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# (*E*)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]prop-2-en-1-one

**Pei-Hua Zhao,[a]* Er-Jun Hao,[b] Ya-Qing Liu[a] and Gui-Zhe Zhao[a]**

[a]Research Center for Engineering Technology of Polymeric Composites of Shanxi Province, College of Materials Science and Engineering, North University of China, Taiyuan 030051, People's Republic of China, and [b]Key Laboratory of Green Chemical Media and Reactions, Ministry of Education, College of Chemistry and Environmental Science, Henan Normal University, Xinxiang 453007, People's Republic of China
Correspondence e-mail: zph2004@yahoo.com.cn

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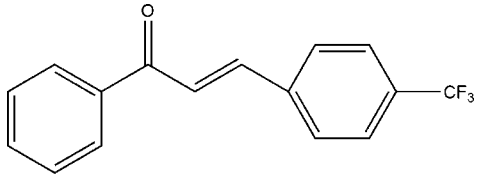
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.078; data-to-parameter ratio = 16.6.

In the title compound, $C_{16}H_{11}F_3O$, the dihedral angle between the two rings is 48.8 (2)°. The crystal packing exhibits no classical intermolecular interactions between the molecules.

## Related literature

For applications of related compounds, see: Shibata (1994); Devincenzo *et al.* (1995); Dimmock *et al.* (1999); Go *et al.* (2005).




## Experimental

### *Crystal data*

$C_{16}H_{11}F_3O$
$M_r$ = 276.25
Monoclinic, $P2_1/c$
$a$ = 14.7469 (5) Å
$b$ = 14.5697 (4) Å
$c$ = 5.8430 (2) Å
$\beta$ = 92.854 (1)°
$V$ = 1253.86 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 113 K
0.20 × 0.18 × 0.08 mm

### *Data collection*

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.976, $T_{max}$ = 0.990
12984 measured reflections
3005 independent reflections
2037 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.078
$S$ = 1.12
3005 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku/MSC, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2055).

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# supporting information

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## (*E*)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]prop-2-en-1-one

**Pei-Hua Zhao, Er-Jun Hao, Ya-Qing Liu and Gui-Zhe Zhao**

### S1. Comment

The title compound belongs to the chalcones, which are Michael acceptors and constitute an important group of natural products that belong to the flavonoid family (Dimmock *et al.*, 1999; Go *et al.*, 2005). Natural and synthetic chalcones have been reported to possess strong antiproliferative effects in ovarian cancer cells and in gastic cancer cells (Shibata, 1994; Devincenzo *et al.*, 1995).

The dihedral angle between two benzene rings is 48.8 (2) ° (Fig. 1). The crystal packing shows no $\pi\cdots\pi$ or other classical intermolecular interactions (Fig. 2).

### S2. Experimental

In 25 ml round-bottomed flask, the acetophenone (5.0 mmol) and sodium hydroxide (7.5 mmol) were dissolved in ethanol (2 ml), and the mixture was stirred at room temperature for 5 min followed by addition of 4-trifluoromethyl-benzaldehyde (5.0 mmol). The reaction mixture was then stirred at room temperature and monitored by TLC until the reaction completed. The solid was filtered, washed with cold water, recrystallized from ethanol, and dried *in vacuo* to give the desired product. Crystals of the title compound were obtained by slow evaporation of the dichloromethane/*n*-hexane solution (1:1) at room temperature. $^1$N NMR(400 MHz, $CDCl_3$, TMS): 7.53 (dd, 2H, J = 7.6, 15.6 Hz), 7.60 (m, 2H), 7.68 (d, 2H, J = 8.0 Hz), 7.75 (d, 2H, J = 8.0 Hz), 7.82 (d, 1H, J = 15.6 Hz), 8.03 (d, 2H, J = 8.4 Hz) p.p.m..

### S3. Refinement

All the H atoms were positioned geometrically (C—H = 0.95 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C).

