Charge Density and Topological Properties of Chosen Aromatic Nitramines

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Aromatic nitramines rearranges under the influence of elevated temperature or diluted mineral acids. The migration is entirely intramolecular, *i.e.* the *N*-nitro group shifts three or five atoms from its original position, still remaining bound to the aromatic residue [1]. The mechanism of the nitramine rearrangement remains still unclear. Analysis of charge density distribution in aromatic nitramines could bring the grounds for electron reasons of their interesting properties *viz.* structure–reactivity relationships and the role of an acidic catalyst. Charge density of chosen aromatic nitramines have been studied to understand those special properties. Conjugation between π-electron systems should divert the charge distribution within the NNO_2 group and give rise to some observable changes in its geometry and chemical properties of the nitramine [2].

In the communication will be shown results of structure determination together with a charge density analysis of N-phenyl-N-methylnitramine together with 1-nitroindoline. Topological properties associated with the bond critical points (*BCP*), molecular geometry, crystal packing and topological properties of those compounds will also be presented.

[1] Daszkiewicz Z., Zaleski J., Nowakowska E., Kyziol J., *Pol. J. Chem*., 2002, **76**, 1113. [2] Anulewicz R., Krygowski T., Gawinecki R., Rasała D., *J. Phys. Org. Chem.,* 1993, **6**, 257.

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