

Formation of Ethane Clathrate Hydrate in Ultrahigh Vacuum by Thermal Annealing

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Supporting information 1:

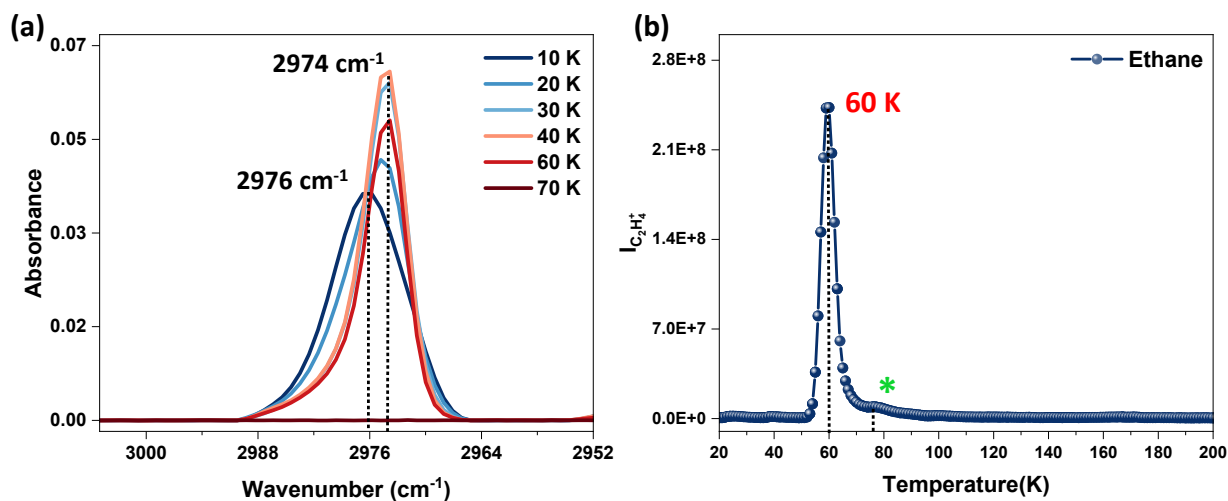


Figure S1. (a) Temperature-dependent RAIR spectra of 150 ML of pure ethane in C-H antisymmetric stretching region. Pure ethane was vapor-deposited on the Ru(0001) at 10 K and annealed with a ramping rate of 2 K min⁻¹. (b) TPD-MS spectrum of 150 ML of pure ethane. The intensity of C₂H₄⁺ (m/z = 28) versus temperature of the Ru(0001) substrate is plotted. The peak at 60 K is attributed to multilayer desorption, and the peak marked by (*) is attributed to monolayer desorption. The pure ethane was vapor-deposited on Ru(0001) at 10 K and further annealed to 200 K with a ramping rate of 30 K min⁻¹.

Supporting information 2:

