



"The Synthesis, Characterization, and Molecular Modeling of Cyclic Arylene Ether Oligomers"

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Abstract

Cyclophanes are a family of bridged cyclic aromatic compounds that have found extensive applications in host-guest chemistry, molecular recognition, biomimetics and most recently as precursors in ring-opening polymerizations.

This research presents the synthesis of several novel cyclic arylene ether oligomers, based on 1,2-bis(4-fluorobenzoyl) benzene with 3, 3'-methylene diphenol and 3,3'-(ethylene dioxy) diphenol, and their characterization by LC-MS/MS, 1-D H-NMR and x-ray crystallography. Electrospray ionization (ES) along with MS/MS was used to characterize cyclic oligomers of molecular weight up to 1600 Da. The thermal properties of these cyclic oligomers were studied by differential scanning calorimetry (DSC) and thermal gravimetric analysis (TGA).

These cyclic oligomers were synthesized in high yield by regulating the reaction time, concentration, temperature and solvent systems. The relevance of reaction conditions was investigated by selected reaction monitoring (SRM).

Molecular dynamics and potential energy calculations were also carried out to understand the molecular characteristics of the bisphenols that lead to the formation of these cyclic species. Furthermore, the molecular modeling studies assisted in predicting the conformations of the small macrocyclic rings. The predicted structures indicated the cavity size and the relative orientation of the oxygen atoms.