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Kinetic study of the degradation of C5 and C6 unsaturated aldehydes and alcohols by ozone

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Emissions of biogenic volatile organic compounds (VOCs) are higher than those from anthropogenic sources. They are therefore likely to have a great influence on atmospheric chemistry both locally and regionally, through their impact on the HO_x balance (HO_x = HO + HO_2), ozone production and ability to form secondary organic aerosols (SOA). Among the volatile organic compounds of biogenic origin are the family of C5 and C6 unsaturated aldehydes and alcohols. Few information exist regarding the fate of these compounds in the atmosphere especially there reaction with ozone.

In this work, we studied the kinetics of the reaction of three unsaturated aldehydes (trans-2-pentenal, trans-2-hexenal and 2-methyl-2-pentenal) and three unsaturated alcohols (1-penten-3-ol, cis-2-penten-1-ol and trans-3-hexen-1-ol) with ozone O_3 in a rigid atmospheric simulation chamber coupled to an FTIR spectrometer at four different temperatures (273, 298, 333 and 353 K) and at atmospheric pressure. The rate constants of the ozonolysis reaction of the unsaturated aldehydes and the unsaturated alcohols studied were determined and the following Arrhenius expression was obtained (cm3 molecule -1 s -1):

k (Trans -2-pentenal)= (3.83 ± 3.71) x 10-16 exp (- (1706 ± 295) / T)
k (Trans-2-hexenal)= (1.43 ± 0.67) x 10-16 exp (- (1369 ± 141) / T)
k(2-Methyl-2-pentenal)= (3.62± 0.22) x 10-18 exp (- (121 ± 20) / T)
k(1-penten-3-ol) = (1.42 ± 1.24) x 10-16 exp (- (642 ± 250) / T)
k(Cis-2-penten-1-ol)= (3.14 ± 0.45) x 10-15 exp (- (1045 ± 40) / T)
k(Trans-3-hexen-1-ol)= (6.38 ± 1.75) x 10-16 exp (- (686 ± 89) / T)

The obtained data will be discussed in terms of structure–reactivity relationship and compared with the reported reactivity with OH radicals. The atmospheric implications derived from this study are discussed as well.