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Structure and intramolecular mobility of N-(thio)phosphoryl(thio)amides: XV. Study of structure and intramolecular dynamics of N 3-phenyl-N 1-(diisopropoxythiophosphoryl)thiosemicarbazide in CD 2Cl2 solution by 1H, 13C and 31P NMR spectroscopy

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Abstract

Structure and intramolecular transformations of N3-phenyl-N 1-(diisopropoxythiophosphoryl--thiosemicarbazide in CD 2Cl2 were studied by one- and two-dimensional 1H, 13C and 31P NMR spectroscopy. The combined analysis of the data of NMR spectroscopy and calculation simulation confirmed a high lability of the studied compounds resulting in the formation of various conformational and tautomeric forms in solutions. The preference of Z,E-conformation of the amide form with cis- and trans-location of two N-H groups and the C=S group relatively to the two C-N bonds was revealed. © 2009 Pleiades Publishing, Ltd.

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