

A TRIMETHYLAMINE STUDY BY NON-RIGID GROUP THEORY

Y. G. SMEYERS, and M. L. SENENT, *Instituto de Estructura de la Materia, C.S.I.C., Madrid, Spain;*
M. VILLA, *Depto. de Quimica, C.B.I., U.A.M.-I., Mexico D.F., Mexico.*

Trimethylamine is a perfect example of a non-rigid molecule with three equivalent internal rotating methyl groups. The three Nitrogen-Carbon axes can be taken as rotating axes around which the angles are considered as variables. The complexity of the problem arises from the multiple number of possible isoenergetic conformations (324). The non-rigid group theory is being used to divide the problem into different subgroups. The symmetry elements of the non-rigid group are proposed and classified into classes. Symmetry adapted functions are deduced on the basis of products of trigonometric functions. Energy calculations for different conformations have been performed and fitted to the totally symmetric function. The energy levels for the triple internal rotation of the molecule of the molecular non-rigid group. Finally, the infrared internal rotation spectrum of trimethylamine is presented.