

## MAPPING THE OH + CO → HOCO REACTION PATHWAY THROUGH INFRARED SPECTROSCOPY OF THE OH-CO REACTANT COMPLEX

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A hydrogen-bonded OH-CO complex has been identified along the reaction coordinate for the OH + CO  $\leftrightarrow$  HOCO  $\rightarrow$  H + CO<sub>2</sub> reaction. The vibrational spectrum of the OH-CO complex has been examined in the OH overtone region at 1.4  $\mu\text{m}$  using infrared action spectroscopy, which relies on detection of OH ( $v = 1$ ) fragments from vibrational predissociation by laser-induced fluorescence. The observed infrared spectrum of OH-CO consists of the pure OH overtone band at 6941.7  $\text{cm}^{-1}$  and combination bands involving the simultaneous excitation of OH stretch and intermolecular vibrations, which appear 50 to 250  $\text{cm}^{-1}$  higher in energy than the pure overtone. The rotational structure of the pure overtone band is indicative of a parallel transition of a linear OH-CO complex having a  $P = 3/2$  projection of the total angular momentum on the intermolecular axis, which arises from the unquenched electronic angular momentum of OH. The OH-CO binding energy,  $D_0 \leq 430 \text{ cm}^{-1}$ , is also established from the quantum state distribution of the OH fragments following pure overtone excitation. The strongest combination bands with 51.1, 57.1, and 247.3  $\text{cm}^{-1}$  of intermolecular energy are attributed to geared bend and H-atom bend excitation, which are the modes that drive the transformation from OH-CO to HOCO. These combination bands exhibit rotational structures that are characteristic of perpendicular transitions ( $\Delta P = \pm 1$ ) to states with vibrational angular momentum from the bending motions of the complex. A complete analysis of the experimental results promises to yield a spectroscopic quality characterization of the OH + CO  $\rightarrow$  HOCO reaction pathway.

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