

Structure and intramolecular flexibility of N-(thio)phosphoryl(thio)amides: VIII. Structure of N-phenyl,N'-(diisopropoxythiophosphoryl)thiourea

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Abstract

© Pleiades Publishing, Ltd., 2014. Structure and intramolecular transformations of N-phenyl,N'-(diisopropoxythiophosphoryl)thiourea has been studied by NMR spectroscopy and the AM1 quantum-chemical simulation. It has been shown that several forms, including two amide forms (EZ and ZE) and two prototropic forms, coexist in a dynamic equilibrium.

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Keywords

E/Z-isomerism, Intramolecular transformation, N-(thio)phosphoryl(thio)urea, Nmr spectroscopy, Phosphorylotropy, Tautomerism