

Low-pressure yields of stabilized Criegee intermediates produced from ozonolysis of a series of alkenes

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Ozonolysis of alkenes is an important oxidation pathway of alkenes in the troposphere because it is involved in the production of organic aerosol and OH radicals. The mechanism of ozonolysis of alkenes involves the formation of a primary ozonide (POZ), which then decomposes into a carbonyl and a high-energy carbonyl oxide (Criegee intermediate). Criegee intermediates are produced with a broad internal energy distribution. High energy Criegee intermediates decompose into atmospherically important compounds (e.g. vinyloxy, OH radical). Stabilized Criegee intermediates (sCIs) undergo reactions to produce secondary ozonides and organic aerosols.

Cavity ring-down spectroscopy (CRDS) is utilized in combination with chemical titration with sulfur dioxide (SO₂) to quantify sCIs. The reactions are carried out under various flow and low-pressure conditions. Reference cross-sections of the products and reactants are fitted with spectral features to obtain product number densities. The yields of sCIs are measured at different low pressures, and the nascent yields are determined by extrapolation to zero pressure. Endocyclic alkenes show no sCI production at the pressures studied. Acyclic alkenes show pressure-dependent sCI yields. Formaldehyde oxide (CH₂OO) from the 1-alkenes studied has a high nascent yield than larger CIs due to its relatively high energy barrier for dissociation. The nascent yield of stabilized CH₂OO increases with increasing carbon number of the carbonyl co-product. The information on the low-pressure yields from the current studies can be used as a benchmark for theoretical calculations.