

***trans*-3,3'-Bis(diphenylhydroxymethyl)stilbene–benzene (3/4)**Shigeru Ohba,^{a*} Takaichi Hiratsuka^b and Koichi Tanaka^b^aDepartment of Chemistry, Keio University, Hiyoshi 4-1-1, Kohoku-ku, Yokohama 223-8521, Japan, and ^bDepartment of Applied Chemistry, Faculty of Engineering, Ehime University, Matsuyama, Ehime 790-8577, Japan

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Key indicators

Single-crystal X-ray study

 $T = 297\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$ R factor = 0.051 wR factor = 0.155

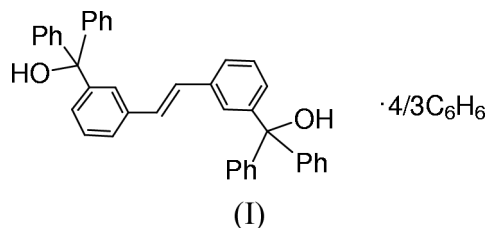
Data-to-parameter ratio = 14.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the crystal structure of the title compound, $3\text{C}_{40}\text{H}_{32}\text{O}_2 \cdot 4\text{C}_6\text{H}_6$, there are one and a half host molecules and two benzene molecules in the asymmetric unit. The host molecules form a ladder structure *via* $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds.

Comment

The photoisomerization of *cis*-3,3'-bis(diphenylhydroxymethyl)stilbene to its *trans*-isomer has been observed in inclusion-complex crystals. In the crystals of the *cis*-host with acetone (1/1), there is an intramolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bond in the host molecule, and the acetone molecule is connected to the host by an $\text{O}-\text{H} \cdots \text{O}$ hydrogen bond (Tanaka *et al.*, 2002). Here, the structure of the title compound, (I), has been determined, in order to investigate the hydrogen-bonding pattern of the *trans*-host in the crystals.



The host molecule in the general position is asymmetric, and the two $\text{C}-\text{CPh}_2\text{OH}$ bond axes ($\text{C}17-\text{C}4$ and $\text{C}27-\text{C}31$) are oriented on the same side of the molecule (Fig. 1). The dihedral angle between the two phenyl rings of the *trans*-stilbene moiety is $45.82(12)^\circ$, and the central $\text{C}21-\text{C}23=\text{C}24-\text{C}25$ torsion angle is $-178.5(3)^\circ$. On the other hand, the half-host molecule has a centre of symmetry at the midpoint of the $\text{C}63=\text{C}63^i$ bond [symmetry code: (i) $2-x, 1-y, 1-z$].

The crystal structure of (I) along c is shown in Fig. 2. The host molecules form a ladder structure along c , and the benzene molecules are accommodated in the columns. The host molecules in general positions along c are connected by the $\text{O}2-\text{H}2 \cdots \text{O}1^{\text{ii}}$ hydrogen bond to form a zigzag chain (Fig. 3 and Table 2) [symmetry code: (ii) $x, y, z-1$]. The half-host molecule acts as both hydrogen donor and acceptor, to connect two zigzag chains *via* $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds to complete the ladder structure (Fig. 2).

Experimental

The title host compound was prepared according to the method of Tanaka *et al.* (2002). Crystals of (I) were grown from an acetone–benzene solution.

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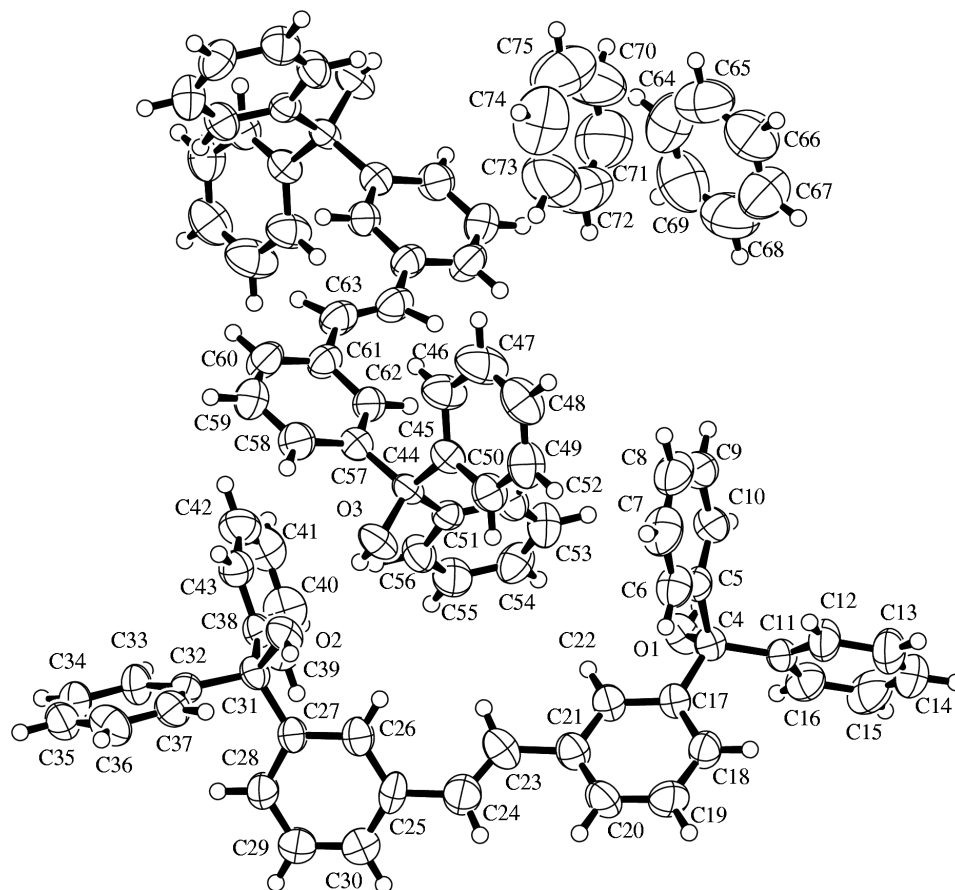


Figure 1

The molecular structure of (I), with displacement ellipsoids plotted at the 50% probability level.

