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

# (1-Adamantyl)diphenylmethanol

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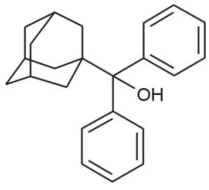
Received 28 May 2010; accepted 7 June 2010

Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.095; data-to-parameter ratio = 13.6.

In the title compound, $C_{23}H_{26}O$, the adamantane cage consists of three fused cyclohexane rings in classical chair conformations with absolute values of the C—C—C angles in the range 106.57 (11)–111.56 (12)°. The dihedral angle between the two phenyl rings is 81.38 (4)°. Although a hydroxy group is present as a conceivable donor, no hydrogen bonds are observed in the crystal structure.

## Related literature

For the preparation and spectroscopic properties of the title compound, see: Vícha *et al.* (2006); Stetter & Rauscher (1960); Molle *et al.* (1984). For related structures, see: Vaissermann & Lomas (1997).




## Experimental

*Crystal data*

$C_{23}H_{26}O$ $M_r$ = 318.44
Monoclinic, $P2_1/n$
$a$ = 6.5370 (12) Å
$b$ = 17.037 (3) Å
$c$ = 15.322 (2) Å
$\beta$ = 91.993 (14)°
$V$ = 1705.4 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 120 K
0.40 × 0.40 × 0.30 mm

*Data collection*

Kuma KM-4-CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.971, $T_{max}$ = 0.978
10354 measured reflections
2996 independent reflections
2133 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
$S$ = 0.93
2996 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

The financial support of this work by the Czech Ministry of Education, project No. MSM 7088352101, and by the Tomas Bata Foundation is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5059).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o1626 [ **doi:10.1107/S1600536810021707** ]

# (1-Adamantyl)diphenylmethanol

**R. Vícha and M. Necas**

## Comment

Adamantane derivatives are well known primarily for their unusual virustatic effect. Nevertheless, the scope of the biological activity of adamantane derivatives is much wider and novel compounds are prepared and tested steadily. The title tertiary alcohol was isolated as unwanted by-product accompanying 1-adamantyl phenyl ketone when no catalyst was employed. The molecule of title compound (Fig. 1) consists of two phenyl rings and an adamantane cage bound to a carbon atom to form a strained tertiary alcohol. Both phenyl rings (C12–C17 and C18–C23) are essentially planar with the maximum deviation from the best planes being 0.0110 (14) Å for C17 and 0.0027 (14) Å for C19. The angle between best planes of these rings is 81.38 (4)°. Both rings are slightly deformed in the plane owing to steric hindrance of the bulky adamantane moiety. The torsion angles describing arrangement of two phenyl rings and the adamantane cage C2—C1—C11—C12 and C1—C11—C12—C13 are -59.06 (14)° and -93.57 (15)°, respectively. Although a hydroxy group is present as a conceivable H-donor, no H-bonds were observed in crystal packing (see Fig. 2). The distance between the closest adjacent O-atoms is 5.2050 (17) Å.

## Experimental

Title compound was isolated from a complex mixture obtained by the reaction of adamantane-1-carbonyl chloride with phenylmagnesium bromide as it has been described previously (Vícha *et al.*, 2006). The crystal used for data collection was grown by slow cooling of a saturated solution of title compound in *n*-hexane.

## Refinement

Carbon bound hydrogen atoms were positioned geometrically and refined as riding using standard SHELXTL (Sheldrick, 2008) constraints, with their $U_{iso}$ values set to $1.2U_{eq}$ of their parent atoms. The oxygen bound hydrogen atom was located in a difference Fourier map and refined isotropically.

## Figures

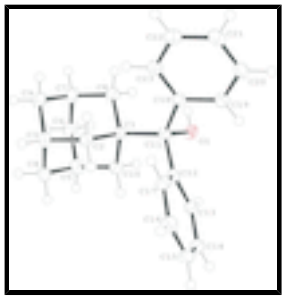

Fig. 1. An ellipsoid plot (50% probability) of the asymmetric unit. Hydrogen atoms are represented as arbitrary spheres.

Fig. 2. A crystal packing viewed along the *a*-axis. Hydrogen atoms are omitted for clarity.

