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Characterisation of the PT-form of *o*-hydroxy acylaromatic Schiff bases by NMR spectroscopy and DFT calculations.

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Streszczenie

A series of *o*-hydroxy Schiff bases showing tautomerism to a varying degree are investigated together with compounds totally at the proton transfer form (enamines). Deuterium isotope effects on ^{13}C chemical shifts are measured at different temperatures. Structural features determining the equilibrium constants are discussed. DFT calculations are done in order to obtain structures. Schiff bases derived from dehydracetic acid (3-acetyl-6-methyl-pyran-2,4-dione) as well as from 1,3,5-triacetyl-2,4,6-trihydroxybenzene are found to be fully at the PT-form. These forms are characterised and the use of these compounds as reference for the PT-form in general is discussed.

Słowa kluczowe

Schiff bases, Theoretical DFT calculations, Deuterium isotope effects on chemical shifts, o-Hydroxy acylaromatics

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