Probing a New Formation Pathway for N-bearing PAHs in the Interstellar Medium Using a 22-Pole Ion Trap

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Synopsis We investigate the reaction of pyrimidine cations with acetylene using a modified 22-pole radio-frequency ion trap. Time-resolved mass spectrometry reveals sequential acetylene addition. The measured kinetics provide rate coefficients for radiative association and subsequent bimolecular reactions, constraining nitrogen-bearing molecular growth in astrochemical environments.

Ion-molecule reactions are considered important pathways to facilitate molecular growth in interstellar and planetary environments. Where low densities can favor reaction mechanisms that differ from those observed under conventional laboratory conditions. Here, we investigate the reaction between pyrimidine cations ($C_4H_4N_2^+$) and acetylene (C_2H_2) using a modified 22-pole radio-frequency ion trap.

Pyrimidine is ionized by electron impact, mass-selected using a quadrupole mass spectrometer, and injected into the 22-pole ion trap, where Helium buffer gas is used for collisional cooling. C_2H_2 is then subsequently introduced into the trap at controlled number densities, and the trapped ions are monitored as a function of storage time using a second quadrupole mass spectrometer. This time resolved approach allows the kinetics of sequential ion–molecule reactions to be followed under reduced-density conditions.

The reaction initially produces an m/z 106 species through bimolecular association of acetylene with pyrimidine ions. At higher acetylene densities and longer storage times, the m/z 106 intermediate undergoes hydrogen abstraction acetylene addition reaction, producing a product at m/z 131. Kinetic modelling of the measured ion populations gives a radiative association rate coefficient of $k_{\mathrm{RA}} = (1.3 \pm 0.3) \times 10^{-10}\ \mathrm{cm}^3, \mathrm{s}^{-1}$ for the initial reaction. The subsequent reactions are characterized by $k_1 = (3.4 \pm 1.1) \times 10^{-13}\ \mathrm{cm}^3, \mathrm{s}^{-1}$ and $k_2 = (2.2 \pm 0.9) \times 10^{-12}\ \mathrm{cm}^3, \mathrm{s}^{-1}$. [1]

Electronic-structure calculations support a sequential reaction mechanism leading to a stable bicyclic nitrogen-bearing cation through an overall exothermic pathway. These results demonstrate the capability of the 22-pole ion-trap technique for studying sequential molecular growth reactions under conditions relevant to astrophysical environment.

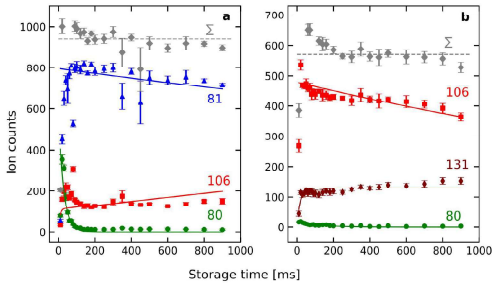

Figure 1. Time-resolved ion counts for pyrimidine and protonated pyrimidine reacting with C_2H_2 at 295 K under (a) low and (b) high acetylene number densities. Solid lines show ODE-model fits; gray dots denote the total ion counts.[1]

References

[1] Payra S S *et al.* 2026 *The Astrophysical Journal* **ApJ 1008 212**

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