HOW SOLVENTS CHANGE THE CONFORMATIONAL LANDSCAPE IN MOLECULES WITH WEAK INTRAMOLECULAR INTERACTIONS: METHYL 2-METHOXYBENZOATE

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The conformational behavior of methyl 2-methoxybenzoate has been explored using rotational spectroscopy. The two conformers identified show for each rotational transition a quadruplet attributable to two sets of splittings due to two tunneling motions, the internal rotation of the ester methyl group and the internal rotation of the entire ester group with respect to the benzene ring, which in addition interconverts both observed conformers. The analysis of such splittings allowed the determination of the potential energy barriers for the tunneling vibrations. The spectra of the complexes of methyl 2-methoxybenzoate with water and formic acid have also been analyzed. In both cases, only the global minimum structure could be identified in the spectra. In contrast with the observations in many other systems, the conformational landscape of the monomer is altered upon complexation. In the complexes the relative stability of the conformers observed in the monomer turn out to be inverted. Ester group torsion and methyl group internal rotation splittings were observed in the monohydrated complex, but not in the complex with formic acid.