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Title: Design and Synthesis of boron- containing organic molecules: Exceptional photophysical, mechanical and optical properties

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Abstract: Organic luminescent materials play a major role in the advancement of materials science. Among the various known organic luminescent materials, boron containing organic molecules (BCOMs) are emerging as a promising class of molecules because of the ease of synthesis and exceptional photophysical properties. One of the popular strategies for the synthesis of BCOMs is to incorporate boron into a π -conjugated system. This approach exploits the electron-deficient nature of boron wherein a lone-pair of electrons from the organic chelate moiety is donated to boron. Boron coordination imparts unique optoelectronic functions and enhances the performance of BCOMs in energy-conversion devices such as organic field-effect transistors, organic photovoltaics, organic light-emitting diodes, organic lasers etc. Tetra-coordinate borate dyes such as boron-dipyrromethenes (BODIPYs) are extensively used for luminescence based applications in biology such as photodynamic therapy, bioimaging etc. Although they exhibit favourable photophysical properties, their low synthetic yield and the tendency for aggregation caused quenching limits their application in materials science. As compared to BODIPYs, compounds obtained by chelating boron to N,O-bidentate ligands like Schiff's bases are comparatively easier to synthesize with good synthetic yields. Further, their fluorescence could be tuned by appropriate functionalization and the solid-state emission could be enhanced through structural variations. This dissertation is devoted to the design and syntheses of novel boron-containing luminescent organic molecules and studying their mechanical and optical properties. Chapter 1 reviews the literature on luminescent BCOMs with an emphasis on tetra coordinate boron containing molecules. We have briefly summarized the structural features and related attributes of tri-coordinate boron compounds followed by a short discussion on optical and self-assembly properties of BODIPYs. The limitations of BODIPYs have also been discussed which demands the development of new fluorophores. Further, we have discussed stimuli responsive properties of BCOMs synthesized from simple N,N-, O,O- and N,O-bidentate ligands. Besides, the self-assembly of BCOMs into gels, liquid crystals and flexible crystals has also been discussed highlighting the effect of self-assembly on their optical and mechanical properties. Chapter 2 describes the synthesis and characterization of difluoride boron complexes of a few Schiff's bases. As the side chains are known to affect the photophysical and selfassembly properties of organic molecules, we have designed and synthesized the difluoride boron complexes A-D (Chart 1) based on salicylideneimine and naphthalideneimine moieties as a core wherein the side chains were systematically varied from alkyl to fluoroalkyl. Further, we have also synthesized two compounds E and F by introducing a side group containing an electron rich moiety with the objective of investigating the role of positional isomerism on the self-assembly and optical properties. Page 2 of 2
Chart 1 Chapter 3 discusses the importance of side groups on the self-assembly of BCOMs. We found that the salicylideneimine-boron complex with an alkyl chain (compound A) formed flexible single crystals whereas fluoroalkyl substituted compound B formed organogels. But when the core was changed from salicylideneimine to naphthalideneimine, the compounds C and D formed single crystals with distinct properties. While the single crystals of C were brittle, the single crystals of compound D exhibited both plastic and elastic bending depending on their dimensions: thick crystals were observed to be plastic whereas the thin crystals were elastic. Next, we studied the self-assembly of the positional isomers E and F, both of which yielded single crystals with different properties: crystals of compound E displayed multiple phenomena such as polymorphism, thermochromism, thermal luminescence switching and thermosensitive properties whereas the crystals of F did not exhibit any of these properties. The distinct features of positional isomers E and F clearly demonstrates the impact of molecular design on their mechanical and luminescence properties. The unique self-assembly and mechanical properties of each of these compounds have been explained through detailed crystallographic and microscopic analysis. Chapter 4 focuses on the photophysical properties of the compounds A-F and the effect of side groups on their optical properties. While the flexible side chains had a minimal effect on the luminescence of the core moieties, the rigid side group in E and F containing an electron rich moiety played a major role in the photophysical properties. It was observed that the fluorescence properties of E and F could be modulated by changing solvent polarity and temperature. Further, we have also explored the potential application of these molecules as optical waveguides, security markers and as sensors. Owing to its flexibility and luminescence properties, crystals of A and D were useful as optical waveguides whereas compound B was used for hydrophobic luminescent marker applications. The reversible thermochromism, thermo-luminescence switching and acidochromic luminescent behaviour of E and F were utilized for anti-counterfeiting applications.

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