INFLUENCE OF MICROSOLVATION BY RARE GAS ATOMS ON THE V_3 BARRIER TO INTERNAL ROTATION IN ACETALDEHYDE: A FREE JET MICROWAVE STUDY

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The rotational spectra of the acetaldehyde-argon and acetaldehyde-kripton van der Waals complexes have been measured by free jet absorption millimeter-wave spectroscopy in the frequency range 60-78 GHz. For acetaldehyde-argon this is an extension to higher frequencies of the already assigned rotational spectrum[a]. For both complexes each rotational transition is split into four hyperfine component lines, which is evidence of the occurring of two different internal motions. The splittings have been interpreted in terms of a coupled Hamiltonian that precisely determines the separation of energy levels due to the tunneling of the rare gas atom between two equivalent minima, while the information on the barrier to internal rotation of the methyl group is obtained from the pattern of the component lines due to this motion. The interaction of the rare gas atom with the acetaldehyde moiety is reflected in the change of the V_3 barrier to internal rotation in going from the molecule to the weakly bound complex. The insertion of the rare gas atom causes a lowering of the barrier by destabilization of the minimum of the V_3 potential well caused by steric hindrance.

[a] I. I. Ioannou and R. L. Kuczkowski *J. Mol. Spectrosc.* **166**, 354, 1994.