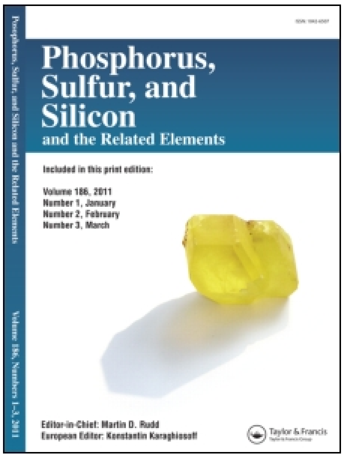

Phosphorus, Sulfur, and Silicon and the Related Elements
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713618290

Tautomerism of Diisopropoxyphosphoryl Benzylisothiourea

Whei Oh Lin[a]; Vanderléa De Souza[b]
[a] Department of Chemistry, Instituto Militar de Engenharia Praia Vermalha, URCA, Rio de Janeiro, RJ [b] PUC-RIO, Brazil

To cite this Article Lin, Whei Oh and De Souza, Vanderléa(1999) 'Tautomerism of Diisopropoxyphosphoryl Benzylisothiourea', Phosphorus, Sulfur, and Silicon and the Related Elements, 147: 1, 219

To link to this Article: DOI: 10.1080/10426509908053590

URL: http://dx.doi.org/10.1080/10426509908053590

Phosphorus, Sulfur and Silicon, 1999, Vol. 147, pp. 219-219
Reprints available directly from the publisher
Photocopying permitted by license only

Published by license under the
Gordon and Breach Science Publishers imprint.
Printed in Malaysia

Tautomerism of Diisopropoxyphosphoryl Benzylisothiourea

WHEI OH LIN[a] and VANDERLÉA DE SOUZA[b]

[a]*Department of Chemistry, Instituto Militar de Engenharia Praia Vermalha, URCA, Rio de Janeiro, RJ, 22290–270 and* [b]*PUC-RIO. Brazil*

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 diisoproxy-phosphorylquanidine[1] as well as the tautomerism of phosphoryl benzylisothiourea. 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 benzylisothiourea was prepared in good yield by a two-phases reaction between diisopropyl phosphite and benzylisothiourea using carbon tetrachloride and water as solvent. The FT-IR spectra of this compound in the solid state show the presence of different δ(NH) (I), δ(HNH) (II) and ν(P=O) normal modes as a result of intramolecular hydrogen bonding; the behavior of the ν(NH), δ(NH), δ(HNH), ν(C=N) and ν(P=O) normal modes of this compound in IR spectra in solutions of CCl_4, $CHCl_3$, $CHBr_3$, CH_2Cl_2, $C_2H_4Cl_2$, $C_2H_4Br_2$ and THF indicates the existence of a tautomerism between the phosphorylamine (I) and N-phosphorylimine (II) structures:

phosphorylamine (I)   N-phosphorylimine (II)

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).