Notification No. : 564/2024 Date of Award : 23-07-2024

Name of the Scholar: Shakeel AlviName of the Supervisor: Dr. Rashid AliName of the Department/Centre:ChemistryTopic of Research: Design, synthesis and properties of functional
truxene based π-conjugated systems

Findings

This work of my Ph.D. thesis has been on the topic Design, synthesis and properties of functional truxene based π -conjugated systems. Truxene, a heptacyclic polyarene with $C_{3\nu}$ symmetry, has gained significant scientific interest due to its exceptional solubility, robust thermal stability, rigid planar structure, and ease of modification. Initially utilized for synthesis and photoluminescence, truxene's applications have expanded into organic electronics, bioinorganic chemistry, medicinal chemistry, materials science, and environmental sciences. Its versatile applications include roles in transistors, organic photovoltaics (OPVs), lasers, molecular wires, sensors, organic light-emitting diodes (OLEDs), organogels, fluorescent probes, liquid crystals, dynamic nuclear polarization, and nonlinear optical (NLO) materials. This work explores novel synthetic routes to C_3 -symmetric pyrrole-based truxene architectures via cyclotrimerization, ring-closing metathesis (RCM), Clauson-Kaas, and Ullmann-type coupling reactions, including the assembly of heterocyclic systems such as oxazole, imidazole, benzimidazole, and benzoxazole within the truxene framework. We also introduce an ecofriendly method for synthesizing diverse pyrrole derivatives through Paal-Knorr condensation using a low-melting mixture of N,N'-dimethylurea and L-(+)-tartaric acid as a dual catalyst/solvent system, which enables high yields and reusability. Furthermore, we detail an efficient approach to indolo-truxene hybrids and report the first synthesis of truxene-based mono-, di-, and tri-substituted dipyromethanes (DPMs), along with their preliminary photophysical properties. Additionally, we present push-pull truxene derivatives incorporating mono-cyanovinyl and 1,3-indanedione groups, synthesized through cyclotrimerization, alkylation, mono-formylation, and Knoevenagel condensation.