Experimental and theoretical NMR study of selected oxocarboxylic acid oximes.

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Streszczenie

^{1}H and ^{13}C NMR spectra of the oxocarboxylic acid oximes 2-hydroxyiminopropanoic acid (**1**), 2-(4-methylthiazol-2-yl)-2-(hydroxyimino)acetic acid (**2**) and 2-cyano-2-(hydroxyimino)acetic acid (**3**) were measured in DMSO-d_6, D_2O and acetone-d_6 solutions. The data indicate the presence of hydrogen bonding in **1** and **2** and a strong electron-withdrawing effect due to the cyano group in **3**. The effect of intra- and intermolecular hydrogen bonding on the hydrogen and carbon chemical shifts in these molecules was studied theoretically. Total energy calculations of the stability of various hydrogen-bonded species, in addition to equilibrium parameters and chemical shifts, were calculated using *ab initio* methods (RHF, MP2) and density functional theory (B3LYP), implemented in the Gaussian 98 software package. The gauge-including atomic orbital (GIAO) method was used to predict magnetic shielding constants. Chemical shift calculations for the most stable species agree fairly well with the observed data, especially for the hydroxyl protons. Substituents adjacent to the α-carbon show some influence of the oximic and carboxyl groups on the ^{13}C chemical shifts, as expected for groups with different polar and anisotropic character.

Adres publiczny

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