Supplementary Material for: *Phase-dependent vacuum ultraviolet photochemistry of diacetylene ices: implications for Titan chemistry*

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S1 Estimation of C_4H_2 ice thickness and column density

The C_4H_2 ice thickness was estimated from the integrated area of the ν_4 C–H stretching band centred at approximately 3273 cm^{-1}. The thickness was then calculated from

$$h = \frac{2.303 \int \mathrm{Abs}(\tilde{\nu})\, d\tilde{\nu}}{\int \alpha(\tilde{\nu})\, d\tilde{\nu}}$$

where $\int \alpha(\tilde{\nu})\, d\tilde{\nu}$ is the integrated extinction coefficient as appropriate for absorption measurements performed in transmission geometry.[1]

The column density (N) is calculated from the integrated band area according to the equation:

$$N = \frac{\int \tau_\nu d\nu}{A}$$

where $\int \tau_\nu d\nu$ is the integrated band and A is the band strength (cm $molecule^{-1}$). Because the depletion curves were analysed using normalised column densities, N_f/N_0, the absolute band strength cancels from the ratio. Therefore, the relative depletion was obtained from the ratio of the integrated areas of the selected C_4H_2 IR band at each fluence to its initial integrated area.

S2 Supplementary Figures

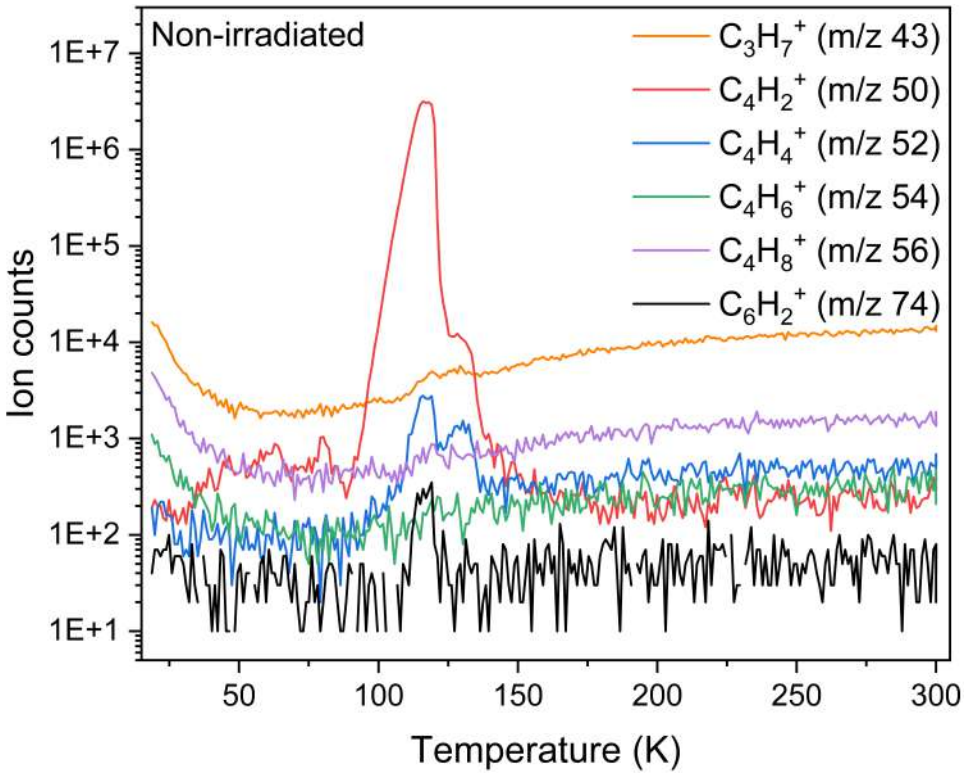

Figure S1. Ion counts for the target ions with m/z 43, 52, 54, 56 and 74 during TPD throughout the temperature ramp to 300 K of C_4H_2 without exposure to VUV irradiation (blank experiment). The m/z 50 corresponding to $C_4H_2^+$ is shown in red as a reference.

