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Mechanistic Investigation into the Decomposition of the Sodium, Potassium, and Calcium Salts of Aromatic Carboxylic Acids and Their Role in Cross-linking Reactions

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Carboxylic acids and their alkali and alkaline earth metal salts play a significant role in controlling tar and liquefaction yields in the pyrolysis and liquefaction of low-rank coals. Carboxylates are thought to be responsible for low temperature cross-linking reactions, and cross-linking reactions have been correlated with loss of carboxyl groups and water. In previous studies, the thermolysis of simple and polymeric model compounds containing aromatic carboxylic acids was investigated to determine if decarboxylation leads to low-temperature cross-linking. In this work, the role of carboxylate salts in cross-linking reactions was investigated by TG-MS. The pyrolysis of the sodium, potassium and calcium salts of benzoic acid and poly(*p*-vinylbenzoic acid *co*-styrene) with various loading of carboxyl groups will be compared to the pyrolysis of the free acid. The impact of the cation on the decarboxylation pathways and the role of carboxylate salts in the low temperature cross-linking of low-rank coals will be discussed.

Key Words: Decarboxylation, Cross-linking reactions, Carboxylate Salts, Model Compound

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