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Vibrational spectroscopy and dynamics of the hydrazoic and thiocyanic acids in protic and aprotic solvents CASSIDY HOUCHINS¹, DANIEL WEIDINGER², JEFFEREY OWRUTSKY, Naval Research Lab — Azide (N_3^-) and thiocyanate (NCS^-) in solvents are benchmark systems for studying fast vibrational energy relaxation (VER) and solvent-solute interactions. To investigate the effects of solute charge as well as solvent-isotope effects on solute vibrational spectra and dynamics, infrared pump-probe studies have been carried out to determine VER times for CN and antisymmetric NNN stretching bands XNCS and XN_3 ($\text{X}=\text{H}, \text{D}$), in protic and aprotic solvents to compare with the well studied N_3^- and NCS^- anions. The study suggests that protonating the anions may be viewed as a limiting case of hydrogen bonding. Results from extending the measurements to other solvents demonstrate that the trend in VER relaxation times with solvent is similar for HN_3 and N_3^- , but there is less of a systematic frequency shift for HN_3 .

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