The aim of this research is to determine the correlation between the pressure required to induce the proton transfer reaction in molecular cocrystals and difference in the acidity of the cocrystal components.

Cocrystals are an interesting group of materials, often possessing properties superior to those of pure components. They found applications as energetic and nonlinear optics materials but mostly are used in the pharmaceutical industry. The design of cocrystals is based on the compatibility of components (coformers) to form complementary hydrogen-bonding patterns. Compounds well known to form intermolecular interactions with each other are Brønsted-Lowry acids and bases. However, depending on their acidity and basicity, they can form salt instead of a cocrystal. In fact, the difference in the acidity of coformers can be used to predict the tendency for cocrystal vs. salt formation at ambient conditions. At the same time, the correlation of the difference in acidity and hydrogen cation transfer from acid to base under conditions different from ambient was not thoroughly investigated. It is worth noting that it was previously shown for oxalic acid dihydrate that pressure can indeed lead to cocrystal–to–salt transformation. Therefore, the purpose of this study is to determine the correlation between the difference in coformers acidity and the pressure required to induce the hydrogen cation transfer in molecular cocrystals.

Experimental work will be carried out with the use of a diamond-anvil cell (DAC). The sample is placed inside the opening of a specially prepared metal gasket mounted inside the DAC. When two parallel diamonds press on the metal gasket, they cause its deformation and increase of pressure inside the chamber. Unfortunately, the construction of the DAC affects the quality and number of collected X-ray diffraction data, hindering the determination of the hydrogen atoms position in the crystal structure, the crucial aspect for differentiating between cocrystal and salt. Therefore, a novel DAC construction with a very high opening angle will be used to ensure the collection of as complete data as possible. This will enable specialistic refinement of hydrogen atoms positions. The X-ray diffraction data will be also supported by Raman spectroscopy. Once the transformation from cocrystal to salt will be confirmed, recrystallization of the sample under pressure will be performed to see if the charged components show an alternative tendency for aggregation in the solid state.

This research will increase the general knowledge on the behaviour of molecular cocrystals under pressure and will enable determination of the correlation between the difference in the acidity of coformers and the pressure required to induce hydrogen cation transfer. Moreover, it can lead to the discovery of new crystal forms unobtainable at ambient conditions. Therefore, the approach used in this study might prove to be a method for obtaining novel materials with interesting properties.