Contribution ID: **54** Type: **Talk**

Investigation of 2-Methylfurane pyrolysis at VUV beam line of Swiss Light Source

Wednesday, 1 October 2014 10:10 (20 minutes)

2-Methylfurane, which can be produced from uneatable biomass, has the potential to be used as alternative fuel in engines. Its combustion chemistry was investigated within the last few years by several groups. But much less knowledge is available about its thermal pyrolysis behaviour, especially the formation of intermediates and pollutants, which can be produced at fuel rich combustion conditions, too.

Therefore the thermal pyrolysis of 2-methylfurane was investigated at the VUV beam line of Swiss Light Source.
Temperature dependent mass spectra of intermediates and products were obtained during thermal pyrolysis, as well as threshold photoelectron spectra. They were used, in addition to the ionisation energies, to identify pyrolysis intermediates and products through comparison with our predicted spectra. The necessary Franck-Condon factors were calculated in the harmonic approximation using quantum chemical calculations results for involved molecules in ground and excited states, as well as ions.
Additionally some reaction pathways describing the formation of identified pyrolysis products were verified through quantum chemical calculations.

Also the dissociative threshold photoionization process of 2-methylfurane ion was investigated. The intermediates and products, as well as reaction pathways were identified. Quantum chemical calculations and RRKM/Master Equation modelling were also preformed to rationalise the experimental results.

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Session Classification: Session 4 Coincidence Spectrometry (Gerber)