

Supplementary Information

Radical Intermediates and Stable Products in Acrolein Pyrolysis

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Heating Power (W)	Reactor Temperature (K)	Reported Temperature (K)
0	RT	RT
10	719	700
20	862	850
30	1004	1000
40	1147	1150
50	1290	1300
60	1432	1450
80	1718	1700

Table S1: The calibrated temperature corresponding to each heating power level used and the reported temperatures.

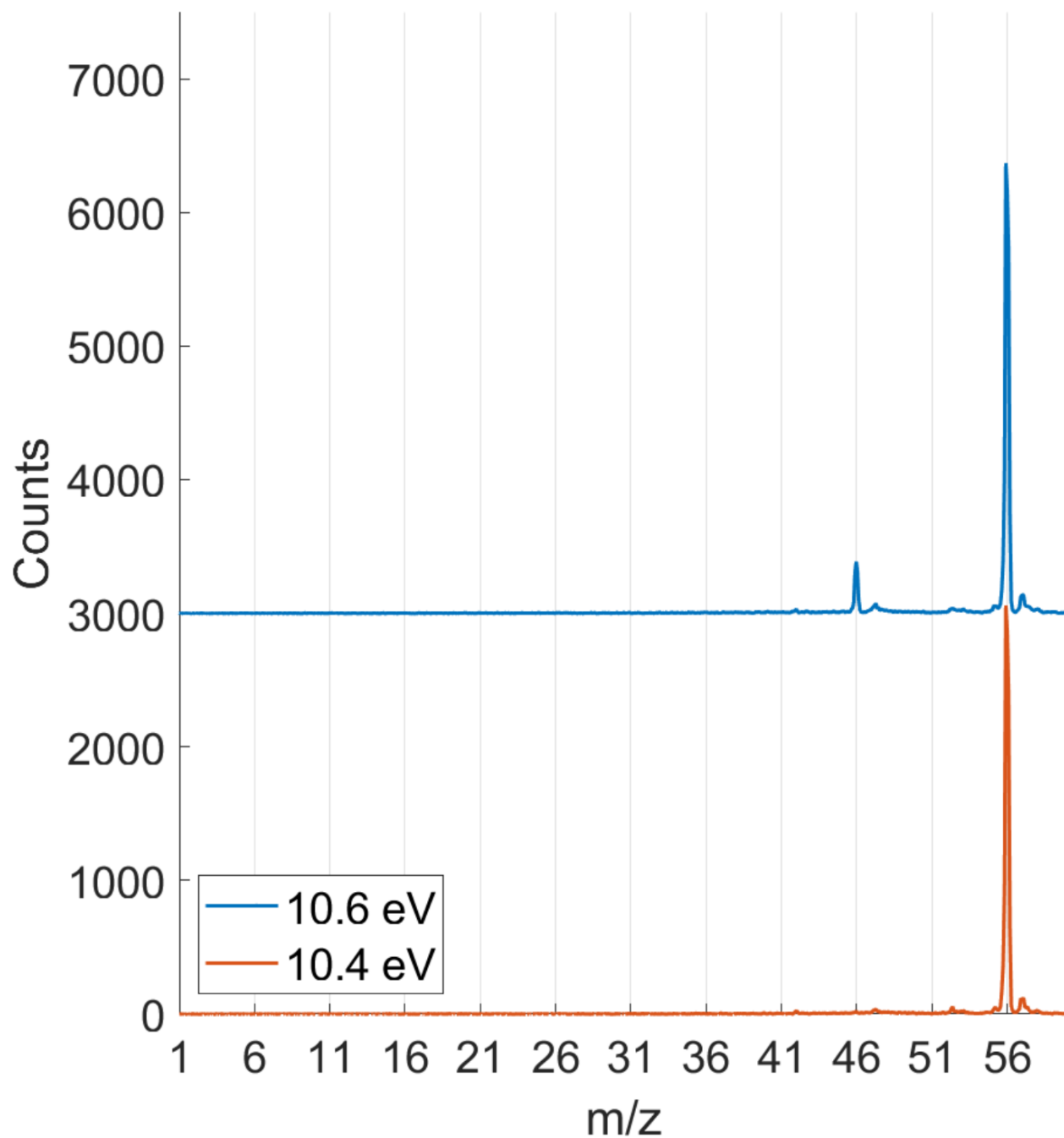


Fig. S1 : Acrolein detection. Room temperature mass spectra of the reaction mixture. Acrolein (m/z 56, IE 10.11 eV) and ethanol (m/z 46, IE 10.48 eV) clearly visible. Upper mass trace shifted upwards by 3000 counts. Molecular beam data.