**(1-Adamantyl)diphenylmethanol**

*Crystal data*

| | |
|---|---|
| $C_{23}H_{26}O$ | $F(000) = 688$ |
| $M_r = 318.44$ | $D_x = 1.240$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Melting point: 400 K |
| Hall symbol: -P 2yn | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 6.5370$ (12) Å | Cell parameters from 10305 reflections |
| $b = 17.037$ (3) Å | $\theta = 3.1$–$27.1°$ |
| $c = 15.322$ (2) Å | $\mu = 0.07$ mm$^{-1}$ |
| $\beta = 91.993$ (14)° | $T = 120$ K |
| $V = 1705.4$ (5) Å$^3$ | Block, colourless |
| $Z = 4$ | 0.40 × 0.40 × 0.30 mm |

*Data collection*

| | |
|---|---|
| Kuma KM-4-CCD diffractometer | 2996 independent reflections |
| Radiation source: fine-focus sealed tube | 2133 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.027$ |
| Detector resolution: 0.06 mm pixels mm$^{-1}$ | $\theta_{max} = 25.0°$, $\theta_{min} = 3.3°$ |
| ω scan | $h = -7 \rightarrow 7$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009) | $k = -20 \rightarrow 20$ |
| $T_{min} = 0.971$, $T_{max} = 0.978$ | $l = -15 \rightarrow 18$ |
| 10354 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 |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.095$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 0.93$ | $w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2996 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 221 parameters | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |

0 restraints $\Delta\rho_{min} = -0.18$ e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.20822 (14) | 0.62332 (7) | 0.54962 (6) | 0.0238 (3) |
| C1 | −0.0671 (2) | 0.63609 (8) | 0.65477 (9) | 0.0192 (3) |
| C2 | −0.2658 (2) | 0.67842 (8) | 0.68106 (9) | 0.0215 (3) |
| H2A | −0.2439 | 0.7359 | 0.6801 | 0.026* |
| H2B | −0.3779 | 0.6657 | 0.6383 | 0.026* |
| C3 | −0.3275 (2) | 0.65309 (8) | 0.77314 (9) | 0.0249 (3) |
| H3 | −0.4570 | 0.6805 | 0.7881 | 0.030* |
| C4 | −0.1578 (2) | 0.67522 (9) | 0.84012 (10) | 0.0297 (4) |
| H4A | −0.1979 | 0.6597 | 0.8994 | 0.036* |
| H4B | −0.1357 | 0.7327 | 0.8396 | 0.036* |
| C5 | 0.0398 (2) | 0.63284 (9) | 0.81687 (9) | 0.0287 (4) |
| H5 | 0.1516 | 0.6474 | 0.8601 | 0.034* |
| C6 | 0.0060 (2) | 0.54372 (9) | 0.81919 (10) | 0.0326 (4) |
| H6A | 0.1342 | 0.5162 | 0.8053 | 0.039* |
| H6B | −0.0334 | 0.5275 | 0.8783 | 0.039* |
| C7 | −0.1637 (2) | 0.52169 (9) | 0.75231 (10) | 0.0275 (4) |
| H7 | −0.1866 | 0.4637 | 0.7537 | 0.033* |
| C8 | −0.0988 (2) | 0.54619 (8) | 0.66034 (9) | 0.0239 (3) |
| H8A | −0.2055 | 0.5299 | 0.6166 | 0.029* |
| H8B | 0.0301 | 0.5191 | 0.6465 | 0.029* |
| C9 | −0.3624 (2) | 0.56423 (9) | 0.77457 (10) | 0.0278 (4) |
| H9A | −0.4726 | 0.5500 | 0.7315 | 0.033* |
| H9B | −0.4054 | 0.5479 | 0.8332 | 0.033* |
| C10 | 0.1005 (2) | 0.65811 (9) | 0.72486 (9) | 0.0241 (3) |
| H10A | 0.2308 | 0.6323 | 0.7105 | 0.029* |
| H10B | 0.1228 | 0.7156 | 0.7241 | 0.029* |
| C11 | 0.0093 (2) | 0.66125 (8) | 0.56147 (9) | 0.0195 (3) |
| C12 | 0.0501 (2) | 0.75000 (8) | 0.55950 (8) | 0.0202 (3) |
| C13 | 0.2443 (2) | 0.78085 (8) | 0.57812 (9) | 0.0235 (3) |
| H13 | 0.3561 | 0.7463 | 0.5898 | 0.028* |
| C14 | 0.2764 (2) | 0.86159 (9) | 0.57982 (9) | 0.0270 (4) |

