SPECTROSCOPY AND DYNAMICS OF THE $H_2$-CN VAN DER WAALS COMPLEX

YALING CHEN and MICHAEL C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*.

The reaction $H_2$ + CN $\rightarrow$ H + HCN is of importance in the combustion of hydrocarbons in air. It is also a prototypical system for studies of polyatomic reaction dynamics. The reaction has a substantial entrance channel barrier ($\approx 1000 \mathrm{cm}^{-1}$), which raises the possibility that pre-reactive $H_2$-CN van der Waals complex may be stable at low temperatures.

We have recently detected $H_2$-CN in a free-jet expansion, using laser excitation of the B-X and A-X transitions. The complex feature associated with the monomer B-X 0-0 transition consisted of a single broad peak. This corresponds to direct excitation to the $H_2$ + CN(B) dissociation continuum. From the onset of the continuum, the ground state well-depth is estimated to be $40 \mathrm{cm}^{-1}$.

Bands of $H_2$-CN associated with the monomer $A^2\Pi$-$X^2\Sigma^+$ 3-0 transition were examined. Complex features associated with $A^2\Pi_{1/2}$ were found to be homogeneously broadened by the spin-orbit predissociation process

$$H_2\text{-CN}(A^2\Pi_{1/2}, v=3) \rightarrow H_2 + CN(A^2\Pi_{3/2}, v=3) \qquad [\Gamma=2.5\text{x}10^{11}\mathrm{s}^{-1}]$$

Excitation of the complex to the $A^2\Pi_{3/2}$ spin-orbit component yielded rotationally resolved bands. A preliminary analysis of the rotational structure yields an $H_2$ to CN separation of 3.7$\mathring{A}$. The rotational lines are homogeneously broadened by the internal conversion predissociation process

$$H_2\text{-CN}(A^2\Pi_{3/2}, v=3) \rightarrow H_2 + CN(X, v=7) \qquad [\Gamma=1.3\text{x}10^{10}\mathrm{s}^{-1}]$$

Double resonance techniques have been used to examine the CN fragments produced by both predissociation channels.

Data for $H_2$-CN and $D_2$-CN (experiments in progress) will be presented and discussed.