

1-(3-Mesityl-3-methylcyclobutyl)-2-phenoxyethanone

Murat Koca,^a Cumhur Kirilmiş^a and Cengiz Arıcı^{b*}

^aDepartment of Chemistry, Faculty of Arts and Science, Adiyaman University, 02040 Adiyaman, Turkey, and ^bDepartment of Engineering Physics, Hacettepe University, Beytepe 06800, Ankara, Turkey

Correspondence e-mail: carici.xray@gmail.com

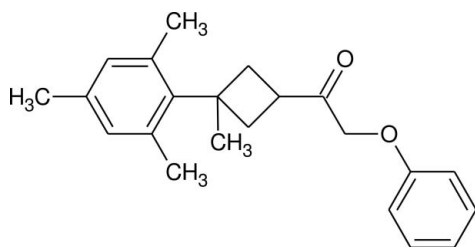
Received 6 January 2010; accepted 1 February 2010

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.047; wR factor = 0.129; data-to-parameter ratio = 18.1.

In the title compound, $\text{C}_{22}\text{H}_{26}\text{O}_2$, the cyclobutane ring is puckered, with a dihedral angle of 24.97 (9)° between the two C_3 planes. In the crystal, intermolecular non-classical $\text{C}-\text{H}\cdots\text{O}$ interactions between the methylcyclobutyl CH group and the O atom of the phenoxy group are found.

Related literature

For related cyclobutanes, see: Çukurovali *et al.* (2005); Dinçer *et al.* (2004); Kirilmiş *et al.* (2005a,b); Sari *et al.* (2002, 2004). For the anti-inflammatory and anti-depressant activity of three-substituted cyclobutane acid derivatives, see: Roger *et al.* (1977); Gerard (1979); Sawhney *et al.* (1978); Brown *et al.* (1974); for anti-microbial activity, see: Suzuki *et al.* (1979); for anti-parasitic activity, see: Slip *et al.* (1974), for herbicidal activity, see: Foerster *et al.* (1979) and for their liquid-crystal properties, see: Dehmlow & Schmidt (1990).



Experimental

Crystal data

$\text{C}_{22}\text{H}_{26}\text{O}_2$
 $M_r = 322.43$
 Triclinic, $P\bar{1}$
 $a = 8.5884$ (12) Å
 $b = 10.1725$ (11) Å
 $c = 11.1018$ (12) Å
 $\alpha = 82.364$ (4)°
 $\beta = 68.170$ (3)°

$\gamma = 86.235$ (2)°
 $V = 892.24$ (19) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
 $0.42 \times 0.33 \times 0.24$ mm

Data collection

Nonius KappaCCD diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker–Nonius, 2002)
 $T_{\min} = 0.969$, $T_{\max} = 0.982$

23641 measured reflections
 3921 independent reflections
 2968 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.129$
 $S = 1.07$
 3921 reflections

217 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.32$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C10}-\text{H10A}\cdots\text{O1}^{\dagger}$	0.99	2.44	3.419 (3)	172 (2)

Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.

Data collection: COLLECT (Bruker–Nonius, 2002); cell refinement: EVALCCD (Bruker–Nonius, 2002); data reduction: EVALCCD program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

This study was supported financially by grant DPT/2003 K 120440-1 from the Scientific and Technical Research Council of Turkey (Project Manager Yıldırım Aydoğdu). The authors extend special thanks to Frank W. Heinemann for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2189).

