



The atmospheric chemistry of acrylic acid initiated oxidation by chlorine atom

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Acrylic acid ($\text{CH}_2=\text{CHCOOH}$) is a typical volatile organic compounds (VOCs), which could be released from polymer and resin productions and produced by marine algae naturally. The release of $\text{CH}_2=\text{CHCOOH}$ into the atmosphere is likely to result in serious environmental problems. As a result, the atmospheric chemistry of $\text{CH}_2=\text{CHCOOH}$ has attracted great attentions. Moreover, Chlorine atom initiated oxidation reaction is significant for the removal of typical volatile organic compounds (VOCs) in the atmosphere. Oxidation of acrylic acid with chlorine atom, as an important atmospheric radical-molecule reaction, are necessary in the computational kinetics and quantum chemistry studies. The mechanisms, kinetics, atmospheric lifetime, and the second further reactions in the presence of O_3 , O_2 , NO , and NO_2 have been investigated by quantum chemistry methods. The results are useful particularly for atmospheric chemistry models.