

*Halogen bonded capsules*Kari Rissanen<sup>1</sup><sup>1</sup>Chemistry, University Of Jyvaskyla, Jyvaskyla, Finland

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In the last 15 years growing attention has been focused to halogen bonding (XB) stimulated by its intriguing properties, such as strong directionality, specificity and strength comparable to hydrogen bonding (HB). Recently, we have applied this "long lost brother" of hydrogen bonding to very strong (OC)<sub>2</sub>N-I•••N halogen bonds using N-iodosuccinimide (NIS) and N-iodosaccharin (NISac) as very strong XB donors and pyridine N-oxides as very strong XB acceptors. Using these XB counterparts led to a new N-X+•••-O-N+ paradigm for halogen bonding[1] and have yielded extremely strong halogen bonded complexes with very high association constants characterised in either CDCl<sub>3</sub> or acetone-d<sub>6</sub> solution by <sup>1</sup>H NMR titrations and in the solid-state by single crystal X-ray analysis. The obtained halogen bond interactions, RXB, in the solid-state are found to be in the order of strong hydrogen bonds, viz. RXB ≈ RHB. Using alternative, yet similarly strong, bifunctional XB donors such as I-I (viz. iodine) or I+ (iodonium cation), both of which can act as bisfunctional XB donors, results in systems like A•••I-I•••D or A•••I(+ )•••A (where A = XB acceptor). Using spatially preorganized and directed XB tetra-acceptors we have managed to create the first dimeric solid-state capsule solely based on halogen bonds [2] and an extremely robust molecular capsules with the help of [N•••I+•••N] halogen bonds.[3] The lecture will highlight the use of XB in these capsules.

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[2] N. K. Beyeh, F. Pan and K. Rissanen, Angew. Chem., Int. Ed. (2015), 54, 7303 - 7307.

[3] L. Turunen, U. Warzok, R. Puttreddy, N. K. Beyeh, C. A. Schalley and K. Rissanen, Angew. Chem. Int. Ed. 55 (2016), 14239 - 14242.

**Keywords:** [Halogen Bonding](#), [Molecular Capsules](#), [X-ray Crystallography](#)