

BEYOND THE BEND: EXPLORING THE CONFORMATIONAL LANDSCAPE OF DECYL, UNDECYL, AND DODECYLBENZENE

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Alkylbenzenes are important components in the combustion process: they make up 20-30% of petroleum fuels and are intermediates on the pathway to soot formation. Understanding their conformational preferences is a vital step in understanding the processes by which fuels begin their journey from small, simple hydrocarbons into the large, graphitic masses of soot. Previous work done in our group, in collaboration with the Sibert group, found that the smallest alkylbenzene which folds its chain back over the ring is octylbenzene. The population of the lone folded structure in octylbenzene is low; however, theory predicts a rapid stabilization of the folded conformations relative to more extended structures as the chain length is increased, suggesting a likely shift in population towards folded structures. This talk will focus on our exploration of this possibility by discussing the UV excitation and single conformation IR spectra of decyl, undecyl, and dodecylbenzene, where increasing chain length allows for multiple stable folded configurations.