ASSIGNMENT OF THE SUB-MILLIMETER WAVE SPECTRUM OF METHYL CARBAMATE, NH_2COOCH_3, IN THE FIRST EXCITED STATE OF THE METHYL GROUP INTERNAL ROTATION

P. GRONER, *Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110-2499.*

The rotational spectrum of methyl carbamate in the first excited torsional state (up to 149 GHz) has been analyzed recently for rotational quantum number J up to 20 together with transitions in the ground state [a]. An extended analysis of the rotational spectrum in the ground state between 10 and 371 GHz with over 6000 transitions with J up to 60 has also been published [b]. In the spectra recorded at that time by the FASSST method, about 3000 transitions belonging to the first torsional excited state of the methyl group have now been assigned and analyzed, about half of them belonging to the E torsional species. Both the newly assigned and previously published transitions have been used to fit less than 45 spectroscopic parameters of an effective rotational Hamiltonian for such systems [c], achieving a dimensionless standard deviation of 1.33. A somewhat unexpected result was the value of the ρ parameter of 0.063628(20) which differed significantly from the value obtained for the ground state of 0.058791(15). The discrepancy will be investigated in the near future. Hopefully, a resolution of the problem can be achieved by a combined fit of all excited and ground state transitions using common ρ and β parameters with β as the angle between the ρ-axis and the a principal axis.

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[b] P. Groner, M. Winnewisser, I. R. Medvedev, F. C. De Lucia, E. Herbst, K. V. L. N. Sastry, Astrophys. J. Suppl. Ser. 169, 28 (2007).
[c] P. Groner, J. Chem. Phys. 107, 4483 (1997).