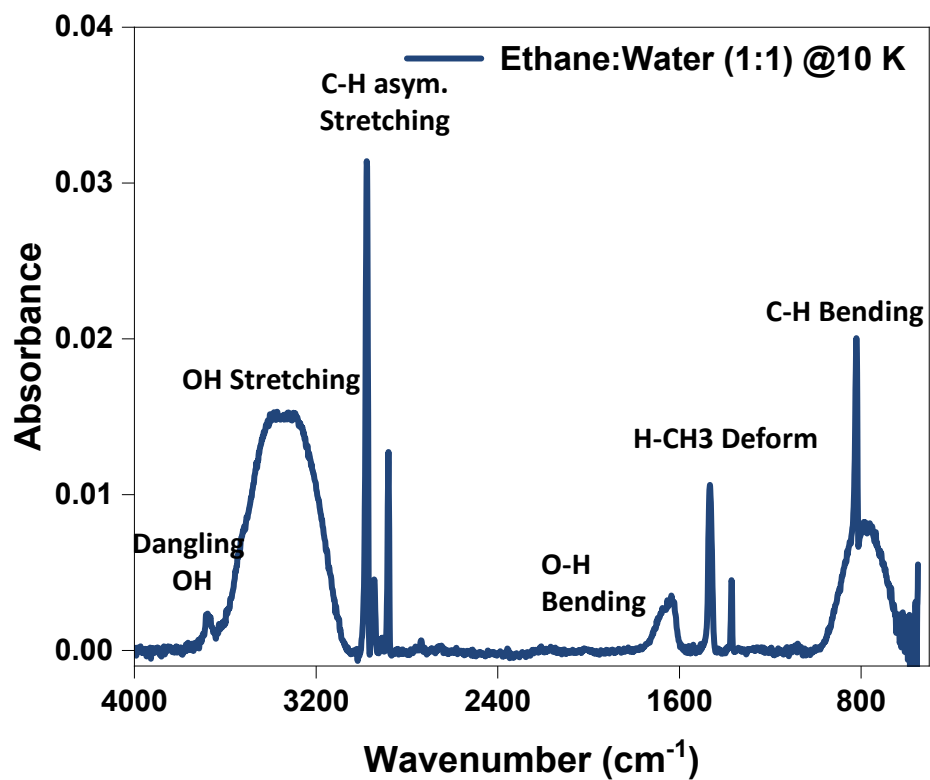


Figure S2. Full-scale RAIR spectrum of 300 ML of ethane:H₂O (1:1) ice mixture at 10 K. Ethane and water vapor were co-deposited on Ru(0001) at 10 K.

Supporting information 3:

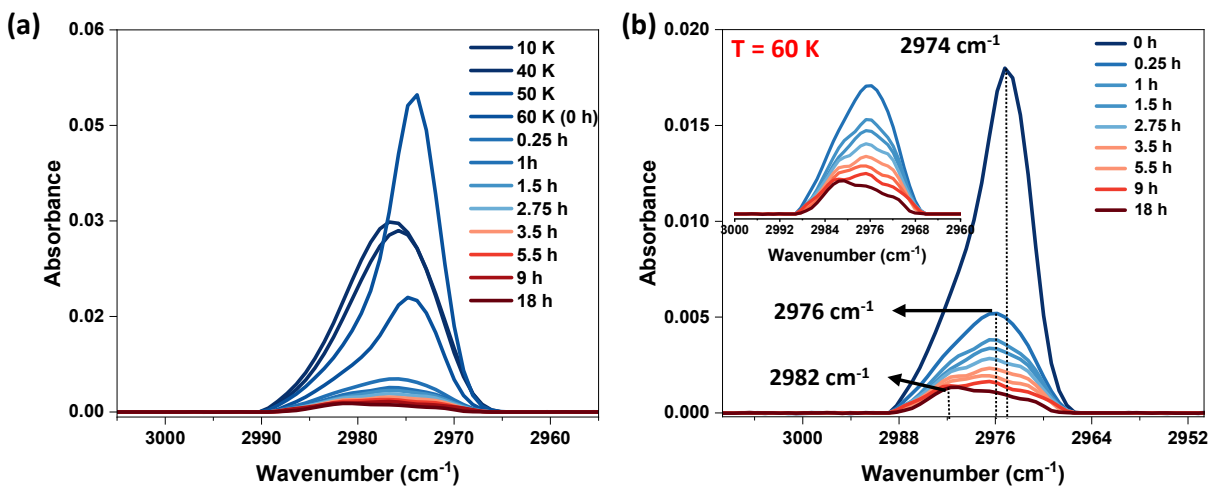


Figure S3. (a) Temperature and time-dependent RAIR spectra of 300 ML of ethane:H₂O (1:1) ice mixture in the C-H antisymmetric region. (b) Time-dependent RAIR spectra of 300 ML of ethane:H₂O (1:1) ice mixture at 60 K, in the left corner, the zoomed spectra from 0.25 h to 18 h are presented. Ethane and water vapor were co-deposited on the Ru(0001) at 10 K and annealed to 60 K at a ramping rate of 2 K min⁻¹.

Supporting information 4:

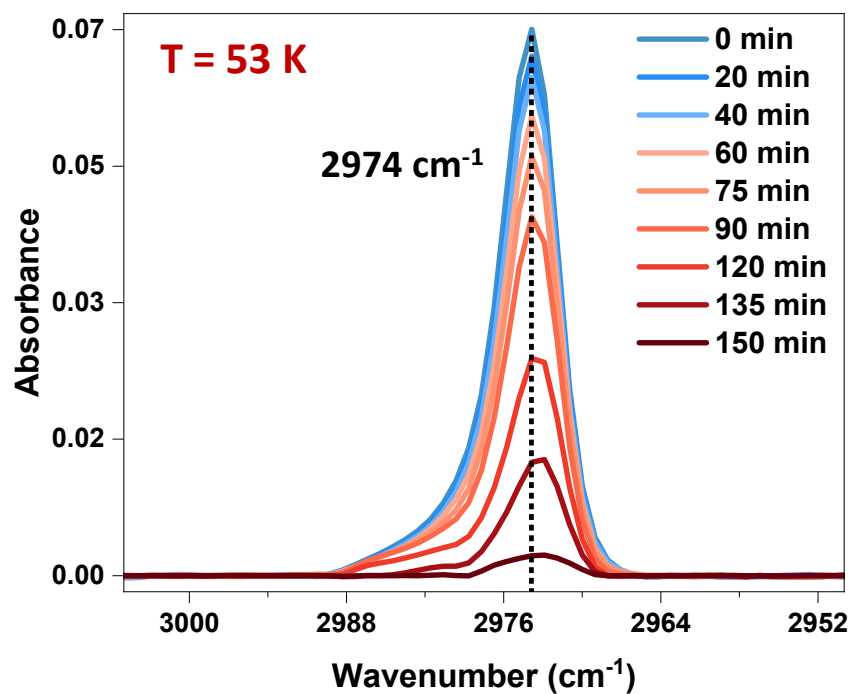


Figure S4. Time-dependent RAIR spectra of 150 ML of pure ethane film at 53 K in the C-H antisymmetric stretching region. Ethane vapor was deposited on Ru(0001) at 10 K and annealed to 53 K at a ramping rate of 2 K min⁻¹.

Supporting information 5:

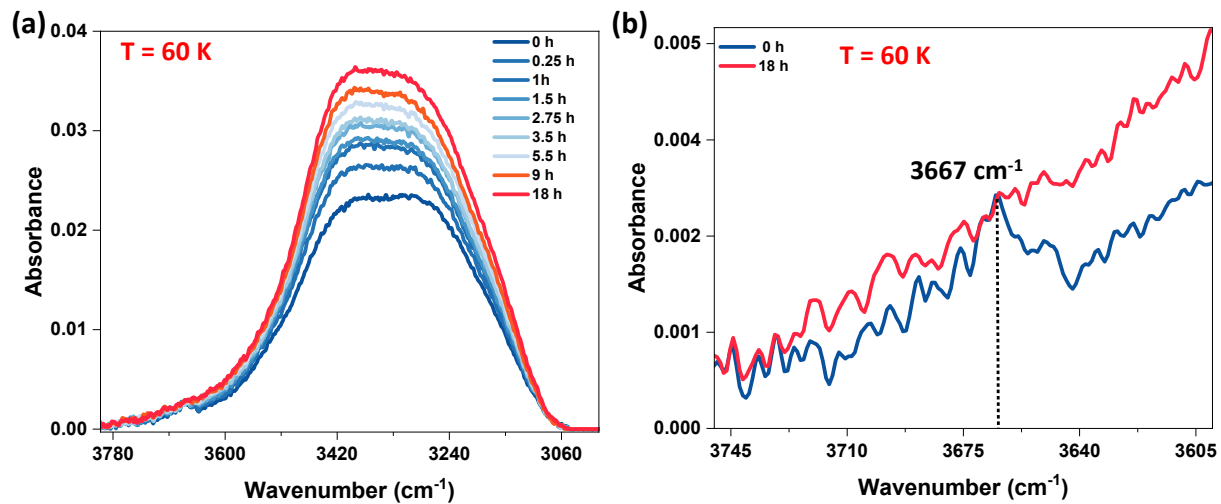


Figure S5. Time-dependent RAIR spectra of 300 ML of ethane:H₂O (1:1) ice mixture in the, (a) O-H stretching region of H₂O, and (b) Dangling O-H stretching region of H₂O. Ethane and water vapor were co-deposited on Ru(0001) at 10 K and annealed to 60 K at a ramping rate of 2 K min⁻¹.

