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Infrared spectroscopy of flavones and flavonols. Reexamination of the hydroxyl and carbonyl vibrations in relation to the interactions of flavonoids with membrane lipids

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Abstract

Detailed vibrational assignments for twelve flavonoids (seven flavones (flavone, 3- and 5-hydroxyflavone, chrysin, apigenin, fisetin and luteolin) and five flavonols (galangin, kaempferol, quercetin, morin and myricetin)) have been made based on own and reported experimental data and calculations at the B3LYP/6-31+G(d,p) level of theory. All the molecules are treated in a uniform way by using the same set of redundancy-free set of internal coordinates. A generalized harmonic mode mixing is used to corroborate the vibrational characteristics of this important class of molecules. Each flavonoid molecule can be treated from the vibrational point of view as made of relatively weakly coupled chromone and phenyl part. It has been shown that the strongest band around 1600 cm⁻¹ need not be attributable to the C=O stretching. The way the vibrations of any of the hydroxyl groups are mixed with ring vibrations and vibrations of other neighboring hydroxyl groups is rather involved. This imposes severe limitations on any attempt to describe normal modes of a flavonol in terms of hydroxyl or carbonyl group vibrations. The role of water molecules in the appearance of flavonoid IR spectra is emphasized. Knowing for the great affinity of phosphate groups in lipids towards water, the immediate consequence is a reasonable assumption that flavonoid lipid interactions is mediated by water.

Keywords flavone, flavonol, vibrational assignment, infrared spectrum, Raman spectrum, B3LYP/6-31+G(d, p) level of theory.

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