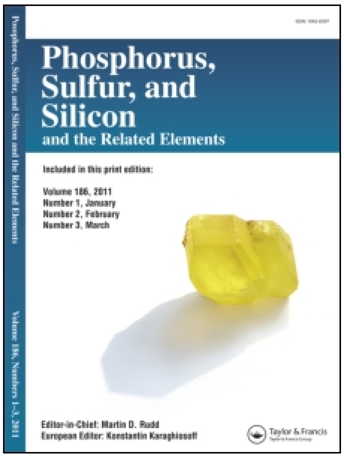

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The Correlation of Structure Features and Valent Phosphorus State with NMR Parameters of Some Five-Membered Heterocycles

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THE CORRELATION OF STRUCTURE FEATURES AND VALENT PHOSPHORUS STATE WITH NMR PARAMETERS OF SOME FIVE-MEMBERED HETEROCYCLES

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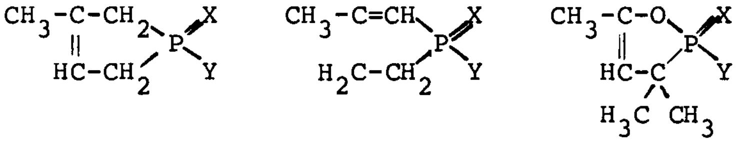
NMR parameters of the phosphorus-containing molecules are known to be affected by the phosphorus coordination number. Very little has been published about the theory proper and about the correlation characteristics of this influence. In order to obtain some information about this problem we have synthesized a number of phospholene and oxaphospholene derivatives containing phosphorus in various valent states.



X = lone-pair, =S, =O, $-O-C(CH_3)=C(CH_3)-O-$
Y = Cl, CH_3, OCH_3, $N(CH_3)_2$

All these compounds have been investigated by means of ^1H, ^{13}C and ^{31}P NMR spectroscopy. A great influence of the increase of the valent phosphorus state on the NMR parameters of rigid five-membered heterocycles has been observed. It has been determined that the pronounced changeable parameters are the chemical shifts of ^{31}P and coupling constants of C-P and P-H. Thus the growth of the phosphorus coordination number provokes the upfield chemical shift of phosphorus, the increase of magnitudes of coupling constants $^1J_{C-P}$ and ethylenic $^3J_{H-P}$, but diminishes ethylenic $^2J_{H-P}$.