From PAHs to carbon clusters in photodissociation regions

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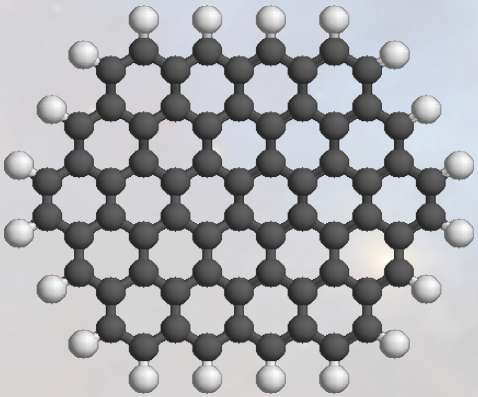
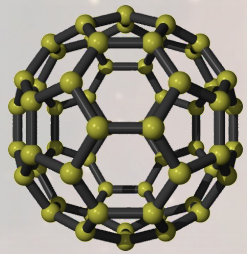


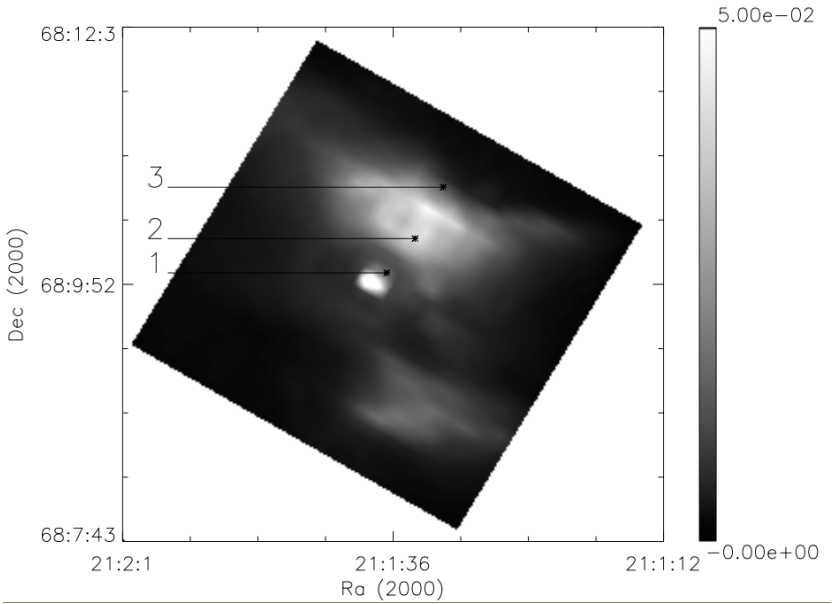


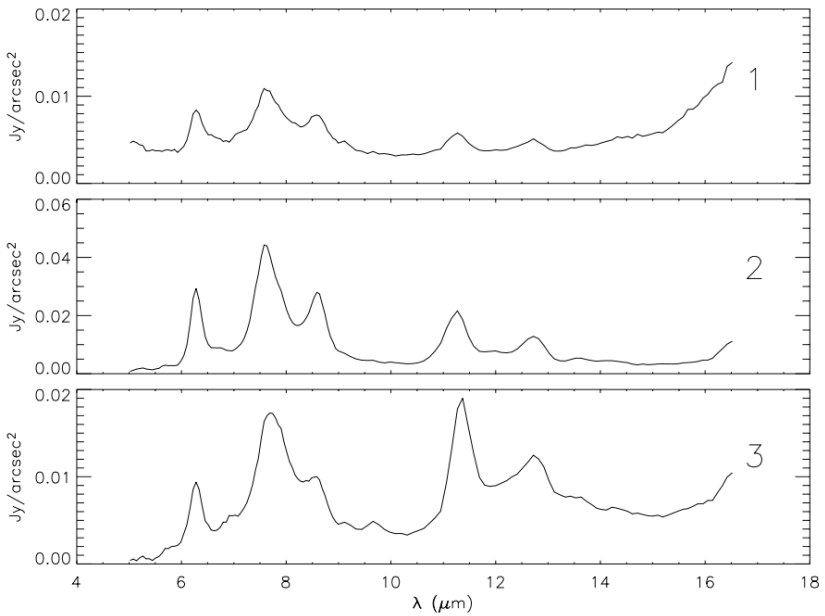
Plan

1. Context: evolutionary scenario of interstellar aromatic carbon
2. Processes driving the evolution of charge and hydrogenation states of PAHs
3. Astrochemical model
4. Conclusion

