Understanding the catalytic pyrolysis mechanism of lignin constituents: the importance of functional groups

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Lignin, rich in aromatic compounds, is renewable and cheap, which makes it an ideal raw material for producing fuels and chemicals.[1] It is a complex and amorphous polymer, and its complex catalytic pyrolysis mechanism results in challenging product-selectivity control. Understanding the reaction mechanism in lignin catalytic pyrolysis is, thus, key to improving product selectivity.[2]

Lignin can be described as a condensate of smaller aromatic units (*p*-hydroxyphenyl and guaiacyl, etc.) with linkages, such as the *β*-O-4 bond, between them.[3,4] Therefore, lignin model compounds, such as guaiacol, vanillin, eugenol, and linkage-bound dimers offer a tractable avenue to investigating the reaction mechanism. We have applied advanced Photoelectron Photoion Coincidence spectroscopy (PEPICO) to investigate a broad variety of lignin model compounds and derived comprehensive reaction pathways based on detecting reactive intermediates isomer-selectively.[5]

In this contribution, we discuss and summarize the influence of the hydroxyl, methoxy, aldehyde, and allyl functional groups on the reaction temperature and the pyrolysis mechanism based on experiments of mono- to tri-substituted aromatics. The goal is to construct a coherent picture based on these model compounds and to reveal universal rules driving lignin catalytic pyrolysis. This will open up new ways to optimizing lignin valorization.

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