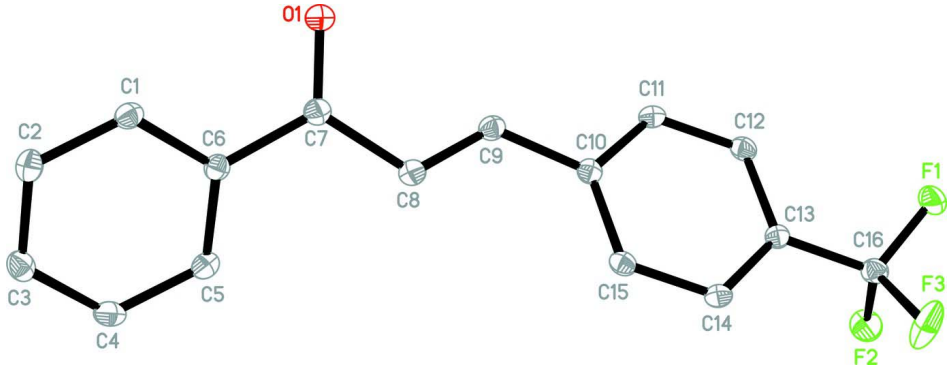


**Figure 1**

The molecular structure of the title compound. Thermal displacement ellipsoids are drawn at the 30% probability level and H atoms are omitted.

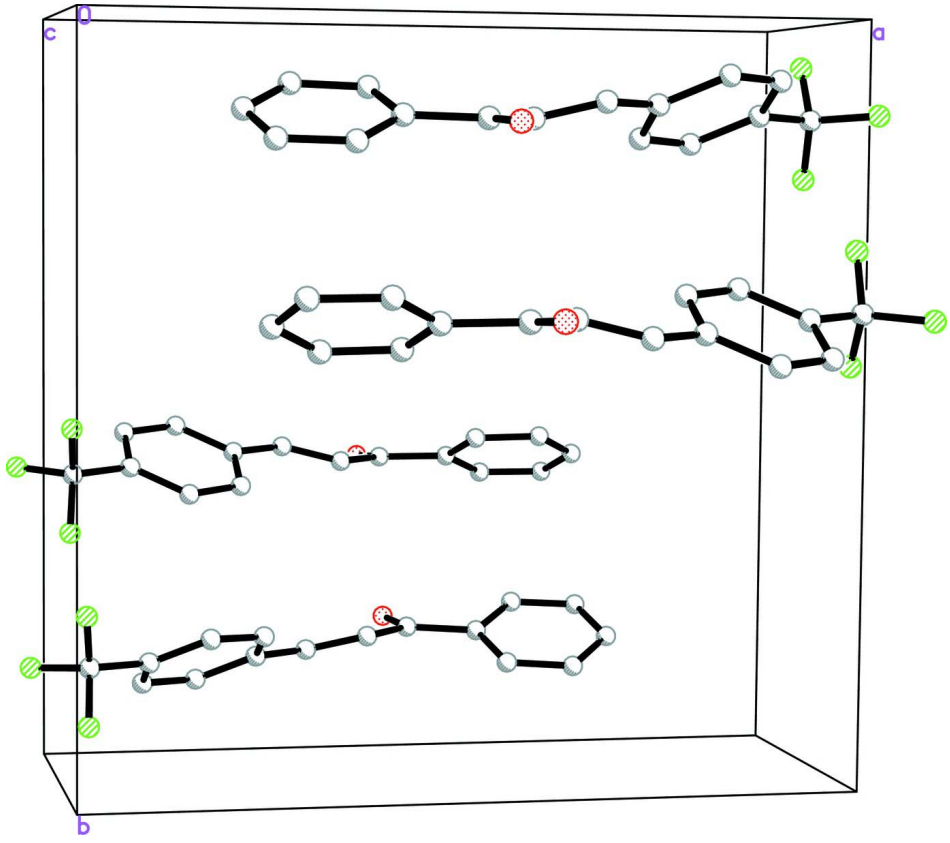


**Figure 2**

The crystal packing of the title compound.

