Coulomb explosion of PAH induced by heavy CR : carbon chain production rates.

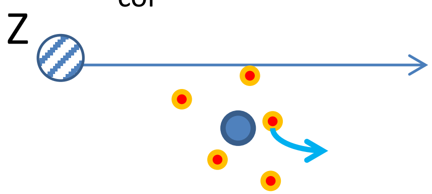
Marin Chabot, Karine Béroff,

Emmanuel Dartois, Thomas Pino, Marie Godard

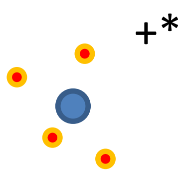
Basic in atomic collision physics at high velocity

Electrons are stripped out.
dE/dx ≈ IP + e- KER

$t_{col} < 10^{-15}$ s

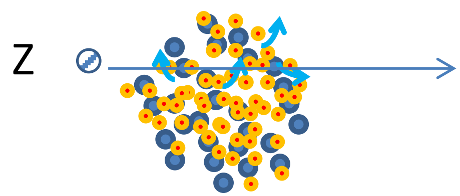


E* : hole in inner shells ≠ dE/dx

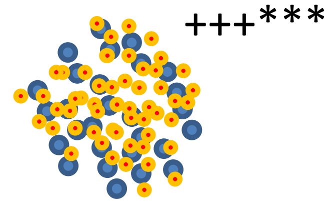


Atomic line emission or auger deexcitation

Electrons are stripped out if e^- range is larger than the size (5 Å for carbon 2g/cc). dE/dx ≈ IP + e- KER

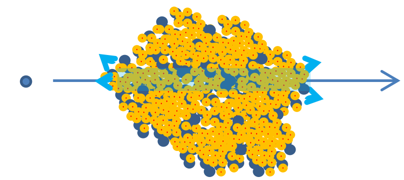


E* : hole in inner shells ≠ dE/dx

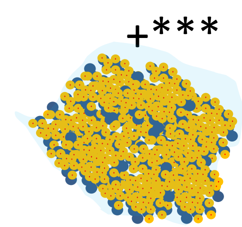


Multi fragmentation / Coulomb explosion

Many electrons are not stripped out.



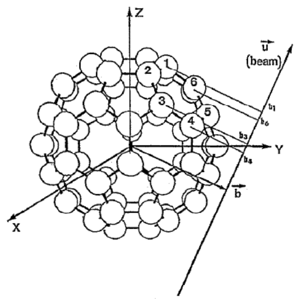
E* = dE/dx



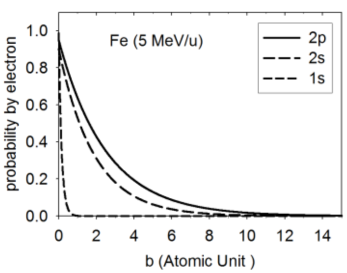
Thermal radiative deeexcitation

Collision model

Q fold ionization cross sections with the Independent Atom an Electron model.



