Tetrahedron Letters No. 1, pp. 3-4, 1960. Pergamon Press Ltd. Printed in Great Britain.

THE CONFORMATION OF CYCLOPENTANE

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(Received 1 December 1959)

FOR several years cyclopentane has been considered not entirely planar owing to torsional stresses between its methylene groups. Experimental investigations into the spatial structure of the molecule, although supporting the above assumption, did not lead to unequivocal conclusions.

Pitzer *et al.*[1] offered arguments and calculations of thermodynamical nature that cyclopentane exists in a number of continuously interchanging molecular forms. Le Fevre and Le Fevre,[2] on the other hand, produced geometric data of a rigid axial-symmetric model based on the measured polarizabilities of the molecule.

Their data, however, appear to be inconsistent with an equilateral pentagon structure of the molecule. I have therefore recalculated the

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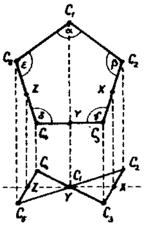
[1] J. E. Kilpatrick, K. S. Pitzer and R. Spitzer, *J. Amer. Chem. Soc.* **69**, 2483 (1947); K. S. Pitzer and W. E. Donath, *J. Amer. Chem. Soc.* **81**, 3213 (1959).

[2] C. G. Le Fevre and R. J. W. Le Fevre, *Rev. Pure and Appl. Chem.* **5**, 261 (1955); C. G. Le Fevre and R. J. W. Le Fevre, *J. Chem. Soc.* 3549 (1956).

cyclopentane model of Le Fevre and Le Fevre with the polarizability values given in their paper.



The corrected values of the C-C-C angles are: α=105.91°; β=ε=102.86°; γ=δ=99.20°. C_2, C_3, C_4 and C_5 lie alternately on both sides of the C_1XYZ plain in a distance of 0.278 Å. The Le Fevres already mention the fact in their latest paper[3] that "... the 5-ring is slightly less non-planar than previously calculated...".

Comparing the thermodynamical model with the mentioned polarizability values it seems probable that the thermodynamical model accords with the real spatial arrangement of the cyclopentane molecule. The polarizability model itself refers rather to the molecular shape distorted by the electric field, when exerted onto the molecule.

The detailed discussion of these calculations is to be published in the Acta Chim. Acad. Sci. Hung.

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[3] C. G. Le Fevre and R. J. W. Le Fevre, J. Chem. Soc. 2340 (1959).