Application of ARAS and MRAS methods to study the kinetics of CF_2 radical formation in pyrolysis of C_3F_7I

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A variety of halogenated hydrocarbons are widely used in various industries. The effectiveness of suppressing combustion by these substances is primarily determined by the processes of chemical inhibition of chain reactions of combustion by the products of their pyrolysis. At the moment, bromine-containing freons [13B1 (CF3Br), 114B2 (C2F4Br2), and 12B1 (CF2ClBr)] remain the most common fire-extinguishing substances. However, awareness of the need to protect the ozone layer in the Earth's atmosphere and the decisions taken by the world community to stop the production of ozone-depleting substances stimulated the search for new, efficient, and environmentally pure fire extinguishing agents. Among the most promising additives, another group of halocarbons, iodine-containing freons, such as CF3I and C3F7I, have become of interest. These halocarbons are characterized by suitable physical properties, as well as being completely ozone-friendly. However, for industrial applications, it is necessary to study the inhibitory and toxic properties of these compounds. Moreover, it is necessary to study the kinetics of dissociation of both the primary substance and its secondary components.

In this work the C3F7I + Ar reaction was studied by sequential application of atomic and molecular resonance absorption spectroscopy (ARAS and MRAS) using resonance line of iodine atom I at 183.04 nm and CF2 radical band at 251.9 nm behind reflected shock waves. As a source of resonance radiation of iodine atoms and CF2 radical, a microwave discharge lamp representing a flowing quartz tube was used, through which a pre-prepared mixtures of 0.4% CF3I in He or 1%CF3H+He were pumped. The experiments were performed at the temperatures from 800 to 1500 K and pressures of 0.6 to 8.3 bar. The initial concentration of C3F7I in Ar was varied from 1 to 1000 ppm.

As a result of the experiments the time profiles of CF_2 and I concentration, forming at C3F7I dissociation were obtained. From these experimental data the temperature dependences of the rate constants of CF_2 and I formation and their activation energy were determined. Moreover, it was found that at a temperature at least below 1500K and a pressure above 0.6 bar, the resulting rate constant C3F7I + Ar = C3F7 + I + Ar is in the high-pressure range. These new data allow presenting in detail the kinetic mechanism of C3F7I decomposition in a wide range of temperatures and pressures.