Spatial and spectral evolution of the aromatic IR bands

Rapacioli et al., A&A 2005



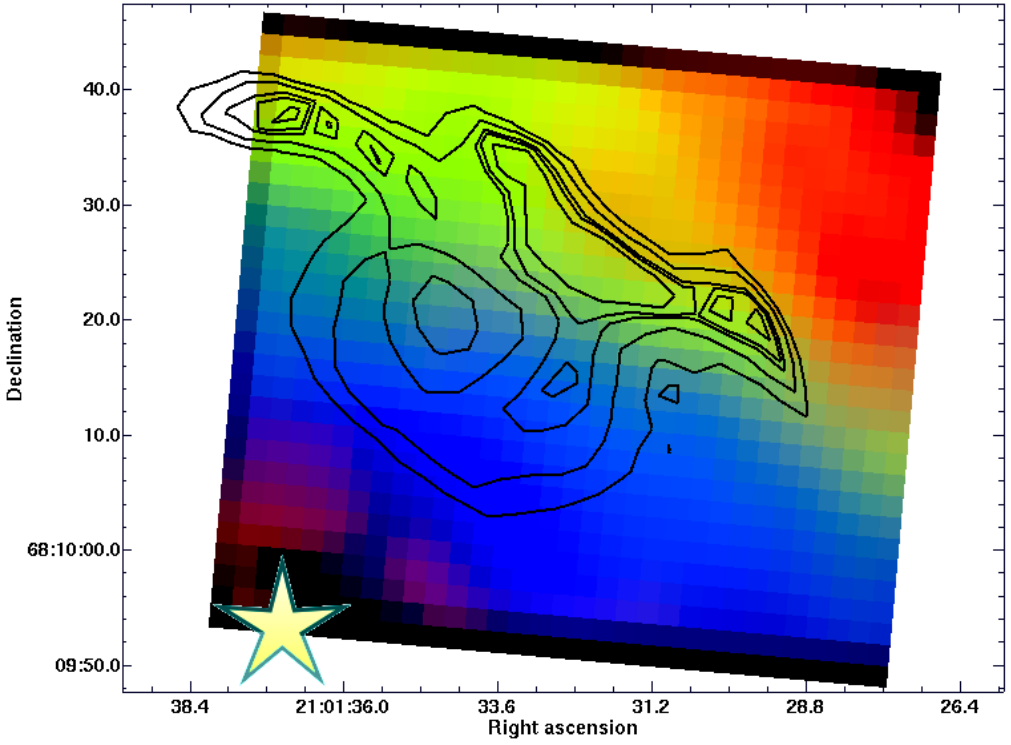


$\longrightarrow$ Clear evolution AIB within NGC 7023

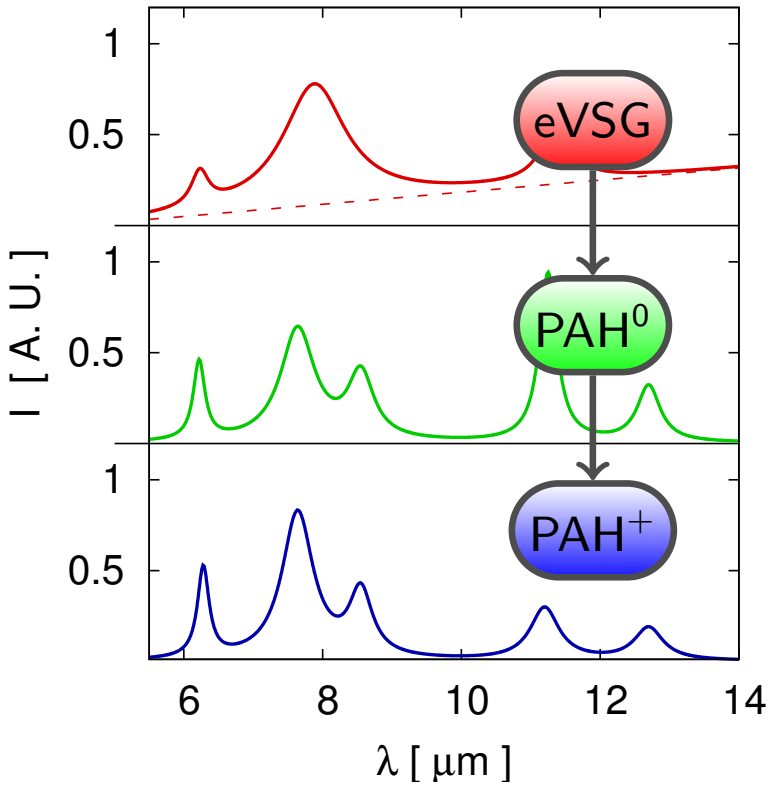
- Evolution of the "PAH" population ?

