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Bridging Experiment and Theory: Insights into the Photoinitiation Efficiency of Acrylate and Methacrylate Derivatives of 2-Mercaptobenzothiazole in Radical Photopolymerization of Selected Acrylates

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Streszczenie

Novel copolymerizable one-component Type I photoinitiators based on 2-mercaptobenzothiazole were considered for initiation of radical polymerization of acrylate monomers. For this purpose, ten diversely substituted compounds were taken into consideration. Based on quantum-chemical calculations in both the ground and excited electronic states, the possible mechanism of generation of initiating radicals was proposed. It was found that S–C bond cleavage led to the formation of thiyl ($RS^{\bullet}$) and carbon-centered radicals ($R^{\bullet}$), and was the preferred pathway for all initiators studied. Time-dependent DFT simulations showed that for all considered compounds, homolytic bond dissociation was feasible. The results obtained from the EPR spectra recorded during in situ irradiation of the photoinitiator revealed that the in silico predicted dissociation pathway is consistent with the experimental observations. The photoinitiation ability of new 2-mercaptobenzothiazole-based compounds was subsequently evaluated through kinetic studies of the photopolymerization of selected acrylate monomers. Their practical performance was further benchmarked against the commercial photoinitiators Irgacure 819 (BAPO) and Irgacure 184 under identical irradiation conditions, demonstrating that several synthesized derivatives achieved comparable or higher final monomer conversions depending on the monomer structure. Among the investigated systems, two acrylate and two methacrylate derivatives exhibited the most promising polymerization performance, with the highest efficiency observed for the system based on 2-hydroxyethyl acrylate (HEA). Correlations between experimental photopolymerization parameters and computational descriptors are semi-quantitative, and—depending on the monomer—highlight the significance of S_1 excitation energy, S–C bond dissociation energy and spin populations in the thiyl and thiazole moieties.

Słowa kluczowe

acrylate derivatives, methacrylate derivatives, 2-mercaptobenzothiazole, initiators, photopolymerization, DFT, EPR spectroscopy, kinetics

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