MS22-P04 | ASSEMBLY, CRYSTAL STRUCTURES AND (NON)LINEAR OPTICAL PROPERTIES OF MULTICOMPONENT MATERIALS CONTAINING SULFONAMIDES

Wojnarska, Joanna (Jagiellonian University, Krakow, POL); Gryl, Marlena (Jagiellonian University, Krakow, POL); Seidler, Tomasz (Jagiellonian University, Krakow, POL); Stadnicka, Katarzyna (Jagiellonian University, Faculty of Chemistry, Cracow, POL)

The constant progress observed in photonics introduces the need for new, more efficient materials. Often, research in materials science focuses on organic crystalline phases as they can possess large and fast responses to the electromagnetic field. The growing demand for innovative ideas motivates scientists to test new molecules as useful components of functional materials.

In this work, we present crystalline phases containing sulfonamides with potential applications in optical devices. Sulfonamides were selected as useful building blocks because many of them possess large values of (hyper)polarizabilities. Additionally, due to their widespread usage in drugs, they are easily accessible and thoroughly examined. The chosen sulfonamide molecules were co-crystallized with selected co-formers to ensure the required polar symmetry necessary for large nonlinear optical properties of even order. The obtained materials were studied using both theoretical and experimental methods. Intermolecular interactions and their influence on molecular assembly were analysed using Bader's QTAIM theory [1] as well as NCI index [2]. The linear (birefringence) and nonlinear optical (second harmonic generation) properties of obtained materials were predicted using the Local Field Theory approach [3] and compared with the experimentally measured responses. The performed analysis of material properties and the arrangement of molecules in crystal architecture enables us to obtain and discuss the structure-property relationship.

[1] R. Bader, Atoms in Molecules: A Quantum Theory, Oxford University Press, USA, 2003.
[2] J. Contreras-Garciá et.al, J. Chem. Theory Comput., 2011, 7, 625-632.
[3] T. Seidler et. al. J. Phys. Chem. C, 2016, 120, 4481-4494.