

Surface science studies of the coverage dependent adsorption of methyl acetate and methyl propanoate on graphite

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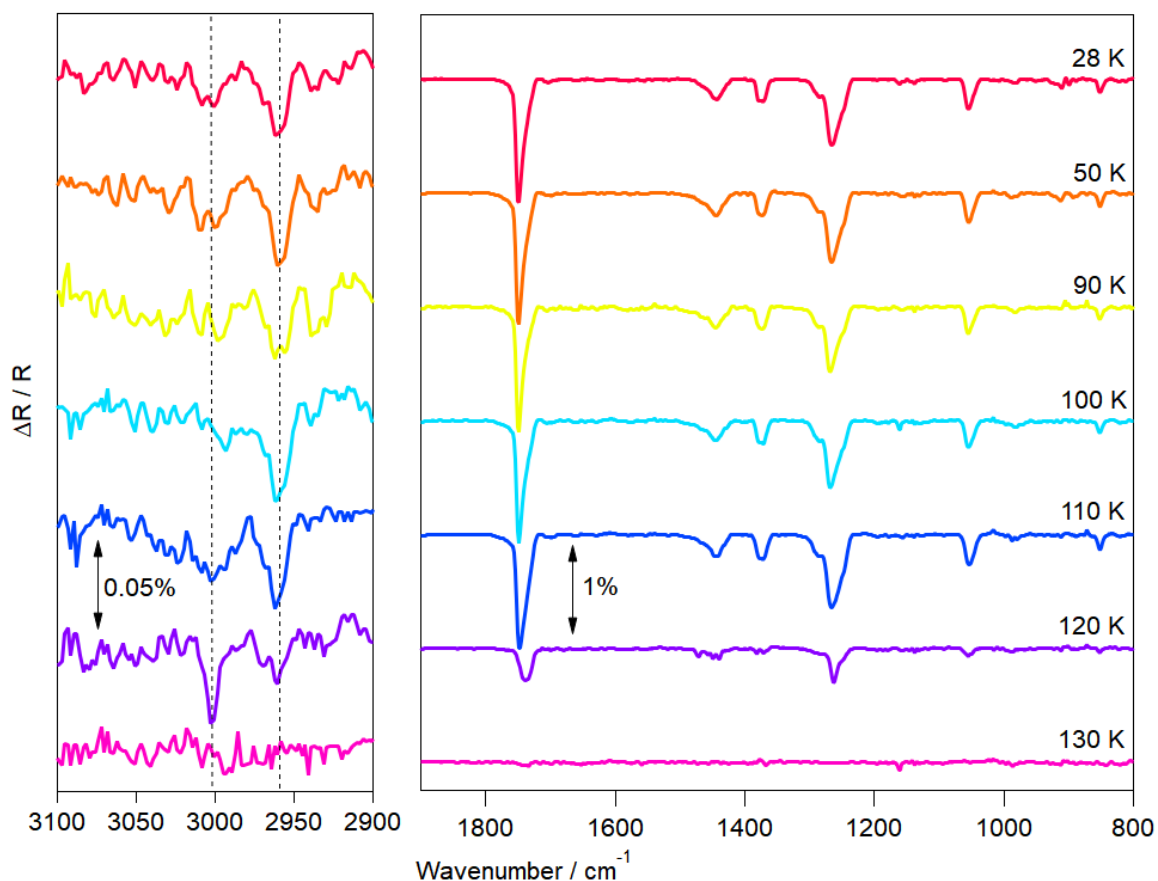


Figure S1: RAIR spectra for the annealing of a 100 L_m methyl acetate ice adsorbed on HOPG. The ice was grown at 28 K and heated at a rate of 0.5 K s⁻¹ in increments of 10 K, holding at each temperature for 3 minutes before cooling back to base temperature to record a spectrum. The left hand panel shows the 2900 – 3100 cm⁻¹ wavenumber region and the right hand panel shows the region from 800 – 1900 cm⁻¹. No vibrational bands are seen in other regions of the spectrum.

