

Propane and Propane-Water interactions: A Study at Cryogenic Temperatures†

Jyotirmoy Ghosh¹, Annapoorani Kobuvayur Hariharan¹, Radha Gobinda Bhui[†], Rabin Rajan Joseph Methikkalam¹, 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

*Corresponding author: Fax: + 91-44 2257-0545/0509

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

Supporting Information:

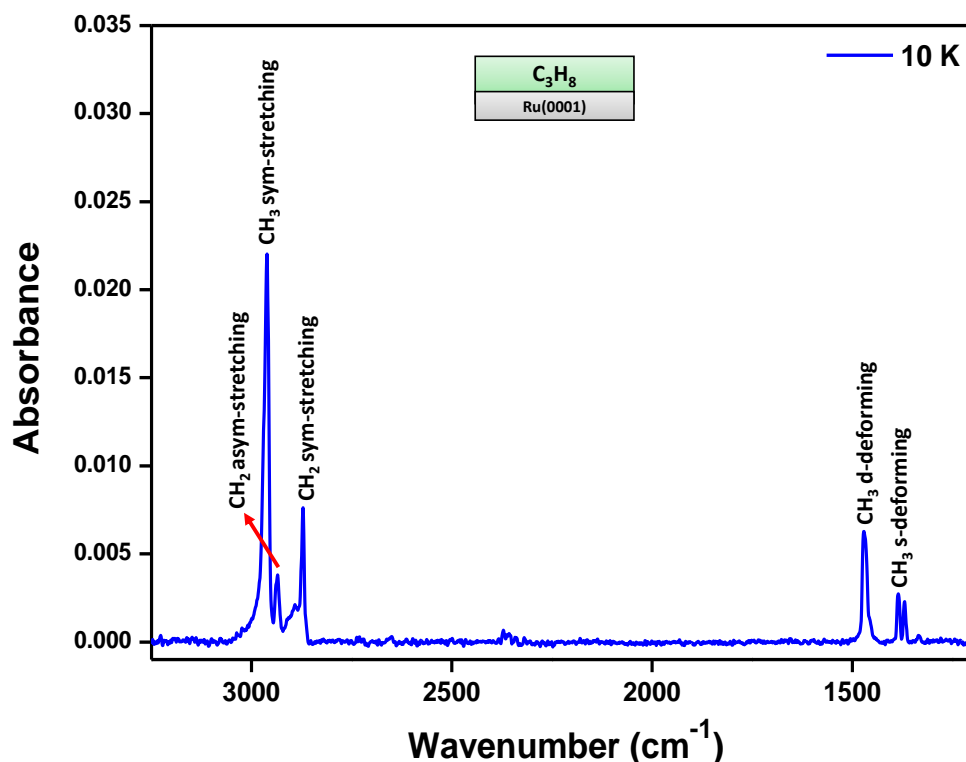


Fig. S1 RAIR spectrum of 150 ML of propane which was deposited on Ru(0001) substrate at 10 K. Different modes of molecular vibrations of propane are assigned in the RAIR spectrum.

Table S1. IR peaks and vibrational band positions for solid and gaseous propane

Sr. no.	Symmetry species	Vibrational mode	Solid phase (Experimental) (cm ⁻¹)		Gas phase ¹ (cm ⁻¹)	Solid phase ² (cm ⁻¹)
			10 K	70 K		
1	A ₁	CH ₃ d-stretch			2977	
2	A ₁	CH ₃ s-stretch	2961.66	2965	2962	
3	A ₁	CH ₂ s-stretch	2871.89	2873	2887	
4	A ₁	CH ₃ d-deformation			1476	
5	A ₁	CH ₂ scissoring			1462	
6	A ₁	CH ₃ d-deformation	1386.44	1388	1392	1382
7	A ₁	CH ₃ rocking	1155.70	1156	1158	1155
8	A ₁	C-C stretch	868.77	867	869	869
9	A ₁	C-C-C deformation			369	
10	B ₁	CH ₃ d-stretch			2968	
11	B ₁	CH ₃ s-stretch		2866	2887	
12	B ₁	CH ₃ d-deformation			1464	
13	B ₁	CH ₃ s-deformation	1369.69	1369	1378	1368
14	B ₁	CH ₂ wagging			1338	
15	B ₁	C-C stretch	1051.09	1049	1054	1050
16	B ₁	CH ₃ rocking	920.31	917	922	918
17	B ₁	CH ₃ d-stretch			922	
18	B ₂	CH ₃ d-stretch			2973	
19	B ₂	CH ₂ a-stretch		2957	2968	
20	B ₂	CH ₃ d-deformation	1471.36		1472	
21	B ₂	CH ₃ rocking			1192	
22	B ₂	CH ₂ rocking	742	747	748	745

