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THE STRUCTURE OF 2,4-DIORGANYL-2,4-DITHIOXO- 1,3,2λ⁵,4λ⁵-DITHIADIPHOSPHETANES IN SOLUTION

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Compounds of the overall composition RPS_2 , so called perthiophosphonic acid anhydrides, prefer a dimeric structure in solution, as it has already been known for the solid compounds. Following compounds $[RP(S)S]_2$ with R=methyl, ethyl, propyl, isopropyl, butyl, tert-butyl, cyclohexyl, phenyl, 4-methoxy-phenyl and 3,5-dimethyl-phenyl were prepared and characterized by NMR spectroscopy. The 3,5-di-tert-butyl-4-hydroxy-phenyl-compound [1] was also investigated. NMR investigations give evidence for the existence of configurational isomers of the 2,4-Diorganyl-2,4-dithio-oxo-1,3,2λ⁵,4λ⁵-dithiadiphosphetanes. In solutions an equilibrium between cis and trans isomers is established. The concentration of the two isomers depends on the kind of R and the solvent used. In general the trans isomer has a higher concentration than the cis isomer. The easy preparation of unsymmetrical compounds by mixing solutions of compounds with different R shows a continuous dissociation and association process of the PSPS-ring. This result underlines the existence of a monomeric compound of low concentration as intermediate. An interesting result is obtained for the isopropyl compound. After dissolving e.g. in $CDCl_3$ almost 90% of the compound is transformed into the other isomer. The progress of the transformation can be followed by NMR spectroscopy. In all other cases the equilibrium state is immediately achieved after preparation of the solution.

[1] G. Ohms, G. Grossmann, N. A. Mukmeneva, E. N. Čerezova, *J. Prakt. Chem.*, in press.