GAS PHASE SPECTROSCOPIC INVESTIGATION OF CHROMATE-ESTERS

SYDNEY H. KAUFMAN and J. MATHIAS WEBER, *JILA, NIST and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309*.

Chromate and dichromate ions are frequently used in the oxidation of alcohols. Chromate esters containing a Cr–O–C bridge are thought to be important intermediates in such reactions. We report the photofragment action spectra of two chromate ester complexes in the UV and visible regions, both of which primarily undergo cleavage of the chromate ester bond resulting in reduction of the chromate from Cr(VI) to Cr(V). Comparison to the UV/Vis absorption spectrum of a methanolic dichromate solution suggests the electronic transitions are the same ligand-to-metal charge transfer transitions in both environments. Comparing the spectral features for different fragment channels leads to insight into the energetics and fragmentation mechanism of these species.