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Directed reactivity in halogen-bonded cocrystals

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Halogen bonds enable chemists to direct the self-assembly of molecules and/or ions in various media. In this presentation, we will describe our efforts to employ halogen bonds to direct chemical reactivity in the organic solid state. Specifically, we describe the use of small molecules as halogen-bonding templates to assemble alkenes lined with I- and F-atoms in positions for intermolecular [2+2] photodimerizations [1]. The photoproducts form stereoselectively and quantitative yield. In our work, we have discovered the ability of halogen bonds to undergo bending deformations in rare single-crystal-to-single-crystal transformations. Applications of the photoproducts as building blocks in supramolecular chemistry and organic synthesis will be discussed.

[1] Sinnwell, M.A.; MacGillivray, L. R. Angew. Chem., Int. Ed. (2016) 55, 3477-3480.

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