

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Determining the Products and Mechanism of the $C_2Cl_3+O_2$ Reaction by Time-Resolved FTIR Emission Spectroscopy HONGMEI SU, TIANCHENG XIANG, SHAOLEI ZHAO, CONGYUN SHI — The reaction products and mechanism of the C_2Cl_3 radical with O_2 have been studied by time-resolved FTIR emission spectroscopy. The chlorinated vinyl radical, C_2Cl_3 , was generated by 248 nm photolysis of a C_2Cl_4 precursor. Vibrationally excited CO, CO_2 and ClCO products were observed. The time evolution of the emission intensity shows that CO_2 and ClCO are primary reaction products. In contrast, CO emission does not decay until *ms* time scale indicating that CO products are due to secondary reactions, most likely, the further dissociation of ClCO. Two primary reaction channels are identified: $C_2Cl_3 + O_2 \rightarrow CO_2 + CCl_3 \rightarrow ClCO + COCl_2$ When reacting with O_2 , the observed products and channels of the chlorinated vinyl radical, C_2Cl_3 , turned out to be very similar to its counterpart, vinyl radical C_2H_3 . Morokuma's DFT study^[1] of the reaction $C_2H_3+O_2$ shows that the main reaction path proceeds through a three-membered CCO ring adduct. The question is, does C_2Cl_3 go through the same reaction path as C_2H_3 ? Does the substitution of H atom by heavier Cl atom make any difference in regard to the reaction mechanism? Further investigation combining *ab initio* calculation is under way.

[1] A.M.Mabel, E.W.G.Diau, M.C.Lin, and K.Morokuma, J.Am.Chem.Soc. 118, 9759 (1996)

Hongmei Su
Institute of Chemistry, Chinese Academy of Sciences

Date submitted: 03 Jan 2006

Electronic form version 1.4