$$P^Q(b, \alpha\beta) = \sum \prod p(i)$$



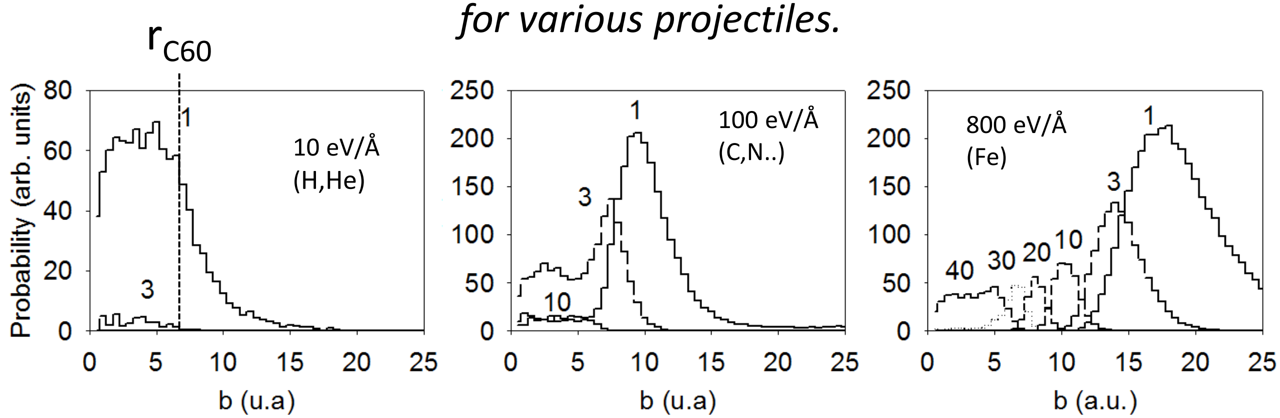
$$\sigma^Q = \iiint b \times P^Q(b, \alpha\beta)\, db\, d\alpha\beta$$

Internal energy following Q fold ionization with the IAE model

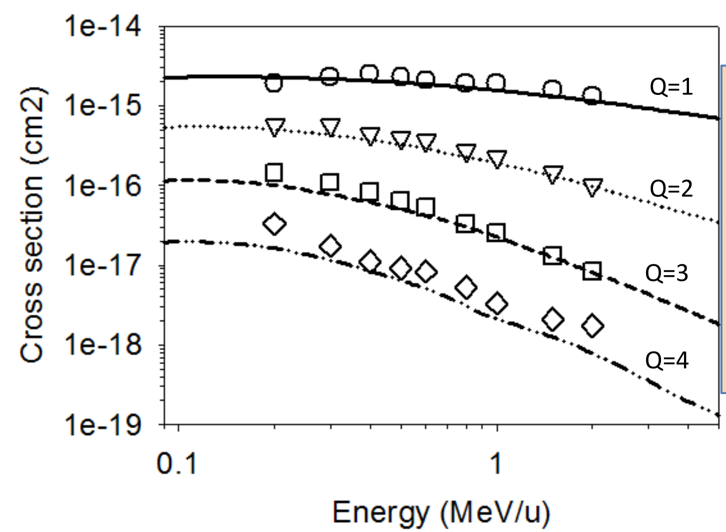
E ~ Q x 20 eV*

Wohrer 1994

*C_{60} **Q** fold ionization probabilities as function of the impact parameter for various projectiles.*



