AN INTERNAL ROTATION PROGRAM FOR MOLECULES WITH C_1 POINT GROUP SYMMETRY

I. KLEINER, *Laboratoire de Photophysique Moléculaire, Université Paris Sud, 91405 Orsay Cedex, France.*; J. T. HOUGEN, R. D. SUENRAM, D. F. PLUSQUELLIC, A. R. HIGHT WALKER, F. J. LOVAS, G. T. FRASER, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD. 20899, USA.*; J. ORTIGOSO, *Instituto de Estructura de la Materia, CSIC, Serrano 119, Madrid, Spain*.

A number of studies recently undertaken at NIST which are aimed at comparing high resolution spectroscopic data with state-of-the art quantum chemistry calculations for small peptide mimetics has led us to write a program that can deal with internal rotor molecules belonging to the C_1 symmetry group. The first molecule of this type to which we are applying the program is ethyl acetamidoacetate, CH_3-CH_2-O-C(=O)-CH_2-NH-C(=O)-CH_3 for which preliminary results were reported at this meeting in 1999 (MH13). About 200 lines in the range of 10-20 GHz have now been measured at NIST using the FTMW spectroscopy. The observed transitions have been assigned to two different conformers which both exhibit A and E states due to the facile internal rotation of the methyl top attached to the carbonyl carbon. The experiments and the ab initio studies indicate that the lowest energy conformer (I) has a plane of symmetry in its equilibrium structure and that only one of the methyl rotors has a barrier low enough to display internal rotation splittings at a resolution of 4 kHz. Using the internal rotation RAM program which has has now applied to a number of internal rotors with a plane of symmetry, we have obtained an excellent fit for the lowest energy conformer. The higher energy conformer (II) does not possess a plane of symmetry and the lost of C_s symmetry requires the introduction of Hamiltonian matrix elements which are complex. Therefore to complete the assignments and the analysis of the FTMW data a new program has been written. Theoretical aspects of this program and preliminary results will be presented.