

1 SUPPORTING INFORMATION

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

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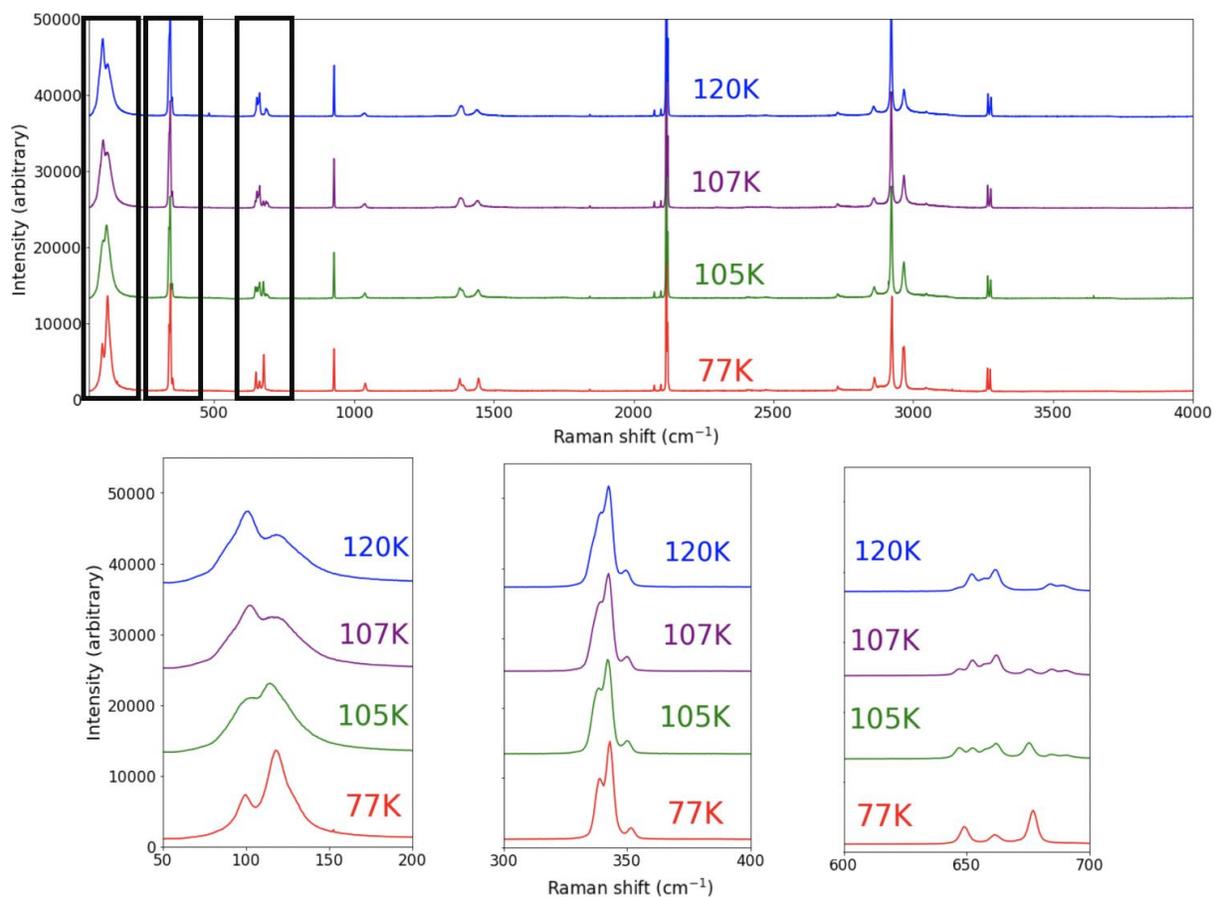
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15 **Figure S-1.** Raman spectroscopy of pure propyne ice deposited at 75 K under low pressure, with  
16 increasing temperatures. A phase transition is observed around 105-107 K. Expanded views of  
17 various spectral regions are shown at the bottom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