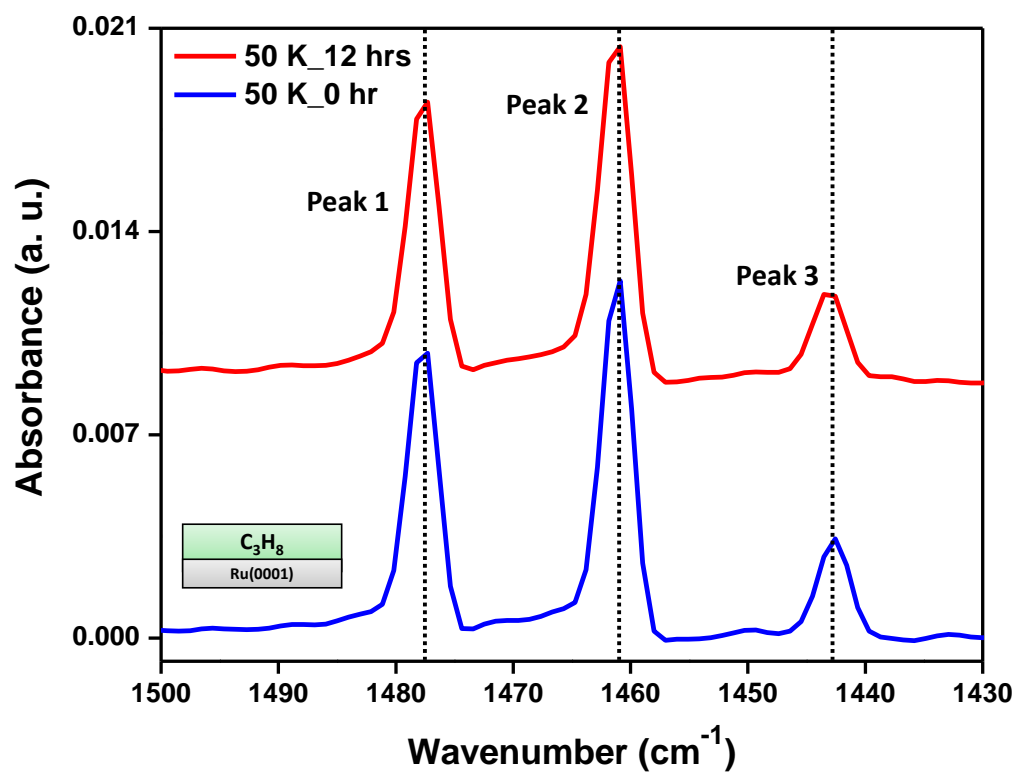


Fig. S2 Study of stability of phase I of propane by RAIR. 150 ML of propane was deposited at 10 K, and it was heated to 50 K for first phase transition. Then, the system was kept at 50 K for 12 hours to check the stability of the phase I.

