C20 | 0.0626 (13) | 0.0462 (14) | 0.0432 (11) | 0.0059 (10) | 0.0140 (10) | −0.0039 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| F1—C6 | 1.371 (3) | C10—C20 | 1.500 (3) |
| F2—C9 | 1.355 (3) | C11—C12 | 1.465 (3) |
| F3—C14 | 1.360 (2) | C11—H11 | 0.9300 |
| F4—C17 | 1.362 (2) | C12—C17 | 1.381 (3) |
| O1—C1 | 1.223 (2) | C12—C13 | 1.392 (3) |
| C1—C10 | 1.493 (3) | C13—C14 | 1.361 (3) |
| C1—C2 | 1.497 (3) | C13—H13 | 0.9300 |
| C2—C3 | 1.341 (3) | C14—C15 | 1.372 (3) |
| C2—C18 | 1.500 (3) | C15—C16 | 1.380 (3) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.462 (3) | C15—H15 | 0.9300 |
| C3—H3 | 0.9300 | C16—C17 | 1.361 (3) |
| C4—C9 | 1.380 (3) | C16—H16 | 0.9300 |
| C4—C5 | 1.386 (3) | C18—C19 | 1.519 (3) |
| C5—C6 | 1.361 (3) | C18—H18A | 0.9700 |
| C5—H5 | 0.9300 | C18—H18B | 0.9700 |
| C6—C7 | 1.366 (4) | C19—C20 | 1.508 (3) |
| C7—C8 | 1.373 (4) | C19—H19A | 0.9700 |
| C7—H7 | 0.9300 | C19—H19B | 0.9700 |
| C8—C9 | 1.359 (3) | C20—H20A | 0.9700 |
| C8—H8 | 0.9300 | C20—H20B | 0.9700 |
| C10—C11 | 1.331 (3) | | |
| O1—C1—C10 | 120.60 (18) | C13—C12—C11 | 124.00 (19) |
| O1—C1—C2 | 120.36 (18) | C14—C13—C12 | 119.5 (2) |
| C10—C1—C2 | 119.03 (19) | C14—C13—H13 | 120.2 |
| C3—C2—C1 | 115.35 (19) | C12—C13—H13 | 120.2 |
| C3—C2—C18 | 125.57 (18) | F3—C14—C13 | 118.2 (2) |
| C1—C2—C18 | 118.93 (17) | F3—C14—C15 | 118.3 (2) |
| C2—C3—C4 | 128.3 (2) | C13—C14—C15 | 123.5 (2) |
| C2—C3—H3 | 115.9 | C14—C15—C16 | 117.7 (2) |
| C4—C3—H3 | 115.9 | C14—C15—H15 | 121.2 |
| C9—C4—C5 | 116.7 (2) | C16—C15—H15 | 121.2 |
| C9—C4—C3 | 119.3 (2) | C17—C16—C15 | 118.7 (2) |
| C5—C4—C3 | 124.0 (2) | C17—C16—H16 | 120.6 |
| C6—C5—C4 | 119.1 (2) | C15—C16—H16 | 120.6 |
| C6—C5—H5 | 120.4 | C16—C17—F4 | 117.7 (2) |
| C4—C5—H5 | 120.4 | C16—C17—C12 | 124.4 (2) |
| C5—C6—C7 | 123.5 (3) | F4—C17—C12 | 117.9 (2) |
| C5—C6—F1 | 117.7 (3) | C2—C18—C19 | 111.88 (17) |
| C7—C6—F1 | 118.8 (2) | C2—C18—H18A | 109.2 |
| C6—C7—C8 | 117.8 (2) | C19—C18—H18A | 109.2 |
| C6—C7—H7 | 121.1 | C2—C18—H18B | 109.2 |
| C8—C7—H7 | 121.1 | C19—C18—H18B | 109.2 |
| C9—C8—C7 | 119.0 (3) | H18A—C18—H18B | 107.9 |
| C9—C8—H8 | 120.5 | C20—C19—C18 | 111.50 (18) |
| C7—C8—H8 | 120.5 | C20—C19—H19A | 109.3 |
| F2—C9—C8 | 118.3 (2) | C18—C19—H19A | 109.3 |
| F2—C9—C4 | 117.9 (2) | C20—C19—H19B | 109.3 |
| C8—C9—C4 | 123.8 (3) | C18—C19—H19B | 109.3 |
| C11—C10—C1 | 115.29 (19) | H19A—C19—H19B | 108.0 |
| C11—C10—C20 | 126.35 (18) | C10—C20—C19 | 111.77 (17) |
| C1—C10—C20 | 118.28 (17) | C10—C20—H20A | 109.3 |
| C10—C11—C12 | 129.4 (2) | C19—C20—H20A | 109.3 |
| C10—C11—H11 | 115.3 | C10—C20—H20B | 109.3 |
| C12—C11—H11 | 115.3 | C19—C20—H20B | 109.3 |
| C17—C12—C13 | 116.12 (19) | H20A—C20—H20B | 107.9 |
| C17—C12—C11 | 119.8 (2) | | |
| O1—C1—C2—C3 | −13.6 (3) | C2—C1—C10—C20 | 11.5 (3) |