| | | | | |
|---|---|---|---|---|
| H14 | 0.4097 | 0.8817 | 0.5925 | 0.032* |
| C15 | 0.1154 (2) | 0.91283 (9) | 0.56323 (9) | 0.0288 (4) |
| H15 | 0.1373 | 0.9679 | 0.5655 | 0.035* |
| C16 | −0.0776 (2) | 0.88315 (9) | 0.54334 (10) | 0.0292 (4) |
| H16 | −0.1885 | 0.9180 | 0.5315 | 0.035* |
| C17 | −0.1100 (2) | 0.80241 (8) | 0.54063 (9) | 0.0247 (3) |
| H17 | −0.2426 | 0.7827 | 0.5258 | 0.030* |
| C18 | −0.1246 (2) | 0.64101 (8) | 0.47894 (9) | 0.0211 (3) |
| C19 | −0.0360 (2) | 0.65919 (8) | 0.39898 (9) | 0.0245 (3) |
| H19 | 0.0992 | 0.6797 | 0.3993 | 0.029* |
| C20 | −0.1413 (2) | 0.64783 (8) | 0.31960 (9) | 0.0274 (4) |
| H20 | −0.0782 | 0.6610 | 0.2666 | 0.033* |
| C21 | −0.3378 (2) | 0.61734 (9) | 0.31742 (10) | 0.0292 (4) |
| H21 | −0.4101 | 0.6092 | 0.2633 | 0.035* |
| C22 | −0.4266 (2) | 0.59892 (9) | 0.39521 (10) | 0.0308 (4) |
| H22 | −0.5614 | 0.5780 | 0.3943 | 0.037* |
| C23 | −0.3220 (2) | 0.61044 (9) | 0.47534 (9) | 0.0263 (4) |
| H23 | −0.3865 | 0.5972 | 0.5280 | 0.032* |
| H1O | 0.191 (3) | 0.5765 (11) | 0.5483 (11) | 0.048 (6)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0194 (5) | 0.0248 (7) | 0.0275 (6) | 0.0000 (4) | 0.0027 (4) | 0.0009 (5) |
| C1 | 0.0199 (7) | 0.0181 (8) | 0.0197 (8) | 0.0010 (6) | −0.0001 (6) | 0.0011 (6) |
| C2 | 0.0228 (8) | 0.0205 (8) | 0.0212 (8) | 0.0009 (6) | 0.0012 (6) | 0.0013 (6) |
| C3 | 0.0262 (8) | 0.0255 (8) | 0.0232 (8) | 0.0028 (6) | 0.0053 (6) | 0.0020 (6) |
| C4 | 0.0374 (9) | 0.0331 (9) | 0.0189 (8) | −0.0015 (7) | 0.0059 (7) | 0.0013 (7) |
| C5 | 0.0303 (9) | 0.0349 (9) | 0.0204 (8) | −0.0023 (7) | −0.0042 (7) | 0.0039 (7) |
| C6 | 0.0335 (9) | 0.0373 (10) | 0.0272 (9) | 0.0060 (7) | 0.0029 (7) | 0.0131 (7) |
| C7 | 0.0314 (9) | 0.0193 (8) | 0.0322 (9) | 0.0004 (6) | 0.0048 (7) | 0.0063 (6) |
| C8 | 0.0232 (8) | 0.0215 (8) | 0.0270 (8) | 0.0010 (6) | 0.0023 (6) | 0.0012 (6) |
| C9 | 0.0291 (9) | 0.0281 (9) | 0.0265 (9) | −0.0014 (6) | 0.0054 (7) | 0.0056 (7) |
| C10 | 0.0227 (8) | 0.0265 (9) | 0.0229 (8) | −0.0006 (6) | −0.0015 (6) | 0.0021 (6) |
| C11 | 0.0175 (7) | 0.0206 (8) | 0.0204 (8) | 0.0013 (6) | 0.0009 (6) | 0.0000 (6) |
| C12 | 0.0245 (8) | 0.0215 (8) | 0.0146 (7) | −0.0016 (6) | 0.0019 (6) | 0.0002 (6) |
| C13 | 0.0255 (8) | 0.0264 (9) | 0.0185 (8) | −0.0014 (6) | −0.0003 (6) | 0.0015 (6) |
| C14 | 0.0321 (9) | 0.0304 (9) | 0.0185 (8) | −0.0098 (7) | −0.0004 (6) | −0.0005 (6) |
| C15 | 0.0441 (10) | 0.0206 (8) | 0.0218 (8) | −0.0056 (7) | 0.0035 (7) | −0.0001 (6) |
| C16 | 0.0370 (9) | 0.0233 (9) | 0.0274 (9) | 0.0032 (7) | 0.0023 (7) | 0.0042 (6) |
| C17 | 0.0253 (8) | 0.0244 (9) | 0.0244 (8) | −0.0011 (6) | 0.0011 (6) | 0.0029 (6) |
