Experimental study of kinetics of C_3H_7I dissociation behind shock waves

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Iodine-containing halocarbons and halogenated hydrocarbons are widely used in various branches of the chemical industry, fire fighting and medicine. Therefore, scientific interest in such substances remains extremely high at the present time. In particular, the C_3H_7I molecule, due to the presence of the weakest bond between halogen and carbon atom (C-I bond), is the most suitable precursor for the alkyl radical C_3H_7. These radicals, as is known, are formed in significant quantities at the combustion and pyrolysis processes of normal alkanes, and without their correct prediction it is impossible to build physically based models of combustion of real hydrocarbon fuels. That is why this work is aimed at studying the kinetic properties of C_3H_7I dissociation. The reaction $C_3H_7I + Ar = C_3H_7 + I + Ar$ (1) has been studied at the temperatures 800–1200 K and pressures 3.5 ± 0.5 bar behind incident and reflected shock waves using the atomic resonance absorption spectroscopy (ARAS) technique on a resonant line of atomic iodine at 183.04 nm. The initial concentration of C_3H_7I in Ar was varied from 0.8 to 1.1 ppm. As a result, the first direct experimental data on the thermal unimolecular decomposition of n-C_3H_7I were obtained. Time profiles of iodine atom concentration were used to determine the temperature dependence of the rate constant of reaction (1) and its activation energy. Based on these data, the value of this rate constant was obtained in the two-parameter Arrhenius form, convenient for use in kinetic databases. It was found also, that under experimental conditions, the obtained values are close to the high-pressure limit.