Supporting Figure 6:

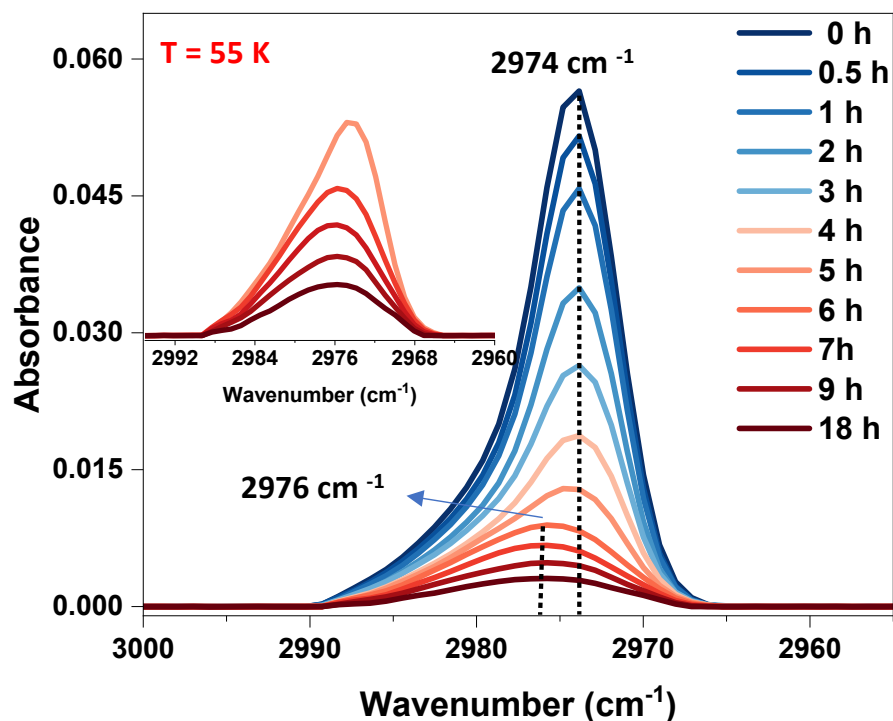


Figure S6. Time-dependent RAIR spectra of 300 ML of ethane:H₂O (1:1) ice mixture at 55 K in the C-H antisymmetric region. The zoomed spectra from 5 h to 18 h are also shown in the left corner of the figure. The ethane-water mixture co-deposited on Ru(0001) at 10 K and annealed to 55 K at a ramping rate of 2 K min⁻¹.

Supporting Figure 7:

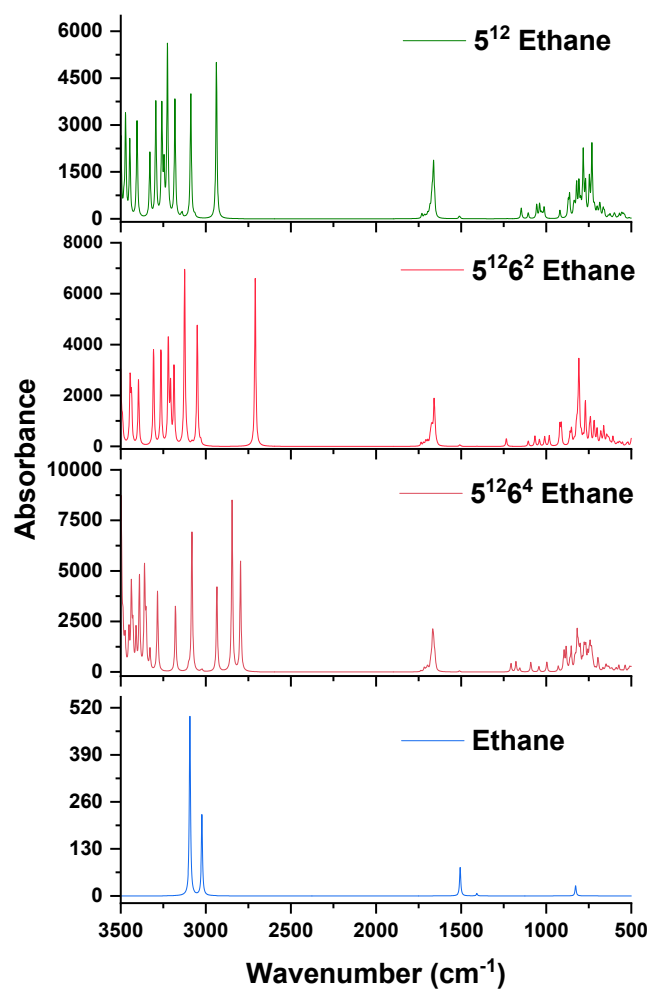


Figure S7. Full-scale computed IR spectra of ethane and ethane entrapped in 5¹²6⁴, 5¹²6², and 5¹² cages. All the data for IR spectra were calculated from the DFT study.