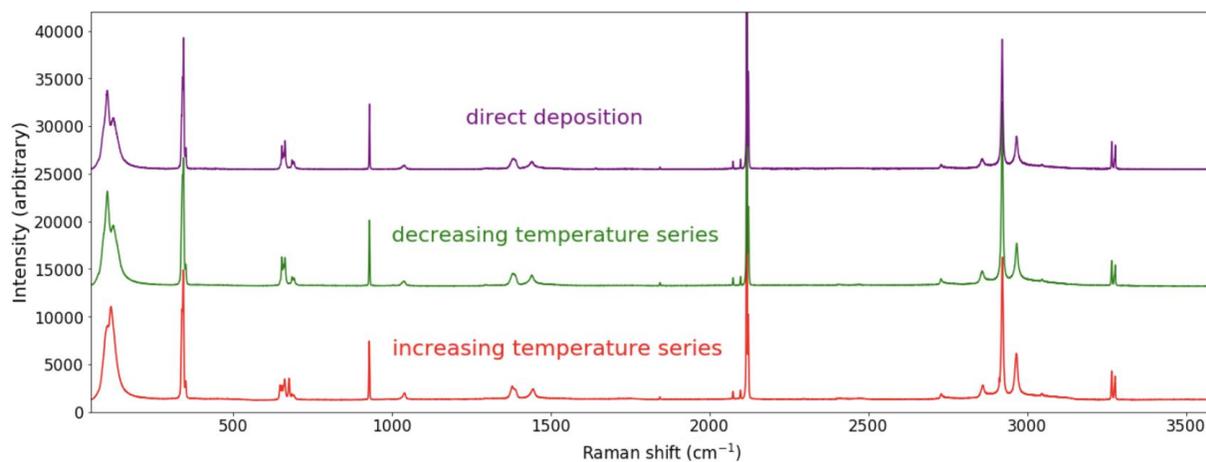
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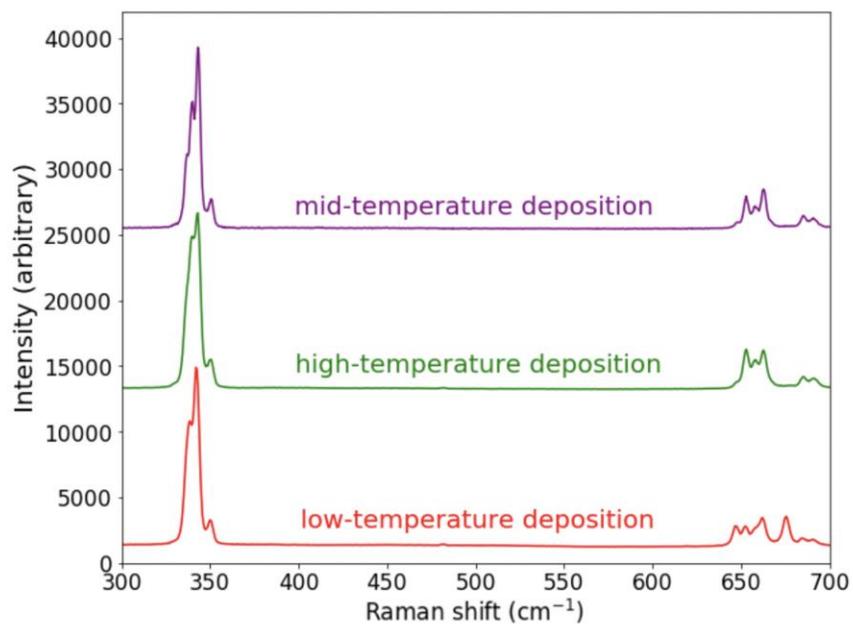
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22 **Figure S-2.** Spectra at 105 K; low-temperature deposition at 75 K (increasing temperature series;  
23 warmed to 105 K), high-temperature deposition at 120 K (decreasing temperature series cooled  
24 to 105 K), and direct deposition at 105 K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

