

1 SUPPORTING INFORMATION

2 Propyne: Determination of physical properties and
3 unit cell parameters under Titan-relevant conditions

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Figure S-1. Raman spectroscopy of pure propyne ice deposited at 75 K under low pressure, with increasing temperatures. A phase transition is observed around 105-107 K. Expanded views of various spectral regions are shown at the bottom panels.

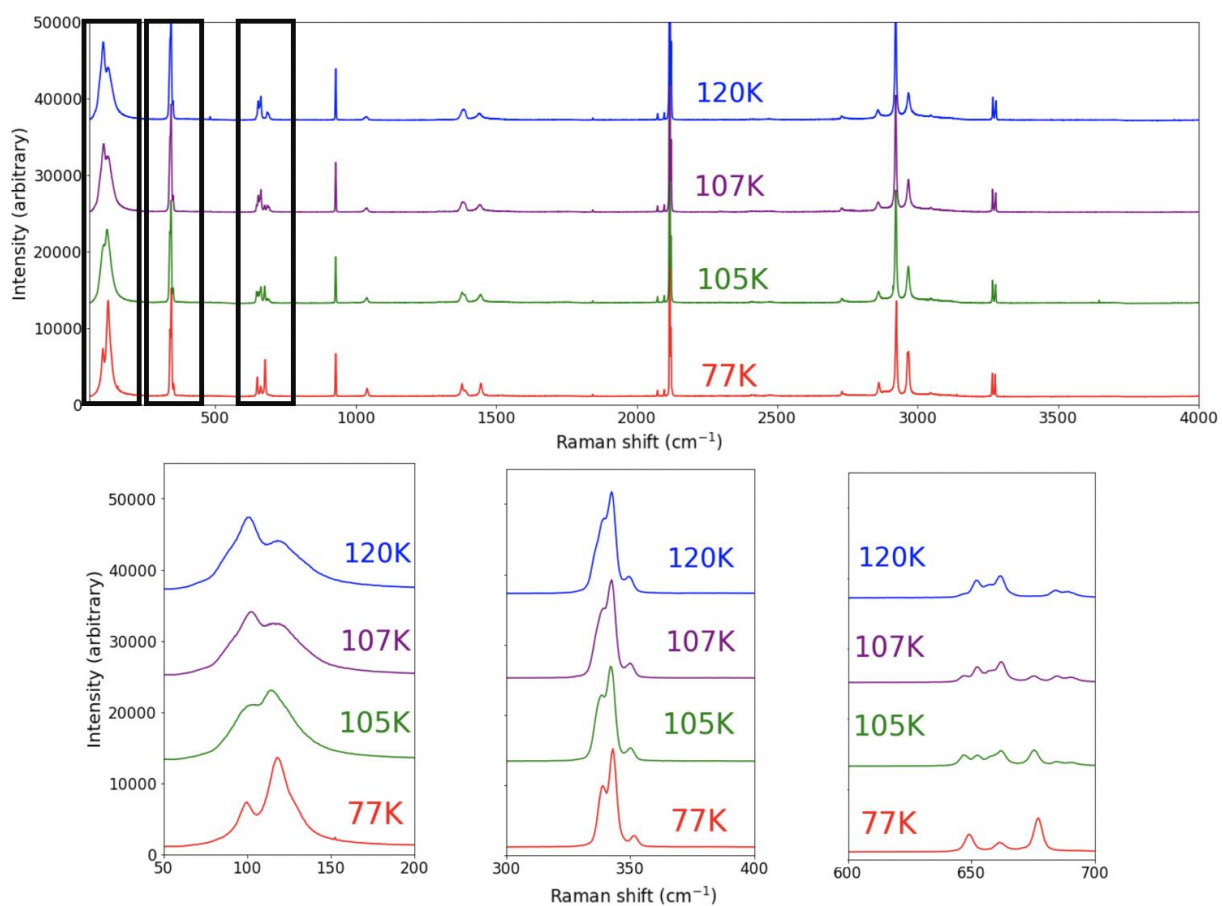
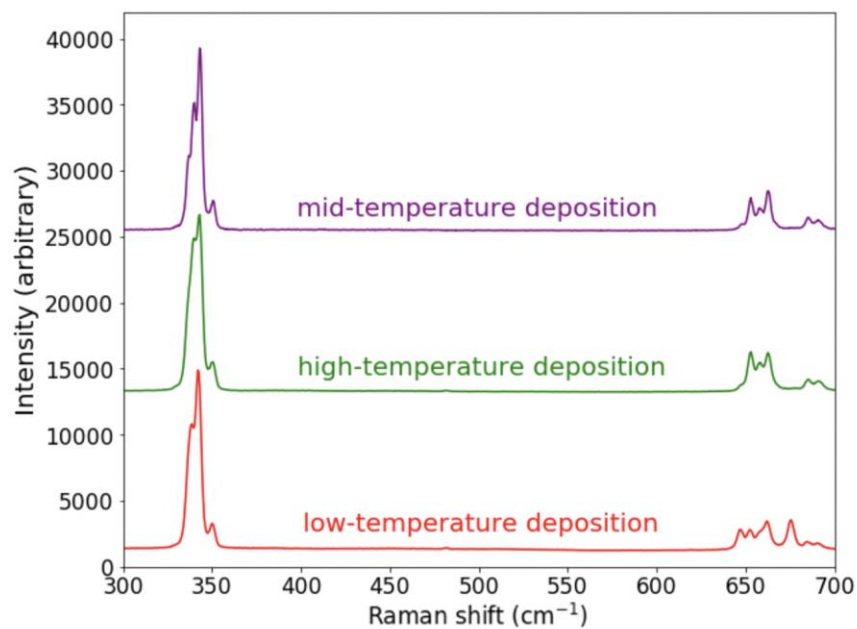
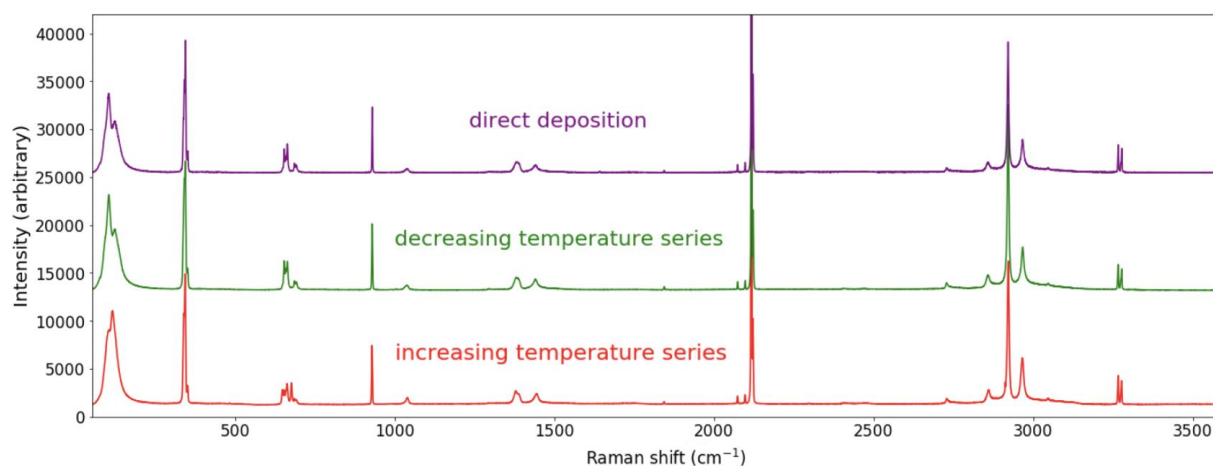


