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# 2-(1-Adamantyl)-1,3-diphenylpropan-2-ol

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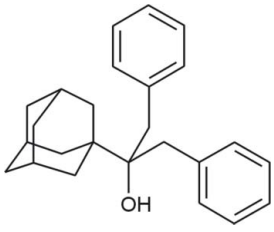
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.033; $wR$ factor = 0.080; data-to-parameter ratio = 14.0.

In the title compound, $C_{25}H_{30}O$, the adamantane cage consists of three fused cyclohexane rings in classical chair conformations, with C—C—C angles in the range 107.15 (9)–111.55 (9)°. The dihedral angle between the benzene rings is 46.91 (4)° and the conformation is stabilized by a weak intramolecular C—H$\cdots\pi$ interaction.

## Related literature

For the preparation and spectroscopic properties of the title compound, see: Vícha *et al.* (2006). For related structures, see: Vaissermann & Lomas (1997); Vícha & Nečas (2010).




## Experimental

### Crystal data

$C_{25}H_{30}O$
$M_r$ = 346.49
Monoclinic, $C2/c$
$a$ = 24.2808 (10) Å
$b$ = 6.3978 (2) Å
$c$ = 25.2555 (14) Å
$\beta$ = 106.183 (5)°
$V$ = 3767.8 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 120 K
0.40 × 0.30 × 0.20 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire2 (large Be window) detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.965, $T_{max}$ = 1.000
17425 measured reflections
3315 independent reflections
2381 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.080
$S$ = 0.96
3315 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

*Cg*1 is the centroid of C20–C25 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C14—H14$\cdots Cg1$ | 0.95 | 2.70 | 3.3172 (13) | 123 |

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2292).

## References

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o2175 [ **doi:10.1107/S1600536810030047** ]

# 2-(1-Adamantyl)-1,3-diphenylpropan-2-ol

**E. Babjaková, M. Necas and R. Vícha**

## Comment

In the title compound, both benzene rings (C13–C18 and C20–C25) are essentially planar with maximum deviations from their respective best planes of 0.0053 (12) Å for C17 and 0.0073 (12) Å for C25. The angle between the best planes of these rings is 46.97 (3)°. The torsion angles that describe the arrangement of the two benzyl substituents and the adamantane cage – C2—C1—C11—O1, C1—C11—C12—C13, C1—C11—C19—C20, C11—C12—C13—C14 and C11—C19—C20—C21 – are 63.42 (11)°, -134.29 (10)°, -174.22 (10)°, -104.43 (13)°, and 107.99 (13)°, respectively. The conformation of the molecules in the crystal is stabilized by a weak C—H···π interaction, C14—H14···*Cg*1 (*Cg*1 is the centre of gravity of C20–C25), with a C14···*Cg*1 distance of 3.3172 (13) Å (see Fig. 2 and Table 1). In analogy to the previously published structure of 1-adamantyl(diphenyl)methanol (Vícha & Nečas, 2010), no H-bonds were observed in the crystal packing. The shortest distance between two adjacent O-atoms is 4.7666 (11) Å. Surprisingly, the more strained molecules of di(1-adamantyl)(2,5-diisopropylphenyl)methanol with two bulky adamantane cages form O—H···O linked dimers in the solid state (Vaissermann & Lomas, 1997).

## Experimental

The title compound was isolated from a complex mixture obtained from the reaction of adamantane-1-carbonyl chloride with benzylmagnesium chloride as described previously (Vícha *et al.*, 2006). The crystal used for data collection was grown by slow evaporation of a solution in hexane at room temperature.

## Refinement

Hydrogen atoms were positioned geometrically and refined as riding using standard *SHELXTL* constraints, with their $U_{iso}$ values set to $1.2U_{eq}$ of that of their parent atoms.

## Figures

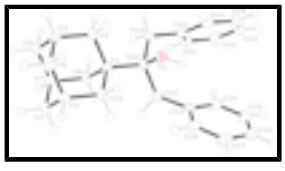

Fig. 1. Ellipsoid plot (50% probability) of the asymmetric unit. Hydrogen atoms are represented as spheres of arbitrary size.

