

Interaction of Acetonitrile with Alcohols at Cryogenic Temperatures

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Supporting Information

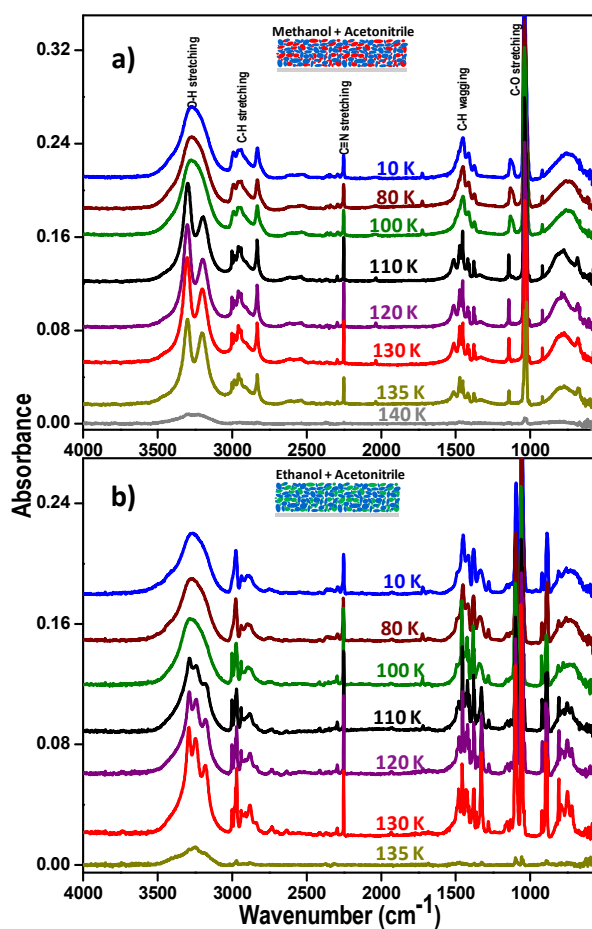


Figure S1: Temperature dependent RAIRS spectra collected for 1:1 co-deposited mixture of a) methanol and acetonitrile and b) ethanol and acetonitrile deposited at 10 K.

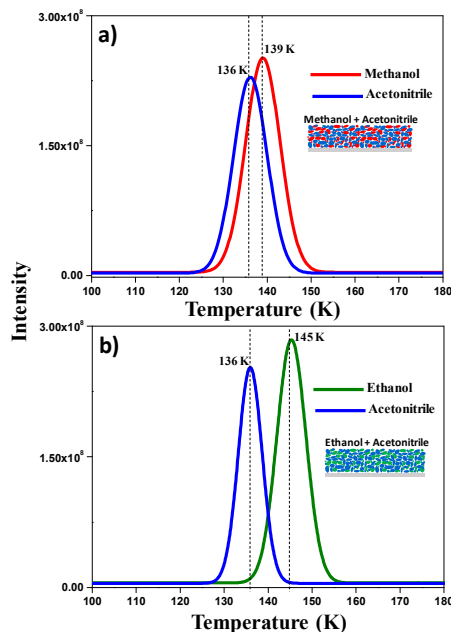


Figure S2: TPD spectra of co-deposited ice mixtures of a) methanol & acetonitrile and b) ethanol & acetonitrile, ramping rate 10 K/min. Mass peaks monitored were m/z 31 and m/z 41, for alcohols (methanol and ethanol) and acetonitrile, respectively.

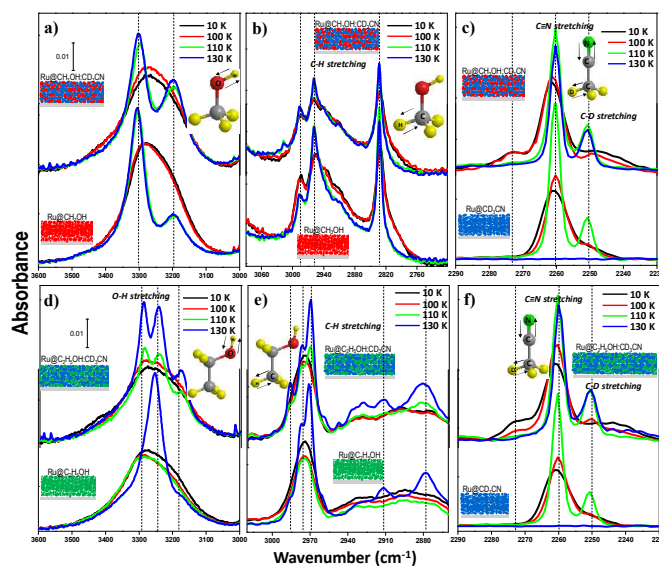


Figure S3: Temperature dependent RAIR spectra obtained from co-deposited mixtures of alcohols (methanol and acetonitrile) with CD_3CN . Spectra (a) and (d) shows the hydroxyl stretching region (b) and (e) show C-H stretching region from methanol and ethanol respectively. They are also compared with pure ice spectra in the same respective regions. Figures (c) and (f) show nitrile and C-D stretching regions from CD_3CN in co-deposited mixtures and are also compared with pure CD_3CN . Schematics within the figures show the ice systems under study. Cartoons of molecules showing the stretching vibrations are shown for better clarity.