References

- Brown, K., Cater, D. P., Cavalla, J. F., Green, D., Newberry, R. A. & Wilson, A. B. (1974). *J. Med. Chem.* **14**, 1177–1181.
- Bruker–Nonius (2002). COLLECT, EVALCCD and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Çukurovali, A., Özdemir, N., Yılmaz, I. & Dinçer, M. (2005). *Acta Cryst.* **E61**, o1754–o1756.
- Dehmlow, E. V. & Schmidt, S. (1990). *Liebigs Ann. Chem.* **5**, 411–414.
- Dinçer, M., Özdemir, N., Çukurovali, A., Yılmaz, İ. & Büyükgüngör, O. (2004). *Acta Cryst.* **E60**, o1523–o1524.
- Foerster, H., Hofer, W., Mues, V., Eue, L. & Schmidt, R. R. (1979). German Patent 2, 822 155.
- Gerard, G. (1979). *Eur. J. Med. Chem.* **14**, 493–497.
- Kirilmiş, C., Koca, M., Arıcı, C., Heinemann, F. W. & Ahmedzade, M. (2005a). *Acta Cryst.* **E61**, o555–o556.
- Kirilmiş, C., Koca, M., Arıcı, C., Heinemann, F. W. & Ahmedzade, M. (2005b). *Acta Cryst.* **E61**, o1176–o1177.
- Roger, E., Pier, C. J., Paulet, V., Gerard, G., Chepat, J. P. & Robert, G. (1977). *Eur. J. Med. Chem. Chem. Ther.* pp. 12501–?????
- Sari, U., Güven, K., Yılmaz, I., Çukurovali, A. & Aksoy, I. (2002). *Anal. Sci.* **18**, 725–726.
- Sari, U., Yılmaz, I., Güven, K., Çukurovali, A. & Aksoy, I. (2004). *J. Chem. Crystallogr.* **34**, 571–575.
- Sawhney, S. N., Arora, S. K. & Sing, J. V. (1978). *Indian J. Chem. Sect. B*, **16**, 605–609.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Slip, P. I., Closier, M. & Neville, M. (1974). *J. Med. Chem.* **17**, 207–209.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Suzuki, N., Tanaka, Y. & Dohmori, R. (1979). *Chem. Pharm. Bull.* **27**, 1–11.

supplementary materials

Acta Cryst. (2010). E66, o523 [doi:10.1107/S1600536810003910]

1-(3-Mesityl-3-methylcyclobutyl)-2-phenoxyethanone

M. Koca, C. Kirilmis and C. Arici

Comment

It is well known that three-substituted cyclobutane acid derivatives exhibit anti-inflammatory and anti-depressant activities (Roger *et al.*, 1977; Gerard, 1979) and liquid-crystal properties (Dehmlow & Schmidt, 1990), moreover their of various thiazoles derivatives showed herbicidal (Foerster *et al.*, 1979), anti-inflammatory (Sawhney *et al.*, 1978; Brown *et al.*, 1974), anti-microbial (Suzuki *et al.*, 1979) or anti-parasitic activity (Slip *et al.*, 1974). Substituted cyclobutane contained similar structures, have been reported in the recent years (Kirilmis *et al.*, 2005a, 2005b; Sari *et al.*, 2002, 2004; Çukurovali *et al.*, 2005; Dinçer *et al.*, 2004).

The four-atom bridge O2/C16/C15/C11 linking the cyclobutane and phenoxy rings is planar (Fig. 1). The torsion angle of O2—C16—C15—C11 is -1.0 (1)°. It corresponds to the (-) synclinal configuration. The cyclobutane ring is similar puckered as in a related compounds; the C9/C7/C10 plane forms a dihedral angle of 24.97 (9)° with the C10/C11/C9 plane in the title compound. The same dihedral angles are presented in the literature: 25.74 (6)° - Çukurovali *et al.*, (2005) and 19.8 (3)° - Dinçer *et al.*, (2004). The mesityl and phenoxy rings are planar. The dihedral angle between these ring is 73.90 (5)°. The maximum deviation from mean plane of the atoms for mesityl and phenoxy rings are -0.046 (6)Å for C5 and 0.016 (3)Å for C17, respectively.

There is one intermolecular non-classical C—H···O hydrogen-bonding interactions in the crystal structure. This interactions lead to close packing between the neighbouring molecules. And the structure is stabilized by van der Waals interactions and symmetry-related molecules are linked to form dimerization chains *via* C—H···O intermolecular non-classical hydrogen bond. Intermolecular van der Waals interactions between the methylcyclobutyl CH group and the O atom of the phenoxy group (Fig. 2, Table 1).

