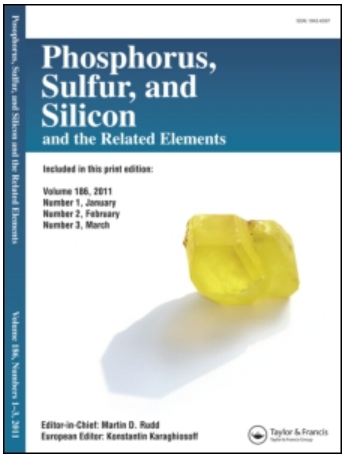

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

Multinuclear NMR Studies of the Substitlent Effects in N-Phenyl-P,P,P-Triarylphospha-λ⁵-Azenes, Triaryl-Phosphines and Triarylphosphine Oxides

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To cite this Article Pomerantz, Martin and Chou, Whe-Narn(1990) 'Multinuclear NMR Studies of the Substitlent Effects in N-Phenyl-P,P,P-Triarylphospha-λ⁵-Azenes, Triaryl-Phosphines and Triarylphosphine Oxides', Phosphorus, Sulfur, and Silicon and the Related Elements, 51: 1, 241
To link to this Article: DOI: 10.1080/10426509008040775
URL: http://dx.doi.org/10.1080/10426509008040775

Phosphorus, Sulfur, and Silicon, 1990, Vols. 51/52, p. 241
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MULTINUCLEAR NMR STUDIES OF THE SUBSTITUENT EFFECTS IN N-PHENYL-P,P,P-TRIARYLPHOSPHA-λ^5-AZENES, TRIARYLPHOSPHINES AND TRIARYLPHOSPHINE OXIDES

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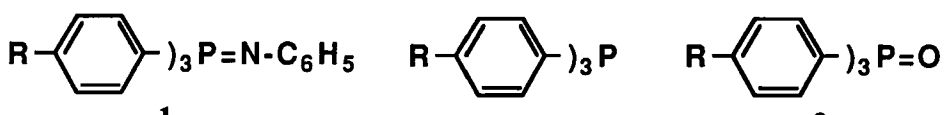
A series of *N*-phenyl-*P,P,P*-triarylphospha-λ^5-azenes (**1**) as well as their ^{15}N labeled analogs was synthesized. The ^{13}C, ^{31}P, and ^{15}N NMR spectra of this series and those of two other series of related compounds, namely triarylphosphines (**2**) and triarylphosphine oxides (**3**), were measured and are reported. Many satisfactory correlations using the mono-substituent parameter (MSP) and the Taft dual-substituent parameter (DSP) treatments with the ^{13}C substituent chemical shifts (SCS), ^{31}P SCS, ^{15}N SCS and the one bond P–N, P–C and C–N coupling constants were observed and will be discussed. Thus, for example, the ^{31}P and ^{15}N chemical shifts in **1** correlated with σ^- with negative slopes while the ^{31}P chemical shifts in **3** correlated with those in **1** with a slope of 2.0. The ^{13}C chemical shifts in **1** correlated excellently with the corresponding ones in **3** with slopes very close to unity. The substituent effects on the chemical shifts of the various nuclei were shown to be mainly due to changes in the charge distribution on those nuclei. In **1** the one bond P–N and P–C coupling constants correlated with σ_p and σ_R respectively. The one bond P–C coupling constants of **1** correlated quite well with those of **3** with a slope of 0.93 while the corresponding correlation of **1** with **2** was quite poor. Taft DSP treatment of $^1J_{PC}$ in **1** and **3** were quite similar, ρ_I and ρ_R were both negative and ρ_R was much larger than ρ_I. Series **2** showed behavior which was different from that shown by **1** and **3** but similar to that shown by other systems with a lone electron pair on the atom bound to the phenyl ring. The substituent effects on the one bond P–N, P–C and C–N coupling constants will be discussed in terms of bonding and hybridization changes between the directly bonded nuclei.



1 **2** **3**