Improved Interpretation of thermal stability models of nitroaromatics by AN efficient selection of descriptors and BY the use of chemical shifts as decriptors

**Bono Lučić1 , Drago Bešlo2, Ana Amić3, Jadranko Batista4, Dražen Vikić-Topić1 and Nenad Trinajstić1,5**

1Ruđer Bošković Institute, NMR Centre, Bijenička c. 54, Zagreb, Croatia (presenting author: [lucic@irb.hr](mailto:lucic@irb.hr))

2Josip Juraj Strossmayer University of Osijek, Faculty of Agriculture in Osijek, Vladimira Preloga 1, Osijek , Croatia

*3University of Mostar, Faculty of Science and Education, Mostar, Bosnia and Herzegovina*

4Juraj Strossmayer University of Osijek, Department of Chemistry, Cara Hadrijana 8a, Osijek , Croatia

5Croatian Academy of Sciences and Arts, Zrinski trg 11, Zagreb, Croatia

Nitroaromatic compounds, like nitrobenzene derivatives can be considered as the typical energetic molecules [1]. Some of them are commonly used as explosives like TNB (1,3,5-Trinitrobenzene) or TNT (2,4,6-trinitrotoluene) [2]. For the suitability of an explosive substance in a specific use, better understanding of physico-chemical attributes of its structure which are related to compound’s stability is a very important task. Many structure-thermal stability models have been developed in the last ten years for this class of compounds. The largest are those published by Fayet et al. [3] based (primarily) on the set of semi-empirical molecular descriptors calculated by the MOPAC program [4], and by Li et al. [2] selected from the large pool of molecular descriptors calculated by the Dragon 5.5 program [5].

To achieve better physico-chemical interpretation of models, in addition to descriptors calcualted and used in previous models we calculated and used additional descriptors like (1) those given in the PubChem database [5], (2) experimental or calculated 1H and 13C chemical shifts of nitroaromatics and (3) the number of specific connectivity terms in molecular skeleton. Also, an improved selection of molecular descriptors was performed in attempt to develop simpler structure-property models (having a smaller number of descriptors). Performing descriptor selection, whenever it was possible and statistically reasonable, we considered the possiblity of inclusion of simpler molecular descriptors into the final models instead of more complex descriptors or those that are computed from 3D structure. As an interesting results we found that the maximal 1H chemical shift of hydrogens attached to aromatic ring is a significant descriptor, as well as the number of multiple bonds in a compound. Obtained results and models were compared with other models from literature showing that presented approach is a promising way of selecting statistically good structure-thermal stability models of nitroaromatics, which are more informative and easy to interpret.

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