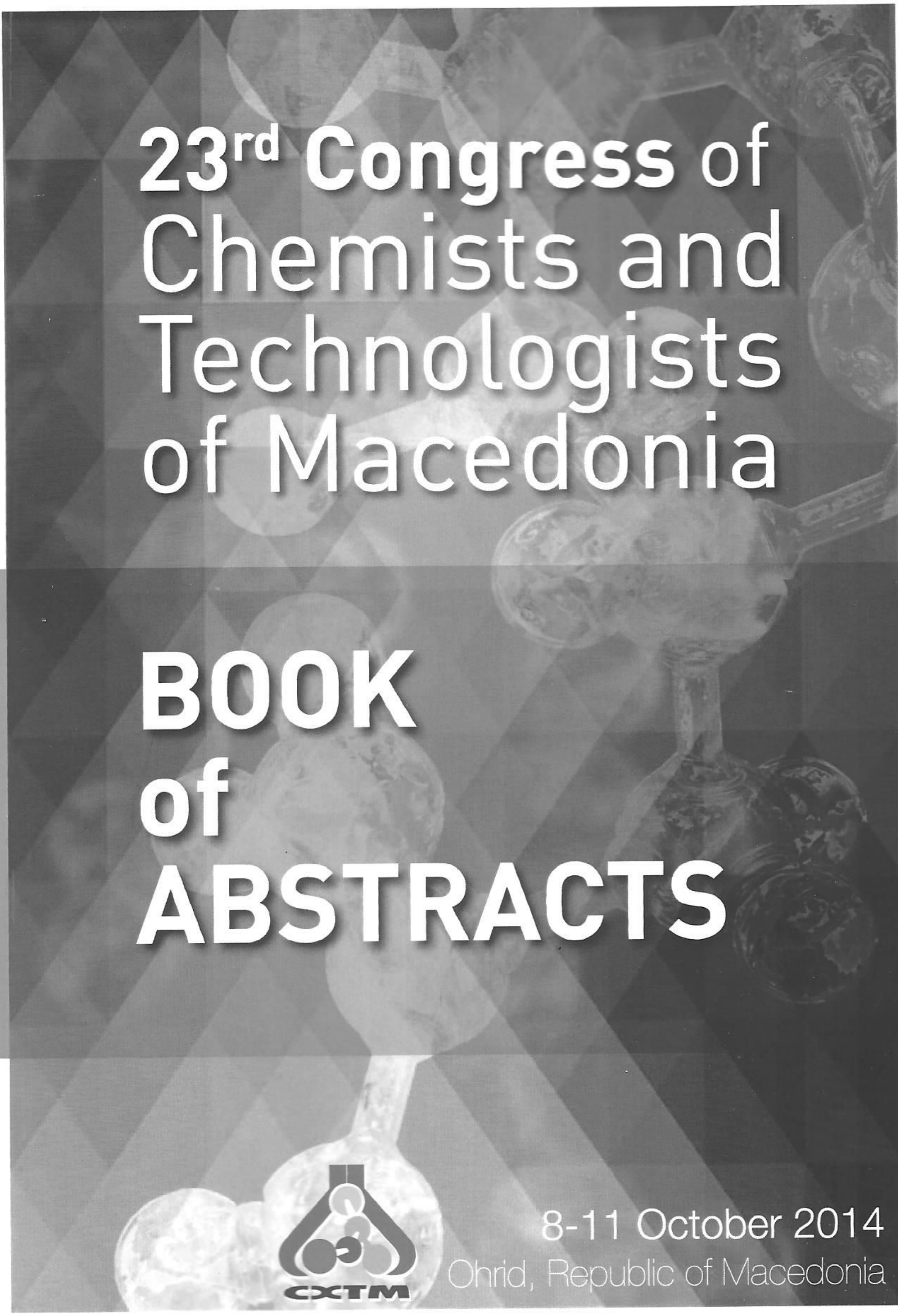

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BOOK of ABSTRACTS

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OCT 003

ACYCLIC AND HETEROCYCLIC COMPOUNDS FROM POLYHALOGENATED NITROBUTADIENES

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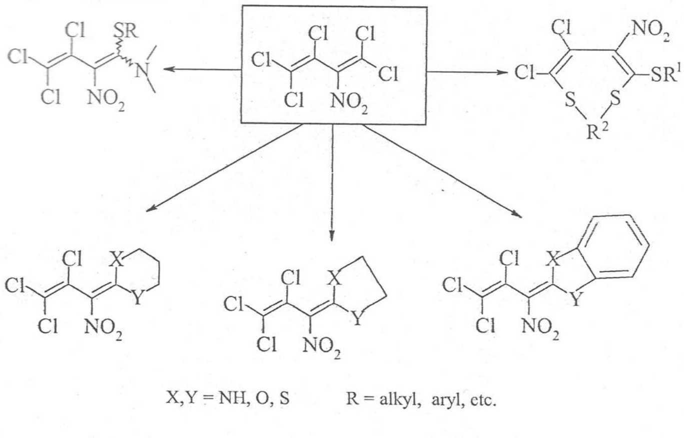
The new class of nitroalkenes called polyhalogenated-1,3-nitrobutadienes, bearing at least one nitro group are in general starting materials [1]. Halogen atoms of nitrovinyl groups exchange their place with nucleophiles via S_NVin reactions. Thus being attacked by an appropriate nucleophile, nitrodiene molecule readily reacts due to position of LUMO preferentially at the dihalogeno-nitrovinyl fragment. In chlorinated compounds, the additional presence of a nitro substituent usually leads to biological activity. The resulting compounds should exhibit biological activity as fungicidal, fungistatic, antibacterial, or anthelmintic agents [2,3]. In the course of our studies, high functionalized acyclic and heterocyclic compounds were obtained by the reactions of some substituted polyhalogenated-1,3-nitrobutadienes with nucleophiles containing some heterocylic amine and thiol functional groups. Reaction products were purified by column chromatography. In all cases, the structure of the products were determined using extensive spectroscopic methods such as elemental analysis, NMR, FT-IR, MS and single crystal X-ray diffraction.



Keywords: 2-nitro-perchloro-1,3-butadiene; polyhalogenated nitrobutadienes; amines; thiols; S_NVin reaction

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OCT 004

