Equilibrium between the aa and ee Conformations of „*Trans*"-1,2-Dichlorocyclohexane

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Electron diffraction observations [1] on "*trans*"-1,2-dibromocyclohexane indicated the presence of approximately equal amounts of the *aa* and *ee* conformations in the gaseous state. Recent dipole moment measurements on "*cis*"- and "*trans*"-1,2-dichlorocyclohexane (both vapour and solution) lead to similar results [2]. We considered the question so important that we started electron diffraction investigations on the 1,2-chlorine derivatives.

The substance designated as "*trans*" was prepared from cyclohexene and chlorine. The product was distilled in a Podbielniak column at 50 mm Hg at the constant temperature of 99° C, it had the refractive index n_D of 1.4885 at 25.5° C. The second substance was kindly placed at our disposal by Dr. Henry C. Stevens, Ohio, U.S.A. and is identical with the "*cis*" compound used for the dipole moment measurements[2].

The radial distribution curves $(\frac{\sigma(r)}{r})$ obtained are reproduced in Fig. 1 together with line diagrams giving the most important interatomic distances calculated for models corresponding to *1a2a*, *1e2e* and *1a2e* configurations. These distances were computed not for strictly tetrahedral valency angles but assuming in the *trans* compound a bending of the *a* C—Cl bonds away from the axis of the carbon ring amounting to 7° and an angle between neighbouring *e* C—Cl bonds of 73.5° (instead of 70.5°). In the case of the "*cis*" compound a corresponding bending of the *a* bond of 8° was assumed.

Curve A of Fig. 1 cannot be explained by only *one* of the line diagrams and must therefore correspond to a mixture of two configurations. As we have all reason to believe that the substance used is a pure chemical substance it must be the "*trans*" compound and consist in the vapour state of a mixture of nearly equal amounts of the *aa* and the *ee* conformations. Curve B is in good agreement with the line diagram drawn for the *ae* configuration ("*cis*" compound).

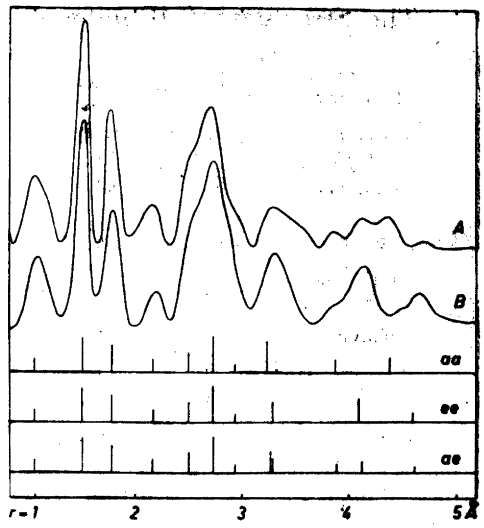

Fig. 1. Curve A: $\frac{\sigma(r)}{r}$*-curve of "trans"-1,2-dichloro cyclo hexane. Curve B:* $\frac{\sigma(r)}{r}$*-curve of "cis"-1,2-dichloro cyclo hexane.*

The results obtained for both *trans* 1,2-dihalides so far studied thus indicate very strongly the presence of nearly equal quantities of the *aa* and *ee* conformations. From an earlier electron diffraction investigation [3] on the vapour of the 1,2-dichloro-4,5-dibromocompound with possible conformations *aa-ee* and *ee-aa* the conclusion was drawn that the conformation having chlorine atoms in *a* positions predominates. These results cannot — it appears — be brought in accordance with simple considerations regarding the interaction between neighbouring not bonded atoms.

We want to express our sincere thanks to Dr. Henry C. Stevens for his kindness in placing a sample of the „*cis*" compound at our disposal.

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