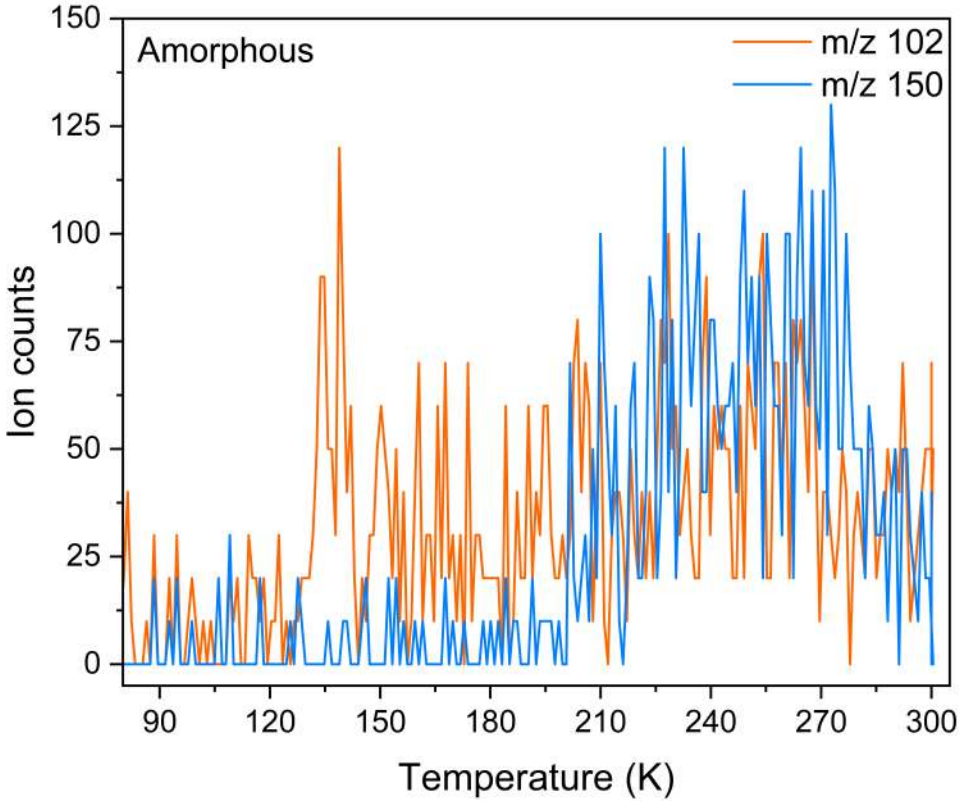

Figure S2. Ion counts for ions with m/z 102 and 150 detected for the amorphous ice irradiated at 20 K.

