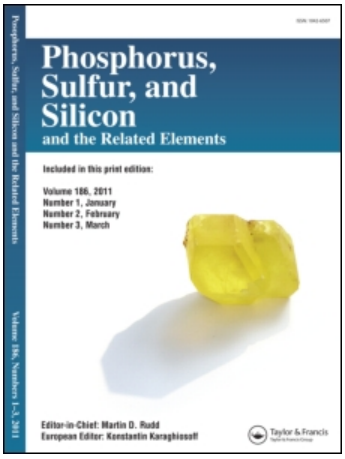


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# $^{31}$P High Resolution Solid State NMR Spectroscopy as a Tool for Structural Studies of Organothiophosporyl Compounds

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**To cite this Article** Potrzebowski, Marek J.(1999) '$^{31}$P High Resolution Solid State NMR Spectroscopy as a Tool for Structural Studies of Organothiophosporyl Compounds', Phosphorus, Sulfur, and Silicon and the Related Elements, 147: 1, 339
**To link to this Article: DOI:** 10.1080/10426509908053649
**URL:** http://dx.doi.org/10.1080/10426509908053649

*Phosphorus, Sulfur and Silicon*, 1999, Vol. 147, pp. 339-339
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# $^{31}$P High Resolution Solid State NMR Spectroscopy as a Tool for Structural Studies of Organothiophosporyl Compounds

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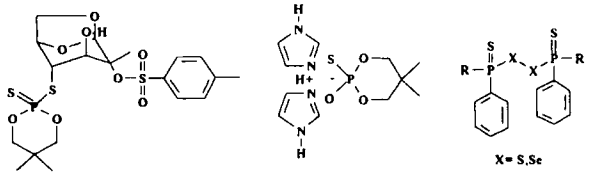
Employing 1,6-anhydro-2-O-(tosyl)-4-S-(5,5-dimethyl-2-tioxa-1,3,2-dioxaphosphorinan-2-yl) β-D-glucopyranose **I**, bis-imidazole 5,5-dimethyl-1,3,2-dioxaphosphorinan-2-tioxa-2-hydroxy complex **II** and bis (organothiophosphoryl) dichalcogenides **III** as models this report presents power of $^{13}$C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



**I** **II** **III**

X= S,Se

From our studies it is concluded that analysis of $^{13}$C and $^{31}$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 Carrol 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 $^{31}$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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