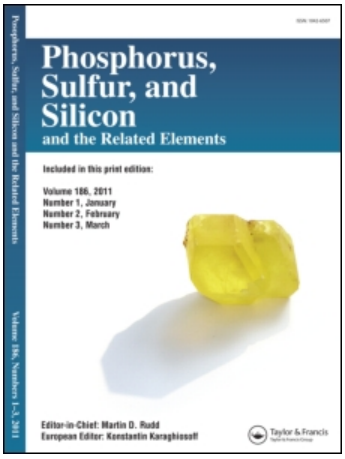

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NMR Spectra and Structure of Phosphorus-Containing Cycles with Acyclic P=Se and Cyclic P-C Bonds

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NMR SPECTRA AND STRUCTURE OF PHOSPHORUS-CONTAINING CYCLES WITH ACYCLIC P=Se AND CYCLIC P-C BONDS

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Using ^{1}H, ^{13}C, ^{31}P, ^{77}Se NMR it has been established that six-membered rings of 5-seleno-5-phenyl-2,2-dimethyl-1,3,5--dioxaphosphorinanes, 5-seleno-1,3,5-diazaphosphorinanes and 5-seleno-5-phenyl(alkyl)-2,2-dimethyl-1,3,2,5-dioxasilaphosphorinanes in the solution are in chair conformation with the equatorial P=Se group, whereas the eight-membered ring of 6-seleno-2,2,6-trimethyl-1,3,2,6-dioxasilaphosphocane is mainly in the chair-chair conformation with the symmetry plane passing through the silicon atom and the axially oriented P=Se group. The selenium nuclear chemical shifts $\delta 77_{Se}$ -266--416 ppm in these compounds depend on the size of the cycle, and on the effect of the substituent of the cycle. The phosphorus nuclear chemical shifts $\delta 31_{P}$ 0-50 ppm depend on the phosphorus valence angle at the cycle and the electron infulence of the closest phosphorus substituents. For the stereoisomer pairs of the six-membered cycles the ^{31}P nuclei in the isomer with the equatorial P=Se group have been shown to be magnetically screened to a greater degree. The spin-spin coupling of the directly bonded nuclei $^{1}J_{PSe}$ -708--752, $^{1}J_{PC}$ 45-48, $^{1}J_{CH}$ 128-152 Hz depends both on the size of the cycle and the character of substituents in it. The values of $^{1}J_{PSe}$ are affected by the position of substituents in the bicycles. The overall values of $^{1}J_{PSe}$ are greater for the axial orientation of the P=Se group than for the equatorial.