MS22-P08 | UNDERSTANDING OF CHROMIC PHENOMENA: THE EXAMPLES OF VIOLURIC ACID - AMINO ACID BASED SALTS AND CO-CRYSTALS

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The color-changing effects play important role in modern technologies, thus chromic materials find enormous applications in thermal printing, optical data storage, biosensor development etc. In crystalline phases, several chromic effects, such as termochromism, piezochromism or crystallochromism can be observed.

Crystallochromic phenomena are well described for single-component crystals in which π···π interactions between molecules are responsible for their absorption properties. In multicomponent materials, evaluation of the color source is more complicated. Our previous study [1] showed that violuric acid (VA) can form colored organic salts which led to formation of red and violet crystals. It has to be pointed out, that in those systems no π···π interactions can be found. In order to examine ability of VA to form colored co-crystals and salts in the presence or absence of π···π interactions, we have chosen amino acids as cocrystallization components. Due to variety of interactions formed by amino acids we can investigate color changes analyzing possible π···π interactions and hydrogen bonds.

Here we present a set of crystalline phases containing violuric acid and selected amino acids. The color phenomenon for those materials is studied using experimental and theoretical methods including X-Ray diffraction, UV-Vis spectroscopy, Fingerprint plots [2] and Non-Covalent Interaction index [3]. This study allowed us to find correlation between crystal packing features and absorption properties of obtained crystalline phases.

[1] Gryl, *et al*. (2019). IUCrJ, 6, 2.
[2] Spackman, *et al*. (2002). *CrystEngCommm*, 4, 378–392.
[3] Contreras-Garciá, et al. (2011). *J. Chem. Theory Comput.* 7, 625-632.