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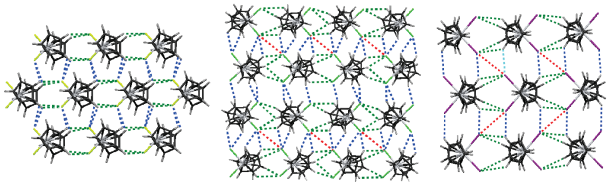

Figure 1. Crystal packing of Cp_2TiF_2 (left), Cp_2TiCl_2 (centre), and Cp_2TiI_2 (right): intrachain C-H···X (green), interchain C-H···X (blue) and X···X (red) interactions.

Keywords: Halogen bonding, Organometallic compounds

MS32-P2 Hydrogen bonds chains supported by halogen-halogen interactions in di- and trihaloimidazoles

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Switchable polarization of NH···N hydrogen bonds remains in a great interest of crystallographersdue to their ferroelectric properties. This effect has been recently reported for dabco salts and halobenzimidazoles. Halogen interactions are kind of electrostatic interaction that can be as strong as hydrogen bods and may force different molecules arrangement in space. What is more X···Xinteractions can significantly shorten NH···N bond length and allow proton transfer along hydrogen bond chains. During our studies we synthesized several haloderivatives of imidazole. Collected X-raydiffraction data at ambient conditions allowed us to determine five novel structures of double and triple substituted imidazoles at ambient conditions as an introduction for further high-pressure studies. The main structural features of all investigated haloimidazoles are: molecules arranged in sheets made of chains linked by NH···N bonds with X···X interactions holding sheets together. Halogen substitution causes steric hindrances which has major effect to the molecules arrangement. What is more, electronegative halogen atoms withdraw more electrons of the imidazole ring than H-atoms strengthening NH···N bonds.

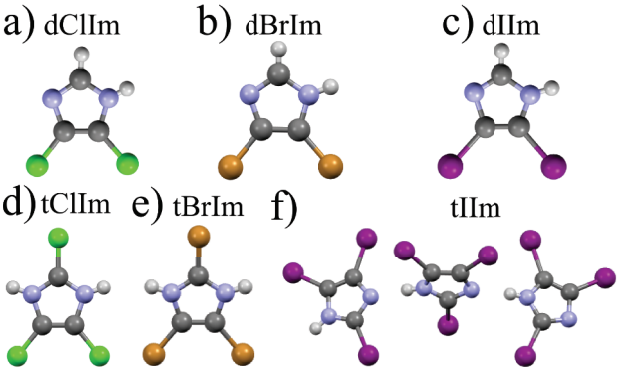

Figure 1. Haloimidazoles studied during research and their acronym symbols: (a) 4,5-dichloroimidazole (b) 4,5-dibromoimidazole (c) 4,5-diiodoimidazole (d) 2,4,5-trichloroimidazole (e) 2,4,5-tribromoimidazole (f) 2,4,5-triiodoimidazole.

Keywords: halogen-halogen interactions, hydrogen bond, imidazole.