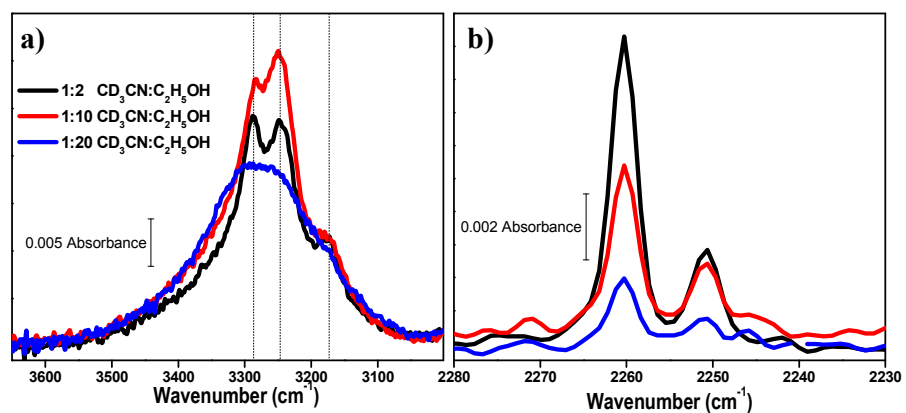


Figure S4: The spectra obtained at 110 K from different co-deposited ethanol and CD₃CN ice samples by varying the ratio of CD₃CN in a) OH stretching region of ethanol b) CN and CD stretching regions of CD₃CN.

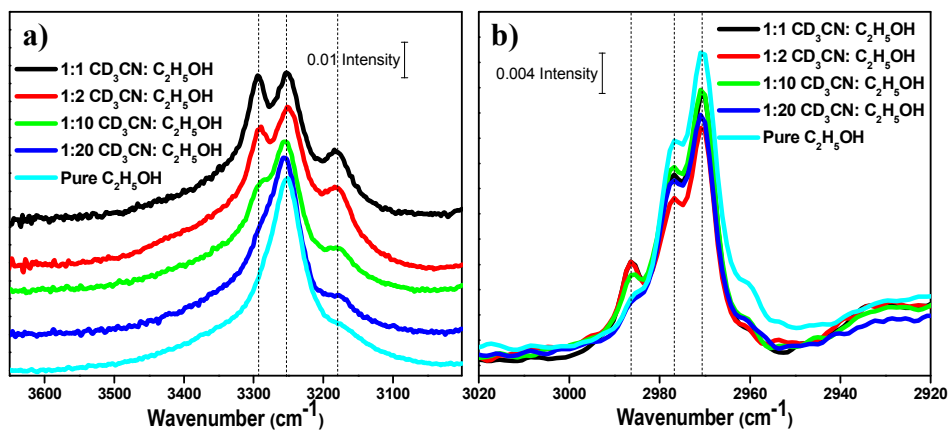


Figure S5: The spectra obtained at 130 K from co-deposited mixtures of ethanol with different ratios of CD₃CN along with pure ethanol spectra at 130 K in a) O-H stretching and b) C-H stretching regions of ethanol.

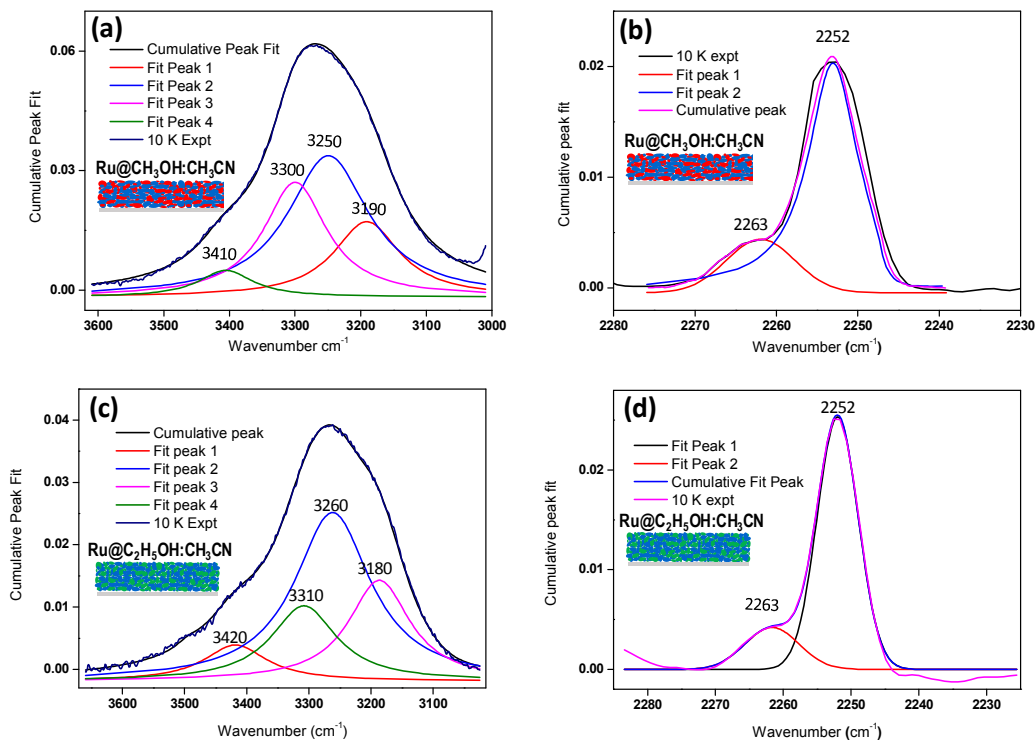


Figure S6: Lorentzian fit of the spectrum of co-deposited mixture at 10 K. (a), (b) For methanol with acetonitrile in OH stretching and CN stretching regions and (c), (d) for ethanol with acetonitrile in OH and CN stretching regions respectively.