Poster Presentation

MS093.P06

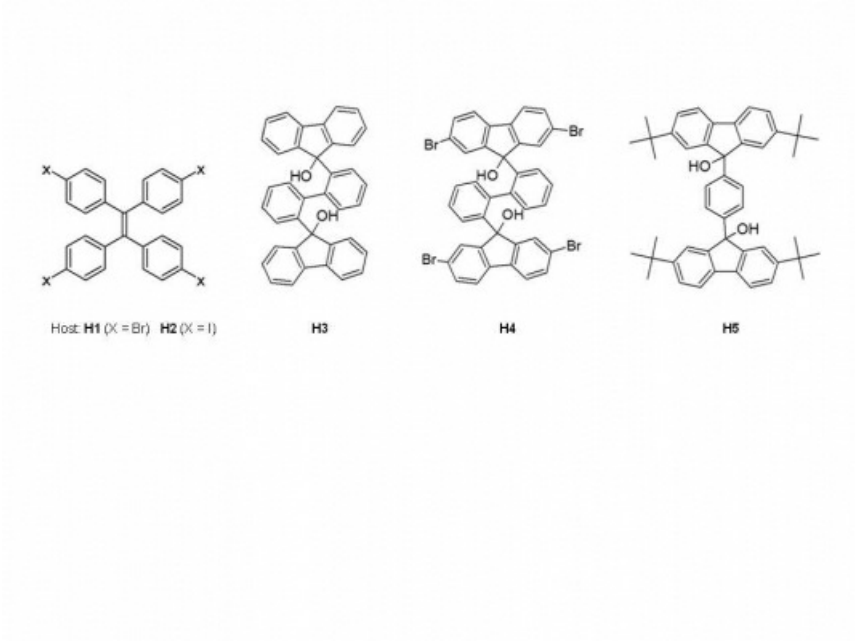
Single crystal XRD structural elucidation of halogenated host-guest compounds

Hong Su[1], Francoise M. Amombo Noa[1], Susan A. Bourne[1], Luigi R. Nassimbeni[1]
[1]*Chemistry Department, University Of Cape Town, Cape Town, South Africa*
E-mail: hong.su@uct.ac.za

Halogen bonding interactions, which are similar to, yet different from hydrogen bonding, have been attracting considerable interest. Both of them are complementary yet competing in the Supramolecular system [1,2]. Elucidation of the structures of various host-guest systems, in which either the host or the guest or both are halogenated, make it possible to identify the finer details of these interactions, so as to formulate useful synthetic crystal engineering strategies that fully utilize the versatile possibilities that these interactions offer.

In the work presented here, the single crystal XRD structures, which occur in the inclusion compounds formed by the hosts tetrakis(4-bromophenyl) ethylene (H1) and its iodo-analogue (H2), 9,9'-(Biphenyl-2,2'-diyl)difluoren-9-ol (H3), 2,2',7,7'-tetrabromo-9,9'-(biphenyl-2,2'-diyl)difluoren-9-ol (H4) and 2,2',7,7'-tetra-tertbutyl-9,9'-(1,4-phenylene)difluoren-9-ol (H5), with the guests 1,2-dichloroethane, methyl iodide and a number of substituted pyridines, are elucidated. In addition, there are also structures of intermediate inclusion compounds which occur during single crystal to single crystal guest exchange transformation, or selected from competition crystallisation experiments. These structures, which exhibit disordered mixed guests, posed special challenges with respect to the refinements of the site occupancy factors of the mixed guests, and a reasonable starting model for the site occupancies is very important for the final refinement to converge [3].

[1] Resnati, G. et al. (2005). Acc. Chem. Res. 38, 386-395.
[2] Aakeroy, C. B. et al. (2015). IUCrJ, 2, 498-510.
[3] Nassimbeni, L. R.; Su, H. (2013). CrystEngComm, 15, 7396-7401.



Keywords: hydrogen bond, halogen bond, intermolecular interaction