X-Ray Crystal Structure of DDT; 1,1-Bis-(p-chlorophenyl)-2,2,2-trichloroethane

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Summary The stereochemistry of DDT has been determined by *X*-ray crystallography.

NUMEROUS steric theories[1] have been postulated to explain the mode of action of the insecticide DDT [1,1-bis-(*p*-chlorophenyl)-2,2,2-trichloroethane]. We now report on its crystal structure; until this present investigation, only limited data have been available.[2]

Colourless needle crystals of DDT were grown from petroleum (b.p. 40—60 °C). *Crystal data:* $C_{14}H_9Cl_5$: $M = 354$, orthorhombic; $a = 9{\cdot}963$ (1), $b = 19{\cdot}200(2)$, $c = 7{\cdot}887(1)$ Å; $U = 1509$ Å^3, $D_m = 1{\cdot}55$ (by flotation); $Z = 4$, $D_c = 1{\cdot}56$, $\mu = 86{\cdot}6$ cm^{-1}; space group, $Pca2_1$. 1400 reflections were collected up to $2\theta = 127°$ by a Picker four circle automatic diffractometer (Cu-K_α radiation, Ni-filtered), using the $\omega - 2\theta$ scanning mode. A standard reflection, measured after every 50 reflections, showed a reduction in intensity of 20% over the collection period. Consequently the measured intensities were corrected for decomposition by rescaling to a common standard, and for *X*-ray absorption. Three chlorine atoms were found from a partial solution of a sharpened Patterson synthesis. Successive electron density syntheses located all non-hydrogen atoms. Two cycles of full-matrix least-squares calculations with isotropic temperature factors, and two cycles with anisotropic ones, reduced the reliability factor R from 0·25 to 0·089. At the present stage of refinement, the bond lengths and angles have standard deviations of about 0·01 Å and 2° respectively.

General views of DDT are illustrated in Figures 1 and 2. The central tetrahedral carbon atom, C(13), links the two *p*-chlorophenyl groups to the trichloromethane group. The angles between the plane of the apex chlorine atoms and the planes of each of the phenyl groups are −5° and +25° respectively, unlike the conventional symmetrical picture of the compound. The trichloromethane group is rotated slightly from the staggered position with respect to the C(13)–C(14) bond, probably to allow maximum non-bonded distance between the chlorine atoms and the phenyl groups (Figure 1).

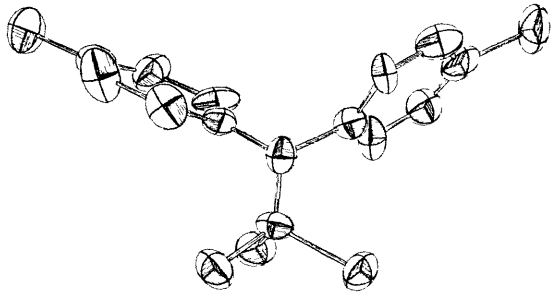

FIGURE 1. *Thermal ellipsoid plot of DDT showing the orientation of the molecule parallel to the* C(13)–C(14) *bond.*

The molecules of DDT pack as separate units in the unit cell with no apparent strong intermolecular forces. Because of this, it is likely that the stereochemistry of the molecule

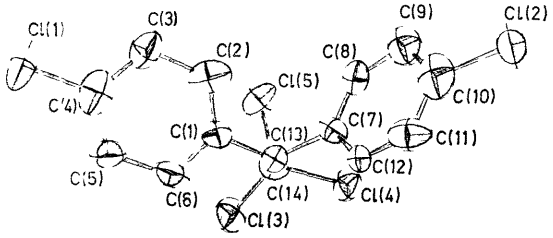

FIGURE 2. *Thermal ellipsoid plot of DDT showing the orientation of the molecule perpendicular to the* C(13)–C(14) *bond.*

found in the biological system is similar to that in the crystal.

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