

Phase transitions in pyridazine-based high-nitrogen-content compounds

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The phenomena of polymorphism and solvation are very interesting issues, due to the fact that different forms of the same compound may have different chemical and physical properties. Therefore it is important to get the knowledge about the conditions of new polymorphs formation and their stability, and understand the mechanisms of phase transitions. This information would allow to obtain specific form of materials in a more controlled way, with desired properties [1]. Also understanding the mechanisms of transformations of intermolecular interactions is essential, as they are the main factor responsible for arrangement of molecules in the crystal structures and their stability. Different factors can affect the intermolecular interactions patterns, which can be reorganized or broken and the new types of bonds can be formed [2].

The investigated pyridazine-based high-nitrogen-content (Fig. 1) are important compounds used in biology, chemistry and pharmacy [3]. The structure, properties and crystallization preferences of materials significantly depend on the thermodynamic conditions in which they are found, the presence of other reagents or the method of obtaining [4,5]. Therefore the pyridazine derivatives have been studied at varied thermodynamical conditions [6-8]. Their structures were determined by single-crystal X-ray diffraction and the obtained results revealed, that the behavior and preferences for new polymorphs and solvates formation of the studied pyridazine derivatives is very different, especially when they are exposed to high-pressure conditions. They exhibit also a high potential for hydrogen bond forming, and considering the number of nitrogen atoms, they are also prone to form N···N intermolecular interactions, which affect the packing of molecules in the crystal structure.

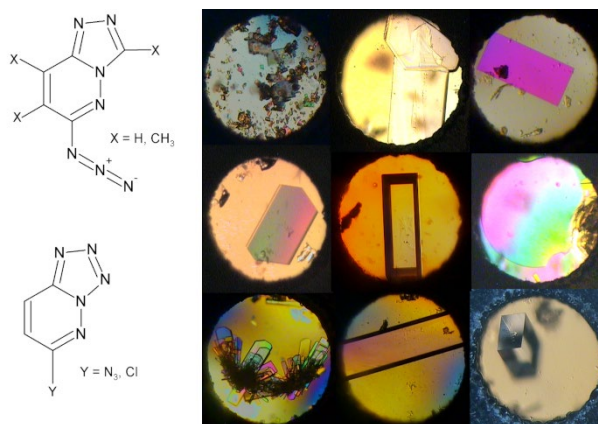


Figure 1. Structural formulas and crystals of the studied pyridazine-based compounds.

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