

Sulfur as Hydrogen Bond Acceptor

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Amino acids consisting of sulfur atom show a variety of interactions in proteins that are hydrogen bonding as well as non-hydrogen bonding.[1,2] Among them the prominent interactions are O-H---S, N-H---S, and C-H---S. Despite the fact that sulfur is a biologically abundant element (amino acids, disulfide bridges, etc.) and is a well established constituent of the therapeutic agents (penicillins, thionucleosides, etc.) and agrochemicals, not much experimental investigations have been done on the X-H—S hydrogen bonding interactions, where X=N or O atom. In recent times we have been investigating the weakly bound complexes between p-cresol, indole and several sulfur containing solvent molecules from the perspective of investigating the H-bonding interaction between XH donor and S acceptor, the salient features of which will be presented.

In the case of X=O we have also investigated the similarities and differences in the XH—O vs XH—S interaction, using a variety of analogous solvent molecules. It turns out that although the XH—S interaction is largely dominated by the dispersion component, it also exhibits a fair amount of the charge transfer component as envisaged by the large red shifts in the XH stretching frequency. The OH—S interaction in the p-cresol-dimethylsulfide complex and the NH—S interaction in indole-dimethylsulfide complex shows yet another aspect of the interaction that in the later interaction the charge transfer component is almost two times as large as that in the OH—S interaction.[3,4]

References:

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