The reason why this research topic was taken

The study of new substances and understanding the nature of physical phenomena that occur in them enables the designation of new materials with potential applications in energetic devices. One group of substances widely studied in recent times are proton conductors. It is expected that they could be used as electrolytes in fuel cells in which the only reaction by-products are water and heat. Such cells could be considered safe for the environment, i.e., meeting all the requirements of green chemistry. Designing proton conductors with high conductivity and thermal stability opens the way to their use in fuel cell design. In the design of substances that meet the above conditions, the key stage is the selection of compounds that do not contain water in their structure. This requirement is dictated by the low thermal stability of hydrated salts, which under the influence of elevated temperature, eliminate water molecules. Proton conductors are usually polymers or ceramic materials, and the latest proton conductors are salts of organic acids and bases, which include, among others, salts of imidazole and methanesulfonic acid. So far, salts of imidazole and aliphatic dicarboxylic acids with different aliphatic chain length have been studied. However, the materials thus obtained were characterized by low conductivity (10^{-4}-10^{-2} $S \cdot m^{-1}$). The advantage of these materials was their high thermal stability up to 373 K.

Based on the above observations, we proposed a new group of proton conductors in which the aliphatic acid anion was replaced with the aromatic acid anion. New salts of imidazole and aromatic acids: orthophthalic and terephthalic acids were obtained. DSC studies confirmed that salts of aromatic acids show good thermal stability: imidazolium orthophthalate melts at 422 K and imidazolium terephthalate at 464 K. In addition, imidazolium orthophthalate had a high conductivity of $2 \cdot 10^{-1}$ $S \cdot m^{-1}$. Analysis of conduction pathways showed that proton transport takes place along helical pathways. This structural motif of the conduction pathway was observed for the first time and is unique for this group of salts of aromatic acids and heterocyclic bases.

The goal of the project

The research will aim to analyze the impact of the chemical nature of anions on the hydrogen bonding network of salts formed. An analysis of hydrogen bond stability as a function of temperature and pressure will be carried out using vibrational spectroscopy. Besides, an analysis of temperature and pressure-induced phase transitions will be performed. An analysis of changes in hydrogen bond parameters under the influence of changes in thermodynamic parameters will also be carried out. Phase diagrams will be designated for systems that will have phase transitions.

Description of research carried out in the project

As part of the project, infrared spectroscopic measurements and diffraction of X-ray as a function of temperature and pressure will be carried out. In order to identify phase transitions, measurements will also be carried out using differential scanning calorimetry as a function of temperature and pressure. In addition, quantum-mechanical calculations will be carried out under appropriate temperature, and pressure conditions. Experimental measurements in conjunction with the theoretical calculations will allow the characterization of the hydrogen bonding network formed in new conductive salts.

The most important expected results

We expect that the results of the project will allow determining how thermodynamic parameters, such as temperature and pressure, influence the parameters of hydrogen bonds within new salts and allow to determine the relationship of HB's pattern with proton conductivity. Understanding the physical and chemical properties of hydrogen bonds will allow concluding on the electrical conductivity and thermal stability of the new conductors. The results of the study will pave the way for the effective design of new materials with high ionic conductivity. The study will also answer the question of how conduction paths will change under the influence of temperature and pressure.