

Experimental Study of the Multichannel $O(^3P) + C_2H_4$ Reaction: Primary Products as a Function of Temperature

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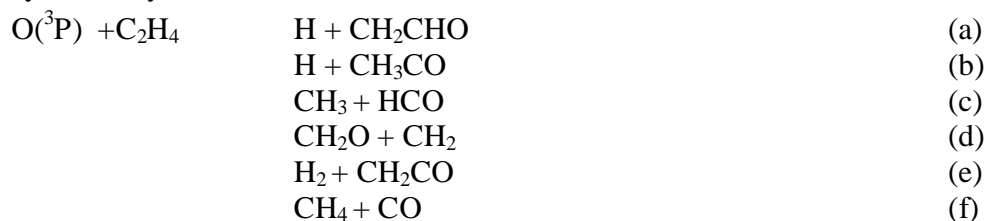
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Reactions of small alkenes, which are known to be intermediates in the combustion of many hydrocarbons, with ground-state oxygen atoms (3P) are important oxidative steps in the combustion mechanisms. The understanding and description of the mechanism of transformation of an organic compound in the combustion process requires first of all the information on kinetics and primary products of its reactions with active species, atoms and radicals, present in the reactive system. Reaction of oxygen atoms with ethylene has been extensively studied, experimentally and theoretically, during the last decades. The total rate constant of the reaction seems to be well established; however the information on the distribution of the reaction products still remains somewhat uncertain, particularly with regard to the temperature dependence. Indeed, almost all previous work, except for a few crossed molecular beam studies, was conducted at room temperature. The objective of the present study was to carry out a systematic experimental investigation of the products of the title reaction as a function of temperature. The total rate constant of the reaction was also determined in an extended temperature range.

Experiments were carried out in a discharge flow reactor using modulated molecular beam mass spectrometer for detection of the reactants and reaction products. The total rate constant of the reaction was determined from the consumption kinetics of oxygen atoms monitored under pseudo-first order conditions in high excess of C_2H_4 over O . The following expression, $k = 3.96 \times 10^{-17} \times T^{1.8} \times \exp(-132/T)$, obtained for the rate constant at $T = 230$ to 902 K and 1 Torr total pressure of helium, is in excellent agreement with current recommendation.

The products of the title reaction have been investigated at temperatures between 298 and 900 K and pressures from 1 to 8 Torr of helium. Under experimental conditions used, the thermodynamically feasible channels of the title reaction are:



Experiments were carried out in presence of molecular bromine in the reactor, which allowed to rapidly transform H atoms (channels (a), (b)) and CH_3 radicals (channel (c)) to stable species, HBr and CH_3Br , respectively, which were detected with mass spectrometry. Formaldehyde (channel (d)) and H_2 (channel (e)) were detected directly at their parent peaks. Preliminary results show that the absolute yields of H , CH_3 and CH_2O are in the ranges 0.25-0.35, 0.45-0.55 and 0.15-0.20 virtually independent of temperature and total pressure under experimental conditions of the study. The yield of H_2 (channel (e)) was measured to be less than 0.02. These results will be discussed in comparison with existing room temperature and crossed molecular beam data and those from theoretical studies.