**(*E*)-1-Phenyl-3-[4-(trifluoromethyl)phenyl]prop-2-en-1-one**

*Crystal data*

$C_{16}H_{11}F_3O$
$M_r = 276.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.7469\ (5)$ Å
$b = 14.5697\ (4)$ Å
$c = 5.8430\ (2)$ Å
$\beta = 92.854\ (1)°$
$V = 1253.86\ (7)$ Å$^3$
$Z = 4$
$F(000) = 568$
$D_x = 1.463$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4102 reflections
$\theta = 2.0–28.0°$
$\mu = 0.12$ mm$^{-1}$
$T = 113$ K
Prism, colorless
0.20 × 0.18 × 0.08 mm

*Data collection*

Rigaku Saturn724 CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.22 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.976$, $T_{max} = 0.990$
12984 measured reflections
3005 independent reflections
2037 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.0°$
$h = -19\rightarrow19$
$k = -14\rightarrow19$
$l = -7\rightarrow7$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.078$
$S = 1.12$
3005 reflections
181 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{min} = -0.27$ e Å$^{-3}$

*Special details*

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 1.01951 (5) | 0.12265 (5) | 1.04772 (13) | 0.0377 (2) |
| F2 | 0.95432 (5) | 0.05980 (5) | 1.32422 (13) | 0.0375 (2) |
| F3 | 0.95565 (5) | 0.20580 (5) | 1.29461 (15) | 0.0493 (3) |
| O1 | 0.47484 (6) | 0.13892 (6) | 0.27878 (15) | 0.0329 (2) |
| C1 | 0.29314 (8) | 0.16320 (7) | 0.3888 (2) | 0.0215 (3) |
| H1 | 0.3095 | 0.1866 | 0.2449 | 0.026* |
| C2 | 0.20299 (9) | 0.16081 (7) | 0.4417 (2) | 0.0243 (3) |
| H2 | 0.1576 | 0.1834 | 0.3353 | 0.029* |
| C3 | 0.17888 (9) | 0.12555 (8) | 0.6496 (2) | 0.0249 (3) |
| H3 | 0.1168 | 0.1235 | 0.6851 | 0.030* |
| C4 | 0.24500 (8) | 0.09312 (8) | 0.8068 (2) | 0.0251 (3) |
| H4 | 0.2280 | 0.0684 | 0.9489 | 0.030* |
| C5 | 0.33571 (8) | 0.09691 (8) | 0.7565 (2) | 0.0225 (3) |
| H5 | 0.3811 | 0.0761 | 0.8655 | 0.027* |
| C6 | 0.36044 (8) | 0.13127 (7) | 0.5461 (2) | 0.0198 (3) |
| C7 | 0.45675 (8) | 0.13432 (8) | 0.4807 (2) | 0.0220 (3) |
| C8 | 0.52985 (8) | 0.13323 (8) | 0.6661 (2) | 0.0230 (3) |
| H8 | 0.5162 | 0.1474 | 0.8193 | 0.028* |
| C9 | 0.61401 (8) | 0.11232 (7) | 0.6158 (2) | 0.0207 (3) |
| H9 | 0.6223 | 0.0939 | 0.4623 | 0.025* |
| C10 | 0.69610 (8) | 0.11424 (7) | 0.7696 (2) | 0.0188 (3) |
| C11 | 0.77584 (8) | 0.07768 (7) | 0.6888 (2) | 0.0202 (3) |
| H11 | 0.7745 | 0.0490 | 0.5426 | 0.024* |
| C12 | 0.85708 (8) | 0.08253 (8) | 0.8182 (2) | 0.0211 (3) |
| H12 | 0.9109 | 0.0571 | 0.7615 | 0.025* |

