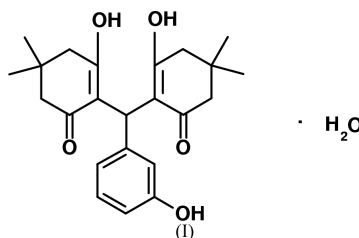


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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.041
 wR factor = 0.115
Data-to-parameter ratio = 17.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2,2'-[(3-Hydroxyphenyl)methylene]bis(3-hydroxy-5,5-
dimethyl-2-cyclohexen-1-one) hydrateThe title compound is a bis-dimedone derivative which
crystallizes as a monohydrate, $\text{C}_{23}\text{H}_{28}\text{O}_5 \cdot \text{H}_2\text{O}$. Its crystal
packing is stabilized by hydrogen bonds involving water.

Comment

Some years ago, we accidentally encountered the twinned
crystal structures of two similar compounds bearing the bis-
dimedone moiety: bis(2-hydroxy-4,4-dimethyl-6-oxo-1-cyclo-
hexenyl)phenylmethane (Bolte *et al.*, 1997) and 2,2'-methyl-
enebis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one) (Bolte &
Scholtyssik, 1997). Since these compounds can easily be
prepared (Hünig *et al.*, 1979), we have decided to synthesize
various derivatives with the objective to find out if these are
also twinned (Bolte *et al.*, 2001). We hoped to find more
twinned crystal structures in order to understand why some of
these simple compounds containing the common bis-dime-
done skeleton are twinned. Unfortunately, none of these,
including the title compound, (I), turned out to be twinned.The two cyclohexenone rings display envelope conforma-
tions with C14 and C24 deviating by 0.644 (2) and 0.653 (2) Å,
respectively, from the plane of the remaining five ring atoms.
Both apices are extended towards the phenyl ring. Two strong
intramolecular hydrogen bonds are formed connecting the two
cyclohexenone rings. The water molecule bridges two
different molecules *via* its H atoms and acts as an acceptor for
the H atom of the hydroxyl group of a third molecule.

Experimental

The title compound was synthesized according to Nagarajan &
Shenoy (1992).

Crystal data

 $\text{C}_{23}\text{H}_{28}\text{O}_5 \cdot \text{H}_2\text{O}$
 $M_r = 402.47$
Monoclinic, $P2_1/n$
 $a = 8.948$ (1) Å
 $b = 27.128$ (3) Å
 $c = 9.045$ (1) Å
 $\beta = 94.30$ (1)°
 $V = 2189.4$ (4) Å³
 $Z = 4$ $D_x = 1.221$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 8192
reflections
 $\theta = 0-25^\circ$
 $\mu = 0.09$ mm⁻¹
 $T = 173$ (2) K
Block, colourless
 $0.70 \times 0.65 \times 0.45$ mm

Data collection

Siemens CCD three-circle diffractometer

 ω scans

Absorption correction: empirical (SADABS; Sheldrick, 1996)

 $T_{\min} = 0.941$, $T_{\max} = 0.962$
41 555 measured reflections
4836 independent reflections
4088 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.028$ $\theta_{\max} = 27.1^\circ$ $h = -11 \rightarrow 11$ $k = -34 \rightarrow 34$ $l = -11 \rightarrow 11$ 486 standard reflections
frequency: 1200 min
intensity decay: none

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.041$ $wR(F^2) = 0.115$ $S = 1.01$

4836 reflections

283 parameters

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.8381P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL97

Extinction coefficient: 0.0036 (10)

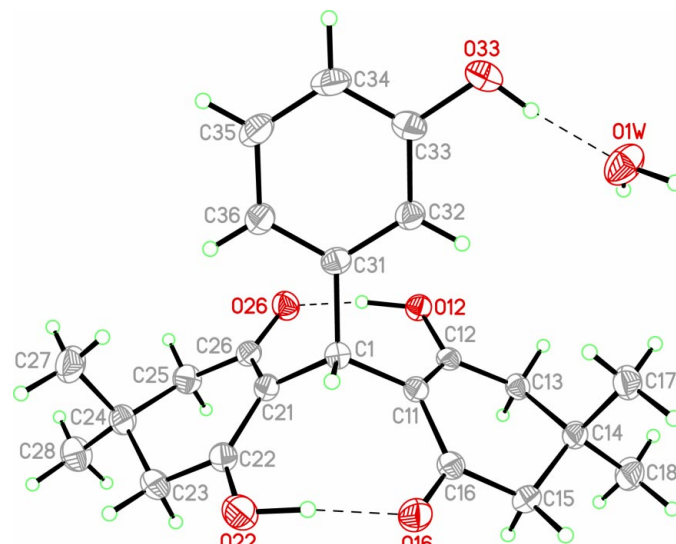


Figure 1

Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

Table 1

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O12—H12 \cdots O26	1.09 (3)	1.49 (3)	2.560 (1)	164 (2)
O22—H22 \cdots O16	1.05 (3)	1.62 (3)	2.664 (1)	171 (3)
O1W—H1W \cdots O16	0.92 (2)	1.88 (2)	2.795 (2)	172 (2)
O33—H33 \cdots O1W ⁱ	0.92 (2)	1.76 (2)	2.684 (2)	174 (2)
O1W—H2W \cdots O12 ⁱⁱ	0.97 (3)	1.90 (3)	2.870 (2)	175 (2)

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

All H atoms bonded to C atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [$U(H) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ or $U(H) = 1.2U_{\text{eq}}(\text{C})$] using a riding model with $C-H(\text{aromatic}) = 0.95$, $C-H(\text{methyl}) = 0.98$, $C-H(\text{secondary}) = 0.99$ or $C-H(\text{tertiary}) = 1.00 \text{ \AA}$. All hydroxyl H atoms were refined isotropically.

Data collection: SMART (Siemens, 1995); cell refinement: SMART; data reduction: SAINT (Siemens, 1995); program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to

refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL-Plus (Sheldrick, 1991).

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