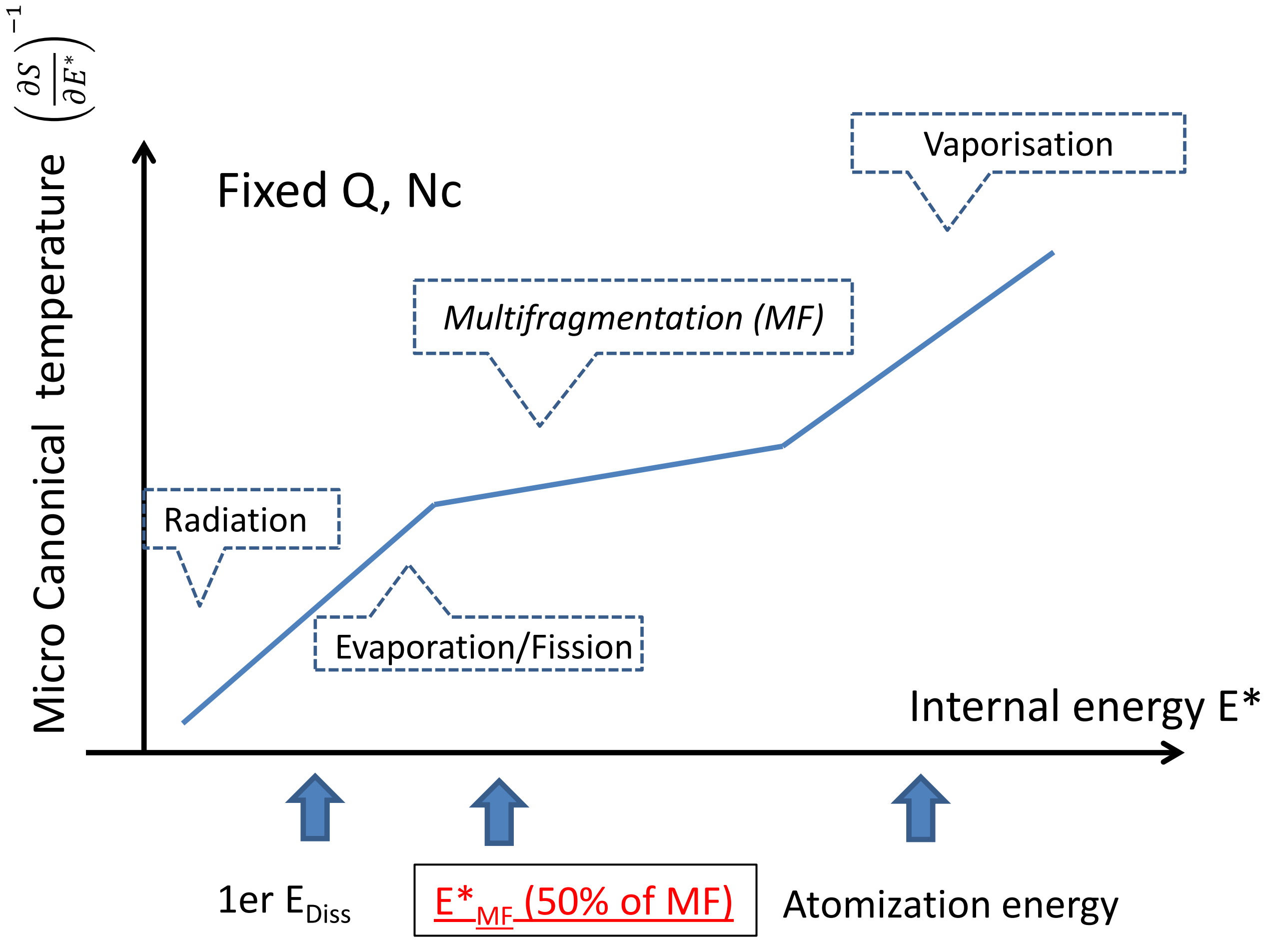
Model vs Experiment (proton on C_{60})



Exp : Tsuchida 1998

Marin Chabot, KIDA conference, Bordeaux 2017

Basic in fragmentation physics for finite systems

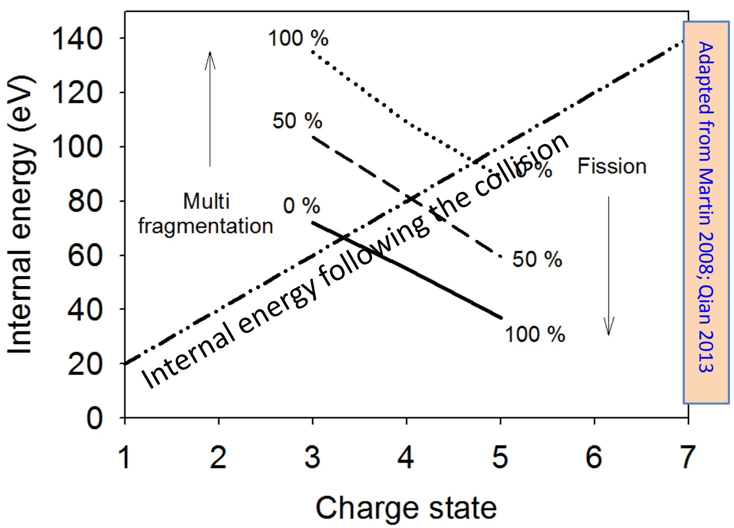


Microcanical formulation is essential (i.e. E, Nc, Q are external quantities and determine the densities of the micro states).

