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Identification of reaction pathways in model flames

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PEPICO spectroscopy was used in flame sampling experiments performed with VUV-photoionization at the Swiss Light Source to identify the fuel radicals and key intermediates in fuel decomposition and in soot formation processes in flames of hydrocarbon fuels.

A key reaction of the fuel decomposition process in pyrolysis as well as in combustion of hydrocarbons is the abstraction of H atoms by small radicals like O, OH and H forming a so-called fuel radical. Because the following reaction steps are highly dependent on the type of radicals formed, the knowledge on H-abstraction pathways is essential for understanding and predicting combustion properties. The flame-sampling PEPICO setup was used to investigate the abstraction of chemically different hydrogen atoms from the hydrocarbon fuels in low-pressure hydrogen flames doped with the different alkanes and alkenes. Ethane, n-butane and i-butane were specifically targeted in a systematic approach to investigate the hydrogen atom abstraction of primary, secondary and tertiary hydrogen atoms. In addition, 1-butene, i-butene and tetramethylethylene were chosen to evaluate the abstraction of allylic and vinylic hydrogen atoms. This set of fuels allows for comparison of different reaction pathways and enables a systematic experimental approach by measuring, identifying and quantifying the fuel radical species in low-pressure flames. Hydrogen was chosen as base fuel to provide sufficient H atoms and to increase the role of hydrogen abstraction or addition in the fuel destruction pathways. Relative H-abstraction ratios for n-butane, i-butane and 1-butene were recorded and give a clear H-abstraction order: tertiary > primary; secondary > primary; allylic > non mesomerically stabilized form. Vinylic radicals were not observed. The comparison of the experimental data to reaction barriers from the literature shows that the mole fraction ratios of the radicals correspond to the ratio of the inverse reaction barriers.

Aromatic hydrocarbons like benzene, toluene, ethylbenzene, and xylene are characterized as volatile organic compounds and can be found with up to 20% (w/w) in typical gasoline blends. These compounds contribute significantly to the fuel mix used today in modern engines. For emissions control a detailed knowledge of important reaction steps during combustion of these aromatics is required. Toluene combustion was investigated in laminar, premixed, flat flames with the PEPICO technique. Two reaction routes are of interest for pollutant formation in toluene combustion: the oxidation and the formation of larger polyaromatic hydrocarbons (PAH). Key intermediates of toluene oxidation were observed, e.g. benzyl radicals and C_5H_5CCH . With regard to PAH formation it was observed, that most PAH are not formed from the fuel but from small resonantly stabilized radicals such as propargyl and allyl radicals. Butadiene and acetylene were added to the toluene fuel, to enhance addition of acetylene and butadiene to the aromatic ring in the flame front. Since both fuels also lead to the formation of small resonantly stabilized radicals the influence on species concentration involved in PAH formation was very small and almost negligible.

Summary

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