Crystal data

$3\text{C}_{40}\text{H}_{32}\text{O}_2 \cdot 4\text{C}_6\text{H}_6$
 $M_r = 1946.52$
 Triclinic, $P\bar{1}$
 $a = 12.972(2) \text{ \AA}$
 $b = 23.653(4) \text{ \AA}$
 $c = 9.304(4) \text{ \AA}$
 $\alpha = 100.61(2)^\circ$
 $\beta = 98.53(2)^\circ$
 $\gamma = 96.030(13)^\circ$
 $V = 2749.0(14) \text{ \AA}^3$

$Z = 1$
 $D_x = 1.176 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 10.0\text{--}11.5^\circ$
 $\mu = 0.07 \text{ mm}^{-1}$
 $T = 297.2 \text{ K}$
 Plate, colourless
 $0.40 \times 0.20 \times 0.05 \text{ mm}$

Data collection

Rigaku AFC-7R diffractometer
 ω scans
 10 329 measured reflections
 9676 independent reflections
 4109 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\text{max}} = 25^\circ$

$h = 0 \rightarrow 15$
 $k = -28 \rightarrow 28$
 $l = -11 \rightarrow 11$
 3 standard reflections
 every 150 reflections
 intensity decay: 0.7%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.155$
 $S = 0.97$
 9676 reflections
 688 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0579P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.005$
 $\Delta\rho_{\text{max}} = 0.25 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C23—C24	1.270 (5)	C63—C63 ⁱ	1.314 (7)
C21—C23—C24	127.9 (4)	C61—C63—C63 ⁱ	127.8 (4)
C23—C24—C25	128.0 (4)		
C20—C21—C23—C24	−22.9 (6)	C23—C24—C25—C26	−24.8 (5)
C21—C23—C24—C25	−178.5 (3)	C62—C61—C63—C63 ⁱ	−13.3 (7)

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

Table 2

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

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O3—H3 \cdots O2	0.75 (3)	2.20 (3)	2.827 (3)	141 (3)
O1—H1 \cdots O3 ⁱ	0.79 (3)	2.03 (2)	2.761 (3)	154 (3)
O2—H2 \cdots O1 ⁱⁱ	0.80 (3)	2.19 (3)	2.774 (2)	129 (3)

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

The hydroxyl H atoms were located from difference syntheses and refined isotropically. The other H atoms were positioned geometrically and fixed, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$. The central C23=C24 bond of the *trans*-stilbene moiety is 1.270 (5) \AA . Such a short bond length may be the result of dynamic disorder caused by a pedal-like motion, as observed in crystals of *trans*-stilbene (Ogawa *et*

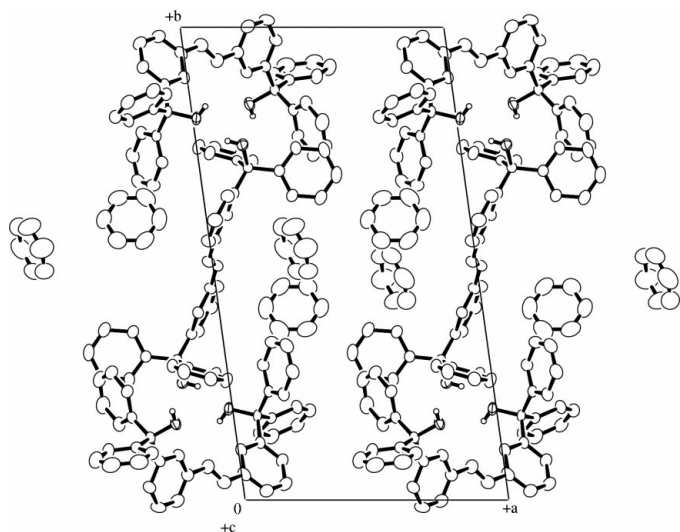


Figure 2
The projection of the crystal structure of (I) along *c*.

al., 1992). The C–C distances of the benzene molecules are 1.30 (2)–1.37 (1) Å, smaller than the standard value. This may be due to the large thermal motion.

Data collection: *WinAFC Diffractometer Control Software* (Rigaku, 1999); cell refinement: *WinAFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *SIR92* (Altomare *et*

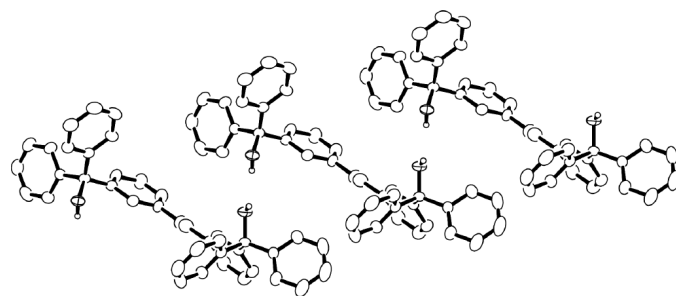


Figure 3
The arrangement of the host molecules in general positions along *c*.

al., 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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