Fragmentation model :

1- Limit of multi-fragmentation induced by the collision

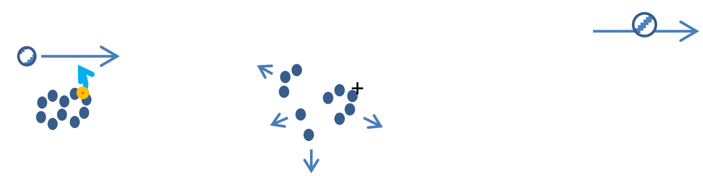
Experiments on $C_{60}{}^{Q+}$ under well-controlled internal energy E, are used as prototype. Since Q and E* are proportional, the MF occurs above a given value of Q/N_c.*



For $Q/N_c > 4/60$ Multi Fragmentation is the dominant de-excitation channel.

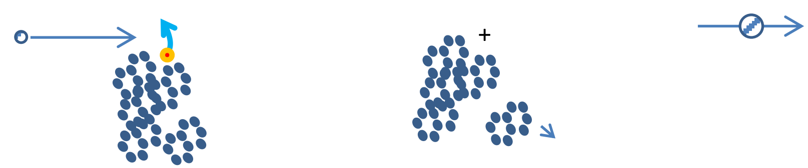
Behavior of lab PAH collided by He (20-30 keV) agrees with $Q/N_{c\,MF} = 4/60$:

- For isolated small laboratory PAH, MF is an abundant channel of deexcitation [P ostma 2010]



He + $C_{14}H_{10}$: Nc=14 ; Q = 1.2 -> Q/Nc = 4.5/60 - > MF dominates
He + $C_{24}H_{12}$: Nc=24 ; Q = 1.3 -> Q/Nc = 3.2/60 -> MF close to dominate

- For cold PAH clusters evaporation is the main deexcitation channel [Holm 2010, Johansson 2011]



He + $(C_{14}H_{10})_m$: Nc=14 x m ; Q = 1.4 -> Q/Nc = 1/m x 4.5 /60 -> no MF (m>3); evap.

Fragmentation model :

2- Fragment sizes

✓ *For C_n^{Q+} (n<11, Q<5) fragments are produced in number equal to [Chabot 2010]:*

$$N_f = \frac{E^*}{E_{bond}} \times \frac{5}{6}\left(1 - \frac{Q}{N_c}\right) + (Q - Q_{max})$$

Mean energy to break a bond

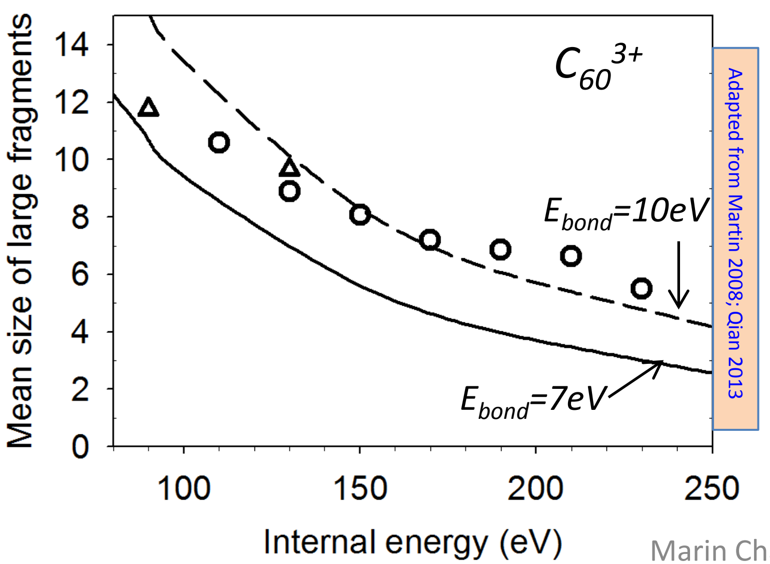
A part of the internal energy goes to KER

