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## 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>

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

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**To cite this Article** Il'yasov, A. V. and Zyablikova, T. A.(1990) 'NMR Spectra and Structure of Phosphorus-Containing Cycles with Acyclic P=Se and Cyclic P-C Bonds', *Phosphorus, Sulfur, and Silicon and the Related Elements*, 51: 1, 232

**To link to this Article:** DOI: 10.1080/10426509008040766

**URL:** <http://dx.doi.org/10.1080/10426509008040766>

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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  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$ ,  $^{77}\text{Se}$  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  $\delta^{77}\text{Se}$  -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  $\delta^{31}\text{P}$  0-50 ppm depend on the phosphorus valence angle at the cycle and the electron influence of the closest phosphorus substituents. For the stereoisomer pairs of the six-membered cycles the  $^{31}\text{P}$  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  $^1J_{\text{PSe}}$  -708--752,  $^1J_{\text{PC}}$  45-48,  $^1J_{\text{CH}}$  128-152 Hz depends both on the size of the cycle and the character of substituents in it. The values of  $^1J_{\text{PSe}}$  are affected by the position of substituents in the bicycles. The overall values of  $^1J_{\text{PSe}}$  are greater for the axial orientation of the P=Se group than for the equatorial.