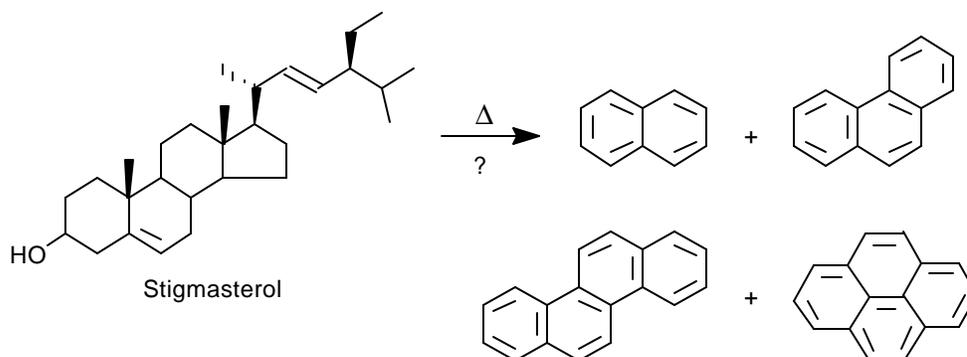


Mechanistic Investigation into the Formation of Polycyclic Aromatic Hydrocarbons from the Pyrolysis of Sterols

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Polycyclic aromatic hydrocarbons (PAHs) are invariably formed in the pyrolysis and combustion of all energy resources. It has been proposed that PAHs are also intermediates in the production of char and soot. As a consequence, formation of PAHs has been of immense practical and scientific interest for the past 100 years. However, the underlying chemistry of PAH formation is still not completely understood. Therefore, we have expanded our mechanistic investigations into the pyrolysis of biomass model compounds, and we are currently focusing on the mechanistic origins of PAHs. Recently, the pyrolysis of many of the components found in biomass, such as the carbohydrates, polyphenols, amino acids, sterols, and terpenes have been investigated. In this presentation, we will focus on the formation of PAHs from the pyrolysis of sterols.

The pyrolysis of stigmasterol and β -sitosterol has been investigated at 500-750 °C by a variety of pyrolysis techniques to identify and quantitate the PAHs that are formed, and to determine the effect of the reaction conditions on PAH yields. Flash vacuum pyrolysis is used to investigate the primary reaction products in the absence of bimolecular reactions. These investigations will determine whether the native ring structure of the sterol leads to the formation of phenanthrene-type structures. The pyrolysis is also investigated by atmospheric pressure flow pyrolysis in which the contact times are varied from 0.15 to 6 sec and the reagent concentration is varied by three orders of magnitude. The role of oxygen on PAH formation is also investigated. The results of our mechanistic investigations on the formation of PAHs from the pyrolysis of sterols will be presented and discussed.



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