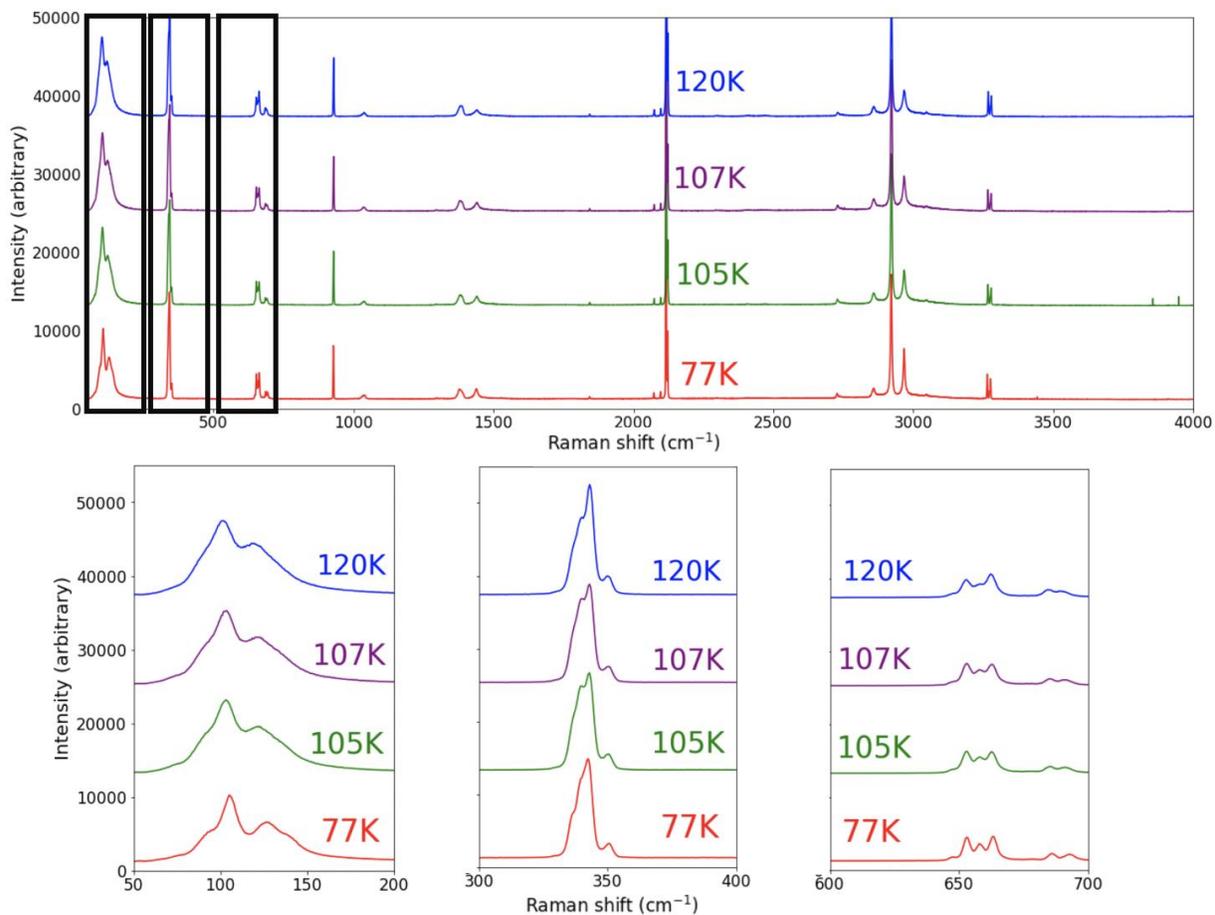


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28 **Figure S-3.** Raman spectroscopy of pure propyne ice deposited at 120 K under low pressure,  
29 with decreasing temperatures. No phase transitions are observed. Expanded views of various  
30 spectral regions are shown at the bottom panels.

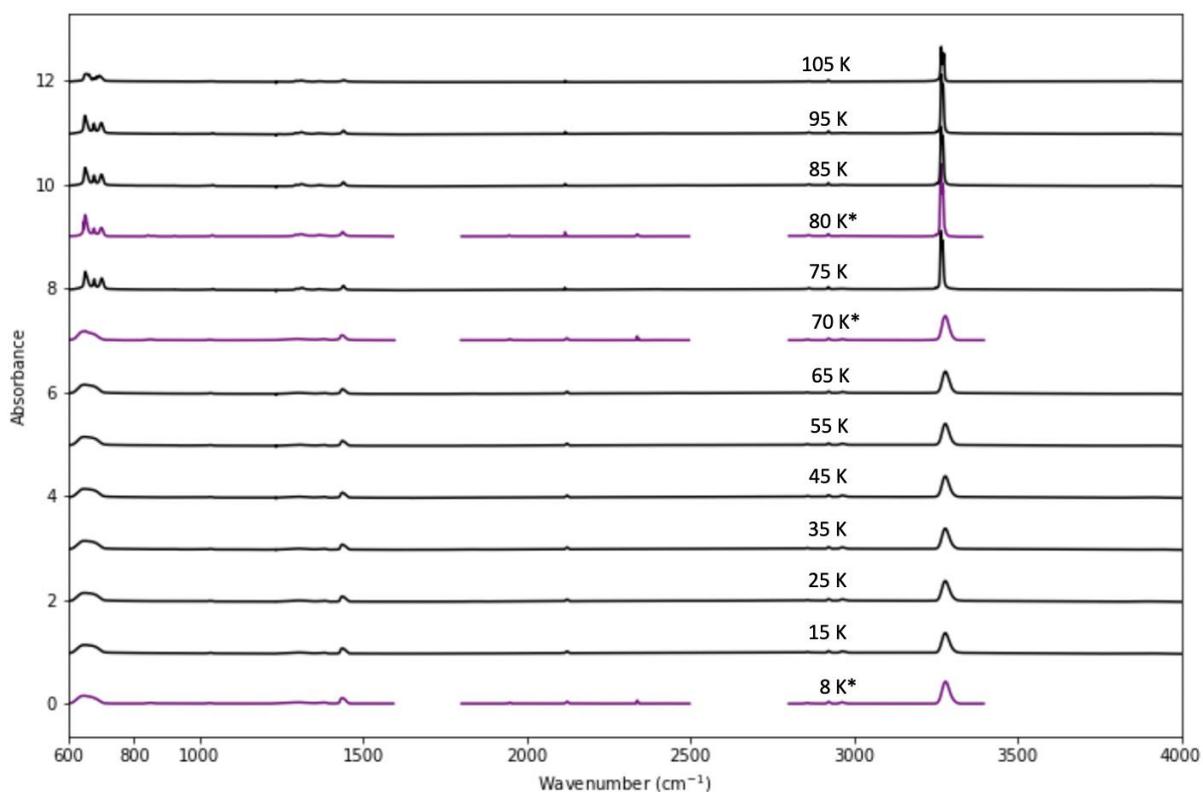


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34 **Figure S-4.** Infrared spectroscopy temperature series of pure propyne deposited at 15 K and  
35 annealed to 105 K, under vacuum. Transition from amorphous to crystalline propyne is observed  
36 between 65 K and 75 K. Spectra highlighted in purple and denoted with an asterisk (8 K, 70 K,  
37 and 80 K) are from previously published work by Hudson et al. 2021<sup>23</sup> (Figures 11-13).



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