



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title: **Recognition of Anionic Guests by Dipodal/Tripodal Receptors: Positional Isomeric and Electronic Effect**

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SHORT ABSTRACT

The thesis provides some substantial outcomes in the domain of 'supramolecular anion recognition chemistry' where the anions/hydrated anions or anionic associations are captured by some series of isomeric dipodal or tripodal artificial acyclic receptors driven by positional or electronic effect of terminal aryl substituents or anion size or molecular host architectures. In general, the present findings from the experimental studies deliver the anionic guest induced capsular, pseudo-capsular, paddle-wheel shaped, linear barrel shaped or polymeric aggregated assembly formation *via* neutral host-guest associations. The results from solid as well as solution state studies have unveiled an interesting binding feature of host towards the guest.

The *o*-phenylenediamine based receptor **L**₁ has been shown to encapsulate the unique triangular [(Cl)₃-DMSO] dual guest association, while its isomeric receptor isomer **L**₂ forms 2:2 noncooperative [(L₂)(Cl⁻)₂] complex. Another *o*-phenylene connected receptor **L**₃ has been found to encapsulate cyclic [(F⁻)₂(H₂O)₂] tetramer as well as unusual (Cl⁻)₂, (Br⁻)₂ and (I⁻)₂ anionic assemblies and divalent carbonate by hydroxide ion induced atmospheric CO₂ fixation. The cyclic [(F⁻)₂(H₂O)₂] tetramer, rugby-ball shaped [SO₄²⁻-(H₂O)₃-SO₄²⁻] adduct, unprecedented [CO₃²⁻-(H₂O)₂-CO₃²⁻] cluster, double divalent sulfate anions as well as unusual asymmetric sulfate anions (naked and cyclic hydrated), linear [(OCOCH₃)(H₂O)]_n polymeric assembly and acyclic (Cl⁻)₂-(H₂O)₂ assemblies have been found to be captured within the neutral self-assemblies of isomeric *m*-phenylenediamine based receptors **L**₄-**L**₈. Furthermore, the *p*-phenylenediamine based linear isomeric receptors **L**₉-**L**₁₅ have been found to entrap cyclic (HCO₃⁻)₂ dimer by F⁻/OH⁻ induced aerial CO₂ fixation and linear polymeric aggregation of (H₂PO₄⁻)_n in most of the cases within the non-cooperative receptor assemblies. On the other hand, the terminal aryl substituted multi-armed isomeric tripodal tris-amine (**L**₁₆-**L**₁₈)/ tris-urea (**L**₁₉-**L**₂₃) receptors demonstrated the cavity induced encapsulation of halide and oxyanions in either protonated or neutral host-guest assemblies. Moreover, the highly electron-rich isomeric tripodal tris-urea receptors **L**₂₄-**L**₂₅ showed ice-like cyclic (H₂O)₆ inside unique hexameric receptor-anion neutral assemblies and among their thiourea analogues **L**₂₆-**L**₂₇, the receptor **L**₂₆ form unimolecular pseudo-capsular assemblies with all anionic guests and the receptor **L**₂₇ form dimeric receptor capsular cages with anions in either 2:2 or 2:1 host-guest fashions.