

**MS33-2-2 Host-guest crystals with a flexible structure**  
**#MS33-2-2**

K. Kravets <sup>1</sup>, A.W. Coleman <sup>2</sup>, K. Suwinska <sup>3</sup>, O. Danylyuk <sup>1</sup>

<sup>1</sup>Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland - Warsaw (Poland), <sup>2</sup>LMI, CNRS UMR 5615, Université Lyon 1, 43 bvd 11 Novembre, 69622 Villeurbanne, France - Villeurbanne (France), <sup>3</sup>Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University, Wóycickiego 1/3, 01-938 Warsaw, Poland - Warsaw (Poland)

**Abstract**

Soft crystals have structural order, but they are able to change their structure in response to some gentle stimuli. [1] The structural transformations can be induced by mechanical stimuli, temperature, vapour exposure, light, etc. The structural response can be accompanied with the change of colour, shape, size, or optical properties. The category of soft crystals embraces organic, inorganic, and inorganic-organic hybrid crystals. Depending on their structure and properties, these crystals have potential applications in sensors, semiconductors, photosynthetic systems, etc.

Herein, we report a soft host-guest crystal complex obtained from macrocyclic host p-sulfonatocalix[8]arene and iproniazid. p-Sulfonatocalix[8]arene is a water-soluble anionic macrocycle with good flexibility due to the large size of the cavity. The host-guest cocrystallization from aqueous solution gave nice crystals suitable for single-crystal X-ray diffraction analysis. The host-guest supramolecular interaction is guided mainly by the ionic forces and charge-assisted hydrogen bonds between cationic iproniazid and anionic sulfonate groups of calix[8]arene. The crystal packing revealed large water channels between layers of calix[8]arenes and iproniazid molecules acting as pillars in the structure. In order to check the structural flexibility of this complex, the loss of solvent water molecules from the crystal was examined. The air-dried crystals of the host-guest complex have the same space group but different arrangement of guest iproniazid molecules in the structure. The desolvation (dehydration) of the host-guest crystal complex proceeds as single crystal to single crystal transformation. The host-guest framework changes from the channel-type to closed structure, and also the change in hydrogen bonding between host and guest is observed.

**References**

[1] M. Kato, H. Ito, M. Hasegawa, K. Ishii. Soft Crystals Flexible response systems with high structural order. Chem - A Eur J., 25 (2019), pp. 5105-5112.