

Interaction of Acetonitrile with Water-Ice: An Infrared Spectroscopic Study

Radha Gobinda Bhui¹, Rabin Rajan J. Methikkalam¹, Bhalamurugan Sivaraman², and Thalappil Pradeep^{1*}

¹DST Unit of Nanoscience (DST UNS) and Thematic Unit of Excellence (TUE), Department of Chemistry, Indian Institute of Technology Madras, Chennai 600 036, India

²Space and Atmospheric Sciences Division, Physical Research Laboratory, Ahmedabad, India.

*Corresponding author: Fax: + 91-44 2257-0545

*E-mail: pradeep@iitm.ac.in

SUPPORTING INFORMATION 1:

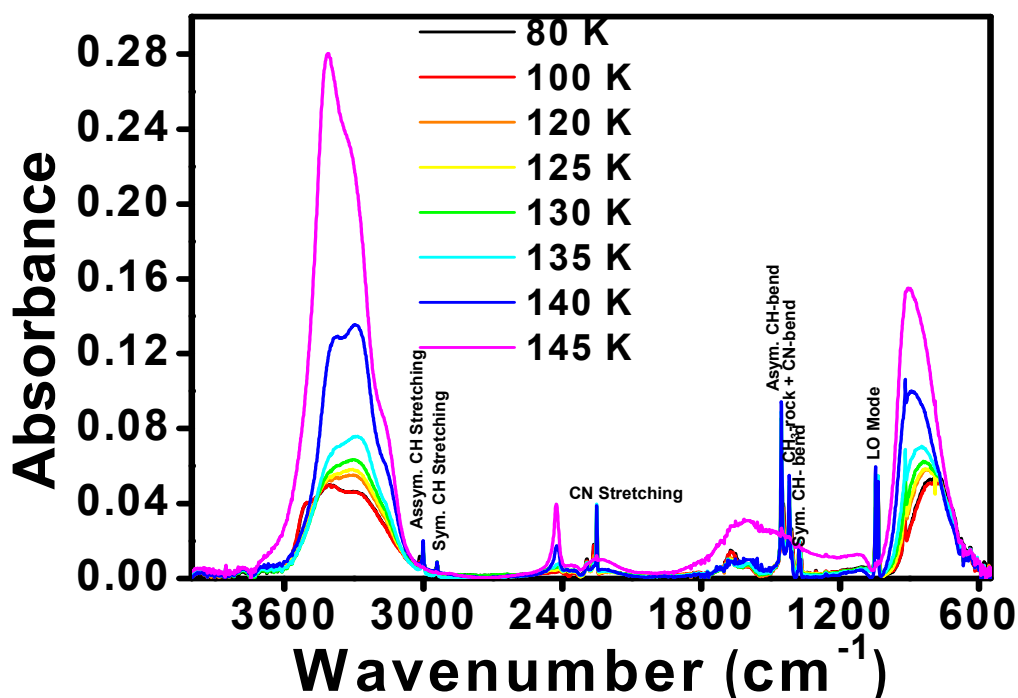


Figure S1: Temperature dependent RAIRS spectra of pure 1:1 ACN-h₃:H₂O deposited on cold Ru(0001) surface at 40 K. Complete desorption of ACN-h₃ takes place at 145 K during crystallization of H₂O.

SUPPORTING INFORMATION 2:

