

# Experimental and kinetic modeling study of the positive ions in ethylene flames

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The flame is weakly ionized plasma. Understanding the behavior of ions in a flame is momentous for the development of new diagnostic methods and new ion-sensitive technologies for controlling combustion processes. In this work, the spatial distribution of positive ions (cationic structure) in premixed ethylene/oxygen/argon flames stabilized on a flat-flame burner at atmospheric pressure was measured by molecular beam mass spectrometry in a wide range of equivalence ratios  $\phi = 0.4\div 1.5$ . Numerical calculations of the cationic structure of these flames as well as profiles of the rate of production of the main flame ions have been carried out using the Cantera software (V.2.5.1) [1]. A detailed ion chemistry mechanism was used for calculations. The mechanism was developed on a basis of ion chemistry models available in the literature [2] and supplemented with reactions for the  $C_3H_5^+$  cation, which is abundant in ethylene flames. A comparison of the experimental and simulation data has shown that the mechanism correctly describes the relative content of the most abundant oxygen-containing cations ( $CH_5O^+$ ,  $C_2H_3O^+$ ) in flames, as well as of the  $C_3H_5^+$  cation detected experimentally in a rich flame ( $\phi=1.5$ ). The chemistry of  $C_3H_3^+$ , a key cation in fuel-rich flames, was also revisited. Two structure isomers of  $C_3H_3^+$  (cyclic and linear) together with the reactions involving these cations and an isomerization reaction are added in the mechanism. The updated mechanism was demonstrated to correctly predict the relative mole fraction of the  $C_3H_3^+$ . Several abundant cations with the general formula  $C_xH_y$  were also detected in the fuel-rich flame ( $\phi=1.5$ ). The obtained data will serve as a basis for further development of the ion chemistry mechanism in fuel-rich hydrocarbon flames.

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[1] D.G. Goodwin, R.L. Speth, H.K. Moffat, B.W. Weber. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes.

[2] D.A. Knyazkov et al. Cationic structure of premixed near-stoichiometric CH<sub>4</sub>/O<sub>2</sub>/Ar flames at atmospheric pressure: New insights from mass spectrometry,

quantum chemistry, and kinetic modeling, *Combustion and Flame* **2022**, *241*, p. 112106.