Evolutionary scenario of PAHs

Rapacioli et al., A&A 2005; Berné et al., A&A, 2007

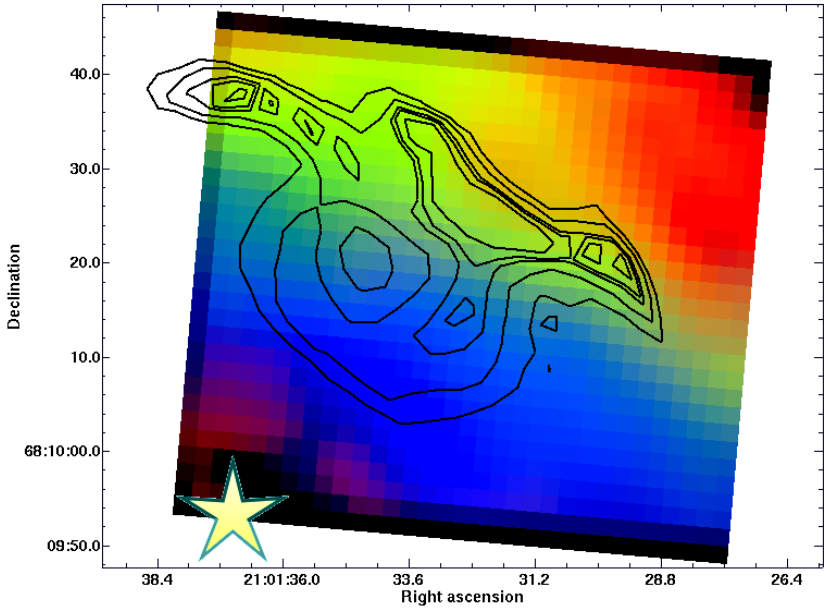


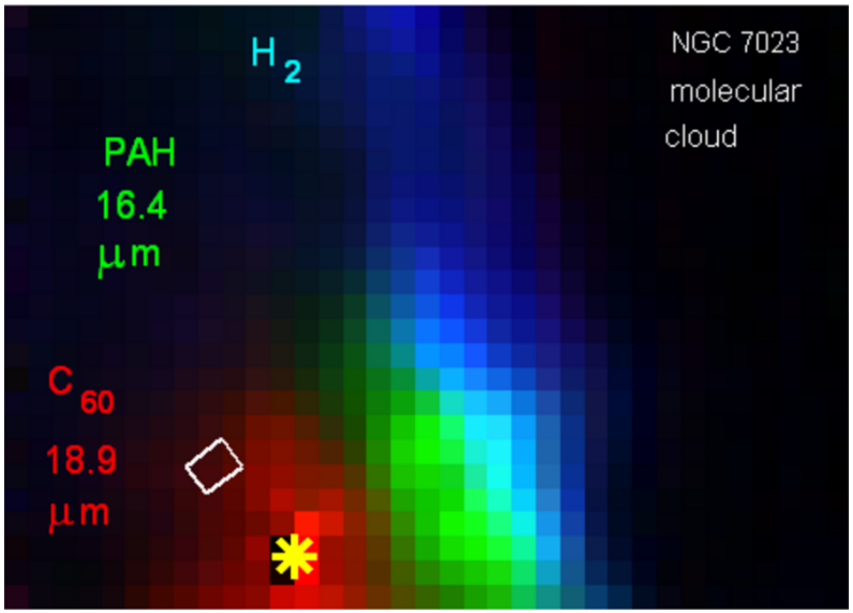
Contours = IRAC 8 μm



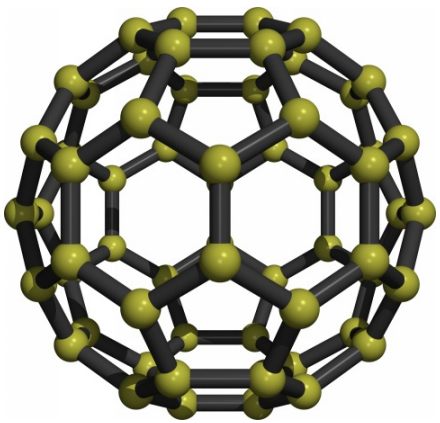
- Influence on the physics of photon dominated regions ?
  $\longrightarrow$ cf. Poster 32 C. Joblin
- Nature of eVSGs (evaporating Very Small Grains): PAH clusters ?
  $\longrightarrow$ cf. Talk P. Rousseau
- Evolution of free PAHs: **charge & hydrogenation states**

C_{60}: a new character in the story ?





[Sellgren et al., ApJ, 2010]



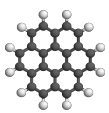
C_{60}

- Which links with PAH evolution ?
  [Berné & Tielens, PNAS, 2012]

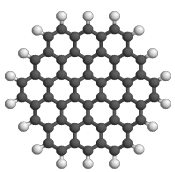
Goals and strategy

Aim: Providing contraints on PAH evolution and their place in the cycle of carbonaceous aromatic matter
Method: Modelling the charge and hydrogenation state of PAHs

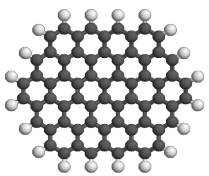
- Selection of a few (presumably) typical species
- Selection of their main chemical properties
- Selection of a well-known environment: NGC 7023
- Development of an astrochemical model dedicated to PAH evolution