| C18 | 0.0252 (8) | 0.0173 (8) | 0.0208 (8) | 0.0013 (6) | −0.0003 (6) | −0.0018 (6) |
| C19 | 0.0273 (8) | 0.0216 (8) | 0.0247 (8) | −0.0017 (6) | 0.0027 (6) | 0.0007 (6) |
| C20 | 0.0401 (9) | 0.0236 (8) | 0.0187 (8) | 0.0016 (7) | 0.0032 (7) | 0.0003 (6) |
| C21 | 0.0357 (9) | 0.0302 (9) | 0.0214 (8) | 0.0010 (7) | −0.0048 (7) | −0.0038 (7) |
| C22 | 0.0283 (9) | 0.0337 (9) | 0.0300 (9) | −0.0060 (7) | −0.0035 (7) | −0.0048 (7) |
| C23 | 0.0261 (8) | 0.0297 (9) | 0.0231 (8) | −0.0033 (7) | 0.0025 (6) | −0.0009 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C11 | 1.4693 (16) | C9—H9B | 0.9900 |
| O1—H1O | 0.806 (18) | C10—H10A | 0.9900 |
| C1—C8 | 1.5482 (19) | C10—H10B | 0.9900 |
| C1—C2 | 1.5507 (18) | C11—C12 | 1.5357 (19) |
| C1—C10 | 1.5535 (18) | C11—C18 | 1.5513 (19) |
| C1—C11 | 1.5895 (18) | C12—C13 | 1.3942 (18) |
| C2—C3 | 1.5425 (18) | C12—C17 | 1.3986 (19) |
| C2—H2A | 0.9900 | C13—C14 | 1.3915 (19) |
| C2—H2B | 0.9900 | C13—H13 | 0.9500 |
| C3—C9 | 1.531 (2) | C14—C15 | 1.384 (2) |
| C3—C4 | 1.532 (2) | C14—H14 | 0.9500 |
| C3—H3 | 1.0000 | C15—C16 | 1.383 (2) |
| C4—C5 | 1.532 (2) | C15—H15 | 0.9500 |
| C4—H4A | 0.9900 | C16—C17 | 1.392 (2) |
| C4—H4B | 0.9900 | C16—H16 | 0.9500 |
| C5—C6 | 1.535 (2) | C17—H17 | 0.9500 |
| C5—C10 | 1.5393 (19) | C18—C23 | 1.3906 (19) |
| C5—H5 | 1.0000 | C18—C19 | 1.4079 (19) |
| C6—C7 | 1.530 (2) | C19—C20 | 1.3901 (19) |
| C6—H6A | 0.9900 | C19—H19 | 0.9500 |
| C6—H6B | 0.9900 | C20—C21 | 1.385 (2) |
| C7—C9 | 1.536 (2) | C20—H20 | 0.9500 |
| C7—C8 | 1.5434 (19) | C21—C22 | 1.380 (2) |
| C7—H7 | 1.0000 | C21—H21 | 0.9500 |
| C8—H8A | 0.9900 | C22—C23 | 1.399 (2) |
| C8—H8B | 0.9900 | C22—H22 | 0.9500 |
| C9—H9A | 0.9900 | C23—H23 | 0.9500 |
| C11—O1—H1O | 108.3 (13) | C3—C9—H9B | 109.7 |
| C8—C1—C2 | 109.33 (11) | C7—C9—H9B | 109.7 |
| C8—C1—C10 | 107.05 (11) | H9A—C9—H9B | 108.2 |
| C2—C1—C10 | 106.57 (11) | C5—C10—C1 | 111.56 (12) |
| C8—C1—C11 | 111.29 (10) | C5—C10—H10A | 109.3 |
| C2—C1—C11 | 113.60 (11) | C1—C10—H10A | 109.3 |
| C10—C1—C11 | 108.69 (11) | C5—C10—H10B | 109.3 |
| C3—C2—C1 | 110.83 (11) | C1—C10—H10B | 109.3 |
| C3—C2—H2A | 109.5 | H10A—C10—H10B | 108.0 |
| C1—C2—H2A | 109.5 | O1—C11—C12 | 105.98 (11) |
| C3—C2—H2B | 109.5 | O1—C11—C18 | 106.15 (10) |
| C1—C2—H2B | 109.5 | C12—C11—C18 | 107.24 (10) |
| H2A—C2—H2B | 108.1 | O1—C11—C1 | 107.44 (10) |
| C9—C3—C4 | 109.77 (12) | C12—C11—C1 | 110.09 (10) |
| C9—C3—C2 | 109.48 (11) | C18—C11—C1 | 119.16 (11) |
| C4—C3—C2 | 109.72 (12) | C13—C12—C17 | 118.12 (13) |
| C9—C3—H3 | 109.3 | C13—C12—C11 | 121.66 (12) |
| C4—C3—H3 | 109.3 | C17—C12—C11 | 120.21 (12) |
| C2—C3—H3 | 109.3 | C14—C13—C12 | 120.80 (14) |

