## **MS32-P08** | INTERMOLECULAR CHALCOGEN···HALOGEN INTERACTION IN ORGANIC

## **MOLECULAR CRYSTALS**

Kazmierczak, Michal (Adam Mickiewicz University, Poznan, POL); Katrusiak, Andrzej (Adam Mickiewicz University, Poznan, POL)

Interactions between chalcogen and halogen atoms are one of the least investigated type of  $\sigma$ -hole bonding in crystals. The focus of academia is shifted to much frequently occurring halogen and chalcogen bonds. Although, structures where formation of chalcogen…halogen contact is possible are relatively common, there is always probability of creation of competing halogen…halogen or chalcogen…chalcogen contacts in such structures. Axiomatic impossibility to avoid this competition, makes chalcogen…halogen interactions less frequent and as a result harder to investigate. Nevertheless, datamining of the Cambridge Structural Database [1,2] allowed us to reveal group of organic molecular crystals with governing chalcogen…halogen interactions. For this population understanding the nature of this cohesion force is crucial for explaining process of molecular aggregation.

[1] Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Crystallogr. B.* **58**, 389–397.

[2] Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater. 72, 171–179.