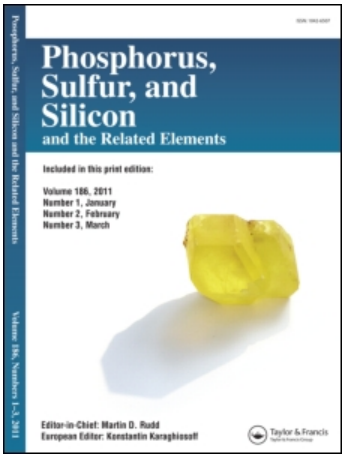

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^{31}P Sold-State NMR Investigations on Phosphonic Acids and Phosphonates

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^{31}P SOLID-STATE NMR INVESTIGATIONS ON PHOSPHONIC ACIDS AND PHOSPHONATES

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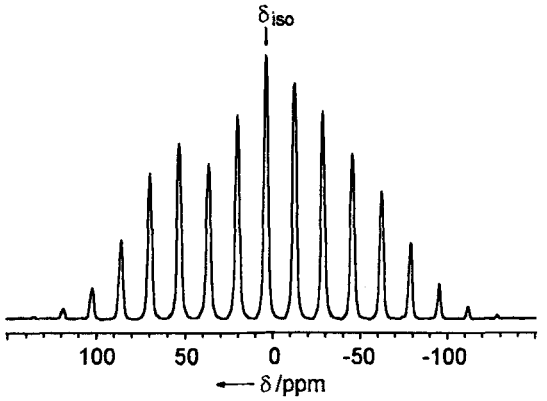
As known from ^{31}P solid-state NMR investigations of inorganic phosphates there is a correlation between chemical shift anisotropy parameters and crystal lattice parameters. For phosphonic acids and phosphonates similar correlations are not known.

The solid-state NMR spectra of various C_6 phosphonic acids $RP(O)(OH)_2$ (R = hexyl, cyclohexyl, 1-hydroxy-cyclohexyl, cyclohex-1-enyl and phenyl) reflect the different geometric and electronic situation at the α-C atom. The principal component at lowest frequency δ_{33} shows the largest changes.



For the two series of acylphosphonates R–C(O)–P(O)(OR')(OX) and hydroxyiminophosphonates R–C(=N–OH)–P(O)(OR')(OX) no correlation between anisotropy parameters and substituent R has been observed. Only variations of the phosphonate group (acid, salt, ester) lead to significant changes.

FIGURE 1 ^{31}P CP/MAS spectrum of Ph-C(O)-P(O)(OH)(ONa)

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