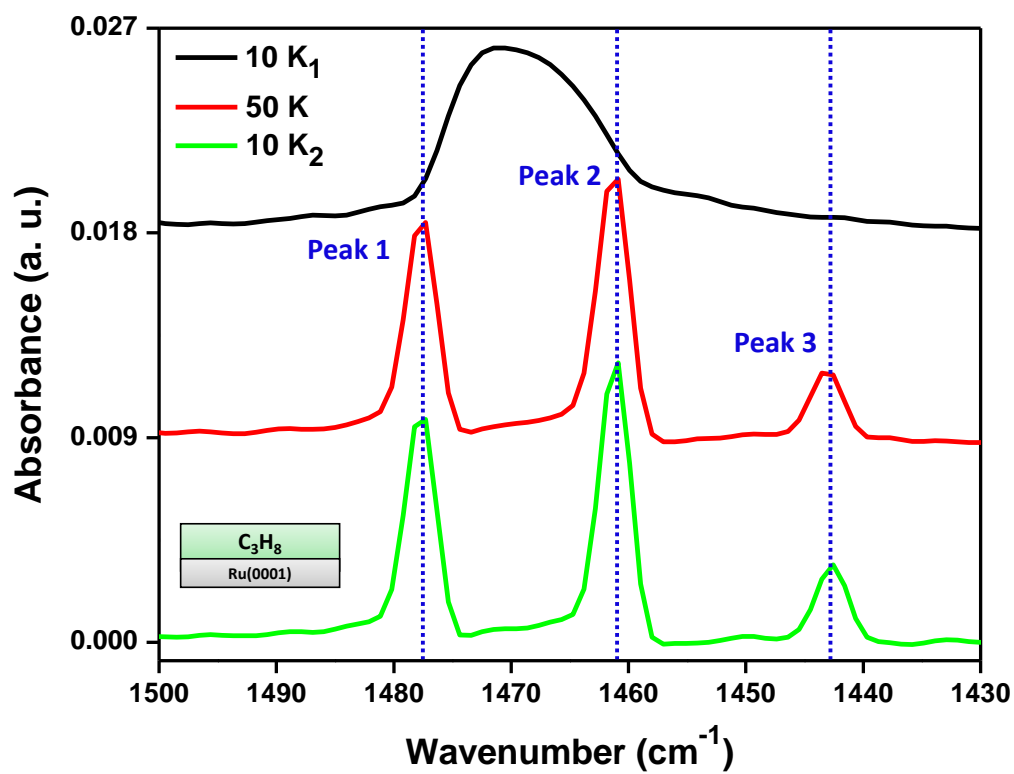


Fig. S3 Study of reversibility of first phase transition of propane by RAIR. 150 ML of propane was deposited at 10 K, and it was heated to 50 K to observe the first phase transition. Again, the system was cooled down at 10 K to check the reversibility of the phase transition.