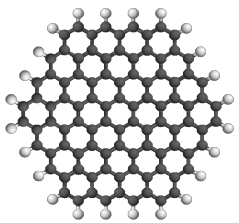
$N_{\mathrm{C}} = 24$
coronene



$N_{\mathrm{C}} = 54$
circumcoronene



$N_{\mathrm{C}} = 66$
circumovalene

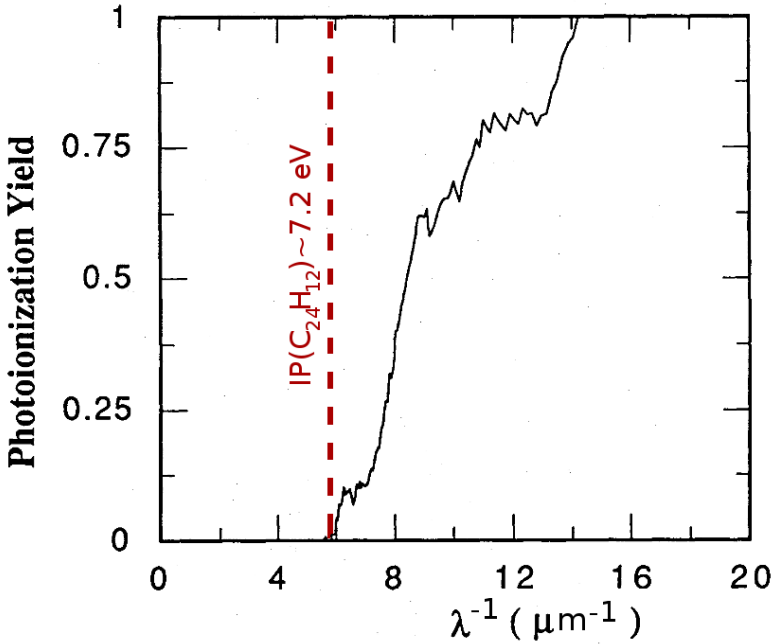


$N_{\mathrm{C}} = 96$
circumcircumcoronene

Plan

Charge state of PAHs

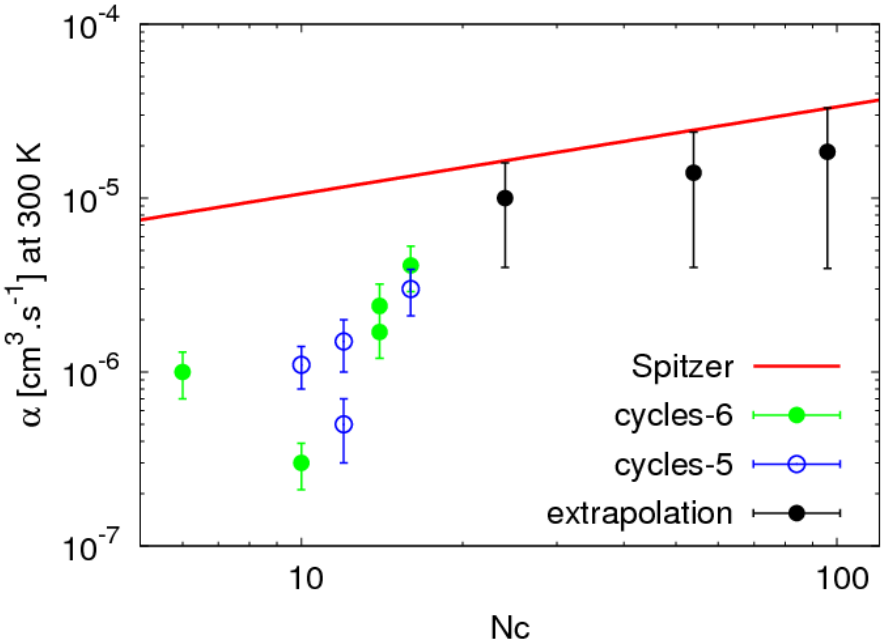
Photoionization



- scale with the number of carbon atoms
- parametrization by the ionization potential

Verstraete et al., A&A, 1990
Bakes & Tielens, ApJ, 1994
Le Page et al., ApJSS, 2001

Recombination with electrons



- measurements up to pyrene
- monocations only

Abouelaziz et al., JCP, 1993
Rebrion-Rowe et al., Int. J. Mass Spectrom., 2003
Novotny et al., JCP, 2005
Biennier et al., Faraday Discuss., 2006

