



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Anion and Ion-Pair Directed Self-Assembly of Urea Functionalized Molecules**

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SHORT ABSTRACT

The thesis consists of five chapters including introduction and experimental sections.

The first experimental work viz Chapter 3 describes the evidence of fluoride induced uptake of atmospheric CO₂ and its stabilization as HCO₃⁻ anion by a structurally simple acyclic 1,3-bis(4-iodophenyl)urea receptor, **L**₁. The in situ formed HCO₃⁻ complex (**1a**) is stabilized by a concert act of hydrogen and halogen bonding donated by the receptors. To the best of our knowledge, 1,3-bis(4-iodophenyl)urea is the simplest of anion receptors that displays a concert act of hydrogen and halogen bonding to stabilize aerial CO₂ as HCO₃⁻. While 1,3-bis(4-bromophenyl)urea, **L**₂ has shown completely lacking if halogen-bonding donor ability throughout its entire results.

The second experimental work viz Chapter 4 is in two parts. Part 1 deals with a set of three nitrophenyl functionalized tripodal urea scaffolds, **L**₃, **L**₄ and **L**₅ and demonstrate the effect of positional isomerism in anion coordination. The *para*-isomer (**L**₃) self-assembles into dimeric (pseudo)molecular capsules as observed in carbonate and terephthalate complexes (**3a** and **3b**). On the other hand, the *meta*-isomer (**L**₄) self-assembles into dimeric capsules only in the presence of inorganic oxyanions (complex **4a**), and assembles into a 2D sheet-like structure in the presence of terephthalate dianion (**4b**). In contrast to **L**₃ and **L**₄, structural authentication of the *ortho*-isomer (**L**₅) in the presence of different oxyanions was not fruitful presumably due to the steric effect provided by the -NO₂ group at the ortho-position, which hinders the facile inclusion and coordination of an anion due to electrostatic factor, as confirmed by 2D-NOESY NMR analysis of the free receptor. Part 2 of the Chapter 4 deals with the *para*-isomer (**L**₃), which in association with 18-crown-6-ether self-assembles into an integrated 1D coordination polymer in the presence of K₂CO₃ (complex **3d**).

The last Chapter is about the recognition of tetrameric mixed phosphate clusters by **L**₃ in its neutral and charged state. Receptor **L**₃ self-assembles, in the presence of excess *n*-TBA(H₂PO₄), into a tetrahedral molecular cage by encapsulation of a tetrameric tetrahedral mixed phosphate cluster (**3e**). Further in the presence of H₃PO₄, **L**₃ self-assembled with side-cleft bonded cyclic planar tetrameric anion-acid cluster (**3f**).