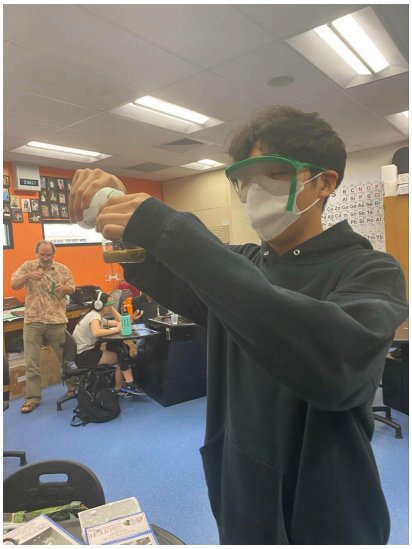
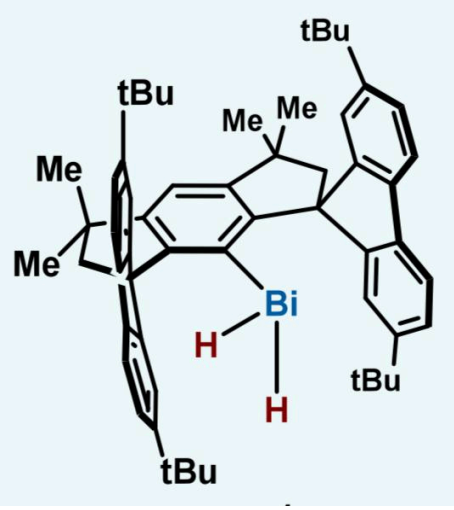
Computational Analysis of Organobismuth Hydride Complex

By: Min Shin ‘26
Mentor: Dr. Sattasathuchana and Dr. Hyvl



Organobismuth compounds are emerging as promising alternatives to traditional transition-metal catalysts, which are widely used to speed up chemical reactions such as radical polymerization (making polymers), hydrogenation (adding hydrogen to molecules), and even breaking down plastics through hydride attack. Compared to transition metals, bismuth is less toxic, more affordable, and more environmentally friendly. Despite this potential, organobismuth catalysts remain relatively underexplored. Current research focuses on discovering new reaction pathways and improving the stability of these complexes, particularly the crucial bismuth–hydrogen (Bi–H) bond, often stabilized by bulky ligands.



My project uses computational chemistry to better understand how these complexes behave. I will optimize molecular structures with quantum mechanical models (Hartree-Fock and DFT) and study bonding with quasi atomic orbital (QUAO) analysis. This will show how different ligands—molecules bound to the bismuth center—affect both the Bi–H bond and overall catalyst stability. In addition, I will calculate the energy needed for homolytic cleavage of the Bi–H bond (breaking it into radicals with unpaired electrons) to evaluate how efficiently the catalyst can cycle between Bi(III) and Bi(II) oxidation states. The radicals are potentially useful in many different reactions as mentioned above (e.g., radical polymerization, hydrogenation, etc.)

By combining structural modeling with bonding analysis, my research aims to guide the design of safer, more efficient bismuth-based catalysts, potentially providing greener alternatives to many transition-metal systems.