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Nonempirical calculations of the effect of molecular fragments on proton chemical shifts in heterocycles

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Abstract

We have calculated the relative changes in the proton chemical shifts for a number of six-membered heterocycles (1,3-dioxan, 1,3-oxazine, 1,3-dithiane, trimethylene sulfite, and also their derivatives). A procedure is proposed for estimating the chemical shifts due to the effect of model molecular fragments. In calculating the chemical shifts expected allowance is made for the way in which the given molecule differs in structure from a similar molecule for which the chemical shift is known. The chemical shifts were calculated in the approximation of gradient-invariant atomic orbitals in a Gaussian basis. The calculations reproduce correctly the effect of alkyl substituents and the trends in the chemical shifts as a function of the orientation of the substituents and of the heterocyclic component of the molecule.

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