In the IR spectra of 1-(3-mesityl-3-methylcyclobutyl)-2-phenoxy-1-ethanone very important bonds were observed as (ν , cm^{-1}); 1711 (sharp C=O stretching) respectively and between 3063 – 2852 (broad aliphatic and aromatic C—H stretching) and 1070 (ether C—O—C stretching). The $^1\text{H-NMR}$ spectra were reported in p.p.m. (δ) relative to tetramethylsilane (SiMe_4) as the internal standard and referenced to deuteriochloroform (CDCl_3). In the $^1\text{H-NMR}$ spectra were H signals obtained as (p.p.m.) 1.7 (s, 3H, cyclobutane- CH_3), 2.2 (s, 9H, CH_3 -mesitylene), 2.5 – 2.9 (m, 4H, cyclobutane CH_2), 3.9 (p, 1H, cyclobutane CH), 4.2 (s, 2H, O— CH_2) and aromatic protons observed at 6.7 – 7.3 (m, 7H, ArH). Elemental Analysis Calc. for $\text{C}_{22}\text{H}_{26}\text{O}_2$ ($322.44 \text{ g mol}^{-1}$): C, 81.95; H, 8.13 Found: C, 81.88; H, 8.05.

Experimental

Elemental analysis were determined on a LECO CHNS-932 auto elemental analysis apparatus. Infrared spectra were obtained by using a Mattson 1000 F T-IR Spectrometer, from 4000 – 400 cm^{-1} in KBr pellet. $^1\text{H-NMR}$ spectra were recorded on a Jeol FX-90Q Spectrometer 90 MHz.

supplementary materials

Synthesis of 1-(3-mesityl-3-methylcyclobutyl)-2-phenoxy-1-ethanone: a mixture of 1-mesityl-1-methyl-3-(2-chloro-1-oxoethyl)cyclobutane (2.64 g, 10 mmol), phenol (1.035 g, 11 mmol) and K_2CO_3 (1.51 g, 11 mmol) in 200 ml dry acetone was refluxed for 8 h. The reaction mixture was poured into water (500 ml), the insoluble portion was filtered off, washed with water and crystallized from ethanol (yield 85%).

Refinement

All H atoms were placed geometrically ($C-H = 0.95-0.99 \text{ \AA}$) and refined in the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$ for CH and CH_2 , and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3 .

Figures

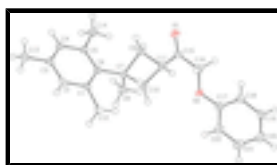


Fig. 1. View of the title molecule with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as a small circles of arbitrary radii.

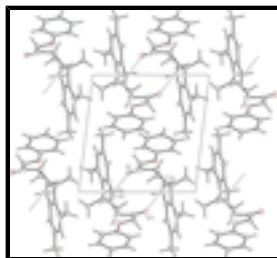


Fig. 2. A packing diagram of title compound with the intermolecular H bonds (dashed lines). Symmetry code: (i) $-x+1, -y+2, -z+1$.

1-(3-Mesityl-3-methylcyclobutyl)-2-phenoxyethanone

Crystal data

$C_{22}H_{26}O_2$	$Z = 2$
$M_r = 322.43$	$F(000) = 348$
Triclinic, $P\bar{1}$	$D_x = 1.200 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.5884 (12) \text{ \AA}$	Cell parameters from 149 reflections
$b = 10.1725 (11) \text{ \AA}$	$\theta = 6.0-20.0^\circ$
$c = 11.1018 (12) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\alpha = 82.364 (4)^\circ$	$T = 100 \text{ K}$
$\beta = 68.170 (3)^\circ$	Block, colourless
$\gamma = 86.235 (2)^\circ$	$0.42 \times 0.33 \times 0.24 \text{ mm}$
$V = 892.24 (19) \text{ \AA}^3$	

