MS32-P15 | SELENOUREAS AS BUILDING BLOCKS IN BINARY AND TERNARY COCRYSTALS

Grguric, Toni (Division of Organic Chemistry and Biochemistry, Ruder Boškovic Institute, Zagreb, HRV); Ward, Jas S. (University of Jyvaskyla, Deparment of Chemistry, Nanoscience Center, Jyvaskyla); Rissanen, Kari (University of Jyvaskyla, Deparment of Chemistry, Nanoscience Center, Jyvaskyla); Džolic, Zoran (Division of Orgainic Chemistry and Biochemistry, Zagreb, HRV)

A halogen bond is an attractive non-covalent interaction between an electrophilic region in a covalently bonded halogen atom and a Lewis base and recently it took a prominent role in supramolecular synthesis [1]. Oxygen and nitrogen atoms were predominantly used as acceptors of halogen bond, although there are few examples of heavier atoms such as S, P, As, Sb as acceptors [2].

In recent paper, thioureas were utilized in construction of ternary cocrystal [3]. Giving that bonding nature of sulfur and selenium should be similar; we selected selenoureas as potential candidates in construction of binary and ternary cocrystals. It is known that selenium atoms can act as a hydrogen bond acceptor or even a chalcogen bond donor, but there are only few examples of selenium atom as a halogen bond acceptor.

Cocrystallization of selenoureas and different perfluorohalocarbons with 18-crown-6 led to formation of ternary cocrystals in which molecules of selenoureas formed 2:1 discrete complex with 18-crown-6 via N–H···O hydrogen bonds, while formed aggregates were further connected via I···Se halogen bonds forming 2D or 3D networks.

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