



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.  
Thesis Title:  
Self-assemblies of Sulphonamide Derived Urea, Thiourea and Conformational Isomers of a Mercury complex  
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The thesis described various solid-state assemblies of urea and thiourea derivatives of sulfa-drugs that had sulphonamide functional group as part of the structural backbone. The hydrogen bonded assemblies of these compounds, solvates, and polymorphic solvates were structurally characterized. The role of dimeric hydrogen bonded moieties within those self-assemblies to modulate the number of solvent molecules in solvates and also providing an aid to understand polymorphs were discussed. A theoretical calculation on dimeric hydrogen bonded assemblies could establish the observed trends in the melting points in a series of positional isomeric compounds. The utilities of these thiourea or urea-based compounds to encapsulate tetrabutylammonium halides, and also in the detection of fluoride ions in solution were described in the thesis. The content had descriptions on the conformational isomers of a mercury complex involving a thiourea based compound linked to an anthracenyl unit where distinctions of the isomers in solution as well as in solid states could be possible. The conformational changes observed from experimental studies were also complemented by theoretical energy optimizations to provide insights to the structure-property relationships