Data collection

Nonius KappaCCD diffractometer	3921 independent reflections
Radiation source: fine-focus sealed tube	2968 reflections with $I > 2\sigma(I)$

graphite $R_{\text{int}} = 0.054$
 Detector resolution: 9 pixels mm^{-1} $\theta_{\text{max}} = 27.1^\circ$, $\theta_{\text{min}} = 3.0^\circ$
 ω -scans with 2.00° and 40 sec per frame $h = -11 \rightarrow 11$
 Absorption correction: multi-scan $k = -13 \rightarrow 12$
 (SADABS; Bruker–Nonius, 2002) $l = -14 \rightarrow 14$
 $T_{\text{min}} = 0.969$, $T_{\text{max}} = 0.982$
 23641 measured reflections

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
 Least-squares matrix: full Secondary atom site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.047$ Hydrogen site location: inferred from neighbouring sites
 $wR(F^2) = 0.129$ H-atom parameters constrained
 $S = 1.07$ $w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.2801P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 3921 reflections $(\Delta/\sigma)_{\text{max}} = 0.001$
 217 parameters $\Delta\rho_{\text{max}} = 0.32 \text{ e } \text{\AA}^{-3}$
 0 restraints $\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.66157 (19)	0.63782 (15)	0.69324 (15)	0.0191 (3)
C2	0.6658 (2)	0.62422 (15)	0.81884 (15)	0.0212 (3)
H2	0.5724	0.5864	0.8899	0.025*
C3	0.8017 (2)	0.66400 (15)	0.84382 (15)	0.0216 (3)
C4	0.9374 (2)	0.71600 (15)	0.73790 (15)	0.0202 (3)
H4	1.0328	0.7416	0.7525	0.024*
C5	0.93938 (19)	0.73229 (15)	0.61020 (15)	0.0181 (3)
C6	0.79712 (19)	0.69657 (14)	0.58680 (15)	0.0168 (3)
C7	0.79622 (18)	0.71572 (15)	0.44807 (15)	0.0175 (3)
C8	0.8730 (2)	0.59338 (16)	0.37804 (16)	0.0238 (4)
H8A	0.8710	0.6069	0.2895	0.036*

supplementary materials

H8B	0.8079	0.5150	0.4267	0.036*
H8C	0.9892	0.5802	0.3731	0.036*
C9	0.86927 (19)	0.84742 (16)	0.36088 (15)	0.0190 (3)
H9A	0.8701	0.9204	0.4114	0.023*
H9B	0.9806	0.8360	0.2918	0.023*
C10	0.62618 (19)	0.75748 (15)	0.42989 (15)	0.0189 (3)
H10B	0.5741	0.6854	0.4069	0.023*
H10A	0.5440	0.7998	0.5038	0.023*
C11	0.72371 (19)	0.85766 (15)	0.31115 (15)	0.0181 (3)
H11	0.7558	0.8179	0.2273	0.022*
C12	0.5091 (2)	0.58448 (17)	0.67897 (17)	0.0255 (4)
H12A	0.5442	0.5430	0.5980	0.038*
H12B	0.4298	0.6575	0.6761	0.038*
H12C	0.4549	0.5185	0.7536	0.038*
C13	0.8009 (2)	0.64947 (18)	0.98136 (16)	0.0283 (4)
H13A	0.7400	0.5695	1.0308	0.042*
H13B	0.7456	0.7273	1.0240	0.042*
H13C	0.9166	0.6421	0.9784	0.042*
C14	1.09987 (19)	0.78228 (18)	0.50263 (16)	0.0233 (4)
H14A	1.1277	0.7295	0.4294	0.035*
H14B	1.1912	0.7741	0.5361	0.035*
H14C	1.0846	0.8756	0.4727	0.035*
C15	0.63834 (19)	0.98988 (16)	0.30363 (15)	0.0196 (3)
C16	0.4891 (2)	1.00148 (15)	0.26088 (16)	0.0217 (3)
H16A	0.3888	1.0322	0.3314	0.026*
H16B	0.5121	1.0673	0.1824	0.026*
C17	0.35862 (19)	0.87125 (16)	0.16126 (15)	0.0193 (3)
C18	0.2842 (2)	0.98135 (16)	0.11452 (16)	0.0231 (4)
H18	0.2968	1.0674	0.1337	0.028*
C19	0.1910 (2)	0.96324 (19)	0.03910 (18)	0.0302 (4)
H19	0.1404	1.0381	0.0062	0.036*
C20	0.1703 (2)	0.8385 (2)	0.01108 (17)	0.0304 (4)
H20	0.1088	0.8280	-0.0425	0.036*
C21	0.2405 (2)	0.72904 (18)	0.06224 (18)	0.0290 (4)
H21	0.2240	0.6427	0.0459	0.035*
C22	0.3340 (2)	0.74507 (17)	0.13673 (17)	0.0253 (4)
H22	0.3819	0.6697	0.1714	0.030*
O1	0.68046 (15)	1.08915 (12)	0.33319 (12)	0.0270 (3)
O2	0.45853 (14)	0.87559 (11)	0.23207 (11)	0.0235 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0195 (8)	0.0117 (7)	0.0253 (8)	-0.0002 (6)	-0.0076 (6)	-0.0015 (6)
C2	0.0221 (8)	0.0149 (8)	0.0224 (8)	-0.0030 (6)	-0.0038 (7)	0.0004 (6)
C3	0.0289 (9)	0.0143 (7)	0.0217 (8)	-0.0001 (6)	-0.0088 (7)	-0.0040 (6)
C4	0.0214 (8)	0.0183 (8)	0.0239 (8)	-0.0011 (6)	-0.0104 (7)	-0.0058 (6)
C5	0.0179 (7)	0.0156 (7)	0.0211 (8)	0.0010 (6)	-0.0066 (6)	-0.0056 (6)

