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Structure and intramolecular lability of N-(thio)phosphoryl(thio)amides: XII. NMR study and computational modeling of the tautomeric forms of N-[dimethoxy(thio)phosphoryl]benzamides

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Abstract

The structure and intramolecular processes in solutions of N-(thio)phosphorylbenzamides were studied by means of 1H, 13C, and 31P NMR spectroscopy. Combined analysis of the NMR data and computational modeling gave evidence for the high lability of the compounds under study, that are capable of forming various tautomeric forms in solutions. The amide form with the NH proton arranged trans with respect to the C=O group was found to be preferred. ©2005 Pleiades Publishing, Inc.

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