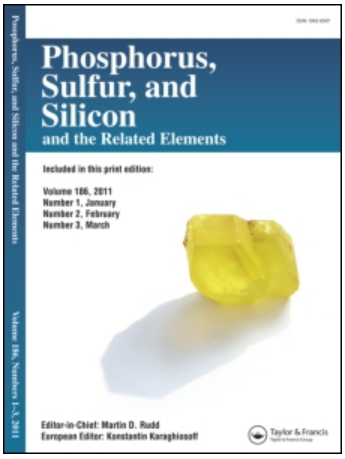

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Substituent Effects on the ^{31}P NMR Chemical Shifts of 1-Amino- and 1-Hydroxy-Alktlphosphonic Acids

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SUBSTITUENT EFFECTS ON THE ^{31}P NMR CHEMICAL SHIFTS OF 1-AMINO- AND 1-HYDROXY-ALKYLPHOSPHONIC ACIDS

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^{31}P NMR chemical shifts are reported for 14 1-amino- and 10 1-hydroxy-alkylphosphonic acids. To derive an exact value of substituent interaction effects the ^{31}P NMR data of some related free phosphonic acids are also reported.

In our latest papers we studied the substituent-induced chemical shifts (α-SCSs) of phosphonate group on ^{13}C NMR in the groups of aminoalkylphosphonic (1) and 1-hydroxyalkylphosphonic acids (2). The varies of the phosphonate α-SCS parameters dependent on the skeleton structure were interpreted in terms of 2p-electrons participation in the valence orbitals of the respective α-carbon. The observed non-additivity of SCS parameters was attributed to intramolecular interaction between the central atoms.

In this poster substituent effects on the ^{31}P NMR chemical shifts are investigated. The correlation between α-SCSs of phosphonate group from ^{13}C NMR spectra calculated in relation to their parent mono-substituted compounds and the ^{31}P chemical shift of the phosphorous concerned will be systematically studied and discussed.

(1) Z.Głowacki and M.Topolski, submitted to Magn.Reson.Chem.
(2) Z.Głowacki and M.Hoffmann, in preparation