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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 known² to be 97°.

On the other hand a conformation having the CSH plane twisted by $26^\circ \pm 3^\circ$ with respect to the benzene ring is in agreement both with the structural parameters (angles and bond lengths) of thiols² 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.