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NMR Determination of the Number of Components of Fast Conformational Exchange in Heterocyclic Systems

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Abstract

A procedure was developed for determination of the number of components (two or more than two) participating in fast conformational exchange in heterocyclic systems. The procedure is based on analysis of temperature dependences of spin-spin coupling constants. It was applied to 5,5-dimethyl-2-methylthio-1,3,2λ5-dioxaphosphinane 2-sulfide which was shown to exist in solution as a mixture of two conformers, chair-ax and chair-eq. The conformational behavior of 2-phenoxy-1,5-dihydro-2,4λ5,3-benzodioxaphosphepine 2-oxide and its 2-thio analog was also considered in terms of the proposed approach.