C6	0.0179 (7)	0.0129 (7)	0.0203 (7)	0.0013 (6)	-0.0069 (6)	-0.0047 (6)
C7	0.0159 (7)	0.0175 (8)	0.0198 (7)	-0.0008 (6)	-0.0066 (6)	-0.0043 (6)
C8	0.0258 (8)	0.0229 (8)	0.0263 (8)	0.0048 (7)	-0.0122 (7)	-0.0099 (7)
C9	0.0168 (7)	0.0216 (8)	0.0177 (7)	-0.0018 (6)	-0.0047 (6)	-0.0035 (6)
C10	0.0174 (7)	0.0177 (8)	0.0237 (8)	-0.0006 (6)	-0.0094 (6)	-0.0039 (6)
C11	0.0187 (7)	0.0190 (8)	0.0182 (7)	-0.0002 (6)	-0.0078 (6)	-0.0048 (6)
C12	0.0228 (8)	0.0225 (9)	0.0302 (9)	-0.0085 (7)	-0.0104 (7)	0.0061 (7)
C13	0.0371 (10)	0.0267 (9)	0.0210 (8)	-0.0066 (8)	-0.0103 (7)	-0.0013 (7)
C14	0.0171 (8)	0.0321 (9)	0.0218 (8)	-0.0037 (7)	-0.0072 (7)	-0.0049 (7)
C15	0.0203 (8)	0.0197 (8)	0.0174 (7)	-0.0029 (6)	-0.0048 (6)	-0.0026 (6)
C16	0.0219 (8)	0.0167 (8)	0.0282 (8)	0.0012 (6)	-0.0099 (7)	-0.0070 (7)
C17	0.0148 (7)	0.0211 (8)	0.0218 (8)	0.0001 (6)	-0.0062 (6)	-0.0036 (6)
C18	0.0218 (8)	0.0190 (8)	0.0277 (8)	-0.0038 (6)	-0.0093 (7)	0.0018 (7)
C19	0.0283 (9)	0.0314 (10)	0.0328 (9)	-0.0060 (7)	-0.0169 (8)	0.0095 (8)
C20	0.0268 (9)	0.0434 (11)	0.0240 (9)	-0.0084 (8)	-0.0121 (7)	-0.0023 (8)
C21	0.0248 (9)	0.0301 (9)	0.0351 (10)	0.0000 (7)	-0.0106 (8)	-0.0154 (8)
C22	0.0215 (8)	0.0204 (8)	0.0365 (9)	0.0040 (7)	-0.0124 (7)	-0.0081 (7)
O1	0.0317 (7)	0.0214 (6)	0.0334 (7)	-0.0009 (5)	-0.0166 (6)	-0.0082 (5)
O2	0.0276 (6)	0.0151 (6)	0.0350 (6)	0.0000 (5)	-0.0196 (5)	-0.0036 (5)

