THE PHENYL TORSION VIBRATION IN FLAVONES IS ONE OF THE KEY FACTORS DETERMINING THEIR CONFORMATIONAL BEHAVIOR: THE EXAMPLES OF FLAVONE AND LUTEOLIN

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The structure and phenyl group internal rotation vibration of the scaffold molecule flavone, its complex with water, and its derivative luteolin have been investigated by laser ablation chirped pulse Fourier transform microwave spectroscopy (LA-CP-FTMW). The investigation of the tunneling splittings detected in the spectrum has allowed the determination of the periodic potential function of the phenyl torsion vibration of flavone. The interaction with water may alter substantially this potential function depending on the site of flavone where interaction takes place. This behavior explains the flexibility and the variety of equilibrium structures found for this molecule in condensed phases.[a,b,c] The shape of the phenyl torsion potential energy function also governs the behavior of luteolin, a flavone derivative with four OH group substituents.

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