

Infrared Conformational Analysis of 1,2-Dichloro-4,5-dibromocyclohexane ($a, a, e, e \rightleftharpoons e, e, a, a$)

K. LUNDE

Universitetets Kjemiske Institutt,
Blindern — Oslo, Norway

Some years ago the compound 1,2-dichloro-4,5-dibromocyclohexane ($a, a, e, e \rightleftharpoons e, e, a, a$) was prepared in this laboratory¹ in order to see which of the two possible conformations, a or b (Fig. 1), would be the preferred one. According to an X-ray investigation by Hassel and Wang Lund² the bromine atoms are in the e, e position (Fig. 1a) in the solid state. Using the electron diffraction method Bastiansen and Hassel³ demonstrated that this conformation was the only detectable also for the molecules in the vapour phase.

This latter result has now been confirmed by the present investigation, using the general assumption that no large shift in the conformational equilibrium should be expected on going from the vapour to the liquid phase. The infrared spectra of the solid compound (nujol mull) and that of the liquid (dissolved in carbon disulphide) were practically identical. Considering the very small quantities of molecular species which can be detected by infrared analysis this result seems remarkable. It indicates a much lower energy content for the free molecules of conformation a than of conformation b (Fig. 1).

to the infrared investigation in inversed conformations: The dichloro-cyclohexane has the conformation e, e and the dibromocyclohexane the conformation a, a in the solid state. It will be seen that this is just the inverted geometrical direction of the halogen atoms in the crystalline 1,2-dichloro-4,5-dibromocyclohexane. The explanation of this phenomenon may be simple: When the energy difference between two conformations of a molecule is small, the lattice packing forces may become the determining factor. Thus, the question of which conformation is present in the crystals will be the question of which conformation gives the most favourable lattice packing.

This argument can, of course, not be used when considering the molecules in their free state. It is therefore surprising to compare the conformational equilibria of the two *trans* 1,2-dihalogenocyclohexanes with the data for the 1,2,4,5-tetrahalogeno compound. In the liquid dihalogenocyclohexanes there are almost equal quantities of the two possible conformations, whereas only *one* conformation has been observed in the case of the tetrahalogeno compound. This unexpected finding cannot be accounted for by simple considerations involving steric interactions.

The author wishes to thank *Sentralinstitutt for Industriell Forskning* for cooperation in recording the spectra and *Norges almenvitenskaplige forskningsråd* for financial support.

1. Hassel, O., Wang Lund, E. and Lunde, K. *Acta Chem. Scand.* **6** (1952) 426.

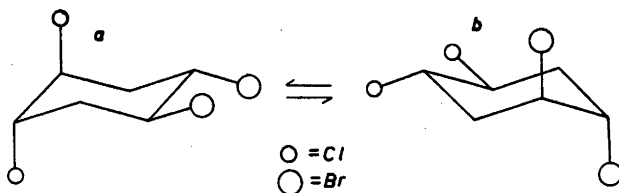


Fig. 1.

Furthermore, it is quite interesting to compare the X-ray results for the solid 1,2-dibromo-4,5-dichloro compound with a recent infrared investigation of the *trans* 1,2-dichloro- and *trans* 1,2-dibromo-cyclohexane⁴. These dihalogenocyclohexanes can be regarded as the two "halves" of the 1,2-dichloro-4,5-dibromo-cyclohexane molecule. They crystallize, however, according

2. Hassel, O. and Wang Lund, E. *Acta Chem. Scand.* **6** (1952) 238.
3. Bastiansen, O. and Hassel, O. *Acta Chem. Scand.* **5** (1951) 1404.
4. Klæboe, P., Lothe, J. and Lunde, K. *To be published shortly.*

Received April 21, 1956.