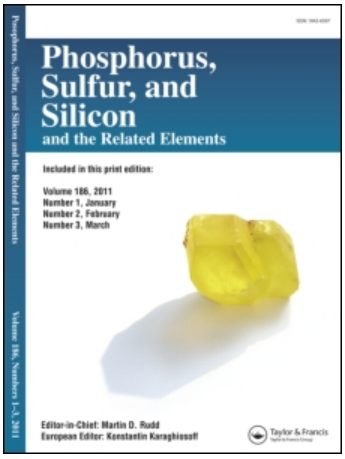

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Nature of Electron Donor Centers of Phosphoalkenes in H-Bond Complexes

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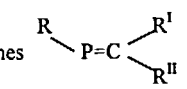
Keywords: Phosphoalkene; phosphorus; electron-donor; protonation; H-bond

Phosphoalkenes  (1), (R, R^I, and R^{II} = H, Hal, Nalk$_2$) show alternative nucleophilic properties towards HX acids or transition metal salts, and depending upon reagent characteristics form addition products through one of P=C double bond atoms. Coordination of a ligand to a cation by its π-electron donor is also observed due to quazidegeneration of higher occupied molecular orbital.

With this in view, it seemed interesting to study proton-acceptor properties of some phosphoalkenes in relation to soft electrophiles – proton donors in H-bond complexes, as well as to reveal the nature of reaction centers. Structures of some molecules in their complexes with a standard proton donor (deuterochloroform) were studied both spectroscopically and quantum chemically. It was found that H-bond formation is more favorable through phosphorus atom with its lone pair orbital in contrast to alternative protonation processes and coordination compounds formation. The electrostatic stabilization of the complex grows with the increase of the excess electron density on the heteroatom. Δν(CD) values of a low frequency shift of the chloroform characterize a relative change of the phosphorus basicity and appear to be proportional to H-bond complex strength. The interdependence of electron and steric effects in the system is discussed.

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