Two-dimensional Supramolecular Structures Mediated by Halogen Bonds: Comparing Cl and Br

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Covalently bonded halogen ligands possess unusual charge distributions, attracting both electrophilic and nucleophilic molecular ligands to form halogen bonds. In many biochemical systems, halogen bonds coexist with hydrogen bonds, being complementary to them due to their similar bond strength and dissimilar directionality. In this study, we directly visualize the individual molecular configuration of chlorinated 1,5-dichloroanthraquinone and brominated 1,5-dibromoanthraquinone molecules on Au(111) using scanning tunneling microscopy. The precise arrangements of observed molecular structures were explained in the context of halogen and hydrogen bonds. We discuss the distances and the strengths of the observed halogen and hydrogen bonds, which are consistent with previous bulk data.

Keywords: Supramolecular self-assembly, Scanning tunneling microscopy, Halogen bond, Hydrogen bond, Chirality