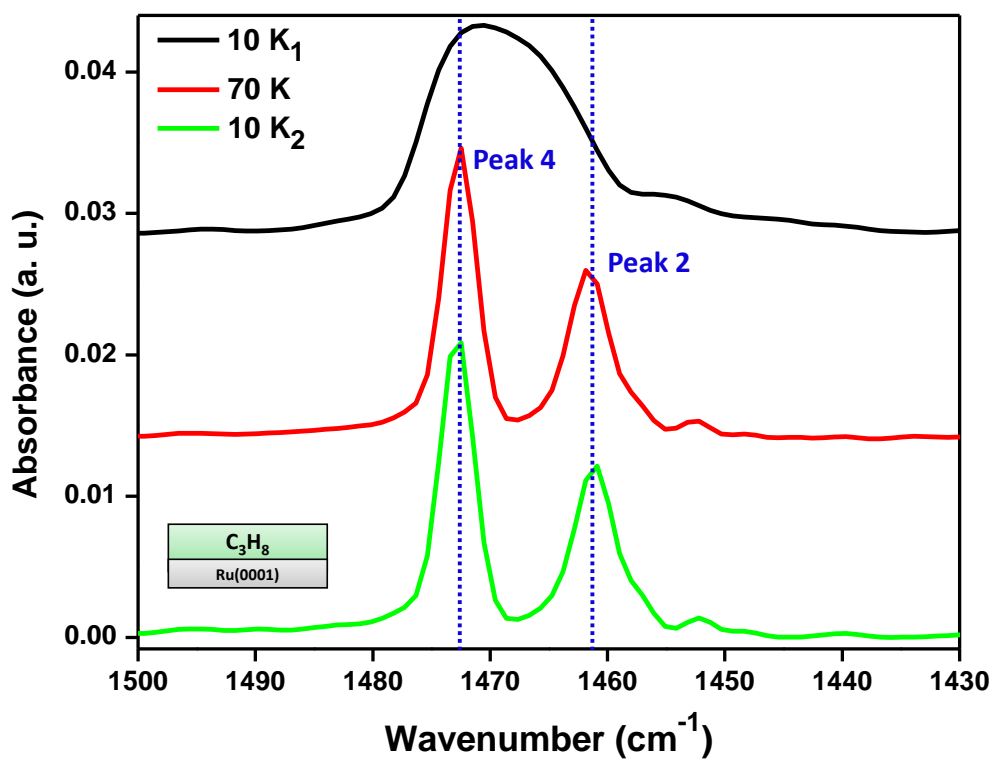


Fig. S4 Study of reversibility of second phase transition of propane by RAIR. 150 ML of propane was deposited at 10 K, and it was heated to 70 K to observe the second phase transition. Again, the system was cooled down at 10 K to check the reversibility the phase transition.

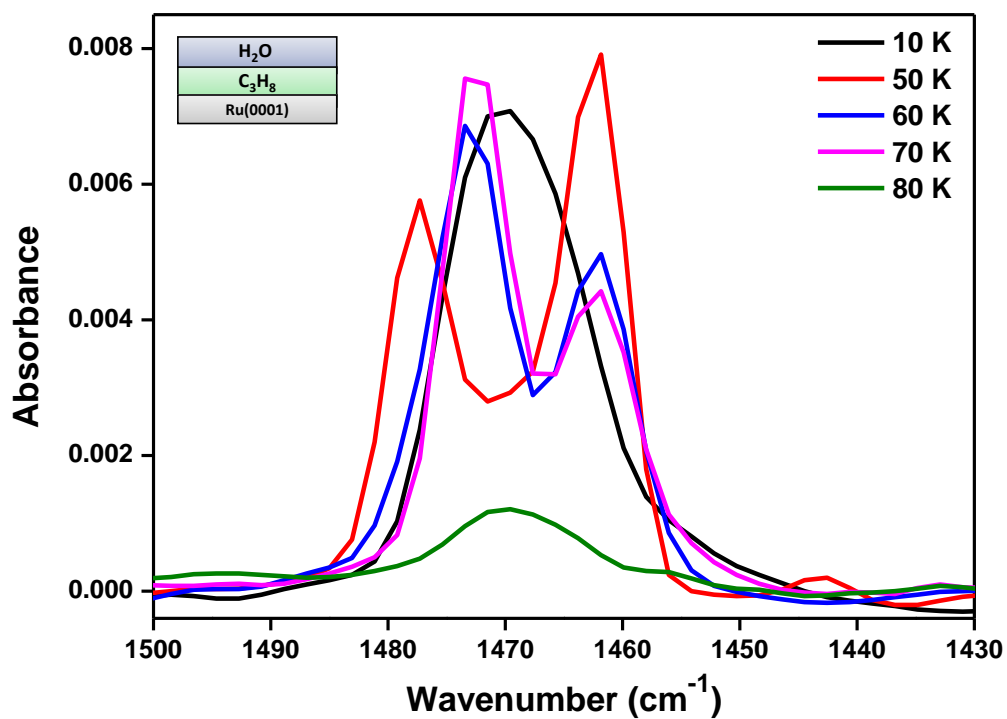


Fig. S5 Temperature dependent RAIR spectra of 150 ML of water deposited on 150 ML of propane at 10 K. After the deposition, the $C_3H_8@H_2O$ system was heated at 2 K/min heating rate and the RAIR spectra were measured at different temperatures.

References

1. T. Shimanouchi, *National Bureau of Standards*, 1972, **Consolidated Volume I**, 1-160.
2. M. A. Goodman, R. L. Sweany and R. L. Flurry, Jr., *J. Phys. Chem.*, 1983, **87**, 1753-1757.