Poster Presentation

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Influence on the self-assembly of sterically-hindered arylsufonamides

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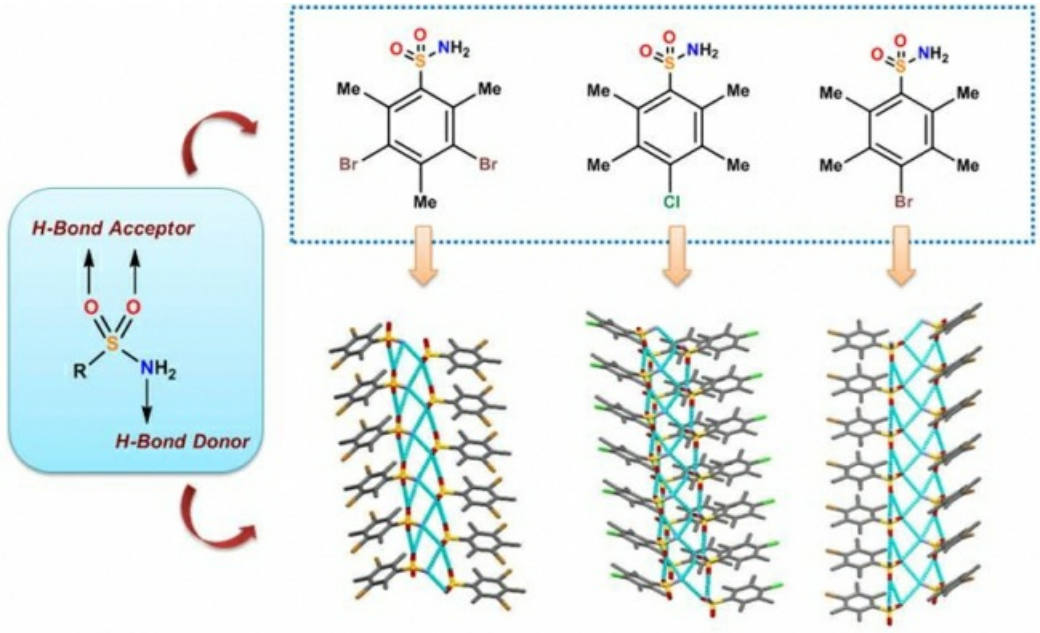
Strong and highly directional hydrogen bonding is the most important of all other noncovalent interactions to program molecular modules to develop macroscopic bulk materials with a pre-defined molecular organization. It is the synthon reproducibility that is the basis for engineering molecular aggregation to develop crystalline solids of importance in diverse areas.

In our laboratories, we have been interested in understanding how sterics influence supramolecular synthons of very important functional groups, namely, acids, alcohols, amides, boronic acids, etc. It has been previously shown that weakly interacting halogens decisively modify the robust supramolecular synthons of carboxylic acid and amide functional groups. [1,2] In a logical continuation of these investigations, we have embarked upon investigation of the self-assembly of sterically-hindered benzenesufonamides and influence of halogens located at different positions. The sulfonamide functional group is uniquely characterized by the presence of two hydrogen bond-accepting oxygen atoms and two hydrogen donors. As each functional group can effectively involve in 4 hydrogen bonds, it is of fundamental importance to examine how the synthons due to this group are influenced both by sterics as well as weakly interacting groups such as halogens. In Figure 1 are shown structures of some sufonamides synthesized and the crystal structures determined along with the crystal packing diagrams for some of them.

The details of crystal structure determinations and comprehensive analysis of the supramolecular synthons observed in a series of sterically-hindered benzenesulfonamides substituted with halogens will be presented

[1] Moorthy, J. N. et al. (2002). J. Am. Chem. Soc., 124 (23), 6530–6531.
[2] Moorthy, J. N. et al. Unpublished results.



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