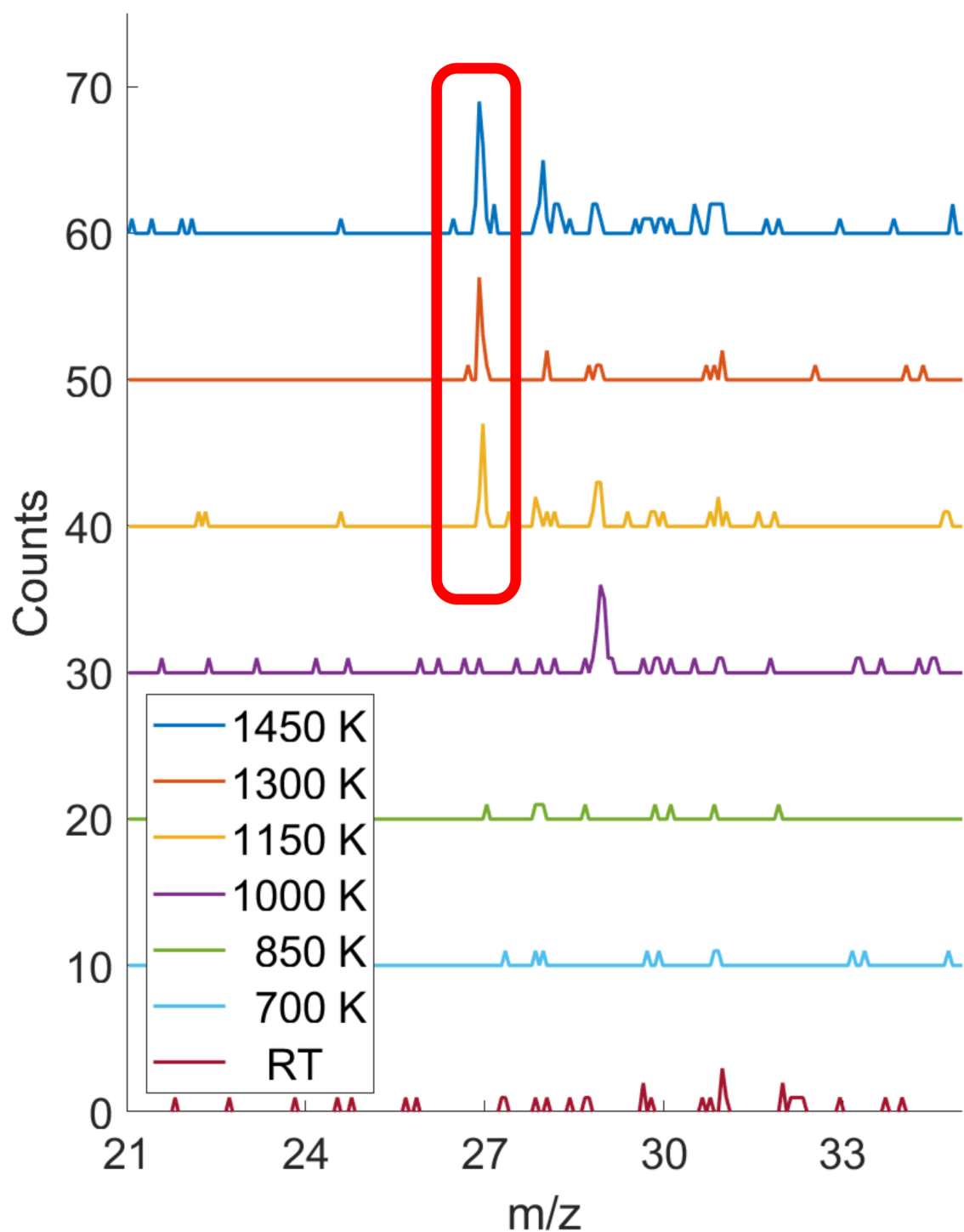


Fig. S2 : Vinyl and CHO radicals. Mass traces of molecular beam data captured at 9.5 eV ionization energy. The signal at m/z 27 (in red rectangle) clearly shows production of the vinyl radical at 1150 K and above. The m/z 29 species observed below the acrolein pyrolysis onset temperature is the ethyl radical (CH_2CH_3 , m/z 29, IE 8.3 eV), a product of ethanol breakdown.

