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Title:	Modular Approaches to Assemble Macrocycles and Pyridinophanes Containing P/N, Al/N, B/N and Zn/N Connectivity in the Framework
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Abstract:	<p>Macrocycles have fascinating ring structures, and attracted significant attention in the field of molecular recognition, catalysis and their coordination complexes exhibit wide structural diversity. Nature being an important source of bioactive macrocycles, many synthetic macrocyclic complexes, that mimic the naturally occurring macrocyclic systems, such as porphyrins, metalloproteins, cobalamine, vancomycin, etc. have been reported. While families of organic macrocycles exert substantial influence across various chemistry disciplines, the exploration of inorganic and hybrid organic-inorganic macrocycles has been limited. Though, the synthesis of macrocyclic system containing inorganic elements is not an easy task and entails the careful tailoring and scrutiny of suitable preorganized building blocks and linker moiety. Their synthesis involves various challenges like variable oxidation states, orbital mismatch, polar nature of bonds, moisture sensitivity and hydrolytic instability etc. Despite these obstacles, the assembly of such macrocyclic frameworks has been achieved through resourceful approaches and significant expertise. This thesis investigates the systematic and rational approaches to assemble novel macrocyclic systems. The first chapter of the thesis gives a brief description and investigates the use of cyclodiphosph(III)azane as an efficient preorganized building block for macrocyclic frameworks. In the past two decades, series of hybrid organic-inorganic cyclodiphosph(III)azane based macrocycles have been experimentally and theoretically highlighted, while the analogous bicyclic counterparts are lagging behind. In the current work, we have investigated the synthesis and characterization of cyclodiphosph(III)azane $[ClP(\mu-NiBu)]_2$, based inorganic-organic hybrid bicyclic macrocycles. Second chapter 2A, presents the versatility of the preorganised building block bis(trimethylsilyl)-N,N'-2,6-diaminopyridine (bap) to synthesise molecular topologies containing -N-Al-N- inorganic bridges. While chapter 2B describes the use of analogous triazine derivatives which shows completely different reactivity. The reaction of bis(trimethylsilyl)-N,N'-2,4-diamino-6-(Me)-triazine (BDMT) and bis(trimethylsilyl)-N,N'-2,4-diamino-1,3,5-triazine (BDT) with borane leads to the dearomatization of triazine ring by the addition of B-H bond across the -C=N- bond. Further the reduced triazine rings self-assembled to afford -N-B-N- bridged macrocyclic framework and DFT calculations were also performed to understand the mechanism involved in dearomatization. Third chapter of thesis deals with the synthesis of zinc containing different molecular topologies including pyridinophane, molecular bowl cluster complexes and bicyclic pyridinophane, where zinc is the constituent member of cyclic core and involve in ring formation. All the new molecules have been characterized by single crystal X-Ray, HRMS and multinuclear NMR. In conclusion, the thesis reveals the successful synthesis and spectroscopic studies of several hybrid organic-inorganic macrocycles with diverse structural motifs and functionalities.</p>
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