Hydrogenation state of PAHs: reactivity with hydrogen

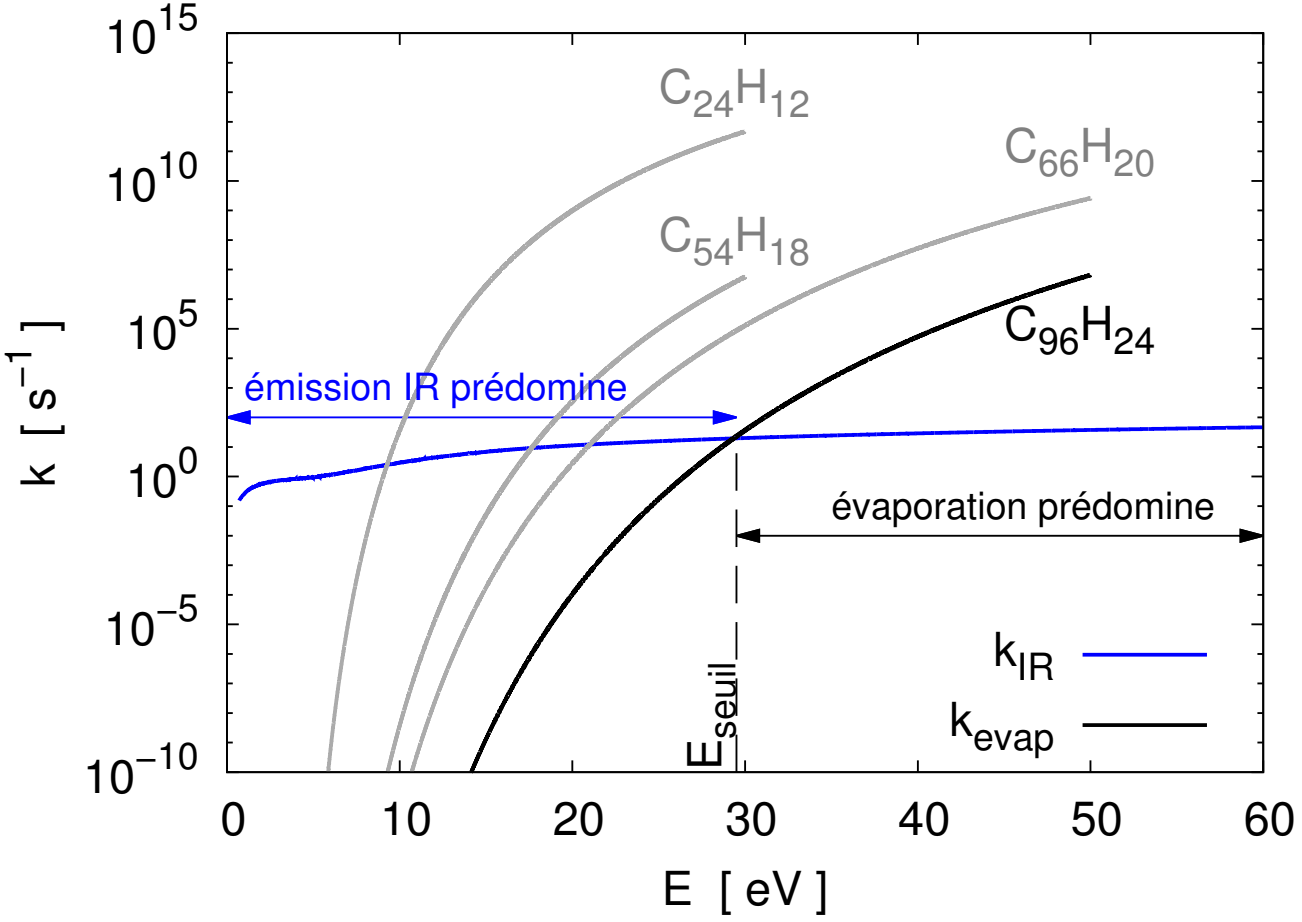
Reaction	k_{diss} [cm^3 s^{-1}]	Ref.	Origin
$C_{24}H_{12}^+ + H$	1.4×10^{-10}	(a)	FA-SIFT
$C_{24}H_{12-2n}^+ + H$	1.4×10^{-10}	(b,c,d)	extrap. $C_{10}H_6^+$ and $C_{16}H_8^+$
$C_{24}H_{12-2n+1}^+ + H$	$\sim 5 \times 10^{-11}$	(b,c)	extrap. $C_{10}H_7^+$
$C_{24}H_{12+n}^+ + H$	$\sim 10^{-12}$	(e)	$C_6H_7^+$, $C_{10}H_9^+$ and $C_{16}H_{11}^+$
$C_{24}H_{12}^+ + H_2$	$< 5 \times 10^{-13}$	(a)	FA-SIFT
$C_{24}H_{12-2n}^+ + H_2$	$< 5 \times 10^{-13}$	(b)	extrap. $C_{10}H_6^+$ and $C_{16}H_8^+$
$C_{24}H_{12-2n+1}^+ + H_2$	$< 4 \times 10^{-12}$	(f)	cold FT-ICR
$C_{24}H_{12+n}^+ + H_2$	-	-	

(a) Betts et al. (ApJ, 2006);
(b) Le Page et al. (ApJSS, 2001);
(c) Le Page et al. (Int. J. Mass Spectrom., 1999);
(d) Le Page et al. (JACS, 1999);
(e) Snow et al. (1998);
(f) C. Joblin, on-going experience.