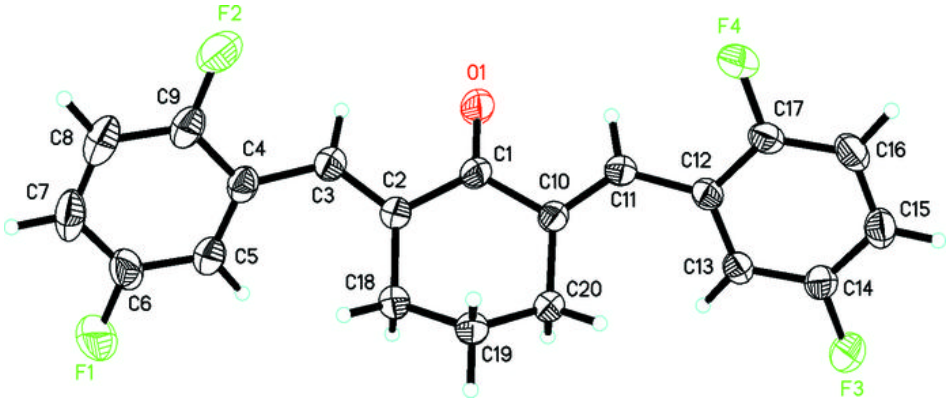
| | | | |
|---|---|---|---|
| C10—C1—C2—C3 | 166.2 (2) | C1—C10—C11—C12 | −178.3 (2) |
| O1—C1—C2—C18 | 170.6 (2) | C20—C10—C11—C12 | 5.2 (4) |
| C10—C1—C2—C18 | −9.7 (3) | C10—C11—C12—C17 | −146.9 (2) |
| C1—C2—C3—C4 | −179.3 (2) | C10—C11—C12—C13 | 36.8 (4) |
| C18—C2—C3—C4 | −3.8 (4) | C17—C12—C13—C14 | 0.1 (3) |
| C2—C3—C4—C9 | 141.8 (2) | C11—C12—C13—C14 | 176.5 (2) |
| C2—C3—C4—C5 | −40.8 (4) | C12—C13—C14—F3 | −178.60 (18) |
| C9—C4—C5—C6 | −1.8 (3) | C12—C13—C14—C15 | 0.2 (3) |
| C3—C4—C5—C6 | −179.3 (2) | F3—C14—C15—C16 | 178.34 (19) |
| C4—C5—C6—C7 | 0.1 (4) | C13—C14—C15—C16 | −0.5 (4) |
| C4—C5—C6—F1 | 177.8 (2) | C14—C15—C16—C17 | 0.5 (4) |
| C5—C6—C7—C8 | 1.1 (4) | C15—C16—C17—F4 | 179.0 (2) |
| F1—C6—C7—C8 | −176.6 (2) | C15—C16—C17—C12 | −0.2 (4) |
| C6—C7—C8—C9 | −0.5 (4) | C13—C12—C17—C16 | 0.0 (3) |
| C7—C8—C9—F2 | −179.5 (2) | C11—C12—C17—C16 | −176.6 (2) |
| C7—C8—C9—C4 | −1.4 (4) | C13—C12—C17—F4 | −179.30 (18) |
| C5—C4—C9—F2 | −179.4 (2) | C11—C12—C17—F4 | 4.1 (3) |
| C3—C4—C9—F2 | −1.7 (3) | C3—C2—C18—C19 | −143.7 (2) |
| C5—C4—C9—C8 | 2.5 (4) | C1—C2—C18—C19 | 31.7 (3) |
| C3—C4—C9—C8 | −179.8 (2) | C2—C18—C19—C20 | −56.2 (3) |
| O1—C1—C10—C11 | 14.5 (3) | C11—C10—C20—C19 | 140.9 (2) |
| C2—C1—C10—C11 | −165.28 (19) | C1—C10—C20—C19 | −35.6 (3) |
| O1—C1—C10—C20 | −168.7 (2) | C18—C19—C20—C10 | 58.3 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16···O1$^{i}$ | 0.93 | 2.46 | 3.343 (3) | 158 |

Symmetry codes: (i) *x*, −*y*+5/2, *z*−1/2.

**Fig. 1**


F2
O1
F4
C9
C17
C8
C4
C1
C16
C12
C7
C3
C2
C10
C11
C15
C5
C13
C18
C20
C14
C6
C19
F1
F3