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An Ionic Model for Pyrolysis Product Formation through the Gas-Phase Ion-Molecule Reaction of $c\text{-C}_3\text{H}_3^+$

Publication: 1994 – 032

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The formation of benzene during the thermal decomposition of hydrocarbons has been attributed to the reactions of C_3H_3^+ with low molecular weight hydrocarbons. Two forms of C_3H_3^+ are observed: *i*) The propargyl isomer, which reacts with dienes to produce a phenyl cation, and *ii*) an unreactive cyclopropenyl isomer ($c\text{-C}_3\text{H}_3^+$). Because the unreactive cyclopropenyl isomer is the predominate ion formed during pyrolysis (>90%), the threshold barrier for endothermic reactions is critical to understanding the mechanism for pyrolysis product formation. Direct observation of the gas phase reactions of $c\text{-C}_3\text{H}_3^+$ with conjugated dienes has been accomplished using Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS).

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