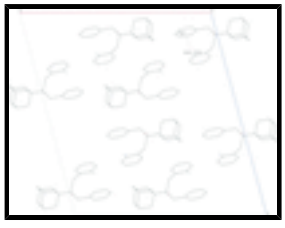

Fig. 2. Crystal packing viewed along the *b*-axis. Intramolecular C—H···π interactions are shown as dotted lines. *Cg*1 is the center of gravity of C20–C25. H-atoms (except those which are involved in C—H···π interactions) have been omitted for clarity.

### 2-(1-Adamantyl)-1,3-diphenylpropan-2-ol

*Crystal data*

| | |
|---|---|
| $C_{25}H_{30}O$ | $F(000) = 1504$ |
| $M_r = 346.49$ | $D_x = 1.222$ Mg m$^{-3}$ |
| Monoclinic, $C2/c$ | Melting point: 396 K |
| Hall symbol: -C 2yc | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 24.2808$ (10) Å | Cell parameters from 6762 reflections |
| $b = 6.3978$ (2) Å | $\theta = 3.0–27.2°$ |
| $c = 25.2555$ (14) Å | $\mu = 0.07$ mm$^{-1}$ |
| $\beta = 106.183$ (5)° | $T = 120$ K |
| $V = 3767.8$ (3) Å$^3$ | Block, colourless |
| $Z = 8$ | 0.40 × 0.30 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur diffractometer with a Sapphire2 (large Be window) detector | 3315 independent reflections |
| Radiation source: Enhance (Mo) X-ray Source | 2381 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.024$ |
| Detector resolution: 8.4353 pixels mm$^{-1}$ | $\theta_{max} = 25.0°$, $\theta_{min} = 3.3°$ |
| ω scan | $h = -28\rightarrow28$ |
| Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009) | $k = -7\rightarrow7$ |
| $T_{min} = 0.965$, $T_{max} = 1.000$ | $l = -17\rightarrow29$ |
| 17425 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 |
| $R[F^2 > 2\sigma(F^2)] = 0.033$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.080$ | H-atom parameters constrained |
| $S = 0.96$ | $w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3315 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 236 parameters | $\Delta\rho_{max} = 0.20$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.21$ 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 $F^2 > 2\sigma(F^2)$ 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 | 0.01323 (3) | 0.97763 (12) | 0.09694 (3) | 0.0262 (2) |
| H1 | 0.0440 | 1.0301 | 0.1163 | 0.039* |
| C1 | −0.05610 (5) | 0.71728 (17) | 0.10148 (5) | 0.0194 (3) |
| C2 | −0.08736 (5) | 0.73762 (19) | 0.03965 (5) | 0.0238 (3) |
| H2A | −0.0807 | 0.8790 | 0.0268 | 0.029* |
| H2B | −0.0715 | 0.6344 | 0.0187 | 0.029* |
| C3 | −0.15200 (5) | 0.70122 (19) | 0.02840 (5) | 0.0251 (3) |
| H3 | −0.1710 | 0.7147 | −0.0120 | 0.030* |
| C4 | −0.17747 (5) | 0.86215 (19) | 0.05970 (5) | 0.0267 (3) |
| H4A | −0.1717 | 1.0049 | 0.0471 | 0.032* |
| H4B | −0.2192 | 0.8381 | 0.0525 | 0.032* |
| C5 | −0.14785 (5) | 0.84099 (17) | 0.12124 (5) | 0.0225 (3) |
| H5 | −0.1640 | 0.9466 | 0.1420 | 0.027* |
| C6 | −0.15777 (5) | 0.62180 (17) | 0.14074 (5) | 0.0246 (3) |
| H6A | −0.1994 | 0.5969 | 0.1341 | 0.030* |
| H6B | −0.1391 | 0.6087 | 0.1808 | 0.030* |
| C7 | −0.13269 (5) | 0.46028 (18) | 0.10926 (5) | 0.0244 (3) |
| H7 | −0.1395 | 0.3168 | 0.1218 | 0.029* |
| C8 | −0.06786 (5) | 0.49578 (17) | 0.12020 (5) | 0.0232 (3) |
| H8A | −0.0519 | 0.3902 | 0.0999 | 0.028* |
| H8B | −0.0487 | 0.4791 | 0.1600 | 0.028* |
| C9 | −0.16199 (5) | 0.48078 (19) | 0.04750 (5) | 0.0279 (3) |
| H9A | −0.2036 | 0.4547 | 0.0401 | 0.034* |
| H9B | −0.1461 | 0.3760 | 0.0269 | 0.034* |
| C10 | −0.08327 (5) | 0.87808 (17) | 0.13238 (5) | 0.0216 (3) |
| H10A | −0.0646 | 0.8674 | 0.1725 | 0.026* |
| H10B | −0.0767 | 1.0210 | 0.1204 | 0.026* |
| C11 | 0.00961 (5) | 0.76258 (18) | 0.11266 (5) | 0.0212 (3) |
| C12 | 0.04245 (5) | 0.72698 (18) | 0.17460 (5) | 0.0230 (3) |
| H12A | 0.0137 | 0.7129 | 0.1956 | 0.028* |
| H12B | 0.0631 | 0.5921 | 0.1776 | 0.028* |
| C13 | 0.08517 (5) | 0.89325 (18) | 0.20235 (5) | 0.0221 (3) |
| C14 | 0.14410 (5) | 0.8651 (2) | 0.21349 (5) | 0.0314 (3) |

