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## Phosphorus, Sulfur, and Silicon and the Related Elements

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### <sup>31</sup>P High Resolution Solid State NMR Spectroscopy as a Tool for Structural Studies of Organothiophosphoryl Compounds

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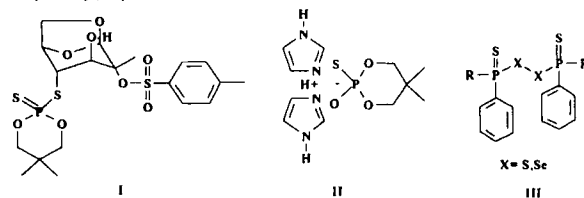
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## <sup>31</sup>P High Resolution Solid State NMR Spectroscopy as a Tool for Structural Studies of Organothiophosphoryl Compounds

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Employing 1,6-anhydro-2-O-(tosyl)-4-S-(5,5-dimethyl-2-tioxa-1,3,2-dioxaphosphorinan-2-yl) β-D-glucopyranose I, bis-imidazole 5,5-dimethyl-1,3,2-dioxaphosphorinan-2-tioxa-2-hydroxy complex II and bis (organothiophosphoryl) dichalcogenides III as models this report presents power of <sup>13</sup>C and <sup>31</sup>P CP/MAS experiment in structural studies organothiophosphoryl compounds [1,2,3].



From our studies it is concluded that analysis of <sup>13</sup>C and <sup>31</sup>P principal elements of chemical shift tensors  $\delta_{ii}$  and shielding parameters ( $\Delta\delta$ ,  $\Omega$ ,  $\eta$  and  $\kappa$ ) can be a source of important information about the nature of "weak" and "strong" hydrogen bonding. A search of the Cambridge Structural Database (CSD) reveals that C-H...S intermolecular contacts are not unusual for thiophosphoryl compounds. We have found more examples of the C-H...S=P contacts than for the analogous C-H...O=P interactions. Formation of C-H...S contacts can be explained in term of hard and soft hydrogen bonds. The S=P as a softer acceptor compared to O=P unit prefers to hydrogen bond with the soft donor C-H. Such explanation is consistent with ideas of Carroll and Bader [4] and the recent results of Braga et al. [5] who surveyed the hydrogen bonding in organometallic crystals. The detailed analysis of the <sup>31</sup>P  $\delta_{ii}$  principal elements of the chemical shift tensor suggests that distinction in values of  $\delta_{33}$  parameters is due to C-H...S=P interactions.

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