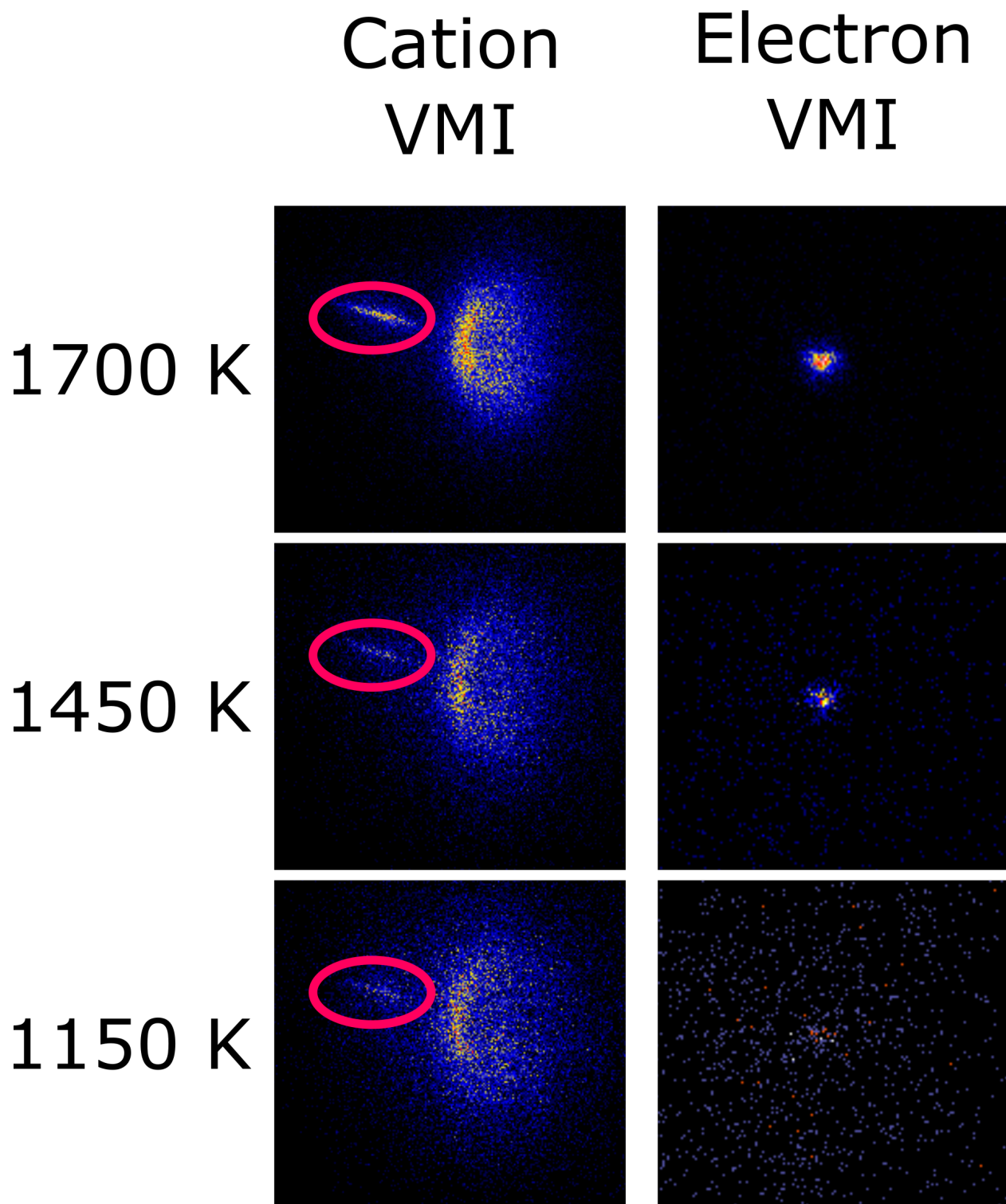


Fig. S3 : CO observation. Left - mass gated cation VMIs for mass 28 at 14 eV VUV energy, at different reactor temperatures. Right - electron VMIs for electrons corresponding to the region of interest, encircled in red in the cation VMIs. This velocity space region of interest is consistent with cations in the molecular beam. (Hemberger et al., 2022)

