



A glimpse to thiol-ene and thiol-yne polymerization mechanisms

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Abstract

Sister polymerization reactions thiol-ene and thiol-yne have been attracting attention due to their unique properties in the polymerization field, such as showing the regular step-growth network nature in the product, low shrinking stress, late gelation point, and click nature. These polymerization techniques have been applied in recent innovative research areas, from dendrimer synthesis to microfluidic devices. Electron-rich monomers are reactive for thiol-ene polymerization, while the effect of thiol structures is limited. In addition to this, the main driving force for chain transfer reaction is the stability of radical intermediate in thiol-ene polymerization. However, the factors affecting the reaction mechanisms for the thiol-yne polymerization (Figure 1.) have not been extensively elaborated yet. The radical hydrothiolation of alkynes by thiols was examined in the early 1930s, and nowadays, this reaction is defined as a click reaction. The application of this method in polymer synthesis results in a product which a regular step-growth network nature. In this study, similarities and discrepancies between the sister's polymerization reactions have been figured out utilizing quantum chemical tools. M06-2X DFT functional was used kinetic and thermodynamic analysis as a cost-effective method which was proven by a benchmark study.

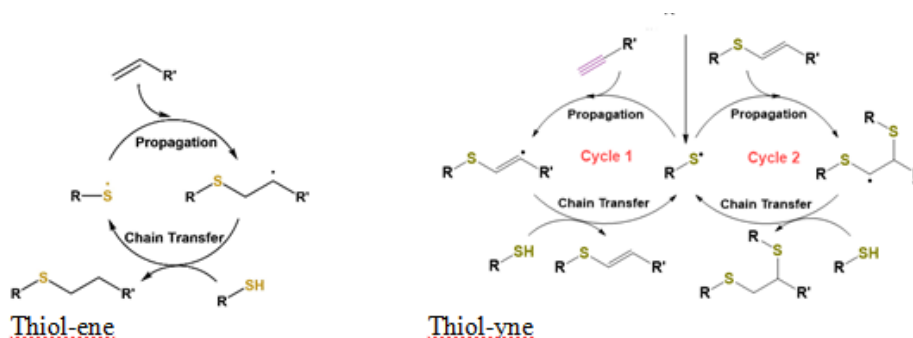


Figure 1- Thiol-ene and Thiol-yne reaction mechanism steps

Biography

Isa Degirmenci has completed his PhD at the age of 30 years from Boğaziçi University, Turkey. He is the Assistant Professor of Boğaziçi University, Turkey. He has been working on reaction mechanisms of thiol-ene and thiol-yne polymerizations utilizing quantum chemical tools. His publication H-index is 10.



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