The Crystal Structure of αα′-Diethylstilbene-4,4′-diol

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THE crystal structure of αα′-diethylstilbene-4,4′-diol (diethylstilbestrol) has been determined because of the interest in its biological activity. A Patterson projection has already shown that the active isomer has the *trans*-configuration;[1] and it has also been established that solvent-free crystals could be grown by sublimation.[2]

X-Ray diffraction data were collected with Cu-K_α radiation by the multiple-film, equi-inclination Weissenberg method and the intensities of 519 reflections were estimated visually. The crystals are orthorhombic with $a = 19{\cdot}18$, $b = 5{\cdot}32$, $c = 15{\cdot}01$ Å, $Z = 4$, $D_c = 1{\cdot}164$ g. cm.$^{-3}$, $D_m = 1{\cdot}162$, space group *Pcab*.

Since the molecular symmetry is $\bar{1}$, the double bond was placed at the origin and the orientation of the benzene ring was established by a Patterson summation and a Fourier synthesis. From these and known chemical evidence, the two ethyl carbon atoms in the asymmetric unit were located. Three cycles of least-squares refinement,[3] with isotropic temperature factors, reduced R for 454 observed reflections to 16·6%. A difference map failed to indicate the hydrogen atom positions.

The bond lengths (Å) and angles (°) are listed below and the Figure gives a perspective view of the molecule.

The standard deviations for bond lengths and angles were 0·02 and 1·5 Å respectively. The positions of all six carbon atoms fall within one root-mean-square radial error of position from the least-squares plane for the benzene ring. The normals for the planes of the benzene rings and that of the central part of the molecule, including the double bond, form angles of 61·43° with each other.

The planes of the two benzene rings are parallel but not coplanar, in contrast to stilbene which was reported to be coplanar as expected for a conjugated molecule.[4] A model confirms that this loss of co-planarity is due to steric effects between the methylene carbon of the ethyl group and the *ortho*-hydrogen atoms. The intramolecular distance C(7) · · · C(8) is 3·14 Å.

The smallest intermolecular contact (3·05 Å) observed was between oxygens of neighbouring molecules which precludes anything but a very weak hydrogen bond.

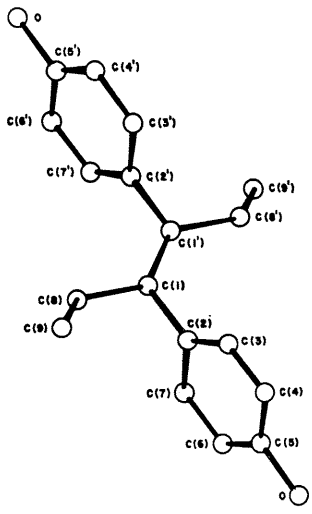

FIGURE. *Molecular stereochemistry of αα′-diethylstilbene-4,4′-diol.*

C(1)–C(1′)	1·33	C(1′)–C(1)–C(8)	124·07
C(1)–C(2)	1·50	C(1)–C(8)–C(9)	109·32
C(2)–C(3)	1·40	C(1)–C(1)–C(2)	122·22
C(3)–C(4)	1·40	C(2)–C(1)–C(8)	113·78
C(4)–C(5)	1·42	C(3)–C(2)–C(7)	116·05
C(5)–C(6)	1·36	C(2)–C(3)–C(4)	125·15
C(6)–C(7)	1·41	C(3)–C(4)–C(5)	116·27
C(2)–C(7)	1·42	C(4)–C(5)–C(6)	122·65
C(1)–C(8)	1·54	C(5)–C(6)–C(7)	119·15
C(8)–C(9)	1·56	C(2)–C(7)–C(6)	121·65
C(5)–O	1·44	C(4)–C(5)–O	119·57
		C(6)–C(5)–O	117·80

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