The highest charge state for stable molecule with E*=0

✓ *Small (S) (n<4) and large fragment (LF) are produced in same quantity, the mean size of LF writes :*

$$S_{LF} = \frac{N_c - {}^1/_2 N_f \times S_s}{{}^1/_2 N_f}$$

<u>Model agrees with measurements on C_{60} and PAH</u>



$C_{24}H_{12}$ PAH collided by He (20 keV) [Lawicki 2011]:

Experiment S_{LF} = *7.5*
Model : S_{LF} = *[10.5 – 7.5] ;* E_{bond} = *[6 – 5] eV*

✓ *Hydrogenation of LF is assumed to be 0, 1, 2 with equal probabilities [Potsma 2010] :*

Application CR - PAH

$$\tau_{S_f} = 4\pi \sum_{Z} f_z \int j_n(E/A, Z) \times \sigma^{S_f}(E/A, Z)\, dE/A$$

- PAH Model :

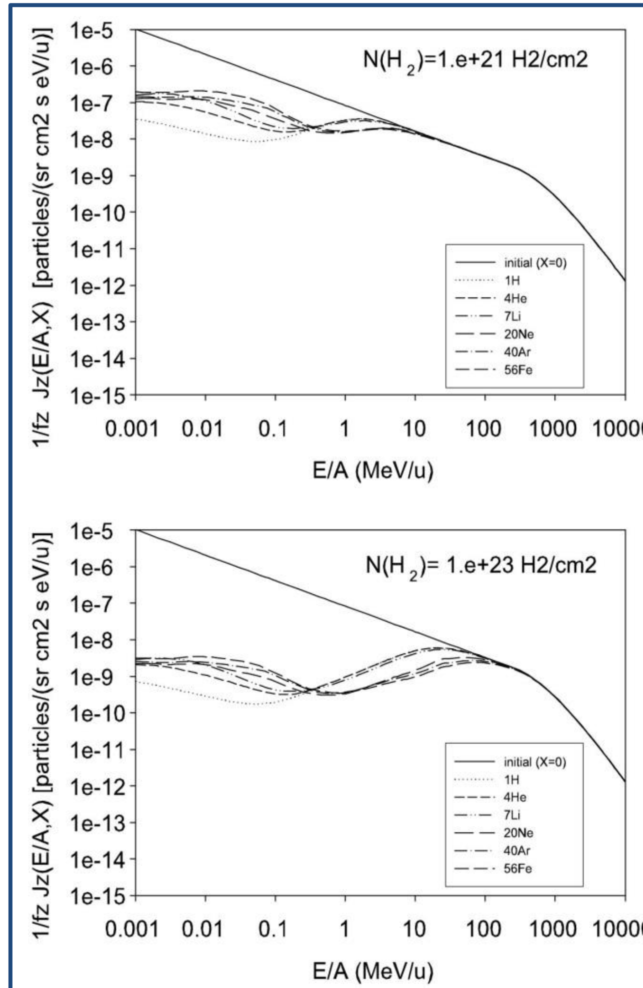
Small : Nc = 54, d=2g/cc
Large : Nc = 216, d=2g/cc
Fluffy : Nc = 216, d=0.25g/cc

- Fractional Abundance (f_z) :

GCR
High Z : GCR with all Z>6 x5

- Spectral density :