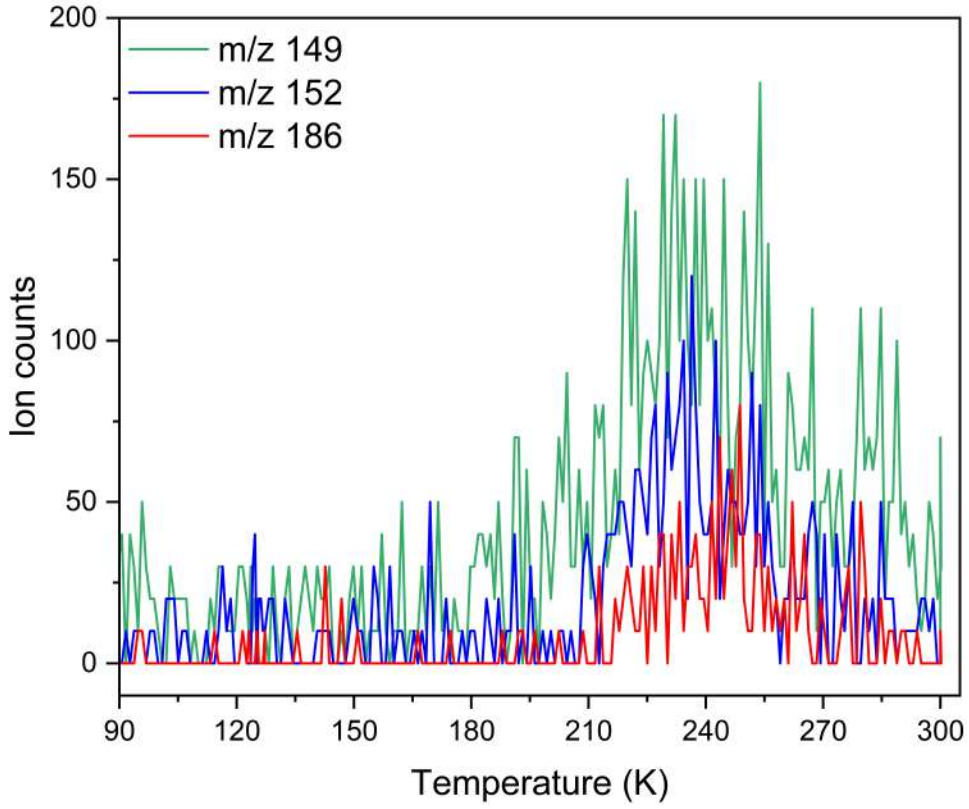

Figure S3. Ion counts for ions with m/z 149, 152 and 186 detected for the crystalline ice irradiated at 70 K.

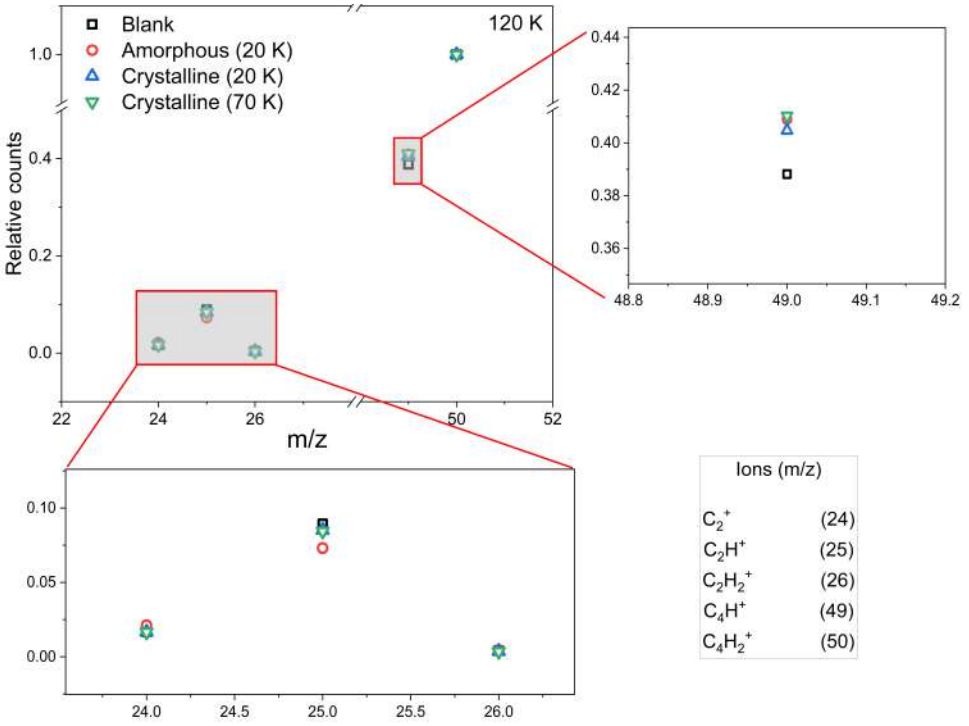

Figure S4. Relative counts for each expected radical formed during the photolysis of C_4H_2.

References

[1] R. L. Hudson, M. J. Loeffler, R. F. Ferrante, P. A. Gerakines and F. M. Coleman, *The Astrophysical Journal*, 2020, **891**, 22.