| | | | | |
|---|---|---|---|---|
| H14 | 0.1586 | 0.7389 | 0.2028 | 0.038* |
| C15 | 0.18185 (5) | 1.0196 (2) | 0.24008 (6) | 0.0395 (4) |
| H15 | 0.2220 | 0.9986 | 0.2472 | 0.047* |
| C16 | 0.16163 (6) | 1.2032 (2) | 0.25620 (5) | 0.0365 (4) |
| H16 | 0.1877 | 1.3086 | 0.2743 | 0.044* |
| C17 | 0.10354 (5) | 1.2327 (2) | 0.24588 (5) | 0.0326 (3) |
| H17 | 0.0893 | 1.3582 | 0.2573 | 0.039* |
| C18 | 0.06578 (5) | 1.08006 (18) | 0.21888 (5) | 0.0270 (3) |
| H18 | 0.0257 | 1.1033 | 0.2115 | 0.032* |
| C19 | 0.03612 (5) | 0.62720 (19) | 0.07513 (5) | 0.0269 (3) |
| H19A | 0.0262 | 0.4791 | 0.0792 | 0.032* |
| H19B | 0.0183 | 0.6678 | 0.0363 | 0.032* |
| C20 | 0.10058 (5) | 0.64448 (19) | 0.08689 (5) | 0.0246 (3) |
| C21 | 0.13650 (5) | 0.4812 (2) | 0.11175 (5) | 0.0289 (3) |
| H21 | 0.1203 | 0.3564 | 0.1213 | 0.035* |
| C22 | 0.19554 (5) | 0.4986 (2) | 0.12276 (6) | 0.0325 (3) |
| H22 | 0.2195 | 0.3857 | 0.1396 | 0.039* |
| C23 | 0.21958 (5) | 0.6795 (2) | 0.10939 (5) | 0.0323 (3) |
| H23 | 0.2601 | 0.6922 | 0.1174 | 0.039* |
| C24 | 0.18452 (5) | 0.8419 (2) | 0.08428 (5) | 0.0324 (3) |
| H24 | 0.2009 | 0.9664 | 0.0748 | 0.039* |
| C25 | 0.12569 (5) | 0.8235 (2) | 0.07287 (5) | 0.0287 (3) |
| H25 | 0.1019 | 0.9355 | 0.0551 | 0.034* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0248 (5) | 0.0256 (5) | 0.0256 (5) | −0.0059 (4) | 0.0027 (4) | 0.0034 (4) |
| C1 | 0.0207 (6) | 0.0180 (6) | 0.0199 (7) | 0.0004 (5) | 0.0061 (5) | −0.0003 (5) |
| C2 | 0.0221 (6) | 0.0273 (7) | 0.0218 (8) | 0.0001 (5) | 0.0058 (6) | −0.0006 (6) |
| C3 | 0.0211 (6) | 0.0317 (7) | 0.0206 (8) | 0.0003 (5) | 0.0025 (5) | −0.0015 (6) |
| C4 | 0.0204 (6) | 0.0260 (7) | 0.0323 (8) | 0.0034 (5) | 0.0049 (6) | 0.0029 (6) |
| C5 | 0.0221 (6) | 0.0195 (6) | 0.0272 (8) | 0.0048 (5) | 0.0092 (6) | −0.0014 (5) |
| C6 | 0.0197 (6) | 0.0262 (7) | 0.0293 (8) | 0.0006 (5) | 0.0091 (6) | 0.0017 (6) |
| C7 | 0.0234 (6) | 0.0168 (6) | 0.0345 (8) | −0.0006 (5) | 0.0105 (6) | 0.0005 (6) |
| C8 | 0.0228 (6) | 0.0199 (6) | 0.0277 (8) | 0.0022 (5) | 0.0083 (6) | −0.0001 (6) |
| C9 | 0.0192 (6) | 0.0286 (7) | 0.0357 (9) | −0.0032 (5) | 0.0072 (6) | −0.0099 (6) |
| C10 | 0.0233 (6) | 0.0190 (6) | 0.0225 (7) | 0.0004 (5) | 0.0065 (5) | 0.0000 (5) |
| C11 | 0.0222 (6) | 0.0209 (6) | 0.0203 (7) | −0.0009 (5) | 0.0057 (5) | 0.0009 (5) |
| C12 | 0.0225 (6) | 0.0236 (6) | 0.0228 (7) | 0.0016 (5) | 0.0059 (5) | 0.0004 (6) |
| C13 | 0.0244 (6) | 0.0277 (7) | 0.0138 (7) | 0.0011 (5) | 0.0047 (5) | 0.0023 (5) |
| C14 | 0.0253 (7) | 0.0422 (8) | 0.0253 (8) | 0.0041 (6) | 0.0046 (6) | −0.0077 (7) |
| C15 | 0.0238 (7) | 0.0638 (10) | 0.0297 (9) | −0.0067 (7) | 0.0054 (6) | −0.0108 (8) |
| C16 | 0.0416 (8) | 0.0420 (8) | 0.0241 (8) | −0.0154 (7) | 0.0062 (7) | −0.0061 (7) |