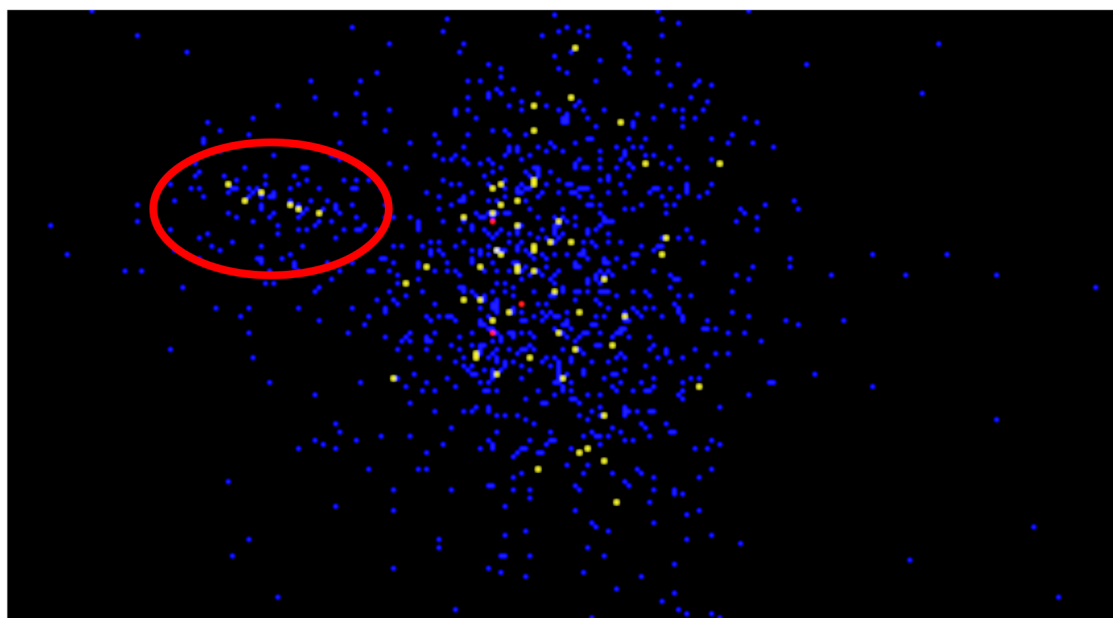
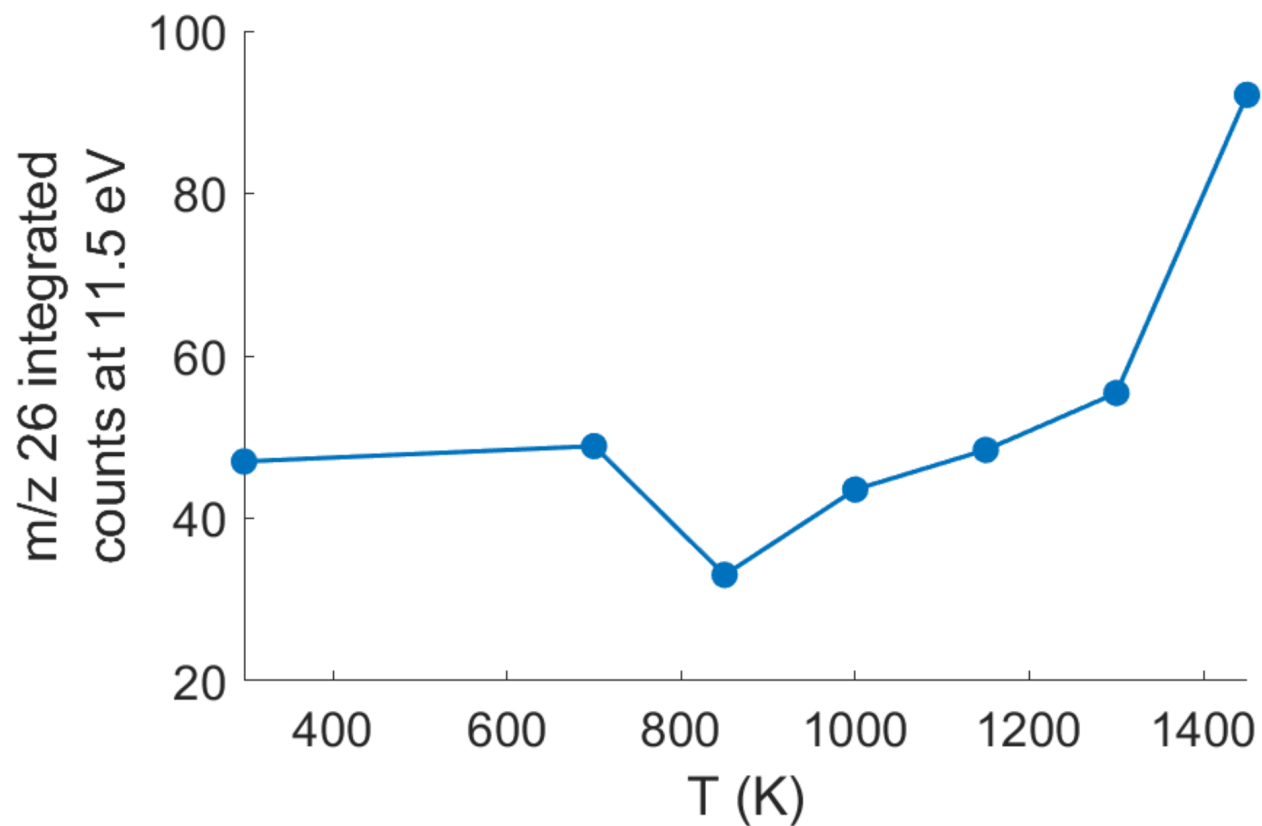


