Abstract

Nitro compounds, including nitrobenzoic acids, are a very important group of chemical compounds from the point of view of industry. This significance arises from their wide range of applications in the production of various materials crucial for the economy, such as polymers, dyes, medicines and explosives. They are also an interesting subject of research in the context of crystal engineering. This is because nitro groups interact with different functional groups through $NO_2\cdots X$ interactions (where X = NO_2, COOH, OH, NH_2, CH_3, H, or π), forming different supramolecular synthons. These interactions often determine the specific properties not only of the nitrobenzoic acids themselves, which exist in crystalline form, but also of multicomponent crystals (including cocrystals, salts, and solvates) formed with their participation.

This doctoral dissertation presents the results of research involving the analysis and theoretical calculations of intermolecular interactions, particularly those involving nitro groups, in crystal structures of: (a) multicomponent crystals involving selected nitrobenzoic acids and aromatic nitrogen bases deposited in the CSD database, (b) nitrobenzoic acids substituted with various functional groups ($–NO_2$, $–NH_2$, –OH, and $–CH_3$) also deposited in the crystallographic CSD database and (c) newly synthesized multicomponent crystals involving nitrobenzoic acids and acridine/acridine derivatives, such as: two salts: acridine with 3-methyl-2-nitrobenzoic acid and acridine with 2-methyl-3-nitrobenzoic acid, the salt of acridine with 2,4-dinitrobenzoic acid (1:2 stoichiometry) and the monohydrate cocrystal salt of acriflavine with 3,5-dinitrobenzoic acid (1:2 stoichiometry). In this doctoral dissertation, supramolecular synthons involving various functional groups, particularly nitro groups, were identified in the crystal structures of analyzed compounds, and their energies were calculated using quantum chemistry methods. The results obtained were discussed, and a classification of the identified synthons was proposed based on the interactions involving nitro groups.