

Disentangling reactive isomers in flames using PEPICO

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One key aspect to the improvement of combustion devices is the knowledge of how a fuel burns. Flame-sampling molecular-beam mass spectrometry (MBMS) has become a standard technique for chemical analysis of reacting gas flows in premixed laminar low-pressure flames. The MBMS measurements typically result in speciation data that contribute as validation data base to the construction and refinement of chemical kinetic reaction mechanisms [1].

The talk discusses measurements performed with the iPEPICO spectrometer at the VUV-beamline of the Paul Scherrer Institute in Villigen, Switzerland coupled to a newly developed molecular-beam interface and flat-flame burner [2] and focuses on its strengths in the detection of reactive radicals. In particular, fuel radicals formed by hydrogen abstraction from the fuel molecule are the starting points for branching in the fuel destruction pathways. Consequently, the measurement of their (relative) concentrations is of particular importance for reaction mechanism development and validation. The spectral information in the mass-resolved threshold-photoelectron spectra adds a new dimension to isomer detection that allows more precise species identification than other isomer detection strategies in combustion research and provides for the first time evidence that vibrationally excited molecules can be sampled by MBMS from flames.

[1] N. Hansen, T.A. Cool, P.R. Westmoreland, K. Kohse-Höinghaus, *Progress in Energy and Combustion Science* 35 (2009) 168-191.

[2] P. Oßwald, P. Hemberger, T. Bierkandt, E. Akyildiz, M. Köhler, A. Bodi, T. Gerber, T. Kasper, *Review of Scientific Instruments* 85 (2014), 025101.

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