Production of Pyrene clusters and measurement of their temperature-dependent evaporation rate

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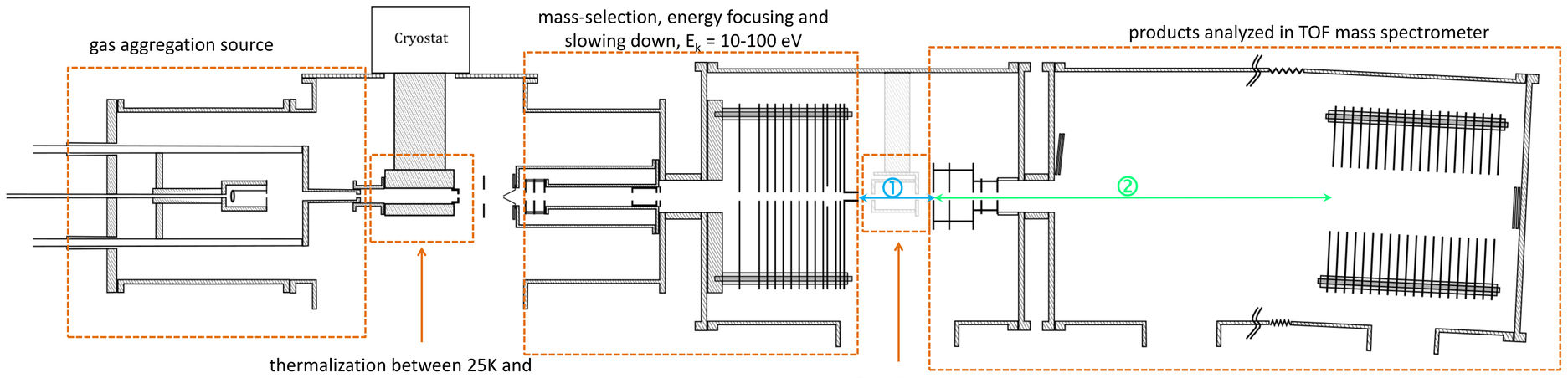
Experimental setup

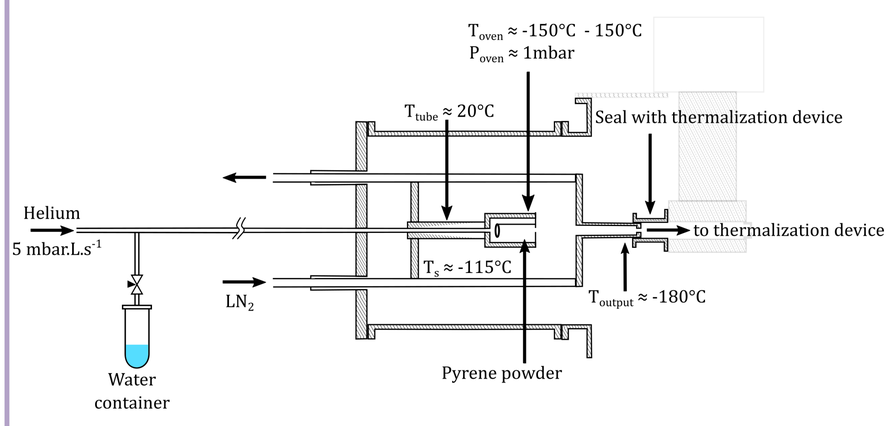


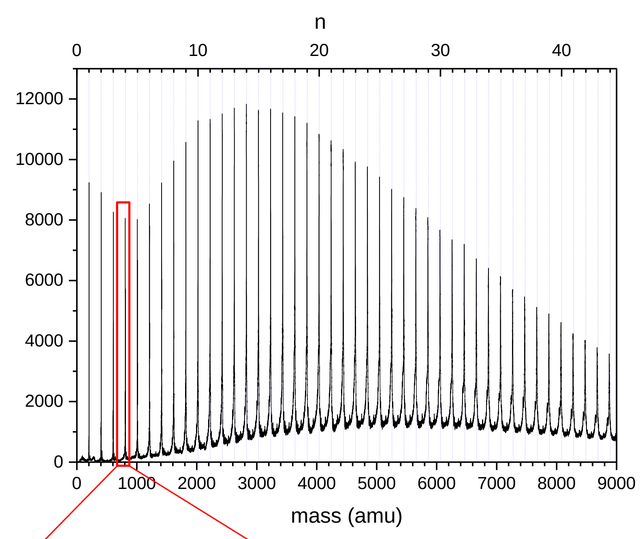
For more details see ref. [1] and [2]

