Russian Journal of General Chemistry 1997 vol.67 N7, pages 1017-1021

Structure and Intramolecular Lability of N-(Thio)phosphoryl(thio)amides III.* 1H, 13C, and 31P NMR Spectroscopic Study of the Structure of N-Diisopropoxy(thio)phosphoryl(thio)benzamides

Karataeva F., Zabirov N., Klochkov V. Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The structure and intramolecular processes in solutions of N-(thio)phosphoryl(thio)benzamides were studied by 1H, 13C, and 31P NMR spectroscopy. Analysis of the NMR data confirmed the strong tendency of these compounds to tautomerism in solution. The amide form with trans orientation of the NH proton and the C=O(S) group with respect to the C-N bond was shown to be preferred. The free energies of activation of tautomerization of the amide forms were determined.