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Probing The Reaction Kinetics of Glycyrrhizic Acid

Glycyrrhizic acid (GA), a prominent triterpenoid saponin found in licorice root, exhibits diverse properties, particularly in the pharmaceutical and food industries. However, its gas phase reaction kinetics and mechanism remain unexplored, primarily because it is considered a typical, readily available, biobased, acidic fuel. This study probes the feasibility of its use as an alternative fuel for various applications such as heating, ventilation, and air-conditioning (HVAC) systems, fuel cells, and other compatible engines, as well as controlled temperature and fame inhibition control systems. We employ a multi-faceted approach combining Molecular Dynamics (MD) simulations, state-of-the-art Machine learning (ML) methods, and kinetic modeling to unravel the complex gas-phase chemistry of glycyrrhizic acid under high-temperature and pressure conditions. Firstly, we investigate the pyrolysis products of glycyrrhizic acid through MD simulations, providing crucial insights into its thermochemical decomposition pathways and determining the future application of the fuel and its related products. Subsequently, employing advanced ML techniques combined with high-level chemical quantum methods, we delve into the thermochemistry of glycyrrhizic acid and its reaction intermediates, enabling a comprehensive understanding of its gas phase reactivity under varying environmental conditions. Building on these insights, we develop a global or skeletal kinetic mechanism to predict critical properties of glycyrrhizic acid, encompassing its reactivity, product distributions, and atmospheric fate. This kinetic model, rooted in fundamental principles derived from MD simulations and ML predictions, offers a powerful tool for elucidating the atmospheric behavior of glycyrrhizic acid and its implications for air quality and environmental chemistry.

Keywords: Glycyrrhizic acid; heating systems; reaction kinetics and modeling; molecular dynamics; biofuels; machine learning.

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