The Crystal Structure of Hexachlorocyclopropane C_3Cl_6

By Tsunehiro TAKANO, Tohru CHIBA, Yoshio SASADA, Masao KAKUDO, Shun'ichi NOZAKURA and Shunske MURAHAHI

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The crystal structure of the hexachlorocyclopropane synthesized at the laboratory of two of the authors was determined by X-ray analysis. Equi-inclination photographs around the b axis were taken with Mo-$K\alpha$ radiation ($k=0, \cdots\cdots, 5$).

The unit cell dimensions obtained are:

$a=12.60$, $b=6.13$, $c=10.94$ Å, $\beta=112.0°$.

The space group is $C_{2h}^5-P2_1/a$, and $Z=4$.

Intensities were measured by a visual comparison with an intensity scale and corrected for Lorentz and polarization factors. However, no correction for absorption was made. The Weissenberg photographs showed a characteristic distribution of intensities; the reflections were very weak for $h+k+l=2n+1$. This suggested that the arrangement of the molecules is approximately body-centered.

Two-dimensional Patterson synthesis projected along [010] and [001] were also computed. The crystal structure was derived uniquely from the Patterson maps and from the requirement of a psuedo-body-centered arrangement of the molecules.

The refinement of the structure projected on the (010) plane was carried out by the least-squares method. After several cycles, the discrepancy index, $R=\sum||F_o|-|F_c||/\sum|F_o|$, became 0.14.

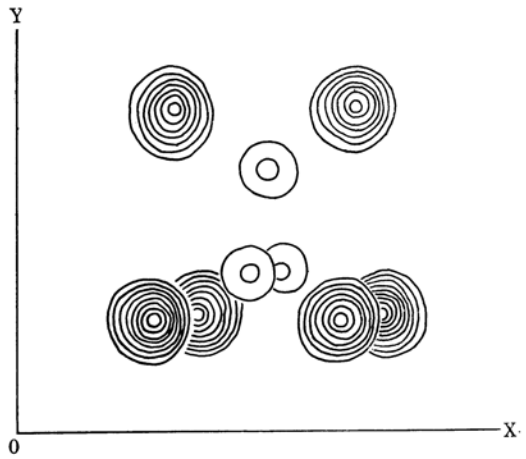

Fig. 1. Composite Fourier diagram of sections parallel to (001).

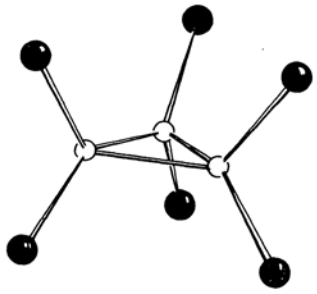

Fig. 2. The molecular configuration of hexachlorocyclopropane.

The three-dimensional Fourier synthesis is shown in Fig. 1. According to the Fourier map, the molecular configuration may be as is shown in Fig. 2.

Intermolecular contacts consist of the ordinary van der Waals distance between chlorine atoms.

The accuracy of the analysis at this stage of refinement is not sufficient to evaluate the bond lengths and bond angles. In order to obtain the details of the structure, a three-dimensional refinement of the atomic parameters is in progress by the least-squares method.

A fullpaper will be published soon.

Institute for Protein Research
Osaka University
Kita-ku, Osaka

Faculy of Science
Osaka University
Kita-ku, Osaka (S. N. & S. M.)