| | | | |
|---|---|---|---|
| C3—C4—C5 | 108.96 (12) | C14—C13—H13 | 119.6 |
| C3—C4—H4A | 109.9 | C12—C13—H13 | 119.6 |
| C5—C4—H4A | 109.9 | C15—C14—C13 | 120.47 (14) |
| C3—C4—H4B | 109.9 | C15—C14—H14 | 119.8 |
| C5—C4—H4B | 109.9 | C13—C14—H14 | 119.8 |
| H4A—C4—H4B | 108.3 | C16—C15—C14 | 119.45 (14) |
| C4—C5—C6 | 109.72 (12) | C16—C15—H15 | 120.3 |
| C4—C5—C10 | 109.11 (12) | C14—C15—H15 | 120.3 |
| C6—C5—C10 | 109.86 (12) | C15—C16—C17 | 120.31 (14) |
| C4—C5—H5 | 109.4 | C15—C16—H16 | 119.8 |
| C6—C5—H5 | 109.4 | C17—C16—H16 | 119.8 |
| C10—C5—H5 | 109.4 | C16—C17—C12 | 120.82 (13) |
| C7—C6—C5 | 109.20 (12) | C16—C17—H17 | 119.6 |
| C7—C6—H6A | 109.8 | C12—C17—H17 | 119.6 |
| C5—C6—H6A | 109.8 | C23—C18—C19 | 117.20 (13) |
| C7—C6—H6B | 109.8 | C23—C18—C11 | 127.72 (13) |
| C5—C6—H6B | 109.8 | C19—C18—C11 | 115.02 (12) |
| H6A—C6—H6B | 108.3 | C20—C19—C18 | 121.63 (14) |
| C6—C7—C9 | 109.53 (12) | C20—C19—H19 | 119.2 |
| C6—C7—C8 | 109.22 (12) | C18—C19—H19 | 119.2 |
| C9—C7—C8 | 109.67 (11) | C21—C20—C19 | 120.27 (14) |
| C6—C7—H7 | 109.5 | C21—C20—H20 | 119.9 |
| C9—C7—H7 | 109.5 | C19—C20—H20 | 119.9 |
| C8—C7—H7 | 109.5 | C22—C21—C20 | 118.85 (14) |
| C7—C8—C1 | 111.07 (11) | C22—C21—H21 | 120.6 |
| C7—C8—H8A | 109.4 | C20—C21—H21 | 120.6 |
| C1—C8—H8A | 109.4 | C21—C22—C23 | 121.22 (14) |
| C7—C8—H8B | 109.4 | C21—C22—H22 | 119.4 |
| C1—C8—H8B | 109.4 | C23—C22—H22 | 119.4 |
| H8A—C8—H8B | 108.0 | C18—C23—C22 | 120.82 (14) |
| C3—C9—C7 | 109.63 (12) | C18—C23—H23 | 119.6 |
| C3—C9—H9A | 109.7 | C22—C23—H23 | 119.6 |
| C7—C9—H9A | 109.7 | | |