Geometric parameters (Å, °)

C1—C2	1.397 (2)	C12—H12A	0.9800
C1—C6	1.410 (2)	C12—H12B	0.9800
C1—C12	1.518 (2)	C12—H12C	0.9800
C2—C3	1.392 (2)	C13—H13A	0.9800
C2—H2	0.9500	C13—H13B	0.9800
C3—C4	1.385 (2)	C13—H13C	0.9800
C3—C13	1.512 (2)	C14—H14A	0.9800
C4—C5	1.399 (2)	C14—H14B	0.9800
C4—H4	0.9500	C14—H14C	0.9800
C5—C6	1.418 (2)	C15—O1	1.2177 (19)
C5—C14	1.514 (2)	C15—C16	1.516 (2)
C6—C7	1.529 (2)	C16—O2	1.4237 (18)
C7—C8	1.535 (2)	C16—H16A	0.9900
C7—C9	1.562 (2)	C16—H16B	0.9900
C7—C10	1.571 (2)	C17—O2	1.3682 (18)
C8—H8A	0.9800	C17—C18	1.389 (2)
C8—H8B	0.9800	C17—C22	1.392 (2)
C8—H8C	0.9800	C18—C19	1.391 (2)
C9—C11	1.536 (2)	C18—H18	0.9500
C9—H9A	0.9900	C19—C20	1.383 (3)
C9—H9B	0.9900	C19—H19	0.9500
C10—C11	1.553 (2)	C20—C21	1.387 (3)
C10—H10B	0.9900	C20—H20	0.9500
C10—H10A	0.9900	C21—C22	1.380 (2)
C11—C15	1.497 (2)	C21—H21	0.9500
C11—H11	1.0000	C22—H22	0.9500
C2—C1—C6	119.74 (14)	C10—C11—H11	111.2

