

THE ROTATIONAL SPECTRA OF FLAVONE AND FLAVANONE: LASER ABLATION AND HEATING METHODS FOR VAPORIZATION.

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Flavonoids constitute a family of natural compounds found in a large number of fruits and vegetables being responsible for many of their vivid colours. Flavonoids are the largest group of phytonutrients, with more than 6,000 types. Flavone (2-Phenylchromone) and flavanone (2,3-Dihydroflavone) define the basic units for whole families of these compounds, anthoxantines and flavanones respectively. Due to their biological activity, their structure–activity relationships are of interest also for medicine and biochemistry. In this work, we present the first study of the microwave spectra of both flavone and flavanone. The spectra of these two molecules have been observed using a CP-FTMW spectrometer with two vaporization methods: conventional heating and a laser ablation (LA) system recently implemented. A conformational search was done for each compound using DFT, corrected with empirical dispersion terms, and MP2 methods. We have observed only one conformer of each system and their monohydrated complexes. Flavanone is a case where DFT and MP2 methods diverge in predicting the global minimum being the experimental data in agreement with the DFT predictions.