

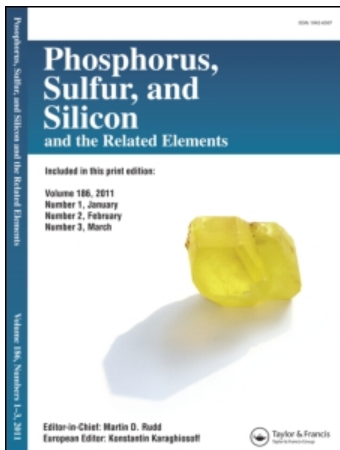
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## Phosphorus, Sulfur, and Silicon and the Related Elements

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### Structure of Low-Coordinated Phosphorus (III) Compounds Including Phosphorus-Nitrogen Multiple Bond: $^{13}\text{C}$ , $^{15}\text{N}$ and $^{31}\text{P}$ NMR Investigation

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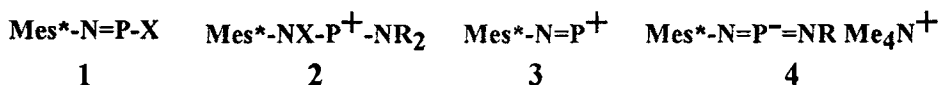
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STRUCTURE OF LOW-COORDINATED PHOSPHORUS (III) COMPOUNDS  
INCLUDING PHOSPHORUS-NITROGEN MULTIPLE BOND:  
 $^{13}\text{C}$ ,  $^{15}\text{N}$  AND  $^{31}\text{P}$  NMR INVESTIGATION

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A wide series of low-coordinated phosphorus (III) compounds including iminophosphines **1**, two- **2** or mono-coordinated **3** phosphorus-containing cations, and anion **4**, where Mes\* = 2,4,6-tris-(*tert*-butyl)phenyl, has been investigated by  $^{13}\text{C}$ ,  $^{15}\text{N}$  and  $^{31}\text{P}$  NMR spectroscopy. The spectral parameters obtained are considered in connection with the *ab initio* (6-31G\*) calculation data of the model compounds.



**1** X= Alk, Ar, NR<sub>2</sub>, OR, SR, PR<sub>2</sub>, Hal; **2** X= H, AlCl<sub>3</sub><sup>-</sup>, GaCl<sub>3</sub><sup>-</sup>

In spite of the absence of the conjugation between the P=N and Mes\*  $\pi$ -systems, essential  $^{13}\text{C}$  shielding variation is found for all carbon-13 nuclei in Mes\* moiety within the series **1-4**. The  $\pi$ -inductive nature of the  $^{13}\text{C}$  shielding variation in the aromatic moiety is suggested. The found peculiarity of the Mes\* substituent to be polarized by electronegative substituents seems to be an additional factor promoting the total stability of low-coordinated phosphorus (III) compounds involving the Mes\* moiety. The  $^{13}\text{C}$  NMR data analysis makes it possible to determine the isomers configuration for compounds **1,2**.

The  $^{15}\text{N}$  and  $^{31}\text{P}$  NMR chemical shifts of corresponding nuclei in Mes\*-N=P-X moiety, as well as phosphorus-nitrogen coupling constants, are shown to be sensitive both to the hybridization type of the P and N atoms and to inductive and resonance properties of the X substituent. The largest deshielding of  $^{15}\text{N}$  nuclei ( $\delta\text{N} = +163.6$  ppm) is found for anion **4**. The P=N bonds have the double character in this compound but they are highly polarized to N atoms.

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