| C17 | 0.0432 (8) | 0.0280 (7) | 0.0233 (8) | 0.0000 (6) | 0.0038 (6) | −0.0012 (6) |
| C18 | 0.0274 (7) | 0.0306 (7) | 0.0210 (8) | 0.0036 (5) | 0.0034 (6) | 0.0006 (6) |
| C19 | 0.0221 (6) | 0.0350 (7) | 0.0240 (8) | −0.0010 (5) | 0.0070 (6) | −0.0058 (6) |
| C20 | 0.0226 (6) | 0.0337 (7) | 0.0187 (7) | −0.0002 (5) | 0.0076 (5) | −0.0076 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C21 | 0.0299 (7) | 0.0269 (7) | 0.0323 (8) | 0.0002 (5) | 0.0126 (6) | −0.0065 (6) |
| C22 | 0.0274 (7) | 0.0351 (8) | 0.0346 (9) | 0.0096 (6) | 0.0082 (6) | −0.0060 (7) |
| C23 | 0.0193 (6) | 0.0439 (8) | 0.0338 (9) | 0.0003 (6) | 0.0077 (6) | −0.0077 (7) |
| C24 | 0.0283 (7) | 0.0403 (8) | 0.0313 (9) | −0.0021 (6) | 0.0129 (6) | 0.0021 (7) |
| C25 | 0.0256 (7) | 0.0394 (8) | 0.0224 (8) | 0.0046 (6) | 0.0086 (6) | 0.0046 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C11 | 1.4414 (13) | C11—C19 | 1.5500 (16) |
| O1—H1 | 0.8400 | C11—C12 | 1.5620 (16) |
| C1—C2 | 1.5397 (16) | C12—C13 | 1.5144 (15) |
| C1—C8 | 1.5454 (15) | C12—H12A | 0.9900 |
| C1—C10 | 1.5459 (15) | C12—H12B | 0.9900 |
| C1—C11 | 1.5680 (15) | C13—C18 | 1.3906 (16) |
| C2—C3 | 1.5331 (15) | C13—C14 | 1.3910 (15) |
| C2—H2A | 0.9900 | C14—C15 | 1.3876 (17) |
| C2—H2B | 0.9900 | C14—H14 | 0.9500 |
| C3—C4 | 1.5296 (16) | C15—C16 | 1.3774 (19) |
| C3—C9 | 1.5316 (17) | C15—H15 | 0.9500 |
| C3—H3 | 1.0000 | C16—C17 | 1.3741 (17) |
| C4—C5 | 1.5258 (17) | C16—H16 | 0.9500 |
| C4—H4A | 0.9900 | C17—C18 | 1.3824 (17) |
| C4—H4B | 0.9900 | C17—H17 | 0.9500 |
| C5—C6 | 1.5276 (15) | C18—H18 | 0.9500 |
| C5—C10 | 1.5323 (15) | C19—C20 | 1.5136 (15) |
| C5—H5 | 1.0000 | C19—H19A | 0.9900 |
| C6—C7 | 1.5299 (15) | C19—H19B | 0.9900 |
| C6—H6A | 0.9900 | C20—C25 | 1.3891 (16) |
| C6—H6B | 0.9900 | C20—C21 | 1.3929 (17) |
| C7—C9 | 1.5289 (17) | C21—C22 | 1.3866 (16) |
| C7—C8 | 1.5373 (15) | C21—H21 | 0.9500 |
| C7—H7 | 1.0000 | C22—C23 | 1.3798 (18) |
| C8—H8A | 0.9900 | C22—H22 | 0.9500 |
| C8—H8B | 0.9900 | C23—C24 | 1.3801 (17) |
| C9—H9A | 0.9900 | C23—H23 | 0.9500 |
| C9—H9B | 0.9900 | C24—C25 | 1.3812 (16) |
| C10—H10A | 0.9900 | C24—H24 | 0.9500 |
| C10—H10B | 0.9900 | C25—H25 | 0.9500 |
| C11—O1—H1 | 109.5 | C5—C10—H10B | 109.4 |
| C2—C1—C8 | 107.87 (9) | C1—C10—H10B | 109.4 |
| C2—C1—C10 | 107.26 (9) | H10A—C10—H10B | 108.0 |
| C8—C1—C10 | 108.34 (9) | O1—C11—C19 | 107.30 (9) |
| C2—C1—C11 | 110.87 (9) | O1—C11—C12 | 111.20 (9) |
| C8—C1—C11 | 112.33 (9) | C19—C11—C12 | 110.36 (9) |
| C10—C1—C11 | 110.01 (9) | O1—C11—C1 | 105.31 (9) |
| C3—C2—C1 | 111.40 (9) | C19—C11—C1 | 111.21 (9) |
| C3—C2—H2A | 109.3 | C12—C11—C1 | 111.29 (9) |
| C1—C2—H2A | 109.3 | C13—C12—C11 | 116.98 (9) |
| C3—C2—H2B | 109.3 | C13—C12—H12A | 108.1 |

