TWO DIMENSIONAL TREATMENT OF THE METHYL, ALDEHYDIC TORSIONS, AND ALDEHYDIC HYDROGEN WAGGING IN GAS PHASE PROPANAL

Y. G. SMEYERS, *Instituto de Estructura de la Materia, C.S.I.C., Madrid, Spain*; V. H. UC and A. VIVIER-BUNGE, *Depto. de Quimica, C.B.I., U.A.M.-I., Mexico D.F., Mexico*.

The potential energy surfaces for the simultaneous methyl and aldehydic torsions, and for the simultaneous aldehydic carbonyl torsion and hydrogen wagging in propanal have been determined at RHF/MP2 level using the 6-311G(3df,p) basis set. The fits of the energy values to symmetry adapted functional forms were carried out in diferent ways: taking into account a large set of energy values, or dropping out the energy values which do not respect the dynamical symmetry of the methyl group. With these potentials, as well as with the kinetic parameters and electric dipole moments variations, the FIR frequencies and intensities for the methyl and aldehyde torsions, and for the aldehydic carbonyl torsion and hydrogen wagging were determined theoretically. It is found that the two dimensional calculations for the *cis* conformer satisfactorily reproduce not only the methyl torsion and aldehyde torsional spectrum, but furnishes also methyl torsionally excited progessions for the aldehyde modes. Most of these transitions occur in the region of 220-100 cm^{-1} and are responsible for the complexity of the spectrum. From these theoretical results a new assignment is provided.