| | | | | |
|---|---|---|---|---|
| C13 | 0.85929 (8) | 0.12479 (7) | 1.0312 (2) | 0.0185 (3) |
| C14 | 0.78038 (8) | 0.16112 (7) | 1.1158 (2) | 0.0202 (3) |
| H14 | 0.7820 | 0.1899 | 1.2619 | 0.024* |
| C15 | 0.69934 (8) | 0.15519 (7) | 0.9860 (2) | 0.0205 (3) |
| H15 | 0.6453 | 0.1793 | 1.0449 | 0.025* |
| C16 | 0.94629 (8) | 0.12902 (8) | 1.1725 (2) | 0.0234 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0177 (4) | 0.0663 (5) | 0.0293 (5) | −0.0017 (4) | 0.0027 (3) | 0.0043 (4) |
| F2 | 0.0314 (5) | 0.0496 (5) | 0.0311 (5) | 0.0037 (3) | −0.0037 (4) | 0.0171 (4) |
| F3 | 0.0378 (5) | 0.0427 (5) | 0.0648 (6) | 0.0105 (4) | −0.0231 (5) | −0.0281 (4) |
| O1 | 0.0250 (5) | 0.0531 (6) | 0.0208 (5) | −0.0003 (4) | 0.0020 (4) | 0.0019 (4) |
| C1 | 0.0247 (7) | 0.0216 (6) | 0.0180 (7) | −0.0040 (5) | −0.0002 (5) | 0.0000 (5) |
| C2 | 0.0216 (7) | 0.0227 (7) | 0.0282 (8) | −0.0008 (5) | −0.0028 (6) | −0.0013 (5) |
| C3 | 0.0217 (7) | 0.0240 (7) | 0.0291 (7) | −0.0045 (5) | 0.0044 (6) | −0.0065 (6) |
| C4 | 0.0313 (7) | 0.0248 (7) | 0.0198 (7) | −0.0074 (6) | 0.0059 (6) | −0.0031 (5) |
| C5 | 0.0254 (7) | 0.0224 (6) | 0.0193 (7) | −0.0015 (5) | −0.0023 (5) | 0.0004 (5) |
| C6 | 0.0206 (6) | 0.0190 (6) | 0.0198 (7) | −0.0023 (5) | 0.0000 (5) | −0.0023 (5) |
| C7 | 0.0222 (7) | 0.0229 (6) | 0.0209 (7) | 0.0002 (5) | 0.0010 (5) | 0.0009 (5) |
| C8 | 0.0234 (7) | 0.0259 (7) | 0.0197 (7) | −0.0017 (5) | 0.0008 (5) | −0.0011 (5) |
| C9 | 0.0239 (7) | 0.0195 (6) | 0.0188 (7) | −0.0013 (5) | 0.0008 (5) | −0.0010 (5) |
| C10 | 0.0206 (6) | 0.0157 (6) | 0.0201 (7) | −0.0012 (5) | 0.0013 (5) | 0.0026 (5) |
| C11 | 0.0248 (7) | 0.0194 (6) | 0.0165 (6) | 0.0011 (5) | 0.0025 (5) | −0.0007 (5) |
| C12 | 0.0201 (6) | 0.0223 (6) | 0.0211 (7) | 0.0033 (5) | 0.0042 (5) | 0.0007 (5) |
| C13 | 0.0197 (6) | 0.0174 (6) | 0.0183 (6) | 0.0006 (5) | 0.0003 (5) | 0.0029 (5) |
| C14 | 0.0238 (7) | 0.0199 (6) | 0.0170 (6) | 0.0020 (5) | 0.0020 (5) | −0.0013 (5) |
| C15 | 0.0199 (7) | 0.0208 (6) | 0.0211 (7) | 0.0031 (5) | 0.0048 (5) | 0.0005 (5) |
| C16 | 0.0224 (7) | 0.0255 (7) | 0.0226 (7) | 0.0032 (5) | 0.0027 (5) | −0.0010 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C16 | 1.3361 (14) | C7—C8 | 1.4896 (16) |
| F2—C16 | 1.3439 (14) | C8—C9 | 1.3249 (16) |
| F3—C16 | 1.3301 (14) | C8—H8 | 0.9500 |
| O1—C7 | 1.2244 (14) | C9—C10 | 1.4715 (16) |
| C1—C2 | 1.3802 (17) | C9—H9 | 0.9500 |
| C1—C6 | 1.3981 (16) | C10—C11 | 1.3946 (16) |
| C1—H1 | 0.9500 | C10—C15 | 1.3967 (16) |
| C2—C3 | 1.3815 (17) | C11—C12 | 1.3866 (16) |
| C2—H2 | 0.9500 | C11—H11 | 0.9500 |
| C3—C4 | 1.3889 (17) | C12—C13 | 1.3874 (16) |
| C3—H3 | 0.9500 | C12—H12 | 0.9500 |
| C4—C5 | 1.3850 (16) | C13—C14 | 1.3914 (15) |
| C4—H4 | 0.9500 | C13—C16 | 1.4920 (16) |
| C5—C6 | 1.3929 (16) | C14—C15 | 1.3860 (16) |
| C5—H5 | 0.9500 | C14—H14 | 0.9500 |

