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Synthesis and Structure of Novel Substituted *N*-Sulfinylanilines

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Abstract—*N*-Sulfinylanilines derived from 4-bromoaniline, 3-nitroaniline, and 4,4'-(ethane-1,2-diyl)dianiline were synthesized. X-ray diffraction analysis of 4-bromo-*N*-sulfinylaniline, 3-nitro-*N*-sulfinylaniline, and 4,4'-(ethane-1,2-diyl)di-*N*-sulfinylaniline was performed. The sulfinyl function in the planar conformation of the Ar-NSO fragment was found to have *Z* configuration. The nature of intra- and intermolecular structure-forming interactions was established.

Keywords: *N*-sulfinylanilines, X-ray diffraction analysis, intra- and intermolecular interactions

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The aromatic sulfinylamine function (Ar-N=S=O) is quite reactive, which is manifested in that it is highly prone to addition across the N=S bond. Especially characteristic of aromatic sulfinylamines are Diels–Alder reactions, where they can act as a dienophile (route *a*) [1, 2], diene (route *b*) [3], or 1,3-dipolarophile (in 1,3-dipolar cycloaddition, route *c*) [4, 5] (Scheme 1). In view of the fact that such reactions

provide a facile synthetic approach to cyclic sulfonamides, in the present work we decided to study in more detail the structure of the starting aromatic sulfinylanilines.

N-Sulfinylanilines **1–3** were prepared in yields of 84–90% by the reactions of the corresponding anilines with thionyl chloride in benzene under reflux (Scheme 2).

Scheme 1.