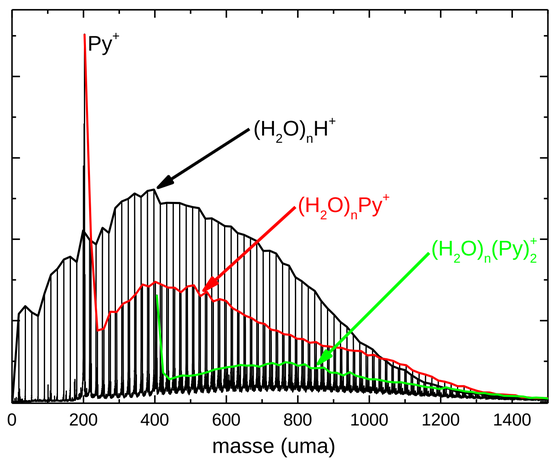
Clusters production

Source conditions

Clusters are produced in a gas aggregation source.
Ionization by either :
- a discharge electrode, I ≈ 100µA, V ≈ 1 kV
- an electron gun, I = 2.5 A, V = -100 V

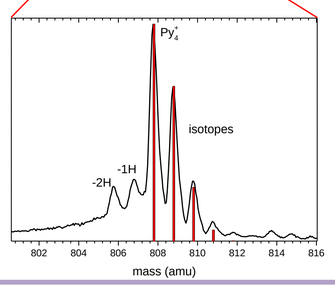






Mass spectra

Observation of dehydrogenation



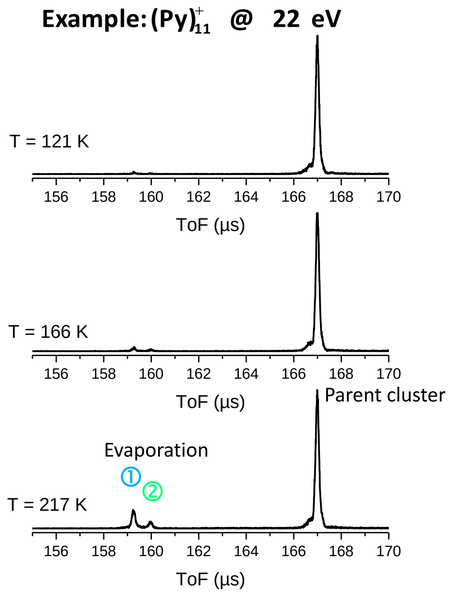
Source allows the production of pure Pyrene clusters or mixed water-Pyrene clusters

Evaporation rates of pure Pyrene clusters

Principle of measurement

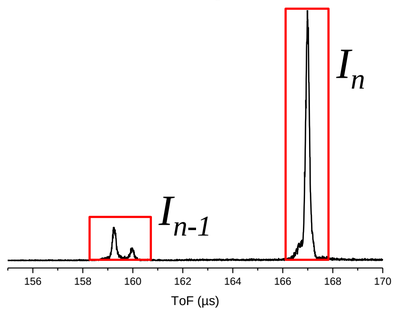
Temperature controlled $(\mathbf{Py})_n^+$ clusters are mass-selected and slowed down.
Mass-spectra show the appearance of evaporation products as the cluster temperature is increased.
Evaporations are detected if they take place between the end of the slowing down and the entrance of the reflectron (①+ ②).
The *n-1* peak has a double structure due to evaporations taking place after the second acceleration and before the reflectron (②).

Example: $(Py)_{11}^+$ @ 22 eV



Evolution of the mass spectra with temperature.

