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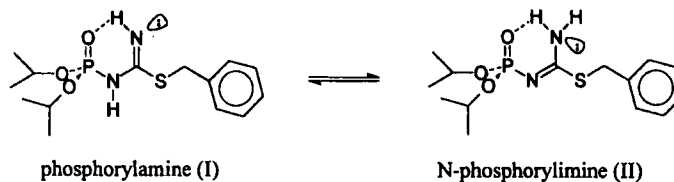
Tautomerism of Diisopropoxyphosphoryl Benzylisothiurea

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As part of our studies in preparation and physical properties of Potential ligands containing 1-phosphoryl(P=O)-3-carbonyl(C=X, X=NH, O, or S) group, we have investigated the intra/inter molecular hydrogen bonding of diisopropoxyphosphorylguanidine[1] as well as the tautomerism of phosphoryl benzylisothiurea. These are of interest as in interpretation of their chelation behavior as well as in development of other potential ligands for specific metal cations.

Diisopropoxyphosphoryl benzylisothiurea was prepared in good yield by a two-phases reaction between diisopropyl phosphite and benzylisothiurea using carbon tetrachloride and water as solvent. The FT-IR spectra of this compound in the solid state show the presence of different $\delta(\text{NH})$ (I), $\delta(\text{HNH})$ (II) and $\nu(\text{P=O})$ normal modes as a result of intramolecular hydrogen bonding; the behavior of the $\nu(\text{NH})$, $\delta(\text{NH})$, $\delta(\text{HNH})$, $\nu(\text{C=N})$ and $\nu(\text{P=O})$ normal modes of this compound in IR spectra in solutions of CCl_4 , CHCl_3 , CHBr_3 , CH_2Cl_2 , $\text{C}_2\text{H}_4\text{Cl}_2$, $\text{C}_2\text{H}_4\text{Br}_2$ and THF indicates the existence of a tautomerism between the phosphorylamine (I) and N-phosphorylimine (II) structures:



References

- [1] W.O. Lin, C.N. Guimaraes, M.C. de Souza and J.B.N. da Costa and H.G. Alt. *Phosphorus, Sulfur, and Silicon*, **92**, 1 (1994).