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Synthesis of Precursors of Cycloparaphenylenes Using Ullmann Coupling

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[n]Cycloparaphenylenes ([n]CPPs) are carbon and hydrogen containing macrocycles which constitute of 'n' number of para-phenylene groups connected via 1,4-biphenyl –C–C– linkages. The chemical, photochemical and electrochemical properties of [n] CPPs make them potential candidates for a broad range of applications. Although [n]CPPs have aesthetically appealing chemical structures, their high energy geometries make them a synthetically challenging class of molecules. Synthesis of [n]CPPs reported thus far associated with expensive catalysts, starting materials and sophisticated reaction conditions. Therefore, this research project was focused on the synthesis of a series of precursors of [n]CPPs; dimer, trimer, tetramer and other oligomeric precursors of 1,4-chlorobenzene using Ullmann coupling with the eventual intention of cyclizing those precursors to obtain a series of [n]CPPs which is feasible in the Sri Lankan context. A number of syntheticattempts followed by the reaction condition optimization attempts were made using 1,4-chlorobenzene as the starting material and activated copper as the catalyst in various solvents at various temperatures to synthesize the [n]CPP precursors. Dimerization of 1,4-chlorobenzene was carried out using activated copper as the catalyst in N-methyl-2-pyrollidone (NMP) solvent at 140 oC. The crude mixture was subjected to column chromatography to obtain clear light yellow color liquid which was characterized using UV-visible, fluorescence and NMR spectroscopy. UV-visible spectra of the obtained product in chloroform exhibited a characteristic absorption peak for the $\pi \rightarrow \pi^*$ transition of the conjugated biphenyl rings which shows λmax at 272 nm. The fluorescence spectra of the obtained product demonstrated a significant enhancement of the fluorescence activity compared to the starting material. The two doublets appeared in between chemical shift values of 7.00 - 8.00 ppm in the 1H NMR spectrum of product in CDCl3 evidenced the formation of the dimer of 1,4-dicholorbenzene, 4,4'-dichlorobiphenyl. In summary, dimerization of 1,4-dichlorobenzene was carried out using Ullmann coupling. Reaction condition optimization and characterization of trimer, tetramer and other oligomers of 1,4-dichlorobenzene are currently underway.

Keywords: [n]Cycloparaphenylenes, Ullmann coupling, 1,4-dicholorbenzene, 4,4'- dichlorobiphenyl