NUCLEOPHILIC SUBSTITUTION REACTIONS OF QUINONES WITH N, S-SUBSTITUTED NUCLEOPHILES

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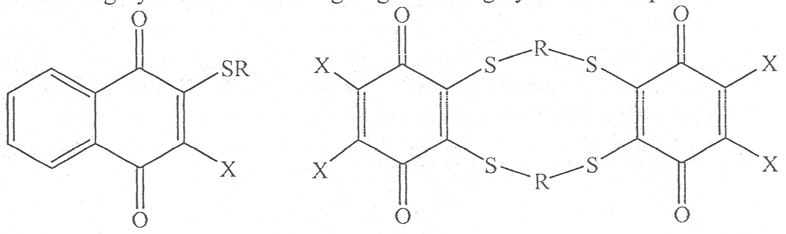
The synthesis of S- and N-substituted napthoquinone- and benzoquinone derivatives have received considerable attention in literature [1]. Nucleophilic addition reactions of 2,3-dichloro-1,4-naphthoquinone have been widely studied in synthetic chemistry [2]. Recently, many studies have demonstrated that naphthoquinone derivatives substituted with sulfur or nitrogen atoms show a particularly marked activity against fungi. Quinones are naturally occurring compounds with specific characteristics that have a great impact on the living cell. The ability to carry electrons makes them an important component of photosynthetic and respiratory electron transfer chain. They are considered as components of biological electron transfer chains located in the membranes of mitochondria, bacteria and chloroplasts. Quinones are good electron acceptors and are known to be efficiency dependent on the redox potentials of the corresponding quinone-hydroquinone system [3]. In this study, the quinone derivatives were synthesized and characterized using elemental analysis and spectroscopic methods (NMR, UV-Vis, FT-IR and MS).

Cyclic thioquinone compounds were directly prepared from reactions of quinone derivatives with some thiols as nucleophiles. Most of these reactions were found to be highly selective resulting in good to high yields of the products.



R = alkyl, aryl, etc. X = Cl, $-OC_2H_5$

Keywords: Quinones; organic synthesis; thiols; amines

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