Identification of Isomers of a Substituted Triarylethylene: the Crystal Structure of 1-*p*-(2-Dimethylaminoethoxyphenyl)-1,2-*cis*-diphenylbut-1-ene Hydrobromide

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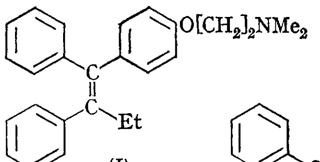
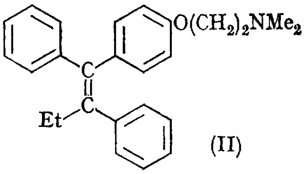
WHILE many substituted triphenylethylenes are known to be oestrogenic,[1] more complex endocrine activity has been reported in certain amino-alkoxytriarylethylenes.[2,3] For example, compound (I) behaves as a conventional oestrogen, whereas its isomer (II) has subtly different properties.[3]



(I)

(*cis*, m.p. 72-74°)



(II)

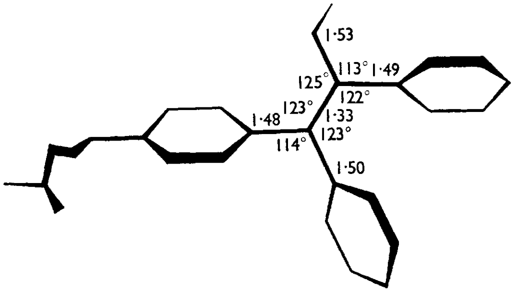
(*trans*, m.p. 96-98°)

The identification of these isomers was based on n.m.r. and dipole moment measurements.[4] The comparison of the u.v. spectra with those of stilbene derivatives, which has been used for a pair of related compounds,[5] is not a satisfactory method.[6]

We determined the crystal structure of the hydrobromide of (I) to identify the isomers: 1-*p*-(2-dimethylaminoethoxyphenyl)-1,2-*cis*-diphenyl-but-1-ene hydrobromide, $C_{26}H_{30}$ BrNO, $M = 452{\cdot}4$, triclinic, $a = 12{\cdot}073$, $b = 14{\cdot}304$, $c = 14{\cdot}169$ Å, $\alpha = 78{\cdot}80°$, $\beta = 93{\cdot}41°$, $\gamma = 91{\cdot}34°$, $U = 2395{\cdot}9$ Å^3, space group $P\bar{1}$ assumed, $Z = 4$, $D_m = 1·27$ (flotation), $D_c = 1·25$ g. cm.$^{-3}$, Mo-K_α radiation, Picker single-crystal diffractometer data.

The structure was solved by standard procedures using 3082 independent reflections with amplitudes greater than 8e. All atoms, other than hydrogen, have been located and their positions refined (with isotropic temperature factors for the light atoms) to an R value of 0·101.

The asymmetric unit contains two crystallographically distinct formula units, conformational isomers, both having the *cis*-arrangement of the unsubstituted phenyl groups with respect to the ethylenic double bond. Thus the suggested identification is unequivocally confirmed.



FIGURE

The Figure illustrates one conformational isomer and includes certain bond distances and angles. There is close agreement between analogous bond distances and angles in the two conformational isomers; the most noticeable difference is the torsion angle about the $-CH_2-CH_2-$ bond, +60° in one isomer and −176° in the other. The phenyl rings are inclined, with reference to the plane of the ethylenic double bond, at angles of 60, 50, 46° in one conformer and 51, 51, 54° in the other; in this respect the two conformers are almost identical. In solution further conformations may be present because of possible rotation about single bonds. However, a conformation with two of the three phenyl rings co-planar with the ethylenic double bond, as recently suggested,[7] is unlikely because of improbably short contact distances between non-bonded atoms.

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