

## CRYOGENIC SOLVENT EFFECTS ON THE INFRARED ABSORPTIONS AND BAND WIDTHS OF CF<sub>3</sub>H

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The spectra of CF<sub>3</sub>H dissolved in liquid argon, nitrogen, and xenon were obtained in the infrared region using a Fourier transform spectrophotometer and a low temperature cell. The equilibrium geometry and vibrational frequencies of CF<sub>3</sub>H in the gas phase and in argon, nitrogen, and xenon solutions were determined by means of ab initio molecular orbital calculations. The calculations were performed using the GAUSSIAN system of programs at the Hartree-Fock level of theory with the 3-21G and 6-31G\* basis sets. Experimental frequency shifts from gas phase to solution spectra are compared with predictions of ab initio molecular orbital calculations. Time correlation functions of the vibrational band profiles are obtained to get information about the dynamic processes at the molecular level.