VIBRATIONAL SPECTROSCOPY AND DYNAMICS OF THE HYDRAZOIC AND ISOTHIOCYANIC ACIDS IN PROTIC AND APROTIC SOLVENTS

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In order 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 vibrational energy relaxation (VER) times for the CN and antisymmetric NNN stretching bands for the pseudohalide acids, XNCS and XN_3 (X=H, D), in protic and aprotic solvents to compare with the well studied azide and thiocyanide anions. The studies indicate that the deuterium effects on the frequency shifts for HN_3 and relaxation times for both HNCS and HN_3 resemble the solvent isotope effects for azide and thiocyanide in water. While it is expected that VER times will be shorter for charged than neutral solutes, this is not observed in all cases.

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