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

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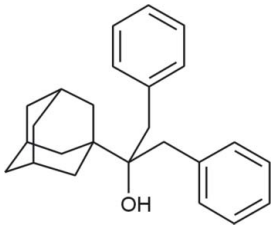
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.080; data-to-parameter ratio = 14.0.

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
β = 106.183 (5)°
V = 3767.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 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).

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supplementary materials

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

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

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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

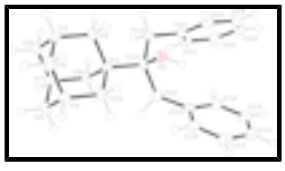


Fig. 1. Ellipsoid plot (50% probability) of the asymmetric unit. Hydrogen atoms are represented as spheres of arbitrary size.

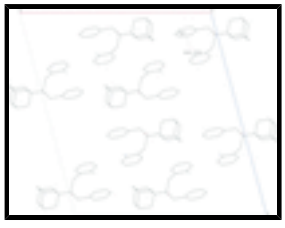


Fig. 2. Crystal packing viewed along the *b*-axis. Intramolecular C—H···π interactions are shown as dotted lines. *Cg*1 is the center of gravity of C20–C25. H-atoms (except those which are involved in C—H···π interactions) have been omitted for clarity.

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	$h = -28 \rightarrow 28$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$k = -7 \rightarrow 7$
$T_{min} = 0.965$, $T_{max} = 1.000$	$l = -17 \rightarrow 29$
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)

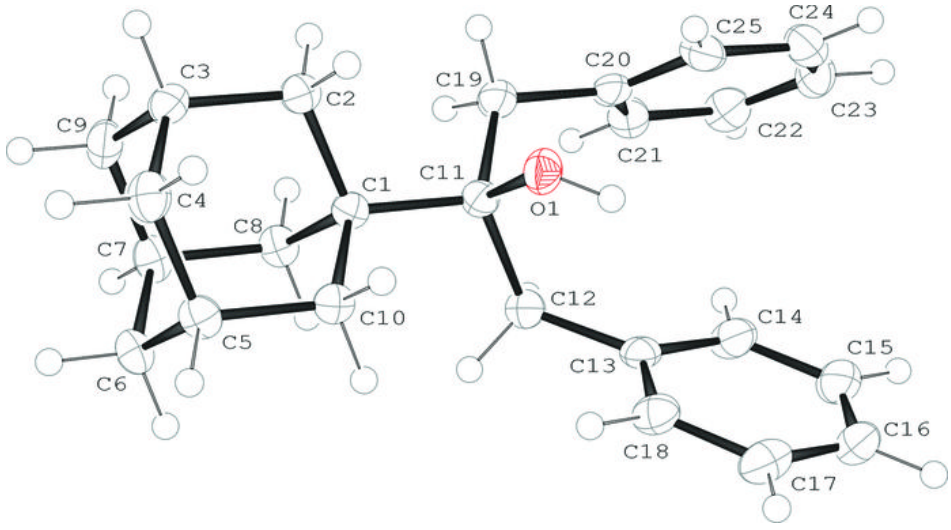
C11—C1—C2—C3	−178.01 (9)	C2—C1—C11—C12	−175.98 (9)
C1—C2—C3—C4	60.09 (13)	C8—C1—C11—C12	−55.21 (12)
C1—C2—C3—C9	−60.06 (12)	C10—C1—C11—C12	65.55 (12)
C9—C3—C4—C5	60.47 (12)	O1—C11—C12—C13	−17.22 (14)
C2—C3—C4—C5	−59.33 (12)	C19—C11—C12—C13	101.75 (11)
C3—C4—C5—C6	−60.57 (11)	C1—C11—C12—C13	−134.29 (10)
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
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C4
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C11
C8
C7
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C5
C6
C19
C20
C25
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C23
C22
C21
O1
C12
C14
C15
C13
C16
C18
C17

Fig. 2