Stability of PAH clusters

Sébastien Zamith,[*1] Ming-Chao Ji,[3] Jean-Marc L'Hermite,[1] Christine Joblin,[3] Léo Dontot,[2] Mathias Rapacioli[2] and Fernand Spiegelman[2]

[1]*Laboratoire Collisions Agrégats Réactivité (LCAR/IRSAMC) UMR5589, Université de Toulouse and CNRS, 118 Route de Narbonne, F-31062 Toulouse, France*
[2]*Laboratoire de Chimie et Physique Quantiques (LCPQ/IRSAMC) UMR5626, Université de Toulouse and CNRS, 118 Route de Narbonne, F-31062 Toulouse, France*
[3]*Institut de Recherche en Astrophysique et Planétologie (IRAP) UMR5277, Université de Toulouse and CNRS, 9 avenue du Colonel Roche, F-31028 Toulouse, France*

[*]*Corresponding author e-mail address: sebastien.zamith@irsamc.ups-tlse.fr*

We have studied the thermal evaporation of positively charged pyrene clusters $(Py)_n$ for sizes between n=2 and n=40. Charged pyrene clusters are produced in a gas aggregation source [1] and are thermalized right after their production. Their temperature can be varied from 25 to 300 K. We use TOF mass spectrometry techniques to mass select the thermalized clusters and characterise their evaporation as a function of their initial temperature. Evaporation manifests itself in the TOF mass spectra as peaks appearing at smaller sizes.
Phase Space Theory (PST) is used to calculate microcanonical evaporation rates, which are in turn used to simulate the temperature dependant evaporation probability.

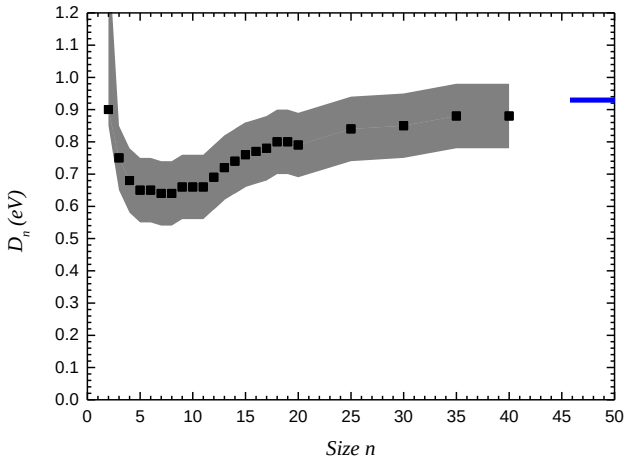

Figure 1 : Dissociation energies of Pyrene clusters obtained by best fit of the experimental data using PST. The grey shaded area represent the uncertainty in the determination of the dissociation energies. The horizontal blue line is the vaporization enthalpy of bulk Pyrene at 298 K [3].

The parameters entering the PST, such as harmonic frequencies, are obtained from DFTB calculations [2]. The only free parameter is the dissociation energy D_n, which is therefore deduced by best fit of the experimental data.

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References

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