supplementary materials

C2—C1—C12	116.96 (14)	C1—C12—H12A	109.5
C6—C1—C12	123.28 (14)	C1—C12—H12B	109.5
C3—C2—C1	122.43 (15)	H12A—C12—H12B	109.5
C3—C2—H2	118.8	C1—C12—H12C	109.5
C1—C2—H2	118.8	H12A—C12—H12C	109.5
C4—C3—C2	117.38 (14)	H12B—C12—H12C	109.5
C4—C3—C13	121.65 (15)	C3—C13—H13A	109.5
C2—C3—C13	120.97 (15)	C3—C13—H13B	109.5
C3—C4—C5	122.47 (15)	H13A—C13—H13B	109.5
C3—C4—H4	118.8	C3—C13—H13C	109.5
C5—C4—H4	118.8	H13A—C13—H13C	109.5
C4—C5—C6	119.57 (14)	H13B—C13—H13C	109.5
C4—C5—C14	116.94 (14)	C5—C14—H14A	109.5
C6—C5—C14	123.43 (13)	C5—C14—H14B	109.5
C1—C6—C5	118.27 (14)	H14A—C14—H14B	109.5
C1—C6—C7	121.45 (13)	C5—C14—H14C	109.5
C5—C6—C7	120.21 (13)	H14A—C14—H14C	109.5
C6—C7—C8	110.39 (12)	H14B—C14—H14C	109.5
C6—C7—C9	117.38 (12)	O1—C15—C11	123.12 (14)
C8—C7—C9	111.83 (13)	O1—C15—C16	117.80 (14)
C6—C7—C10	118.07 (12)	C11—C15—C16	119.06 (13)
C8—C7—C10	110.26 (12)	O2—C16—C15	109.41 (13)
C9—C7—C10	87.08 (11)	O2—C16—H16A	109.8
C7—C8—H8A	109.5	C15—C16—H16A	109.8
C7—C8—H8B	109.5	O2—C16—H16B	109.8
H8A—C8—H8B	109.5	C15—C16—H16B	109.8
C7—C8—H8C	109.5	H16A—C16—H16B	108.2
H8A—C8—H8C	109.5	O2—C17—C18	124.76 (14)
H8B—C8—H8C	109.5	O2—C17—C22	115.14 (14)
C11—C9—C7	89.84 (11)	C18—C17—C22	120.10 (15)
C11—C9—H9A	113.7	C17—C18—C19	118.77 (16)
C7—C9—H9A	113.7	C17—C18—H18	120.6
C11—C9—H9B	113.7	C19—C18—H18	120.6
C7—C9—H9B	113.7	C20—C19—C18	121.37 (17)
H9A—C9—H9B	110.9	C20—C19—H19	119.3
C11—C10—C7	88.89 (11)	C18—C19—H19	119.3
C11—C10—H10B	113.8	C19—C20—C21	119.17 (16)
C7—C10—H10B	113.8	C19—C20—H20	120.4
C11—C10—H10A	113.8	C21—C20—H20	120.4
C7—C10—H10A	113.8	C22—C21—C20	120.27 (16)
H10B—C10—H10A	111.1	C22—C21—H21	119.9
C15—C11—C9	117.93 (13)	C20—C21—H21	119.9
C15—C11—C10	114.89 (13)	C21—C22—C17	120.25 (16)
C9—C11—C10	88.64 (11)	C21—C22—H22	119.9
C15—C11—H11	111.2	C17—C22—H22	119.9
C9—C11—H11	111.2	C17—O2—C16	118.20 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C10—H10A···O1 ⁱ	0.99	2.44	3.419 (3)	172 (2)

Symmetry codes: (i) $-x+1, -y+2, -z+1$.

Fig. 1

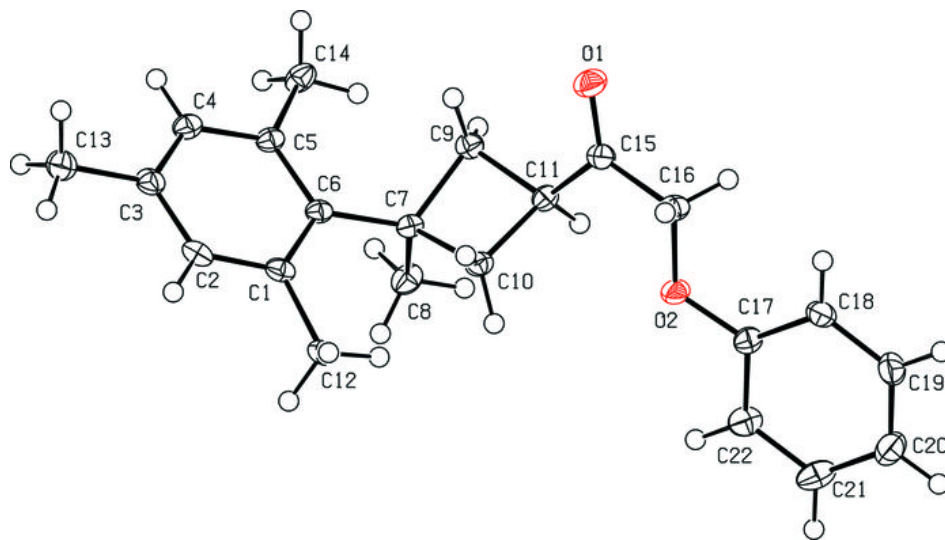


Fig. 2