| | | | |
|---|---|---|---|
| C1—C2—H2B | 109.3 | C11—C12—H12A | 108.1 |
| H2A—C2—H2B | 108.0 | C13—C12—H12B | 108.1 |
| C4—C3—C9 | 109.56 (10) | C11—C12—H12B | 108.0 |
| C4—C3—C2 | 110.03 (10) | H12A—C12—H12B | 107.3 |
| C9—C3—C2 | 108.99 (9) | C18—C13—C14 | 117.77 (11) |
| C4—C3—H3 | 109.4 | C18—C13—C12 | 119.81 (10) |
| C9—C3—H3 | 109.4 | C14—C13—C12 | 122.40 (11) |
| C2—C3—H3 | 109.4 | C15—C14—C13 | 120.59 (12) |
| C5—C4—C3 | 108.84 (9) | C15—C14—H14 | 119.7 |
| C5—C4—H4A | 109.9 | C13—C14—H14 | 119.7 |
| C3—C4—H4A | 109.9 | C16—C15—C14 | 120.59 (12) |
| C5—C4—H4B | 109.9 | C16—C15—H15 | 119.7 |
| C3—C4—H4B | 109.9 | C14—C15—H15 | 119.7 |
| H4A—C4—H4B | 108.3 | C17—C16—C15 | 119.53 (12) |
| C4—C5—C6 | 109.76 (10) | C17—C16—H16 | 120.2 |
| C4—C5—C10 | 109.94 (10) | C15—C16—H16 | 120.2 |
| C6—C5—C10 | 109.16 (9) | C16—C17—C18 | 120.06 (13) |
| C4—C5—H5 | 109.3 | C16—C17—H17 | 120.0 |
| C6—C5—H5 | 109.3 | C18—C17—H17 | 120.0 |
| C10—C5—H5 | 109.3 | C17—C18—C13 | 121.46 (12) |
| C5—C6—C7 | 109.34 (9) | C17—C18—H18 | 119.3 |
| C5—C6—H6A | 109.8 | C13—C18—H18 | 119.3 |
| C7—C6—H6A | 109.8 | C20—C19—C11 | 114.97 (10) |
| C5—C6—H6B | 109.8 | C20—C19—H19A | 108.5 |
| C7—C6—H6B | 109.8 | C11—C19—H19A | 108.5 |
| H6A—C6—H6B | 108.3 | C20—C19—H19B | 108.5 |
| C9—C7—C6 | 109.44 (10) | C11—C19—H19B | 108.5 |
| C9—C7—C8 | 109.43 (10) | H19A—C19—H19B | 107.5 |
| C6—C7—C8 | 110.04 (10) | C25—C20—C21 | 117.97 (11) |
| C9—C7—H7 | 109.3 | C25—C20—C19 | 120.90 (11) |
| C6—C7—H7 | 109.3 | C21—C20—C19 | 121.13 (11) |
| C8—C7—H7 | 109.3 | C22—C21—C20 | 120.84 (12) |
| C7—C8—C1 | 110.35 (9) | C22—C21—H21 | 119.6 |
| C7—C8—H8A | 109.6 | C20—C21—H21 | 119.6 |
| C1—C8—H8A | 109.6 | C23—C22—C21 | 120.17 (12) |
| C7—C8—H8B | 109.6 | C23—C22—H22 | 119.9 |
| C1—C8—H8B | 109.6 | C21—C22—H22 | 119.9 |
| H8A—C8—H8B | 108.1 | C22—C23—C24 | 119.65 (12) |
| C7—C9—C3 | 109.32 (9) | C22—C23—H23 | 120.2 |
| C7—C9—H9A | 109.8 | C24—C23—H23 | 120.2 |
| C3—C9—H9A | 109.8 | C23—C24—C25 | 120.11 (13) |
| C7—C9—H9B | 109.8 | C23—C24—H24 | 119.9 |
| C3—C9—H9B | 109.8 | C25—C24—H24 | 119.9 |
| H9A—C9—H9B | 108.3 | C24—C25—C20 | 121.25 (12) |
| C5—C10—C1 | 111.28 (9) | C24—C25—H25 | 119.4 |
| C5—C10—H10A | 109.4 | C20—C25—H25 | 119.4 |
| C1—C10—H10A | 109.4 | | |
| C8—C1—C2—C3 | 58.61 (12) | C8—C1—C11—C19 | 68.28 (13) |
| C10—C1—C2—C3 | −57.89 (12) | C10—C1—C11—C19 | −170.96 (10) |

