

Experimental Investigation of the Low Temperature Oxidation of the Five Isomers of Hexane

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The low-temperature oxidation of the five hexane isomers (n-hexane, 2-methyl-pentane, 3 methyl-pentane, 2,2-dimethyl-butane and 2,3-dimethyl-butane) was studied in a jet-stirred reactor (JSR) at atmospheric pressure under stoichiometric conditions between 550 and 1000 K. The evolution of reactant and product mole fraction profiles were recorded as a function of the temperature using two analytical methods: gas chromatography and synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS). Experimental data obtained with both methods were in good agreement for the five fuels. These data were used to compare the reactivity, the nature of the reaction products and their distribution. At low temperature (below 800 K), n-hexane was the most reactive isomer. The two methyl-pentane isomers have about the same reactivity, which was lower than that of n-hexane. 2,2 dimethyl-butane was less reactive than the two methyl-pentane isomers, and 2,3-dimethyl-butane was the least reactive isomer. These observations are in good agreement with research octane numbers given in literature. Cyclic ethers with ring including 3, 4, 5 and 6 atoms have been identified and quantified for the five fuels. While the cyclic ether distribution was notably more detailed than in other literature JSR studies of branched alkane oxidation, some expected oxiranes were missing amongst the cyclic ethers expected from methyl-pentanes. Using SVUV-PIMS, the formation of C2-C3 monocarboxylic acids, ketohydroperoxides, and species with two carbonyl groups has also been observed, supporting their potential formation from branched reactants in line with what was previously demonstrated from linear fuels. Possible structures and ways of decomposition of the most probable ketohydroperoxides were discussed.

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Primary author: Prof. BATTIN-LECLERC, Frédérique (CNRS)

Co-authors: Prof. QI, Fei (University of Science and Technology of China); Dr HERBINET, Olivier (Université de Lorraine); Dr WANG, Zhandong (University of Science and Technology of China)

Presenter: Prof. BATTIN-LECLERC, Frédérique (CNRS)

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