Abstract

In this PhD dissertation, synthesis and structural studies of esters and salts of hypodiphosphoric acid are described. Three salts of the new ADP analogue – adenosine 5′-hypodiphosphate (AhDP) were obtained, structurally characterized and revealed similarity of AhDP to ADP in terms of molecular structure and intermolecular interactions. In order to complete the characteristics of the intermolecular interactions in nucleoside ester hypodiphosphate crystals, model compounds (i.e. salts of purine and pyrimidine nucleosides, purine bases and cytosine, and sodium salts) were obtained and analyzed in terms of intermolecular interactions. In the class of nucleoside connections, 13 crystals containing protonated nucleosides: adenosine, cytidine, 2′-deoxycytidine and cytarabine were obtained and characterized, and 10 crystals containing protonated adenine, xanthine, theophylline, theobromine, caffeine and cytosine were described among the nitrogen base salts. Additionally, 7 crystals of sodium hypodiphosphate salts were obtained and characterized.

Based on the obtained ester crystals along with salts of nucleosides and nitrogen bases, the crystallochemistry of the hypodiphosphate group in this type of organic connections was characterized. The main types of interactions were determined, including direct hydrogen bonds of the base–hypodiphosphate type (B–PP) and hypodiphosphate–hypodiphosphate (PP–PP) and interactions involving the lone electron pair of the hypodiphosphate oxygen atom and the electrons of the aromatic ring (lp–π interactions). Anionic substructures formed as a result of PP–PP hydrogen bonds were analyzed and the preferred structural motifs were determined.

Structure analysis of a series of salts containing hypodiphosphate anions in different ionization states provided structural and supramolecular characterization of hypodiphosphates in their sodium salts. In particular, coordination of hypodiphosphate anions to Na^+ cations along with the coordination environment of cations and anions was characterized, and the results were compared with the published data for potassium salts.