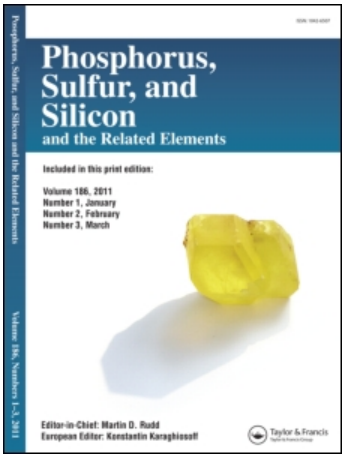

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THE CONFORMATION OF THIOPHENOL IN SOLUTION DETERMINED BY LIQUID CRYSTAL NMR SPECTROSCOPY

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THE CONFORMATION OF THIOPHENOL IN SOLUTION DETERMINED BY LIQUID CRYSTAL NMR SPECTROSCOPY.

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It has been possible to obtain the proton NMR spectrum of thiophenol and 4-chlorothiophenol dissolved in the nematic phase of a liquid crystalline solvent. The computer iterated spectral analysis allowed the authors to determine the direct dipolar couplings that depend solely on the ratio of the interprotonic distances.[1]

It has been ascertained that a planar conformation does not match the experimental data: to do so one should assume a CSH angle of 107° whereas this angle in thiols is known[2] to be 97°.

On the other hand a conformation having the CSH plane twisted by 26° ± 3° with respect to the benzene ring is in agreement both with the structural parameters (angles and bond lengths) of thiols[2] and with the liquid crystals NMR experiment. It seems therefore that thiophenol and its para derivatives are not planar in solution.

1) L. Lunazzi, in "Determination of Organic Structures by physical methods" Vol. 6 Chapter 6 pp. 335-413. Academic Press. New York 1976.

2) J.C. Paul in "The Chemistry of thiol group" S. Patai Ed., Part I Chapter 2. J. Wiley and Sons, London 1974.