FTIR AND ULTRAFAST INFRARED SPECTROSCOPY OF THE DICYANAMIDE ANION IN SOLUTION

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Steady state and time-resolved IR spectroscopy have been used to study the vibrational band positions, vibrational energy relaxation (VER) rates, and reorientation times of the antisymmetric C≡N stretching band of dicyanamide ($N(CN)_2^-$) anion near 2100 cm^{-1} in several bulk solvents. The transient signals indicate a complicated relaxation mechanism, consistent with there being a Fermi resonance enhanced combination band in the region. The solvent-induced spectral blue shifts and VER rates both increase for solvents with stronger solute-solvent interactions. The gas-phase vibrational frequency is estimated by extrapolating to zero solvent shift by scaling the solvent shift to those previously observed for azide (N_3^-). $N(CN)_2^-$ exhibits a strong correlation between vibrational frequency and VER rate, so that, as with N_3^-, an estimate of the relative VER rate can be obtained from the static spectra.