X-Ray Crystal Structure of a New Insecticide: 1,1-Di-(*p*-ethoxyphenyl)-2,2-dimethylpropane

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Summary The stereochemistry of the title compound, a new insecticide, has been determined by *X*-ray crystallography.

SEVERAL series of promising new insecticides have been designed[1] using a general steric model which also included the structure of DDT and its analogues.[2] This three dimensional model was obtained from parallel beam projections of atomic models of active compounds. It was therefore of interest to determine accurately representative structures of the new insecticides by *X*-ray crystallographic techniques. Consequently, the title compound was selected to obtain a valid comparison for future predictive synthesis.

Colourless, tubular crystals were obtained from ethanol. *Crystal data:* $C_{21}H_{28}O_2$; $M = 312$, orthorhombic; $a = 22{\cdot}912$ (2), $b = 10{\cdot}424(1)$, $c = 7{\cdot}869(1)$ Å; $U = 1{\cdot}879$ Å^3, $D_m = 1{\cdot}11$ (by flotation); $Z = 4$, $D_c = 1{\cdot}10$; $\mu = 5{\cdot}40$ cm^{-1}; space group, $Pca2_1$. 1400 reflections were collected up to $2\theta = 115°$ by a Picker four-circle automatic diffractometer (Cu-K_α radiation, Ni-filtered) using an ω–2θ scanning mode. The structure was solved by direct methods, using phases

determined and refined by the tangent formula.[3] The parameters were refined by least squares to give the conventional and weighted R values of 0·040 and 0·035 respectively.

General views of the three dimensional structure of the insecticide established by the X-ray analysis are illustrated in the Figures. C–C distances range from 1·38 to 1·40 Å in the phenyl groups, 1·55 and 1·56 Å about C(13), 1·52 to 1·53 from C(14) to the methyl carbons, and 1·50 to 1·51 Å in the ethoxy-groups. C–O distances are 1·36 and 1·38 Å adjacent to the phenyl group and 1·42 to 1·44 Å in the

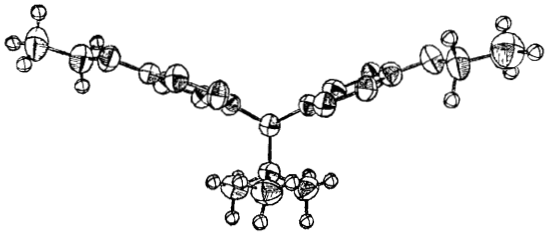

FIGURE 1. *Thermal ellipsoid plot of* 1,1-*di*-(p-*ethoxyphenyl*)-2,2-*dimethylpropane showing orientation of molecule parallel to the* C(13)–C(14) *bond.*

ethoxy-groups. Angles about C(13) are: C(1)–C(13)–C(7), 113·7°; C(1)–C(13)–C(14), 113·4°; C(7)–C(13)–C(14), 112·9°; and some adjacent to C(13)–C(14), 113·4°; C(6)–C(13)–C(14), 112·9°; and some adjacent to C(13) are C(6)–C(1)–C(13), 126·1°; C(8)–C(7)–C(13), 125·8°; C(13)–C(14)–C(16), 114·6°. The angles about the two oxygens are C(4)–O(1)–C(18), 117·7°; C(10)–O(2)–C(20), 116·3°. Approximate estimated standard deviations for an interatomic distance is 0·005 Å and for an angle 0·3°.

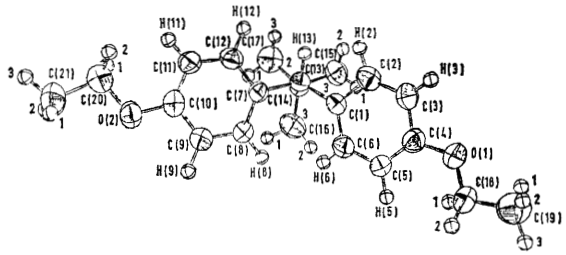

FIGURE 2. *Thermal ellipsoid plot of* 1,1-*di*-(p-*ethoxyphenyl*)-2,2-*dimethylpropane showing orientation of molecule perpendicular to the* C(13)–C(14) *bond.*

The projections of each of the two phenyl planes perpendicular to the C(13)–C(14) bond are approximately co-planar to each other and also with the plane of the trimethyl group. Least-squares-planes calculations show that each ethoxy group is approximately co-planar with its attached phenyl group.

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