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

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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 ($\approx 1000 cm^{-1}$), 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 $40 cm^{-1}$.

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

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

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

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

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.