TIME-RESOLVED FTIR STUDY ON THE REACTION OF CH_2Br WITH NO_2

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Time-Resolved Fourier Transform Infrared (TR-FTIR) emission spectroscopy has been used extensively to study the dynamics of gas-phase free radical reactions. Radicals of CH_2Br are believed to be important reactive intermediates involved in atmospheric pollution chemistry. It is expected that this highly reactive and exothermic reaction of CH_2Br with NO_2 has multiple reaction channels and interesting chemical transformations. However, except a few kinetics measurements, it has been lack of the knowledge of its reaction products, channels, dynamics and mechanisms up to now. In this work, we have employed step-scan TR-FTIR emission spectroscopy to investigate these aspects of the CH_2Br + NO_2 reaction. By probing the infrared fluorescence emitted from vibrationally excited molecules in real time, the elementary reaction products and their vibrational state distribution can be identified from TR-FTIR emission spectroscopy, revealing the information of the product channels and reaction dynamics. Here, we have observed multiple elementary reaction products of H_2CO, HBr, CO_2, CO, NO from the CH_2Br + NO_2 reaction, identified the corresponding reaction channels and analyzed the product vibrational state distributions. The reaction mechanism and dynamics is elucidated from these experimental results combined with B3LYP/6-311G(d,p) level of DFT calculations on the reaction energetics.