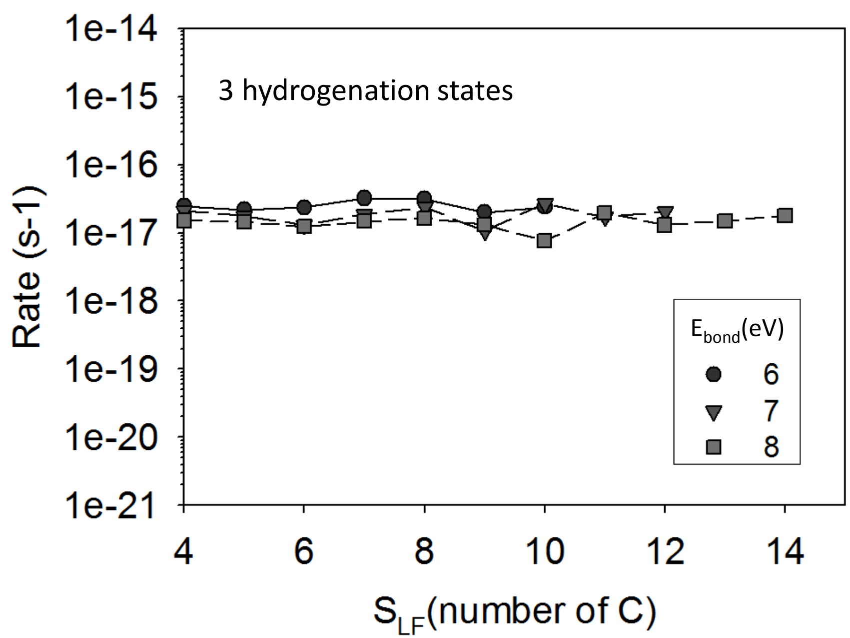
Standard (i.e. after passing through 1 Av):
ζ_{H_2} = 6.3 10^{-17} s^{-1}
With a strong low energy component (only in diffuse medium):
ζ_{H_2} = 1.3 10^{-15} s^{-1}



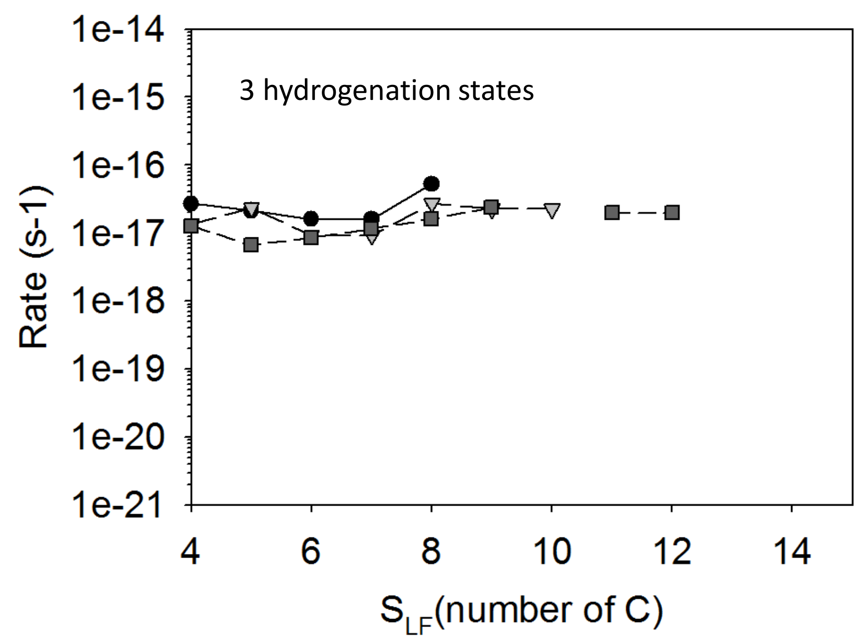
Chabot 2016

Results (1/2)

