OZONOLYSIS OF ALKENES: THEORETICAL STUDIES OF OH, HO_2 AND EPOXIDE PRODUCED FROM DECOMPOSITION OF PRIMARY OZONIDE

WAI-TO CHAN AND IAN P. HAMILTON, *Department of Chemistry, Wilfrid Laurier University, Waterloo, Ontario, Canada N2L 3C5*.

Ozonolysis of alkenes is initiated by the cycloaddition of ozone to the double bond to form a primary ozonide (POZ). Decomposition of the vibrationally excited POZ is a major source of various organic pollutants. The dominant mechanistic pathway is generally believed to be a concerted cleavage of the C=C and the O–O bonds to form a Criegee intermediate (CI) and an aldehyde followed by unimolecular decompostion of the vibrationally excited CI. We report *ab initio* calculations of the ethene and propene POZ using DFT-BH&HLYP, CCSD(T) and QCISD(T) methods. Our results suggest the favoured pathway to be the non-concerted cleavage of the POZ to a diradical oxy-peroxy intermediate forming CI and aldehyde. Competitive channels for formation of OH, HO_2 and epoxides are also studied. The possibility of verification of the mechanism of POZ fragmentation via spectroscopic detection of prompt formation of OH and HO_2 is discussed.