**Fig. 1**

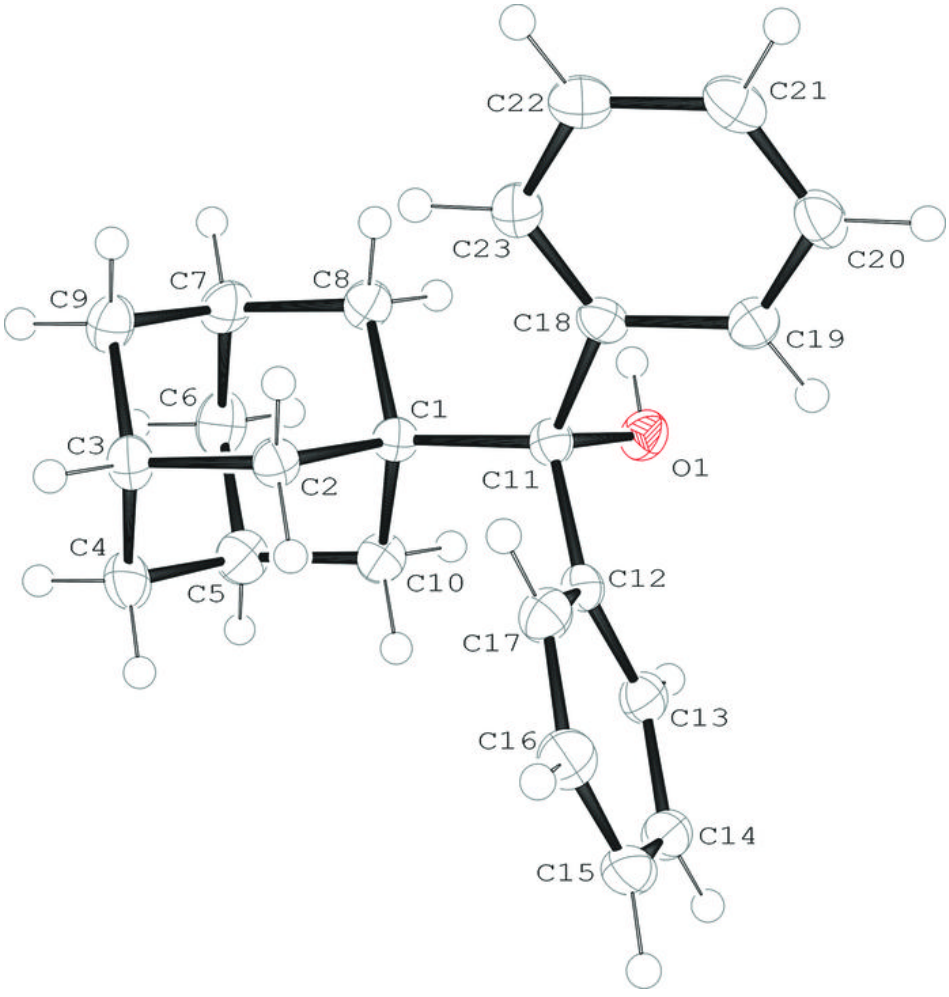
C22
C21
C23
C20
C9
C7
C8
C18
C19
C6
C1
C3
C2
C11
O1
C4
C5
C10
C12
C17
C13
C16
C14
C15

**Fig. 2**