Standard GCR on *large* PAH



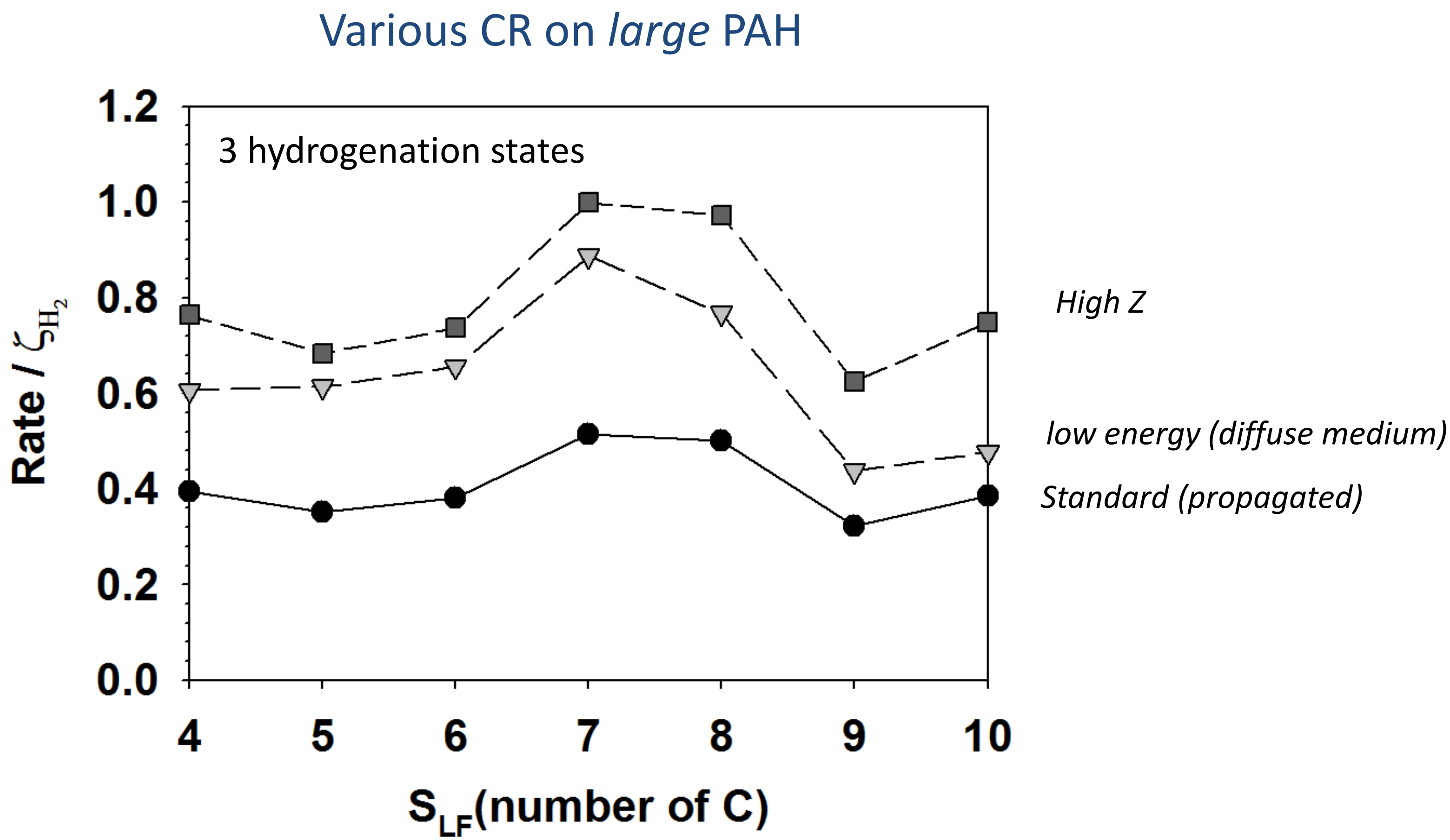
Standard GCR on *small* PAH



The size of chains extend up to 10 – 15 carbon atoms.

The production rates are independent of the carbon chain sizes.
They are not very sensitive to the exact nature of the PAH.

Results (2/2)



Production rates of the carbon chains scale with the ionization rate of H_2 within factor 2.

Conclusions

- *CR on PAH produce carbon chains. Rates are in the order of 0.1 to 1 zeta. Confidence interval is one order of magnitude.*
- *This carbon chains formation process is low but for Nc > 6, much larger than the effective rates in a pure gas phase chemistry at steady state.*
- *DRAFT of this work is available on arXiv for discussions.*

  http://arxiv.org/abs/1709.07803