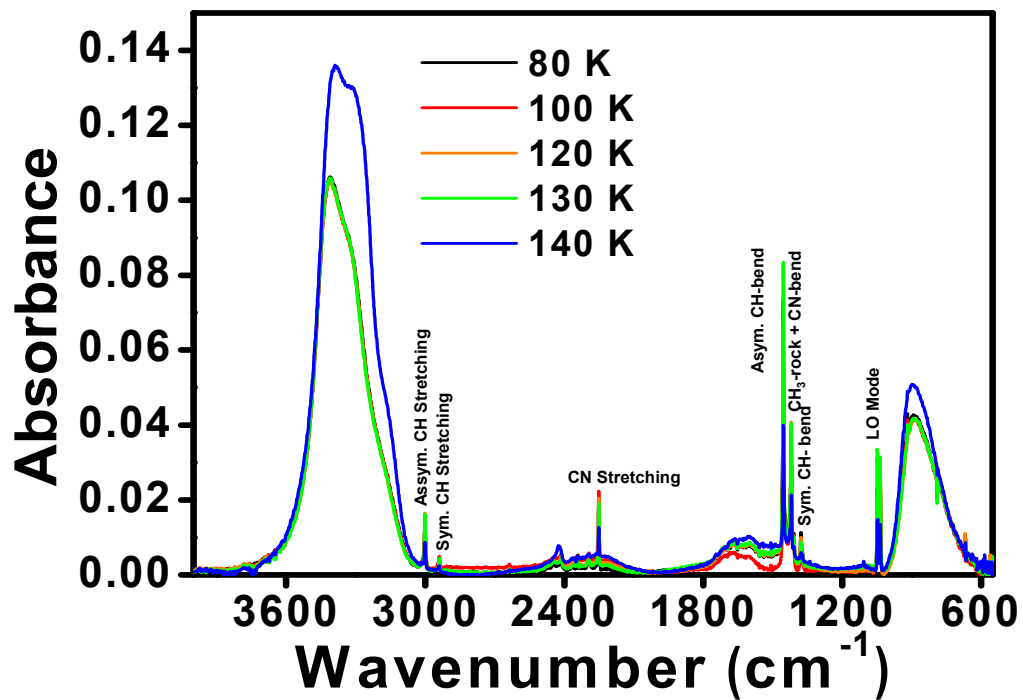


Figure S2: Temperature dependent RAIRS spectra of ACN-h₃@H₂O deposited on cold Ru(0001) surface at 40 K. Desorption of ACN-h₃ takes place during crystallization of H₂O at 140 K and it desorbs completely at 145 K.

SUPPORTING INFORMATION 3:

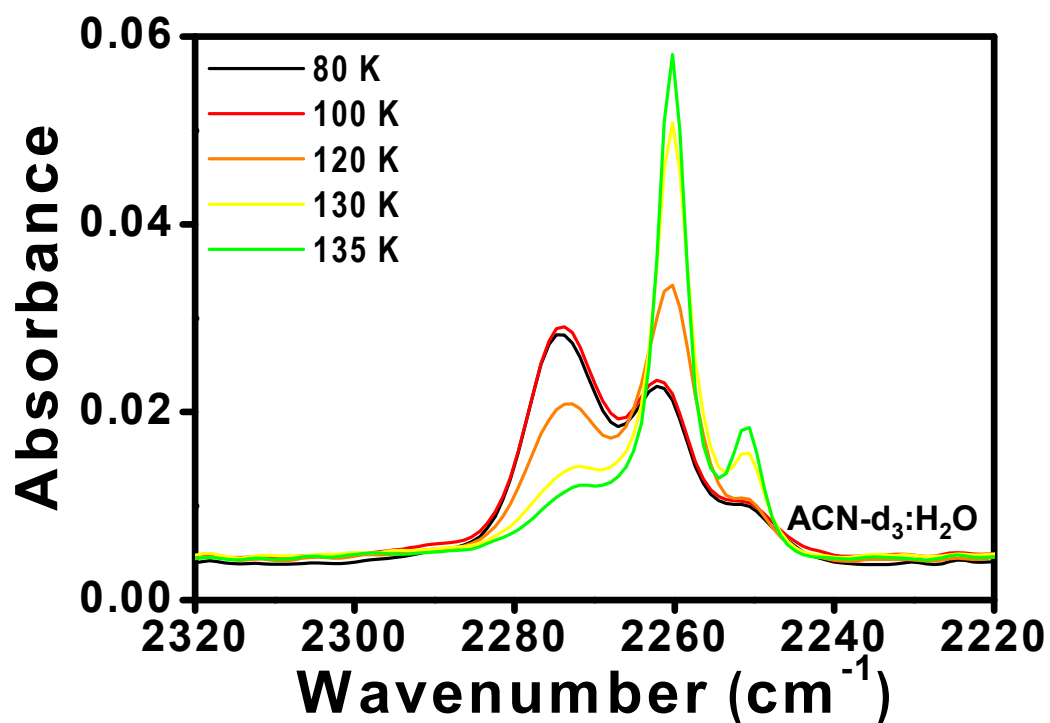


Figure S3: Temperature dependent RAIRS spectra of 1:1 ACN-d₃:H₂O deposited on cold Ru(0001) surface at 40 K. Spectra show the appearance of hydrogen bonded C≡N stretching at 2274 cm⁻¹ and the peak disappears upon warming.

SUPPORTING INFORMATION 4:

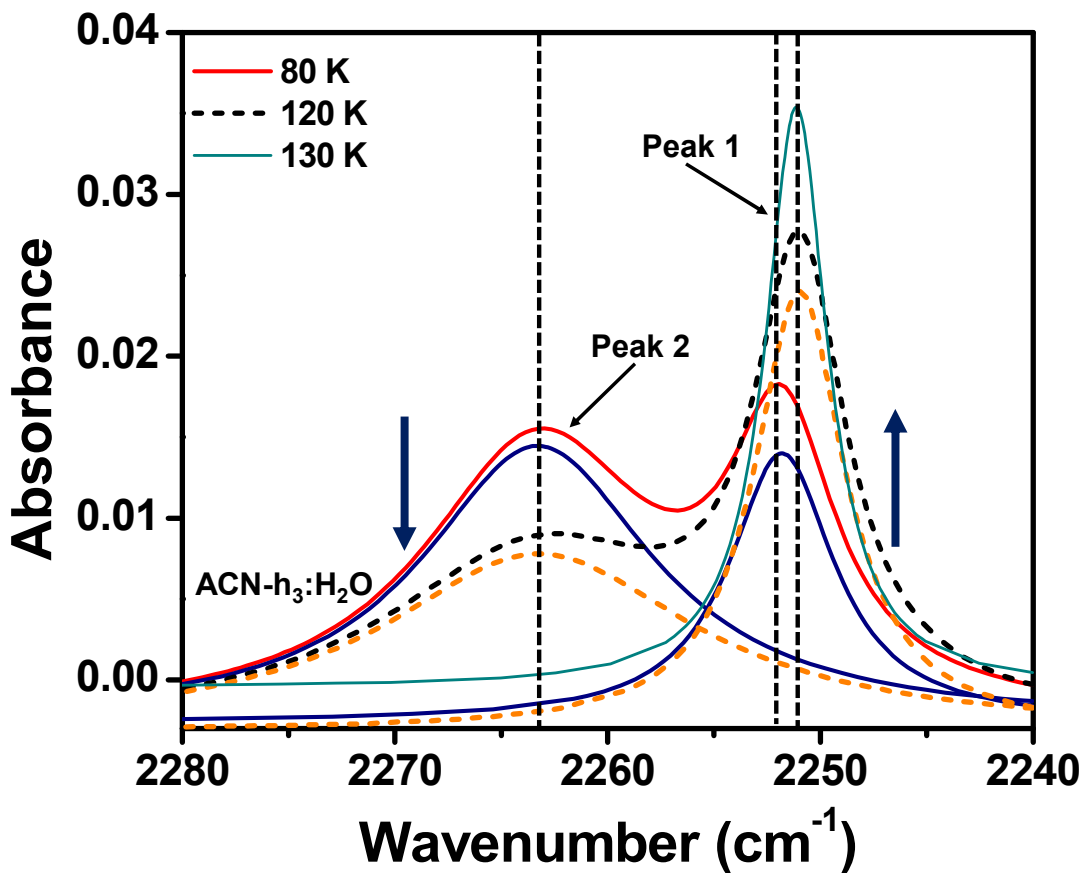


Figure S4: Lorentzian fit of the spectra of 1:1 ACN-h₃:H₂O at three different temperatures. Both fitted and cumulative spectra are shown in the figure. Two peaks in the cumulative spectrum at each temperature are fitted with two components, peak 1 corresponds to the free ACN molecules and peak 2 corresponds to H-bonded ACN molecules. Fitted spectrum and cumulative spectrum were overlapping at 130 K. Hence, only fitted spectrum is shown in the figure at 130 K.

SUPPORTING INFORMATION 5:

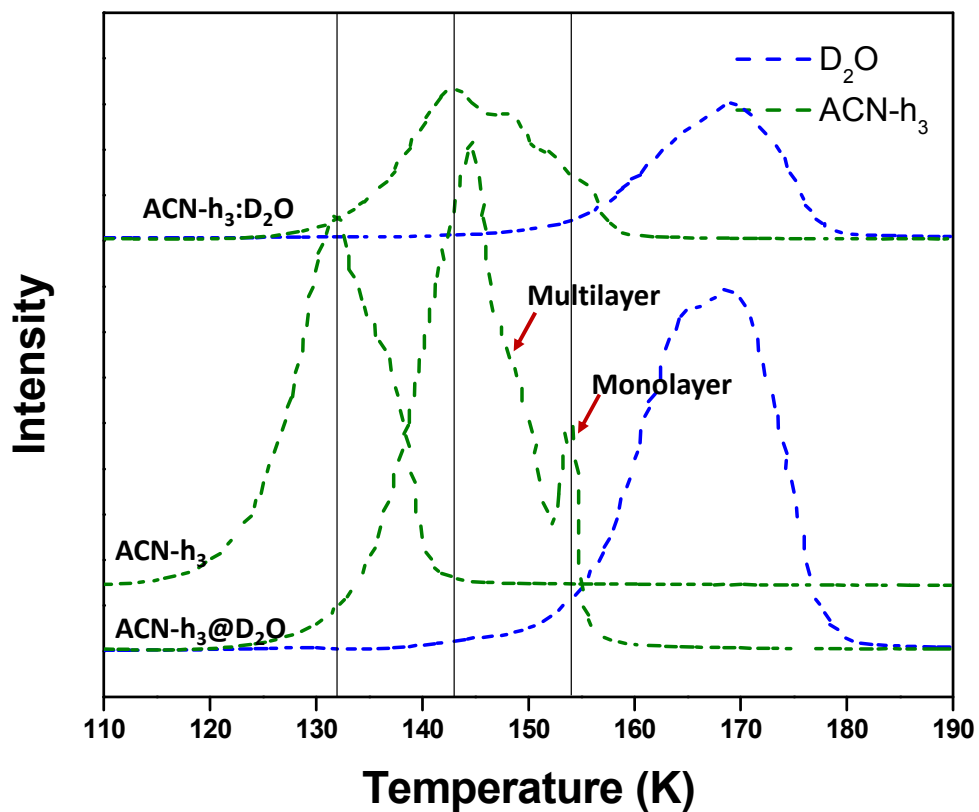


Figure S5: TPD spectra of three different sets of experiments are presented here. Desorption of pure ACN-h₃ is observed at 132 K whereas both co-deposited and overlayer deposited systems desorb at ~145 K, during crystallization of water-ice. Ramping rate was 20 K/min.