ARAS-study of the interaction of pentanol isomers with oxygen behind shock waves

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Pentanol isomers (n-$C_5H_{11}OH$, i-$C_5H_{11}OH$) are promising applicants for the complete replacement of gasoline fuel. Several scientific groups are conducting research on the development of the chemical-kinetic mechanism of combustion of this biofuel, but it still needs significant improvements. The main goal of this work is the experimental study the interaction of pentanol isomers with oxygen at the high temperatures 1800-3000 K and pressures 2-3 bar. The kinetics of reaction of pentanol molecules with oxygen atoms formed at N_2O dissociation in mixture 10 ppm N_2O + 10 ppm n-$C_5H_{11}OH$ or i-$C_5H_{11}OH$ in argon behind reflected shock waves is studied. The quantitative measurements of the time profiles of the concentration of oxygen atoms in the ground electronic state $O(^3P)$ were carried out by the precise method of atomic resonance absorption spectroscopy (ARAS) on the resonant vacuum-UV line of an oxygen atom at 130.5 nm. Along with the experimental measurements, a detailed kinetic analysis was carried out using the OpenSMOKE++ code, with a simulation of oxidation processes using current kinetic mechanisms and a corresponding sensitivity analysis of considered reactions. The data obtained during a comprehensive study provide new valuable information on the features of the interaction of pentanol isomers with oxygen at high temperatures, which will help both in verifying existing mechanisms and in creating new reliable kinetic schemes in a wide range of temperatures and pressures.

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