No measurement for PAHs larger than coronene ($C_{24}H_{12}^+$)
No measurement for neutral PAHs
No measurement for highly superhydrogenated PAHs

Hydrogenation state of PAHs: photodissociation

$$\mathrm{PAH} \xrightarrow{h\nu} \mathrm{PAH}^* \longrightarrow \mathrm{PAH}_{-\mathrm{H}} + \mathrm{H} \quad k_{\mathrm{diss}}$$
$$\longrightarrow \mathrm{PAH} + \mathrm{IR} \quad k_{\mathrm{IR}}$$



Assuming statistical dissociation
[Jochims et al., 1994]

$E_{threshold} > 13.6$ eV:

- successive absorption of several photons before complete cooling
- dissociation close to threshold energy
[Joblin et al., in prep.]

$$k_{\mathrm{diss}}(E) = A_{\mathrm{diss}} \frac{\rho(E - E_0)}{\rho(E)} \; ; \; E_0^{\mathrm{even/odd}} = 4.8/3.2 \text{ eV} \; ; \; A_{\mathrm{diss}} = 6.8 \times 10^{17} \text{ s}^{-1}$$

Plan

Basics of the astrochemical model

- Fixed astrophysical conditions: (from Meudon PDR code, cf. Talk F. Le Petit)
  - → profile of UV spectrum and intensity
  - → profile of local density, H, H_2, electrons
  - → profile of temperature

- Kinetic modelling

$$\frac{\partial X_i(E)}{\partial t} = P_i - L_i$$

  - time evolution
  - rate equations

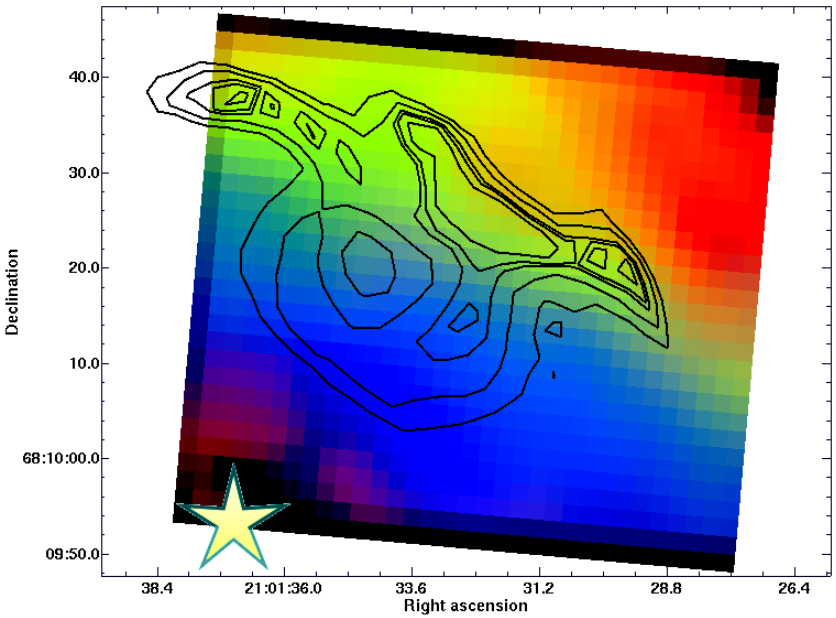
- Photodissociation: accounting for the internal energy evolution of PAHs

