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ACCEPTED MANUSCRIPT

A CONCEPT FOR STIMULATED PROTON TRANSFER IN 1-(PHENYLDIAZENYL)NAPHTHALEN-2-OLS

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Abstract:

A series of aryl azo derivatives of naphthols (1-3) were studied by means of UV-Vis and NMR spectroscopy in different solvents as well as by quantum chemical calculations and X-ray analysis. Previous studies have shown that Sudan 1 (1) exists as a tautomeric mixture. The effect of the solvents is minimized by the existing intramolecular hydrogen bond. Therefore, the influence on the tautomeric state in structurally modified 1 has been investigated. Structure 2 contains an additional OH-group, which deprotonates easily and affects the position of the tautomeric equilibrium by changing the electronic properties of the substituent. The implementation of a sidearm in 3 creates a condition for competition between the nitrogen from the azo group and from the piperidine unit for the tautomeric proton. In this case the use of acid as a stimulus for controlling the tautomeric process was achieved.

Keywords: tautomerism, molecular switches, molecular spectroscopy, azo dyes

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