MICROWAVE SPECTRA AND AB INITIO STUDIES OF THE NE-ACETONE COMPLEX

JIAO GAO, JAVIX THOMAS, YUNJIE XU, WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

Microwave spectra of the neon-acetone van der Waals complex were measured using a cavity-based molecular beam Fourier-transform microwave spectrometer in the region from 5 to 18 GHz. Both ^{20}Ne and ^{22}Ne containing isotopologues were studied and both *c*- and weaker *a*-type rotational transitions were observed. The transitions are split into multiplets due to the internal rotation of two methyl groups in acetone. Electronic structure calculations were done at the MP2 level of theory with the 6-311++g (2d, p) basis set for all atoms and the internal rotation barrier height of the methyl groups was determined to be about 2.8 kJ/mol. The *ab initio* rotational constants were the basis for our spectroscopic searches, but the multiplet structures and floppiness of the complex made the quantum number assignment very difficult. The assignment was finally achieved with the aid of constructing closed frequency loops and predicting internal rotation splittings using the XIAM code.[a] Analyses of the spectra yielded rotational and centrifugal distortion constants, as well as internal rotation parameters, which were interpreted in terms of structure and internal dynamics of the complex.

[a] H. Hartwig and H. Dreizler, Z. Naturforsch. A **51**, 923 (1996).