MATRIX ISOLATION AND COMPUTATIONAL STUDIES OF THE PHOTOLYSIS OF DIHALOETHANES: PROBING THE PATHWAYS LEADING TO RADICAL AND MOLECULAR PRODUCTS

AIMABLE KALUME, LISA GEORGE AND SCOTT A. REID, *Department of Chemistry, Marquette University, Milwaukee, WI 53233*; PATRICK Z. EL-KHOURY AND ALEXANDER TARNOVSKY, *Department of Chemistry and Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH 43403*.

The importance of haloalkanes in atmospheric chemistry is well appreciated. In this talk, we will report on matrix isolation and computational studies of the photolysis of dihaloethanes following selected wavelength laser irradiation. The photolysis products are characterized by matrix isolation infrared and UV/Visible spectroscopy, supported by ab initio calculations. Results will be reported for the dibromo- and diiodoethanes. In our initial experiments, pulsed deposition of 1,2-dibromoethane:Ar samples (1:1000) onto a KBr window at 5 K yielded almost exclusively the anti-conformer (30:1 anti:gauche). Irradiation of this conformer at 220 nm yielded infrared absorptions assigned to: a) the gauche-conformer, b) the 2-bromoethyl radical, and c) the ethylene-Br_2 complex, which was confirmed in separate experiments where the complex was formed by deposition of ethylene:Br_2:Ar (1:1:1000) samples. The observed infrared and UV/Visible absorptions of these species are in excellent agreement with computational predictions. We will report on related studies of 1,1-dibromoethane and the corresponding diiodoethanes, with emphasis on the search for the bridged C_2H_4I radical.