| | | | |
|---|---|---|---|
| C11—C1—C2—C3 | −178.01 (9) | C2—C1—C11—C12 | −175.98 (9) |
| C1—C2—C3—C4 | 60.09 (13) | C8—C1—C11—C12 | −55.21 (12) |
| C1—C2—C3—C9 | −60.06 (12) | C10—C1—C11—C12 | 65.55 (12) |
| C9—C3—C4—C5 | 60.47 (12) | O1—C11—C12—C13 | −17.22 (14) |
| C2—C3—C4—C5 | −59.33 (12) | C19—C11—C12—C13 | 101.75 (11) |
| C3—C4—C5—C6 | −60.57 (11) | C1—C11—C12—C13 | −134.29 (10) |
| C3—C4—C5—C10 | 59.52 (12) | C11—C12—C13—C18 | 77.21 (14) |
| C4—C5—C6—C7 | 60.41 (12) | C11—C12—C13—C14 | −104.43 (13) |
| C10—C5—C6—C7 | −60.15 (13) | C18—C13—C14—C15 | −0.20 (19) |
| C5—C6—C7—C9 | −59.80 (12) | C12—C13—C14—C15 | −178.59 (12) |
| C5—C6—C7—C8 | 60.48 (13) | C13—C14—C15—C16 | 0.4 (2) |
| C9—C7—C8—C1 | 60.66 (12) | C14—C15—C16—C17 | 0.1 (2) |
| C6—C7—C8—C1 | −59.63 (13) | C15—C16—C17—C18 | −0.8 (2) |
| C2—C1—C8—C7 | −58.44 (12) | C16—C17—C18—C13 | 1.0 (2) |
| C10—C1—C8—C7 | 57.36 (12) | C14—C13—C18—C17 | −0.49 (18) |
| C11—C1—C8—C7 | 179.08 (10) | C12—C13—C18—C17 | 177.94 (12) |
| C6—C7—C9—C3 | 59.81 (12) | O1—C11—C19—C20 | 71.11 (13) |
| C8—C7—C9—C3 | −60.84 (12) | C12—C11—C19—C20 | −50.21 (13) |
| C4—C3—C9—C7 | −60.35 (12) | C1—C11—C19—C20 | −174.22 (10) |
| C2—C3—C9—C7 | 60.09 (12) | C11—C19—C20—C25 | −72.41 (15) |
| C4—C5—C10—C1 | −60.40 (12) | C11—C19—C20—C21 | 107.99 (13) |
| C6—C5—C10—C1 | 60.05 (13) | C25—C20—C21—C22 | 0.84 (19) |
| C2—C1—C10—C5 | 58.06 (12) | C19—C20—C21—C22 | −179.55 (11) |
| C8—C1—C10—C5 | −58.14 (12) | C20—C21—C22—C23 | 0.34 (19) |
| C11—C1—C10—C5 | 178.72 (9) | C21—C22—C23—C24 | −0.9 (2) |
| C2—C1—C11—O1 | 63.42 (11) | C22—C23—C24—C25 | 0.3 (2) |
| C8—C1—C11—O1 | −175.82 (9) | C23—C24—C25—C20 | 0.9 (2) |
| C10—C1—C11—O1 | −55.05 (12) | C21—C20—C25—C24 | −1.47 (19) |
| C2—C1—C11—C19 | −52.49 (12) | C19—C20—C25—C24 | 178.92 (11) |