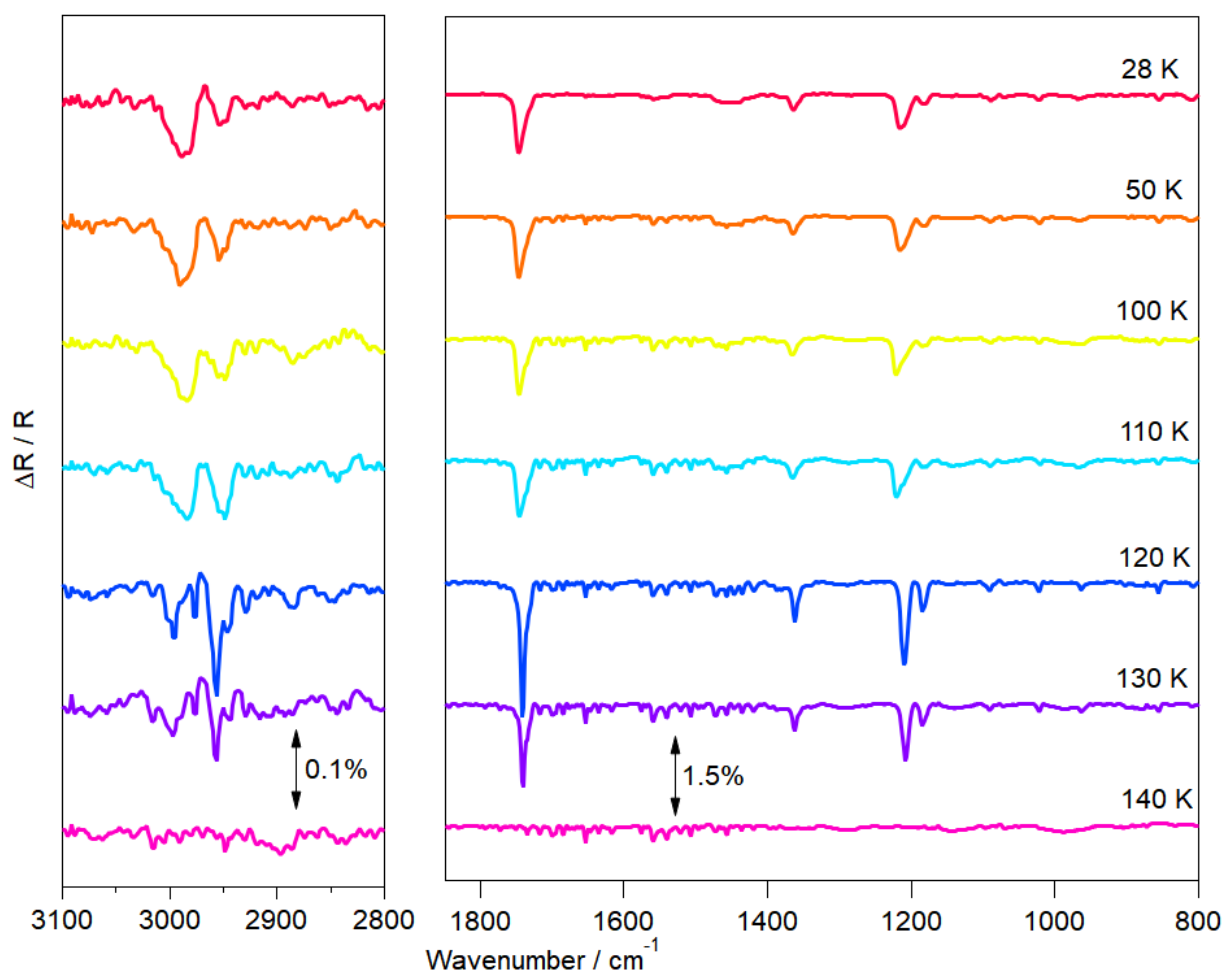


Figure S2: RAIR spectra for the annealing of a 100 L_m methyl propanoate ice adsorbed on HOPG. The ice was grown at 28 K and heated at a rate of 0.5 K s^{-1} in increments of 10 K, holding at each temperature for 3 minutes before cooling back to base temperature to record a spectrum. The left hand panel shows the 2800 – 3100 cm^{-1} wavenumber region and the right hand panel shows the region from 800 – 1900 cm^{-1} . No vibrational bands are seen in other regions of the spectrum.

