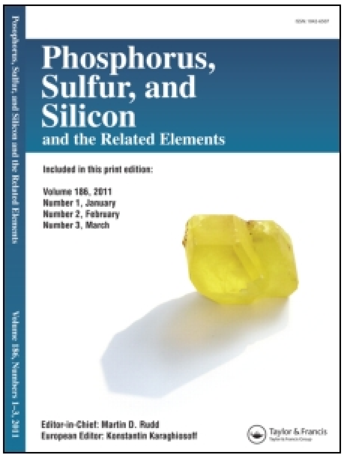

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Vibrational Spectra of Cyclic Organophosphorus Compounds and Their Conformations in the Liquid and Solid States

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VIBRATIONAL SPECTRA OF CYCLIC ORGANOPHOSPHORUS COMPOUNDS AND THEIR CONFORMATIONS IN THE LIQUID AND SOLID STATES

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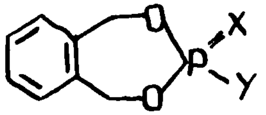
The Raman and IR spectra of 5,6-benzo-1,3,2-dioxaphosphepines



X= lone pair, O, S, Se
Y= NR_2, Ph, OPh, OMe

have been studied in the solid and liquid states, in solutions of different polarity, the temperature and concentration being varied. The assignments of the spectra have been made. The main spectral features that depend on molecular conformations are the intense highly polarized lines of the symmetric vibrations ("breathing") of the seven-membered ring in the 700-800 cm^{-1} region, $\nu_{P=X}$ (X=S, Se) at 530-650 cm^{-1}, the vibrations of o-xyllilenic fragment in the regions of 1050-1070 cm^{-1} ($\delta_{C{\cdots}C-C}$) and 1200-1220 cm^{-1} ($\nu_{C{\cdots}C-C}$). The $\delta_{C{\cdots}C-C}$ and $\nu_{C{\cdots}C-C}$ vibrations appeared to be a reliable conformational test for the identification of the chair and twist forms, the frequencies being equal to ~1050 and ~1220 cm^{-1} in the first case and ~1070 and ~1200 cm^{-1} in the second. As for the equilibrium of the chair-like forms the frequencies of the axial P=X bonds are always lower than the equatorial. For most of the compounds the complex three and even four-component equilibrium of the chair-like and flexible (twist) forms have been found in liquids and solutions. In the crystal phase only the chair form is stable, the P=X bond orientation being dependent on the substituents at phosphorus.