VIBRATIONAL DYNAMICS OF TRICYANOMETHANIDE

DANIEL WEIDINGER, CASSIDY HOUCHINS, and JEFFREY C. OWRUTSKY, *Code 6111, Naval Research Laboratory, 4555 Overlook Ave SW, Washington, D.C. 20375*.

Time-resolved and steady-state IR spectroscopy have been used to characterize vibrational spectra and energy relaxation dynamics of the CN stretching band of the tricyanomethanide (TCM, $C(CN)_3^-$) anion near 2170 cm^{-1} in solutions of water, heavy water, methanol, formamide, dimethyl sulfoxide (DMSO) and the ionic liquid 1-butyl methyl imidazolium tetrafluoroborate ([BMIM][BF_4]). The band intensity is strong ($\sim$1500 $M^{-1}cm^{-1}$) and the vibrational energy relaxation times are relatively long ($\sim$5 ps in water, 12 ps in heavy water, and $\sim$30 ps in DMSO and [BMIM][BF_4]). They are longer than those previously reported for dicyanamide in the same solvents. Although the static TCM frequency generally shifts to higher frequency with more strongly interacting solvents, the shift does not follow the same trend as the vibrational dynamics. The results for the experimental frequencies and intensities agree well with results from *ab initio* calculations. Proton and electron affinities for TCM are also calculated because they are relevant to potential applications of this anion in low viscosity ionic liquids.