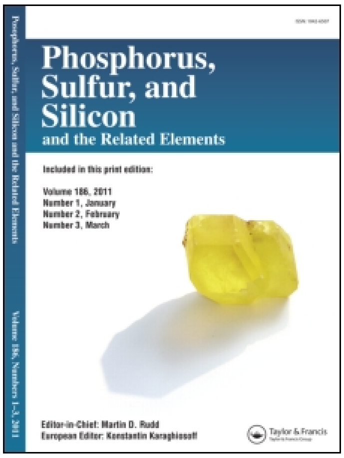

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SULPHONATION OF THE TEN DIMETHYLNAPHTHALENES AND 2-METHYLNAPHTHALENE: ISOMER DISTRIBUTION AND CORRELATIONS WITH MOLECULAR ORBITAL THEORY

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SULPHONATION OF THE TEN DIMETHYLNAPHTHALENES AND 2-METHYLNAPHTHALENE: ISOMER DISTRIBUTION AND CORRELATIONS WITH MOLECULAR ORBITAL THEORY.

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The isomer distribution for the mono- and di-sulphonation of 2-methylnaphthalene (2-MN) and all ten dimethylnaphthalenes (DMN's) with SO_3 in nitromethane as solvent were determined at 0° and/or 12°C. From the substitution pattern it is evident that steric factors play a more important role in the sulphonation than in most other electrophilic substitutions. In the disulphonations the substitution of the second sulpho group occurs in part in the same ring as the first one. This may infer that the directing effect of the first (pyro)sulphonic acid group is relatively small. The positional order of substitution for the monosulphonation of a given substrate is in excellent agreement with that predicted by the localization energies, calculated by a simple Hückel m.o. treatment, utilizing the inductive model for the methyl substituent, provided that allowance is made for steric factors.