

## Summary

Lublin 2019

MARIA CURIE-SKŁODOWSKA UNIVERSITY

Institute of Chemical Sciences

Department of General Chemistry, Coordination Chemistry and Crystallography

### **TWO-COMPONENT CRYSTALLINE MOLECULAR COMPLEXES OF SELECTED BENZOFURAN DERIVATIVES**

Author: mgr Ilona B. Materek

Doctoral supervisor: prof. dr hab. Anna E. Koziół

Auxiliary supervisor: dr Liliana A. Mazur

The first part of the presented work is a review of the literature and describes issues related to the field of supramolecular chemistry, crystal engineering, solid phase interactions, as well as the synthesis and methods of characterization of crystalline molecular complexes. The data available in the literature and the structural database search allowed the creation of the concept and research goals of this dissertation.

In the presented doctoral thesis, I have devised a method for the synthesis of two-component crystalline molecular complexes of two benzofuran derivatives (BZF) with selected co-formers, which were dicarboxylic acids, monocarboxylic compounds and others, such as hydroquinone or saccharin. In total, according to the devised method of synthesis, I received 31 new crystalline phases. Powder diffraction patterns were registered for each of them to confirm the phase compliance of products after grinding and after recrystallization. The crystal structure of the obtained complexes was determined by X-ray crystallography. Structural studies of the obtained crystalline phases included primarily the analysis of their stoichiometry in the solid phase, as well as the analysis of the geometry of BZF molecules in co-crystals and cations  $[\text{HBZF}]^+$  in salts, and the analysis of interactions stabilizing the molecular system of  $\text{BZF}\cdots\text{co-former}$  (supramolecular synthons, hydrogen bonds,  $\pi$ - $\pi$  and  $\text{CH}\cdots\pi$  interactions).

Methods of association of molecules in the crystal lattice have also been interpreted. The Hirshfeld surfaces of BZF molecules and cations  $[\text{HBZF}]^+$  together with fingerprint plots have been calculated for all obtained crystalline phases. In this part of the dissertation there were also considered weak intermolecular interactions  $\text{C-H}\cdots\text{O}$  and  $\pi$ - $\pi$  stacking. Quantitative analysis was performed for the most important types of intermolecular interactions. Structural studies were supplemented with infrared spectra and thermal analysis.