Fig. S4 : Acetylene observation. m/z 26, assigned as acetylene, observed at 1450 K and 11.5 eV VUV energy . Molecular beam data (Above). The mass gated cation VMI for the 1450 K, 11.5 eV measurement. The molecular beam region is circumscribed in a red ellipse (Below).

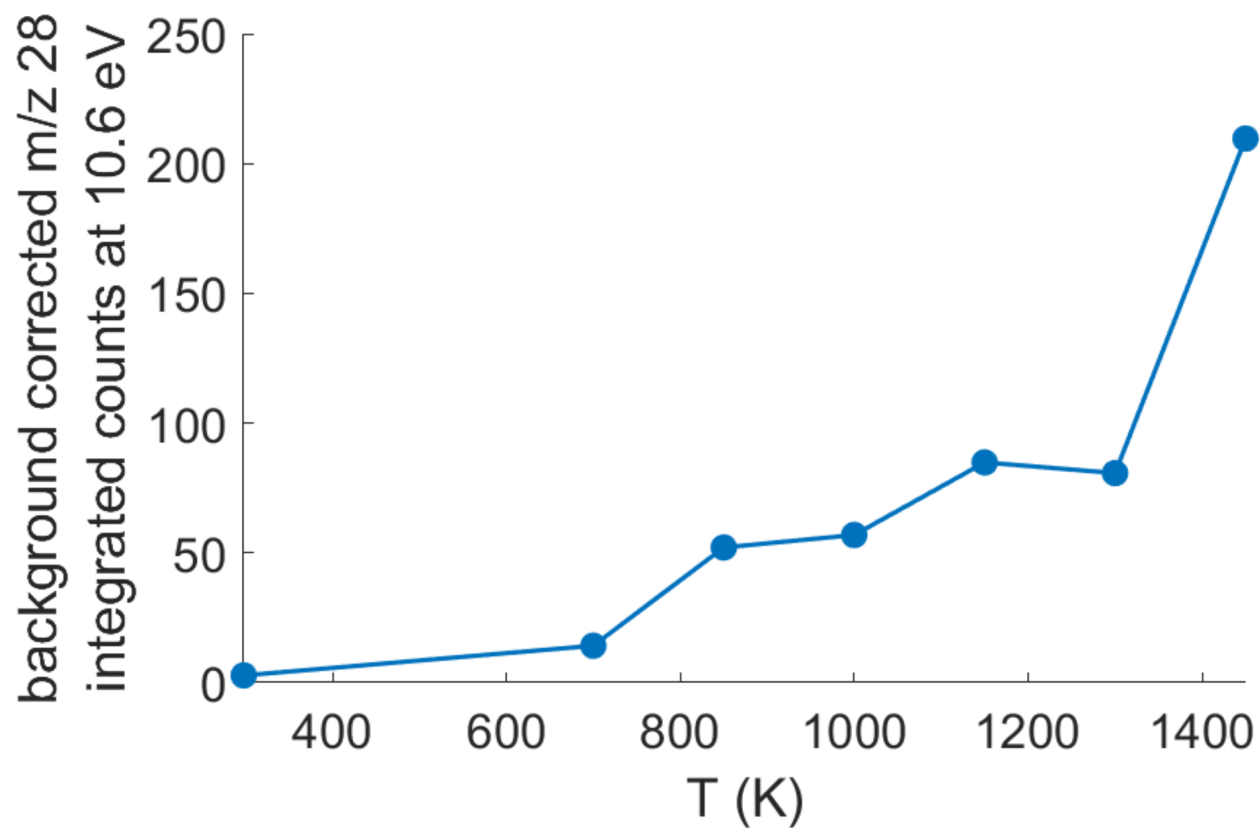


Fig. S5 : Ethylene observation. m/z 28, assigned as ethylene, observed at ionization energy of 10.6 eV, after subtraction of the signal at 10.4 eV, to control for background gas. Molecular beam data.

