PHOTOELECTRON STUDIES OF METHYLNITRENE, CH_3N

BARNEY ELLISON, *Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215*.

Complex organic radicals are important intermediates in many combustion and environmental processes. In combustion processes, the organic radical CH is known to cleave N_2 into HCN and N atoms. Most N atoms are further oxidized to NO which exhausts into the atmosphere. Thus the reaction of CH with N_2 to produce N atoms connects internal combustion engines with NO production. Some fraction of these N atoms, however, reacts with CH_3 in the flame to produce CH_3N. Methylnitrene is very unstable and decomposes to generate CH_2NH or H_2 + HCN. We will discuss the use of negative ion photoelectron spectroscopy to characterize methylnitrene.

$$CH_3N^- + \hbar\omega_{488\ nm} \rightarrow CH_3N + e^-$$

We find EA(CH_3N) = 0.022 ± 0.009 eV. In addition to detaching the methylnitrene anion to the ground state of CH_3N ($\widetilde{X}\ ^3A_2$), we also detect the first electronically excited state of methylnitrene, $\tilde{a}\ ^1E$. We measure $\Delta E(\tilde{a}\ ^1E - \widetilde{X}^3A_2)$ = 1.352 ± 0.011 eV. The reaction dynamics of nitrene rearrangements will be discussed:

$$CH_3N(\widetilde{X}\ ^3A_2) \rightarrow \text{no reaction}$$
$$CH_3N(\widetilde{a}^1E) \rightarrow CH_2NH$$