*Hydrogen-bond geometry (Å, °)*

*Cg*1 is the centroid of C20–C25 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14···Cg1 | 0.95 | 2.70 | 3.3172 (13) | 123. |

**Fig. 1**

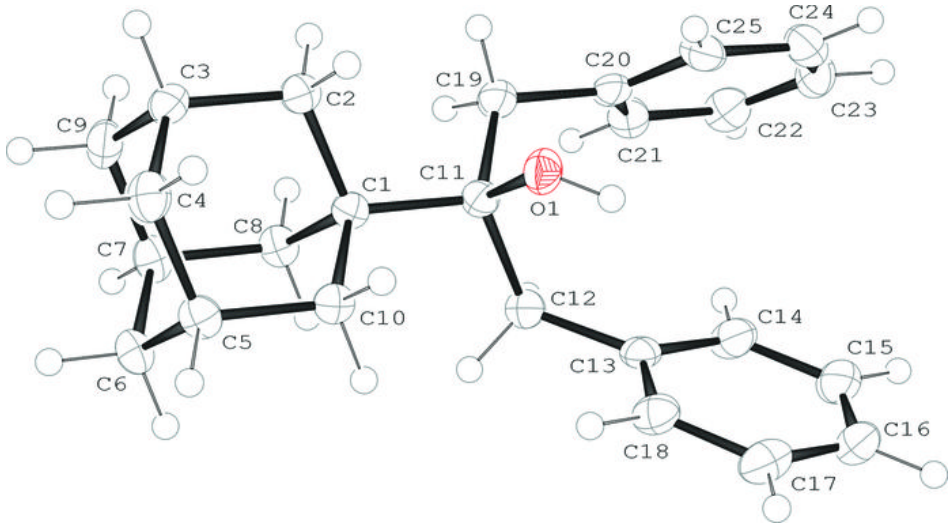
C3
C2
C9
C4
C1
C11
C8
C7
C10
C5
C6
C19
C20
C25
C24
C23
C22
C21
O1
C12
C14
C15
C13
C16
C18
C17

**Fig. 2**