| | | | |
|---|---|---|---|
| C6—C7 | 1.4897 (16) | C15—H15 | 0.9500 |
| | | | |
| C2—C1—C6 | 120.29 (12) | C10—C9—H9 | 116.1 |
| C2—C1—H1 | 119.9 | C11—C10—C15 | 118.58 (11) |
| C6—C1—H1 | 119.9 | C11—C10—C9 | 117.90 (11) |
| C1—C2—C3 | 119.95 (12) | C15—C10—C9 | 123.42 (11) |
| C1—C2—H2 | 120.0 | C12—C11—C10 | 121.06 (11) |
| C3—C2—H2 | 120.0 | C12—C11—H11 | 119.5 |
| C2—C3—C4 | 120.34 (12) | C10—C11—H11 | 119.5 |
| C2—C3—H3 | 119.8 | C11—C12—C13 | 119.55 (11) |
| C4—C3—H3 | 119.8 | C11—C12—H12 | 120.2 |
| C5—C4—C3 | 119.98 (12) | C13—C12—H12 | 120.2 |
| C5—C4—H4 | 120.0 | C12—C13—C14 | 120.32 (11) |
| C3—C4—H4 | 120.0 | C12—C13—C16 | 119.73 (11) |
| C4—C5—C6 | 119.99 (11) | C14—C13—C16 | 119.94 (11) |
| C4—C5—H5 | 120.0 | C15—C14—C13 | 119.70 (11) |
| C6—C5—H5 | 120.0 | C15—C14—H14 | 120.1 |
| C5—C6—C1 | 119.43 (11) | C13—C14—H14 | 120.1 |
| C5—C6—C7 | 122.13 (11) | C14—C15—C10 | 120.78 (11) |
| C1—C6—C7 | 118.44 (11) | C14—C15—H15 | 119.6 |
| O1—C7—C8 | 121.12 (11) | C10—C15—H15 | 119.6 |
| O1—C7—C6 | 120.32 (11) | F3—C16—F1 | 106.62 (10) |
| C8—C7—C6 | 118.56 (11) | F3—C16—F2 | 105.91 (10) |
| C9—C8—C7 | 119.56 (11) | F1—C16—F2 | 105.12 (9) |
| C9—C8—H8 | 120.2 | F3—C16—C13 | 113.26 (10) |
| C7—C8—H8 | 120.2 | F1—C16—C13 | 113.02 (10) |
| C8—C9—C10 | 127.71 (12) | F2—C16—C13 | 112.27 (10) |
| C8—C9—H9 | 116.1 | | |
| | | | |
| C6—C1—C2—C3 | −0.92 (17) | C15—C10—C11—C12 | −0.73 (17) |
| C1—C2—C3—C4 | 0.55 (17) | C9—C10—C11—C12 | 175.76 (10) |
| C2—C3—C4—C5 | 0.65 (17) | C10—C11—C12—C13 | −0.31 (17) |
| C3—C4—C5—C6 | −1.48 (17) | C11—C12—C13—C14 | 0.78 (17) |
| C4—C5—C6—C1 | 1.10 (17) | C11—C12—C13—C16 | 179.16 (10) |
| C4—C5—C6—C7 | −178.18 (10) | C12—C13—C14—C15 | −0.18 (17) |
| C2—C1—C6—C5 | 0.10 (17) | C16—C13—C14—C15 | −178.57 (10) |
| C2—C1—C6—C7 | 179.41 (10) | C13—C14—C15—C10 | −0.88 (16) |
| C5—C6—C7—O1 | 158.69 (12) | C11—C10—C15—C14 | 1.33 (16) |
| C1—C6—C7—O1 | −20.61 (16) | C9—C10—C15—C14 | −174.95 (10) |
| C5—C6—C7—C8 | −22.32 (16) | C12—C13—C16—F3 | 145.25 (11) |
| C1—C6—C7—C8 | 158.38 (10) | C14—C13—C16—F3 | −36.36 (16) |
| O1—C7—C8—C9 | −18.27 (17) | C12—C13—C16—F1 | 23.86 (15) |
| C6—C7—C8—C9 | 162.75 (11) | C14—C13—C16—F1 | −157.75 (10) |
| C7—C8—C9—C10 | 175.00 (10) | C12—C13—C16—F2 | −94.84 (13) |
| C8—C9—C10—C11 | 171.53 (11) | C14—C13—C16—F2 | 83.55 (13) |
| C8—C9—C10—C15 | −12.17 (19) | | |