Figure S-2. Spectra at 105 K; low-temperature deposition at 75 K (increasing temperature series; warmed to 105 K), high-temperature deposition at 120 K (decreasing temperature series cooled to 105 K), and direct deposition at 105 K comparisons. Direct deposition at 105 K has a crystalline structure.



28 **Figure S-3.** Raman spectroscopy of pure propyne ice deposited at 120 K under low pressure,
 29 with decreasing temperatures. No phase transitions are observed. Expanded views of various
 30 spectral regions are shown at the bottom panels.

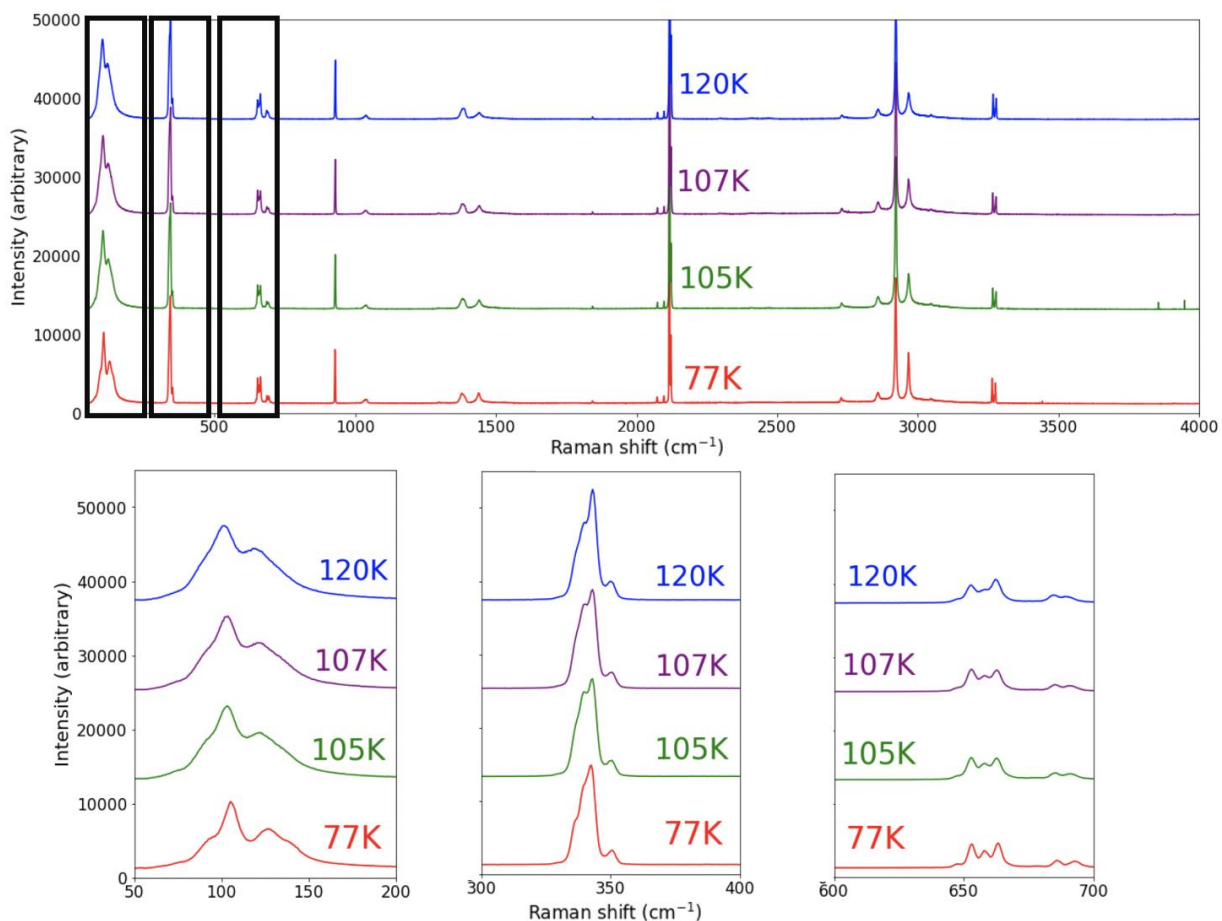


Figure S-4. Infrared spectroscopy temperature series of pure propyne deposited at 15 K and annealed to 105 K, under vacuum. Transition from amorphous to crystalline propyne is observed between 65 K and 75 K. Spectra highlighted in purple and denoted with an asterisk (8 K, 70 K, and 80 K) are from previously published work by Hudson et al. 2021²³ (Figures 11-13).

