

Abstract

Compounds with the characteristic supramolecular structure of the host–guest type are found in the area of continuous interest of the scientific world. Such compounds are attractive in the context of their physico–chemical and structural properties that can be properly designed and modified. An interesting group of compounds are copper(I) coordination compounds with Schiff bases based on 4-amino-1,2,4-triazole. They tend to form binuclear cationic units and to form crystal structures with the presence of one–dimensional channels occupied by solvent molecules. On the basis of a small amount of data in the literature, it has been observed that this tendency is related to the presence of the halogen atom located in the *para*- position of the phenyl ring of the Schiff base, which by directional interactions determines such a supramolecular structure. The presence of channels in the crystal structure is attractive in the context of the exchange of guest molecules, which is used in heterogeneous catalysis, selective molecular separation, gas storage or chemical sensors.

The main goals of the presented dissertation were the synthesis and characterization of copper(I) coordination compounds with triazole Schiff bases in order to study the influence of additional halogen atoms in the phenyl ring of the ligand, on the structural motif of copper(I) coordination compounds, taking into account the influence of the anion geometry.

In this work 28 copper(I) coordination compounds with halogen derivatives of Schiff's bases were obtained (an additional 16 were obtained as a result of post–synthetic modification). Among them there are 11 one–dimensional coordination polymers. Six of them are characterized by the presence of one–dimensional channels in which the guest molecules are located. Preliminary studies have shown that these systems are capable of exchanging molecules in channels. The remaining compounds are discrete systems in which the binuclear cationic units are X–shaped. Among these systems, four are characterized by the presence of one–dimensional channels occupied by guest molecules. In these cases, desolvation leads to huge changes in the self–organization of these binuclear units, resulting in the closure of the channels. This process is reversible and the reopening of the channels is possible by placing the crystal in a solvent vapour. The selectivity of these systems for sorption of solvent molecules are changed depending on the modification of these systems, which are halogen atoms (their position and type) in the phenyl ring of the ligand. The binuclear copper(I) coordination

compounds were also obtained and their self-assembly results in dense packing (no channels). It is caused by the size of the halogen atom located in the *para*- position of the phenyl ring of the ligand. The dissertation showed that the expansion of the phenyl ring of Schiff's bases by introducing additional atoms promotes the formation of one-dimensional coordination polymers. It has also been proven that the geometry of the anion is of great importance in the design of these systems. Properly selected Schiff's base and an appropriately good anion resulted in the obtaining of the copper(I) coordination compound, in which the geometrical parameters make it possible to carry out the [2 + 2] photochemical reaction in the crystal.