

Functionalized Boron Nanoparticles: Characterization of Thiol-ene Click Chemistry

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Carboranes are a family of cluster compounds comprised of boron, carbon, and hydrogen that are being investigated in a number of applications, including self-assembling monolayers (SAMs), cancer treatment, and non-catalytic synthetic agents. Various functionalities have been attached to carboranes to facilitate their utilization. Thiol-ene “click” chemistry between thiol-functionalized m-carborane and a variety of maleimide derivatives provides a facile path to a wide variety of functionalized boron nanoparticles. The reaction rate shows a strong dependence on the solvent as well as on the position of the thiol group on the carborane. To test the reaction rate dependences, absorbance measurements were taken over time in a temperature controlled spectrophotometer for each selected solvent. Preliminary testing revealed reactivity differences greater than an order of magnitude between m-carborane-1-thiol and m-carborane-9-thiol. In order to better understand observed differences in reactivity, the chemical kinetics are modeled to clarify the reaction mechanisms and to quantify the rate constants and activation energies. Future research entails computational and electron density modelling to further investigate the cause of the reaction kinetic differences.

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