

ABSTRACT

In recent times the both chemical and pharmaceuticals industries more often use co-crystals - the structures composed of few chemical compounds, which are also known as the solid solutions. These objects become more popular because of the relative easiness of controlling their composition. Moreover, an additional element (a chemical compound) in the crystal structure may influence the properties of the second substance, in particular its solubility and its bioaccessibility [1]. In this context the co-crystallization of at least two solid substances is treated as the way of producing the solid form of particular properties. [2].

The main compounds used in the presented studies were derivatives of pyridine, 1,3,5-triazine and 1,2,4,5-tetrazine. They belong to the group of azaaromatic compounds, in which the basic aromatic ring characterized by the deficit of π electrons, which depending on the substituents can be modified. Therefore such a ring as well as constituting nitrogen atoms can play a role of donor or acceptor of the electron density in various non-covalent interactions. Structural analysis of such interactions, as hydrogen, halogen and chalcogen bonds, was the main aim of the presented work. For this purpose the following methods have been used: X-ray diffraction analysis, quantum chemistry methods, IR spectroscopy, Hirshfeld surfaces analysis.

The dissertation is focused on X-ray determination and analysis of 16 novel crystal structures. On the base of the obtained results the following findings can be indicated: the previously unknown molecular structure of 2-aminopyridine *N*-oxide has been confirmed by X-ray methods; in the analyzed group of co-crystals sulfonamide group can act as a double hydrogen bond donor to the both *N*-oxide- and nitro- groups; in the pentachloropyridine *N*-oxide crystal the C-Cl...Cl halogen bonds and *N*-oxide...*N*-oxide interactions are responsible for the formation of molecular bands ordered into the herringbone motif; 2-mercaptopyridine *N*-oxide can be used as a mild reducing agent undergoing oxidation to the disulfide form; the existence of a half-protonated form of disulfide, stabilized by charge assisted hydrogen bond CAHB(+) has been revealed; $R_2^2(8)$ motif resulting from N-H...S hydrogen bonds is a typical molecular synthon of thiourea and trithiocyanuric acid derivatives; sulfur atoms of trithiocyanuric acid may act as acceptors of halogen bonds (e.g. C-Br ... S) as well as donors of chalcogen bonds type C-S ... O in the crystal structures; there are typical hydrogen bonds with the pyridyl nitrogen as acceptor and novel C-Br ... N halogen bonds in the crystal structures of 1,2,4,5-tetrazine derivatives.

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*Badania strukturalne i analiza oddziaływań stabilizujących
w kryształach wybranych pochodnych związków azaaromatycznych*

Literature:

- [1] C. Sun, X. Zhang, H. Huang, P. Zhou, *Bioorg. Med. Chem.*, 2006, **14**, 857.
[2] Z. Zhong, R. Xing, S. Liu, L. Wang, S. Cai, P. Li, *Carbohydr. Res.*, 2008, **343**, 566.