

2nd World Congress on Petrochemistry and Chemical Engineering

October 27-29, 2014 Embassy Suites Las Vegas, USA

Fast pyrolysis of lignin

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Lignocellulosic biomass is the most abundantly available renewable energy resource available in nature. While conversion of cellulose to fuels and valuable chemicals has received a lot of attention, this is not true for lignin. However, lignin conversion has significant potential for the sustainable production of aromatic chemicals currently obtained from crude oil. Unfortunately, the determination of the structures of lignin degradation products is still a challenge. Therefore, multiple stage tandem mass spectrometry (M^{Sn}) with collision-activated dissociation (CAD) coupled with negative ion mode ESI or APCI was used to examine the fragmentation behavior of seven lignin model compounds (ranging from dimers to octamers) with 5-5 and/or β -O-4 linkages by using a linear quadrupole ion trap mass spectrometer. Examination of the observed fragmentation patterns revealed characteristic ion groups that, when combined with their CAD products (MS_3 experiments), can be used to sequence unknown oligomers. The primary fast pyrolysis products of the same lignin model compounds were then determined by coupling a very fast heating pyroprobe with a linear quadrupole ion trap mass spectrometer through a custom-built adaptor. The primary pyrolysis products evaporated into an atmospheric pressure chemical ionization (APCI) source where they were instantly quenched and ionized by negative ion mode APCI and directed into the mass spectrometer. Their elemental compositions were determined by high resolution measurements and their structures were verified by using the sequencing method discussed above. The most abundant primary products were found to be lignin dimers. Further, the results suggest that most of the pyrolysis reactions occur via concerted mechanisms and not radical mechanisms. Quantum chemical calculations support these conclusions.

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