EXPERIMENTAL CHARACTERIZATION OF THE WEAKLY ANISOTROPIC CN $X^2\Sigma^+$ + Ne POTENTIAL FROM IR-UV DOUBLE RESONANACE STUDIES OF THE CN-Ne COMPLEX[a]

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A fluorescence based IR-UV double resonance technique is used to obtain rotationally resolved infrared spectra of the CN-Ne van der Waals complex in the CN stretch overtone region. Several hindered rotor combination bands are observed, with the spectra displaying evidence of Coriolis coupling in both line intensities and positions of the closely spaced vibrationally excited states. A depertubation analysis is performed through modification of the rotational Hamiltonian to generate accurate rotational constants and account for the shifted line positions and band shapes observed. The energy spacings between hindered rotor states are used to deduce information on the anisotropic CN $X^2\Sigma^+$ + Ne intermolecular potential from which radially averaged anisotropy terms (V_{10} and V_{20}) are extracted. The angular potential is compared to that produced by *ab initio* calculations using MRCI+Q extrapolated to the complete one-electron basis set limit. Experiment and theory are in excellent agreement, both indicating a nonlinear CN-Ne *(X)* minimum energy configuration and nearly free-rotor behavior. Similar studies on CN-Ar and CN-H_2 are currently in progress and analogous data analysis is ongoing.

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