

Density functional theory, semiempirical, and genetic algorithm exploration of the reactivity of silyl ketenes

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Poly(silyl ketene)s have been proposed as a class of polymers with a potential range of desirable properties, such as degradability. Under appropriate circumstances, both the C=C and C=O moieties within the silyl ketenes can undergo reactions, leading to different chemical reactivities and, ultimately, different products. Therefore, it is important to establish the fundamental reactivities of silyl ketene monomers to improve the ability to plan targeted syntheses of desirable products. This work presents computational studies that build on earlier work [1] studying the activation of silyl ketene monomers by reaction with nucleophiles. Depending on the interplay between nucleophile and monomer, activation occurs via nucleophilic addition to or deprotonation of the monomer, respectively. Systematic studies were performed to characterize the different reaction pathways and to help rationalize trends in reactivities.

- (1) Yuanhui Xiang, Sarah Mitchell, Arnold L Rheingold, Daniel S Lambrecht, and Emily Pentzer, Oligomerization of Silyl Ketene: Favoring Chain Extension over Backbiting, *Macromolecules*, 2019, 52, 6126-6134