Pyrolysis Mechanisms of Coal Model Compounds

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In the thermochemical conversion of coal, product formation is controlled by the relative rates of bond breaking, hydrogen donation, cross-linking, rearrangements, and mass transport. As a consequence of the structural complexity and heterogeneity of coal, it has been difficult to determine the reaction pathways at molecular level. Thus, the pyrolysis of compounds that model key structural features found in coal has been studied to gain insight into the reaction pathways in coal, provide fundamental data for the development of kinetic models to describe the processing of coal at the molecular level, and provide fundamental knowledge to guide the design of more efficient strategies for the conversion of coal to higher value products. Over the past decade, our research group has focused on the impact of restricted mass transport on free radical reactions, reaction pathways of oxygen functional groups in low rank coal and lignin, and the role of carboxylic acids in cross-linking reactions in low-rank coal. Highlights from these mechanistic studies will be presented and its relevance to the thermal processing of coal discussed.

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