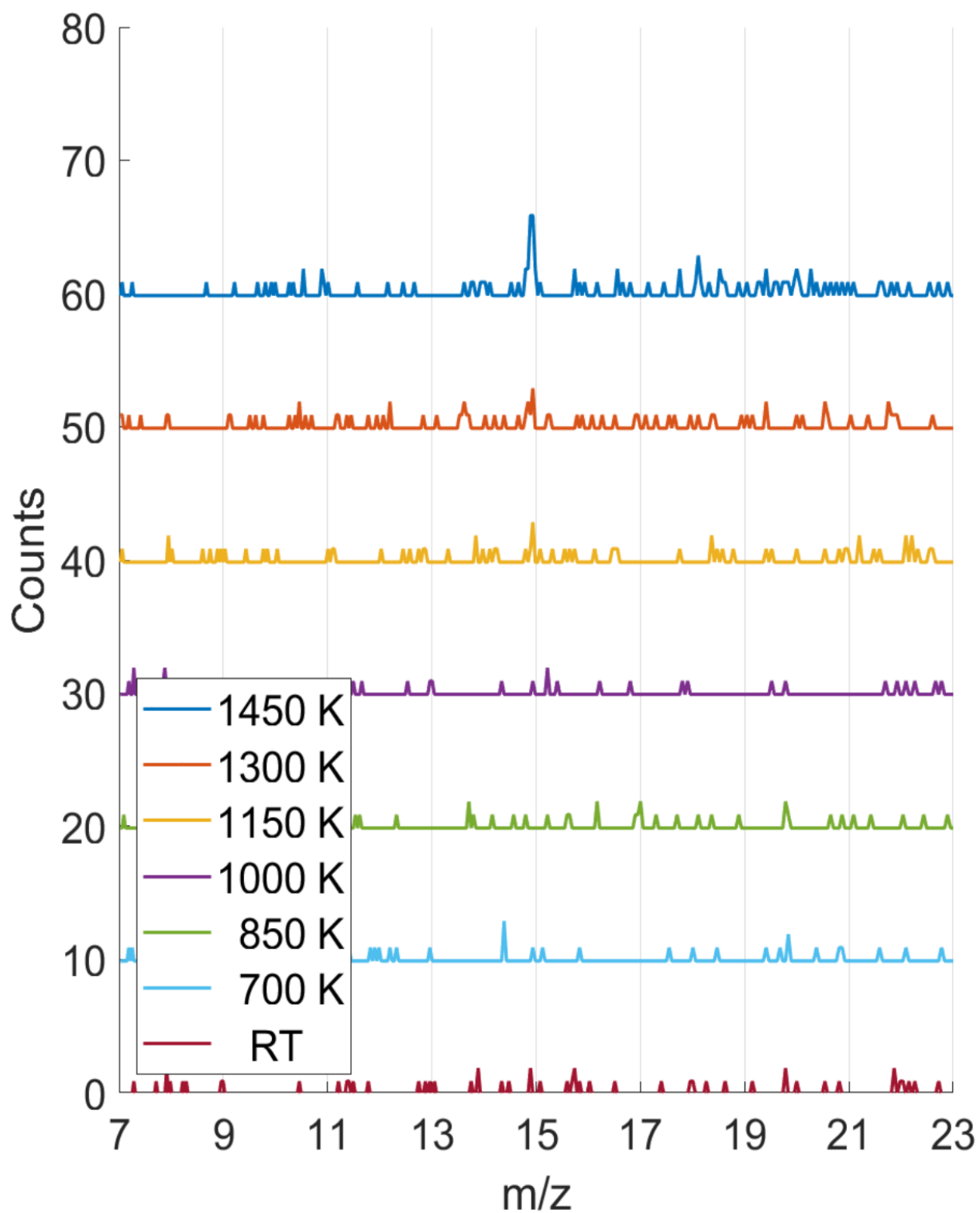


Fig. S6 : MS traces for m/z 15. m/z 15 observed at 1450 K. Each mass trace is shifted upwards from the one below by 10 counts. Molecular beam data at 10 eV ionization energy.