

INVESTIGATION OF THE HYDROGEN BONDED OH-ACETYLENE REACTANT COMPLEX BY OH OVERTONE AND ASYMMETRIC C-H STRETCH EXCITATION

MARGARET E. GREENSLADE, JAMES B. DAVEY, MARK D. MARSHALL, and MARSHA I. LESTER,
Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323.

The entrance channel leading to the addition reaction between the hydroxyl radical and acetylene is examined by spectroscopic characterization of the OH-acetylene reactant complex. The structure of the reactant complex is determined from infrared action spectra in the OH stretch overtone region near $1.4 \mu\text{m}$ and the asymmetric C-H stretching region near $3.0 \mu\text{m}$. Analysis of the rotationally resolved parallel band at 6885.5 cm^{-1} (origin) resulting from OH overtone excitation yields the $(B + C)/2$ rotational constant and confirms the T-shaped, π -hydrogen bonded structure predicted by *ab initio* theory. The perpendicular transition associated with C-H stretch excitation was expected to be similar to that previously reported for the near-prolate HF/HCl-acetylene asymmetric tops. However, the resultant spectrum centered at 3278.6 cm^{-1} consists of seven peaks of various intensities and widths, some peaks with shading and others symmetrical. A model, which will be detailed in the following talk, has been developed to examine the origin of this result, namely the partial quenching of the OH orbital angular momentum in the complex. The stability of the OH-acetylene reactant complex is deduced from the OH product states populated following vibrational predissociation of the complex. The OH ($v = 0$ or 1) products are probed by laser-induced fluorescence on various $A-X$ transitions. Results obtained following infrared excitation in both spectral regions are consistent with an upper limit for the binding energy of $D_0 \leq 950 \text{ cm}^{-1}$.