REVEALING THE EQUILIBRIUM STRUCTURE OF METHACRYLAMIDE BY MICROWAVE SPECTROSCOPY: INTERPLAY OF THEORY AND EXPERIMENT

K. G. LENGSFELD, S. HERBERS, J. WANG, J.-U. GRABOW, Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, Hannover 30167, Germany

Methacrylamide is an important starting material for the production of various polymer resins. In contrast to the polymer, the structures and properties of the monomer are hardly known. In particular, there is little data on the structure of methacrylamide in the gas phase. In this study, the two conformers, s-cis and s-trans, were studied to determine their structures. For the s-cis conformer, the structure could be determined with accuracy below one picometer. In the s-trans conformer, the coupling of the methyl group internal rotation, in combination with the coupling of a vibration that interconverts two equivalent structures, causes problems. High-resolution investigations are necessary to address this challenge. The figure on the left shows the optimized geometry of the s-trans conformer and on the right its $J_{K''''K''''}^{''} - J_{K''''K''''}^{''} = 1_{11} - 0_{00}$ transition.