THERMAL DECOMPOSITION OF THE LIGNIN MODEL COMPOUNDS: SALICYLALDEHYDE AND CATECHOL

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The nascent steps in the pyrolysis of the lignin components, salicylaldehyde (o-HOC_6H_4CHO) and catechol (o-HOC_6H_4OH), have been studied in a set of heated micro-reactors. The micro-reactors are small (roughly 1 mm ID x 3 cm long); transit times through the reactors are about 100 μsec. Temperatures in the micro-reactors can be as high as 1600 K and pressures are typically a few hundred Torr. The products of pyrolysis are identified by a combination of photoionization mass spectrometry and matrix isolation infrared spectroscopy. The main pathway by which salicylaldehyde decomposes is a concerted fragmentation: o-HOC_6H_4CHO (+ M) $\rightarrow$ H_2 + CO + C_5H_4=C=O. At temperatures above 1300 K, fulveneketene loses CO to yield a mixture of HC≡C−C≡C−CH_3, HC≡C−CH_2−C≡CH, and HC≡C−CH=C=CH_2. These alkynes decompose to a mixture of radicals (HC≡C−C≡C−CH_2 and HC≡C−CH−C≡CH and H atoms. H-atom chain reactions convert salicylaldehyde to phenol: o-HOC_6H_4CHO + H $\rightarrow$ C_6H_5OH + CO + H. Catechol has similar chemistry to salicylaldehyde. Electrocyclic fragmentation produces water and fulveneketene: o-HOC_6H_4OH (+ M) $\rightarrow$ H_2O + C_5H_4=C=O. These findings have implications for the pyrolysis of lignin itself.