SHORT COMMUNICATIONS

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Note on the crystal structure of *s*-tetramesitylethane (TME).

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Attempts to obtain an accurate structure for the TME molecule, $C_{38}H_{46}$, were hampered by the occurrence of disorder in the crystals. In spite of this it could be shown that the molecule has a staggered conformation.

The carbon skeleton of *s*-tetramesitylethane (TME) is shown in Fig. 1(*a*). The aim of the structure determination was to obtain the conformation of the molecules and to check how the bond lengths and angles of the ethane group are affected by the repulsion between the bulky mesityl groups. The crystal data and intensities were measured at room temperature. At lower temperatures reversible changes take place in the crystals as could be deduced from Guinier photographs and from zero-layer line Weissenberg photographs.

Crystal data

Monoclinic, $a = 11{\cdot}832$ (2), $b = 7{\cdot}980$ (2), $c = 17{\cdot}383$ (2) Å, $\beta = 112{\cdot}14$ (1)° [from zero-level Weissenberg photographs with NaCl calibration, $\lambda(\text{Cu } K\alpha_1) = 1{\cdot}54051$, $\lambda(\text{Cu } K\alpha_2) = 1{\cdot}54433$, $a(\text{NaCl}) = 5{\cdot}640$ Å]. Space group *Pc* (from systematic absences), $Z = 2$.

The intensities of 2439 independent reflexions with $\theta < 25°$ and $I(\text{net}) > 0$ measured with Zr-filtered Mo radiation ($\lambda = 0{\cdot}7107$ Å) on a Nonius automatic three-circle single-crystal diffractometer (θ–2θ scan) were available for the structure determination. Corrections for Lorentz and polarization effects were made in the usual way. The structure was found from a Patterson synthesis and refined by block-diagonal least-squares analysis (Cruickshank, 1961). Function minimized: $\sum w[|F_o| - |F_c|]^2$ with $w = 1$. After several refinement cycles it appeared, however, that the structure shows disorder. The large values of the thermal parameters can be explained by assuming that each observed molecule is a superposition of two molecules. Fig. 1(*b*) shows a schematic projection of the two molecules (one in full and one in dashed lines) along the line $p_1 - p_2$ (or $p'_1 - p'_2$) parallel to the best plane *B* through the skeleton $p_1p_2p - qq_1q_2$ of the average structure. The mesityl groups of the two molecules are rotated such that they coincide with each other as much as possible. Owing to the disorder the bond lengths and angles of the ethane group cannot be determined sufficiently accurately to detect possible deformations. Therefore we decided to restrict the refinement to the coordinates and anisotropic thermal parameters of the composite C atoms of the average structure ($R = 0{\cdot}126$).

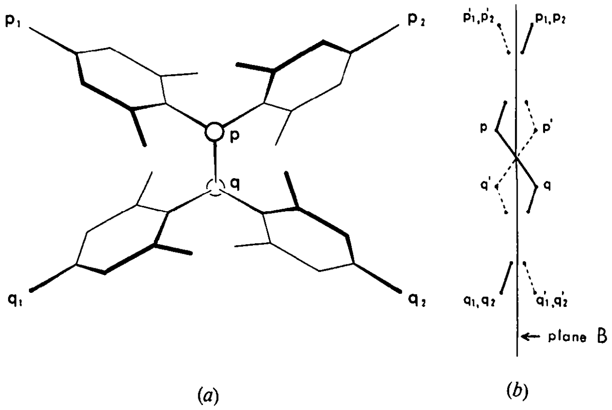

Fig. 1. Carbon skeleton of the TME molecule. (*a*) Schematic drawing of the molecule. (*b*) Schematic projection of the superimposed molecules along the best plane *B* through the skeleton $p_1p_2p - qq_1q_2$ of the average structure. Only the lines $p \ldots p_1$ *etc.* of the mesityl groups are shown.

The schematic drawing of TME given in Fig. 1(*a*) shows that the molecule has the staggered conformation. Apart from the rotation of the mesityl groups around the C(ethane)–C(mesityl) bonds the molecule has a pseudo-inversion centre. In the average structure these rotations vary from 58 to 65°. The mesityl groups are closely packed; eight distances between *ortho* methyl groups and C atoms of neighbouring six-membered rings are smaller than 3·2 Å. The conformation of the TME molecules in the solid state agrees with the conformation obtained by Lankamp (1970) from an n.m.r. study of the molecules in solution.

References

Cruickshank, D. W. J. (1961). In *Computing Methods and the Phase Problem in X-ray Crystal Analysis*. Oxford: Pergamon Press.

Lankamp, H. (1970). Thesis, Free University, Amsterdam.