



Study of Spontaneous Thermal Polymerization of Alkyl Acrylates Using Computational Quantum Chemistry

Masoud Soroush, Department of Chemical and Biological Engineering, Drexel University

Conventional thermal initiators are fairly expensive raw materials in resins and coatings production, and spontaneous thermal polymerization does not require any added conventional initiators. Polymer resins and coatings that do not include any residual groups from conventional initiators are more resistant to UV radiation. High-temperature spontaneous thermal polymerization allows for the production of low-molecular-weight resins that require less organic solvents to be sprayable and brushable. A monomer that undergoes self-initiation needs a stricter handling procedure. Therefore, a better understanding of the spontaneous polymerization reactions is of safety, environmental and economic importance. Using density functional theory calculations and polymer-sample spectroscopic analyses, we have been able to (a) conclusively confirm that ethyl acrylate, n-butyl acrylate and methyl methacrylate initiate free-radical polymerization at high temperatures, and (b) determine the initiation mechanisms.