Extraction of the evaporation rate *W(T)*



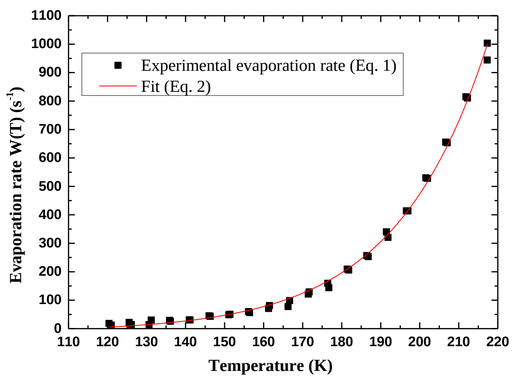
$$I_n = (I_n + I_{n-1})e^{-W(T)t}$$

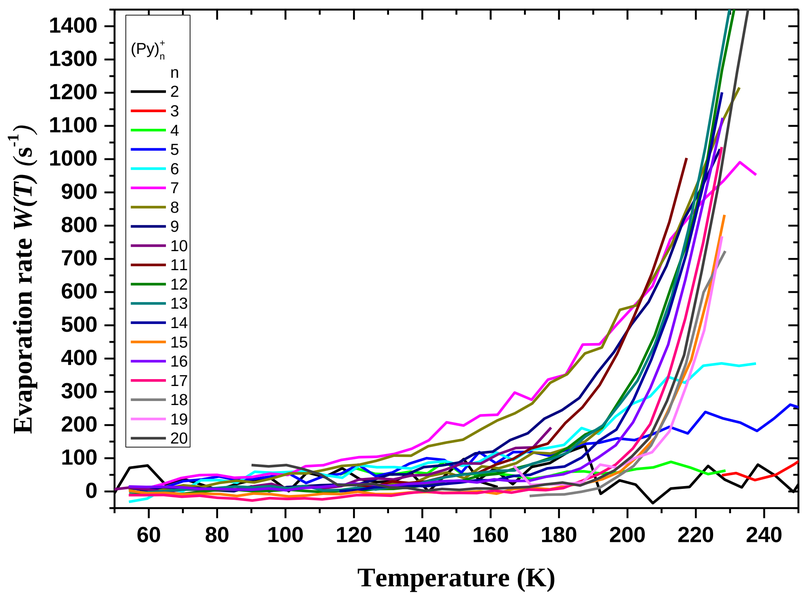
$$\Rightarrow W(T) = -\ln\left(\frac{I_n}{I_n + I_{n-1}}\right) \times \frac{1}{t} \quad \text{(Eq. 1)}$$

t is the time of flight in the region ①+ ② .
For n=11 pyrene clusters @ 22eV, *t* = 160 µs.

Experimental data are fitted by the empirical function:

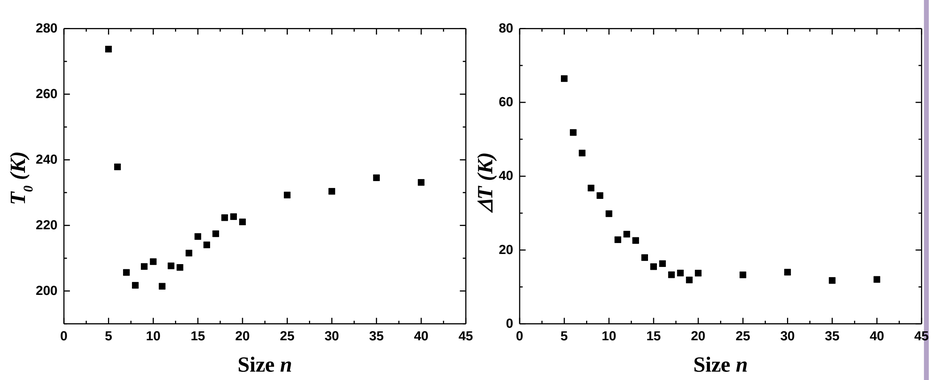
$$f(T) = W_0 + 500e^{(T-T_0)/\Delta T} \quad \text{(Eq. 2)}$$





Above: evaporation rates for all sizes as a function of temperature.

Below: these curves are fitted with Eq. 2 to extract the threshold temperature T_0 and the width ΔT:



For n=2-4, no evaporation observed up to 273K. Above n=6, the threshold temperature T_0 increases with size. Around n=20, evaporation rates stop evolving with size. *W(T)* get steeper as the size increases.

What's next ?

- Phase space theory and/or RRKM calculations are needed to interpret our results
- Collision induced dissociation of pyrene clusters could also give threshold energies for dissociation
- Study of mixed water-pyrene clusters

References

[1] F. Chirot, S. Zamith, P. Labastie, and J.-M. L'Hermite, Rev. Sci. Instrum. **77**, 063108 (2006)
[2] I. Braud, S. Zamith, and J.-M. L'Hermite, Rev. Sci. Instrum. **88**, 043102 (2017)

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