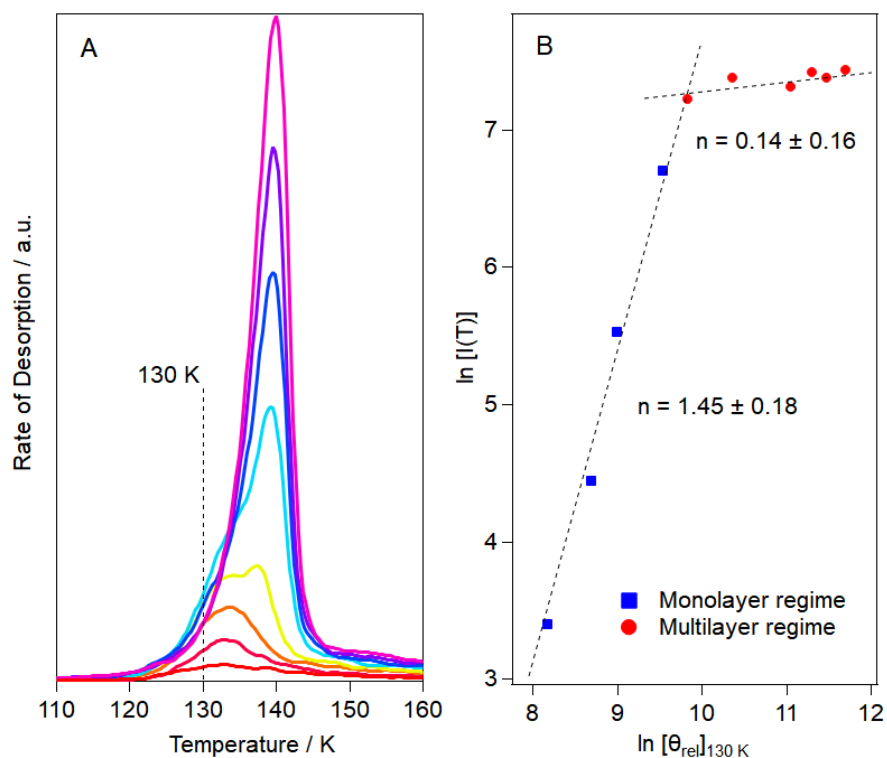


Figure S3: (A) TPD data for methyl propanoate adsorbed on HOPG with the common temperature of 130 K labelled. (B) An example order plot for the desorption at 130 K.

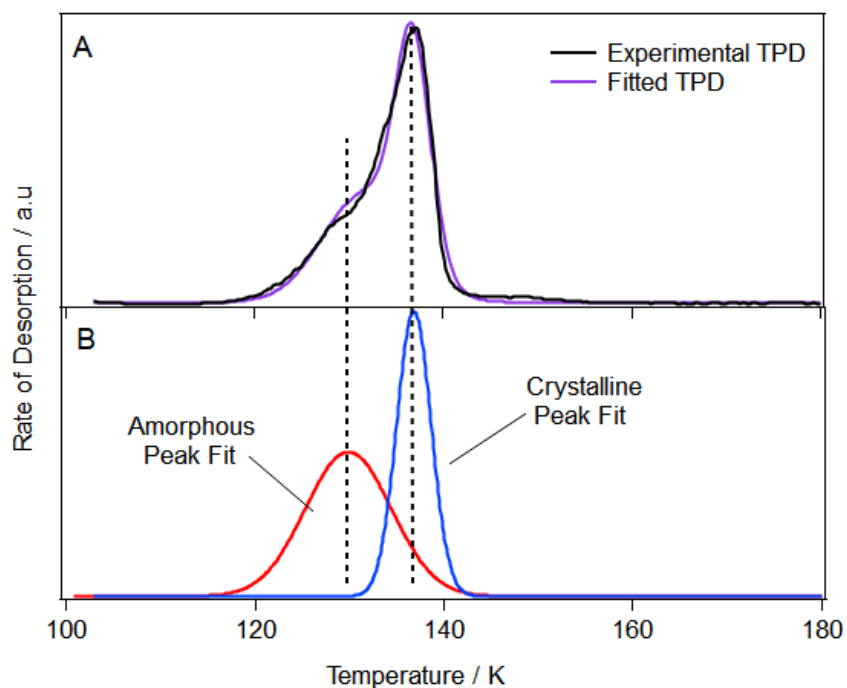


Figure S4: An example peak fit for the separation of amorphous and crystalline methyl acetate desorption for a 180 L_m ice grown at 120 K on HOPG. (A) The experimental data compared to the fitted trace. (B) The separated amorphous and crystalline peaks.

Table S1: Molecular constants used in the transition-state-theory analysis.

	Mass / amu	Principle moments of inertia / amu Å ²			Symmetry factor (σ)
		I _x	I _y	I _z	
Methyl acetate	74	163.83	121.04	49.16	1
Methyl propanoate	88	278.46	235.18	52.73	1