

IR ABSORPTION AND CALCULATED FREQUENCIES OF FORMALDEHYDE DISSOLVED IN LIQUID Kr

SURESH SUNUWAR, CARLOS MANZANARES, *Department of Chemistry and Biochemistry, Baylor University, Waco, TX, USA.*

Using a Fourier transform infrared spectrophotometer and a low temperature cryostat, we have obtained the IR spectra of formaldehyde dissolved in liquid krypton between 125 K and 137 K. Monomeric formaldehyde in gas phase was prepared by thermal decomposition of para-formaldehyde. Peak positions (ν), wavenumber shifts ($\Delta\nu$), and full widths at half maximum ($\Delta\nu_{1/2}$) are reported. Influence of the solvent on fundamental vibrational frequencies are studied using the polarizable continuum model (PCM). When used in combination with calculated anharmonic frequencies, the PCM model shows qualitative agreement with frequency shifts in liquid Kr. The importance of formaldehyde IR characterization around 100 K will be discussed in reference to its detection in the interstellar medium ^a, the IR detection of the ν_1 vibration in the protostar W33A^b, and although the Cassini infrared spectrometer (CIRS) was not able to detect methanol, formaldehyde, and acetonitrile in Titan's atmosphere, upper limits on their abundances and formation conditions have been proposed. ^{c,d}

^aB. Zuckerman et al., Observations of Interstellar Formaldehyde, *Astrophys. J.*, 1970, 160: 485–506.

^bE. Roueff et al., Infrared Detection of Gas Phase Formaldehyde Towards the High Mass Protostar W33A, *A&A*, 2006, 447: 963–969

^cC.A. Nixon et al., Upper Limits for Undetected Trace Species in the Stratosphere of Titan. *Faraday Discuss.* 2010, 147: 65–81.

^dB.N. Tran et al., Titan's Atmospheric Chemistry: Photolysis of Gas Mixtures Containing Hydrogen Cyanide and Carbon Monoxide at 185 and 254 nm, *Icarus*, 2008, 193: 224–232