THERMAL DECOMPOSITION OF ACETALDEHYDE STUDIED BY MATRIX IR AND PIMS SPECTROSCOPY

ANGAYLE VASILIOU, KRZYSZTOF PIECH, G. BARNEY ELLISON, *University of Colorado, Boulder, CO 80309-0215*; MARK R. NIMLOS, *Center for Renewable Chemical, Technologies & Materials, NREL, 1617 Cole Blvd., Golden, CO 80401*; JOHN W. DAILY, *Department of Mechanical Engineering, University of Colorado, Boulder, CO 80309-0427*; JOHN F. STANTON, *Institute for Theoretical Chemistry, Department of Chemistry, University of Texas, Austin, TX 78712-0165*.

In all previous experimental studies of the thermal decomposition of acetaldehyde (CH_3CHO), the products were presumed to be CH_3 + CHO. These species result from cracking of the weakest bond. Other routes are possible: ($DH_{298}(CH_3{-}CHO)$ = 84.8 $\pm$ 0.2 kcal mol^{-1}; $DH_{298}(CH_3CO\text{-}H)$ = 89.4 $\pm$ 0.3 kcal mol^{-1}; $DH_{298}(H\text{-}CH_2CHO)$ = 92 $\pm$ 2 kcal mol^{-1}. This work explores the possibility of other thermal decomposition pathways, that result via C-H bond scission. We have used a resistively heated SiC tubular reactor with a 65 μsec residence time to study the thermal cracking of acetaldehyde. The decomposition products are identified by two independent techniques: 118.2 nm (10.487 eV) VUV photoionization mass spectroscopy and infrared absorption spectroscopy in a cryogenic matrix. The observed dissociation channels seem to be:

$$CH_3CHO + \Delta \rightarrow CH_3CO + H$$

$$\rightarrow CH_2{=}CHOH$$

$$\rightarrow CH_2{=}C{=}O$$

$$\rightarrow CH_3 + HCO$$