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Structure and Intramolecular Lability of N-(Thio)phosphoryl(thio)amides. IV. 1H, 13C and 31P NMR Study of Dynamic Processes in Solutions of N,N′-Bis(diisopropoxythiopnosphorylaminothiocarbonyl)-1,10-diaza-18-crown- 6 Ethers

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Abstract

1H, 13C, and 31P NMR spectroscopy was used to study the structure of N,N′-bis(diisopropoxythiophosphorylaminothiocarbonyl)-1,10-diaza-18-crown- 6 ethers in CD3CN, CD2Cl2, and (CD3)2CO solutions. A tautomeric equilibrium was detected, involving the amide (with C=S trans to P=S), two prototropic, and one phosphorylotropic forms. It is found that the macroheteroring has two conformations: with trans,cis, and trans N-substituents. The conformational equilibrium is solvent-dependent.