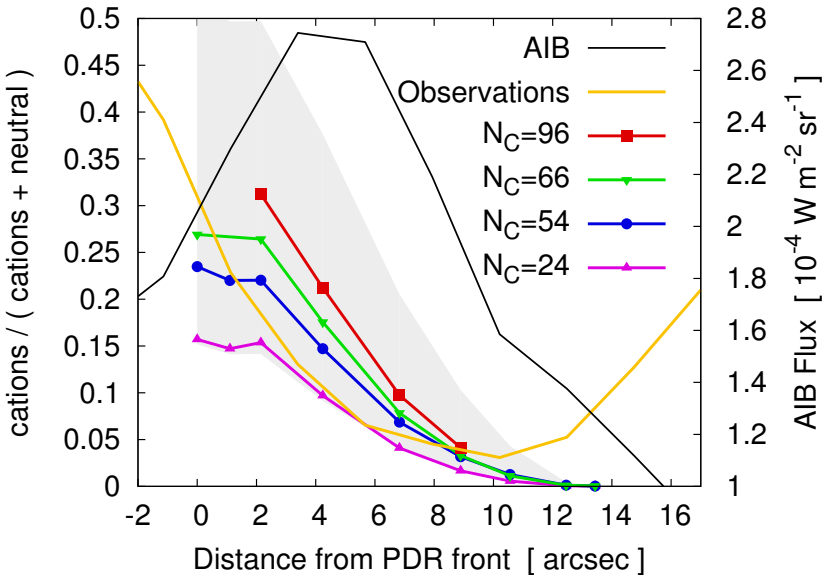
$$X(E) + h\nu_{\mathrm{UV}} \xrightarrow{[1-Y_{\mathrm{ion}}(E)]k_{\mathrm{abs}}(E)} X(E') \quad (1)$$

$$X(E) \xrightarrow{k_{\mathrm{IR}}(E)} X(E'') + h\nu_{\mathrm{IR}} \quad (2)$$

$$X(E) \xrightarrow{k_{\mathrm{diss}}(E)} X^{-\mathrm{H}}(0) + \mathrm{H} \quad (3)$$

Results: charge state in NGC 7023 NW





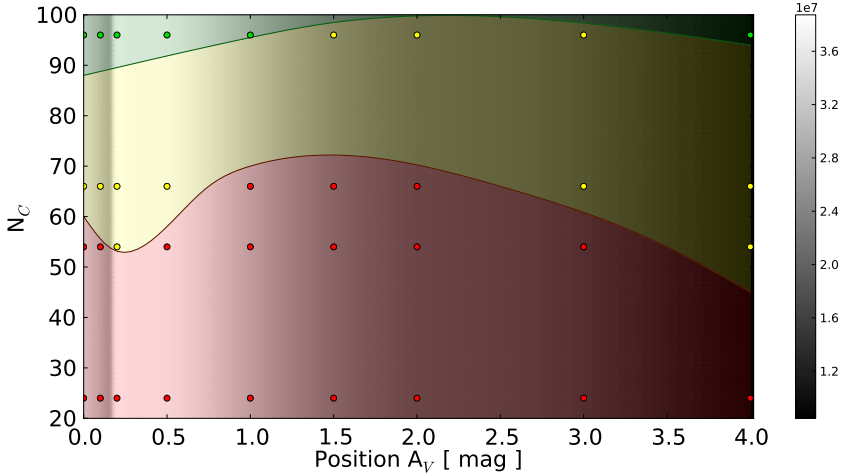
[Montillaud et al., submitted]

Main source of uncertainty: recombination of PAH^+ with electrons

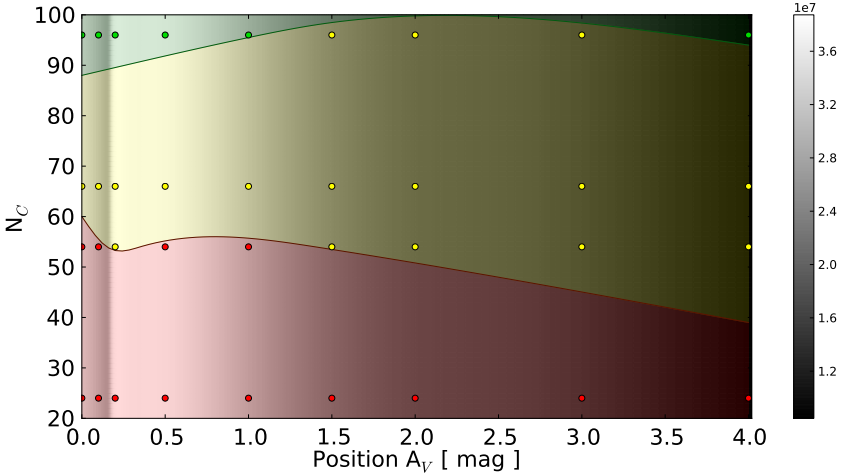
Results: hydrogenation state in NGC 7023 NW

[Montillaud et al., submitted]

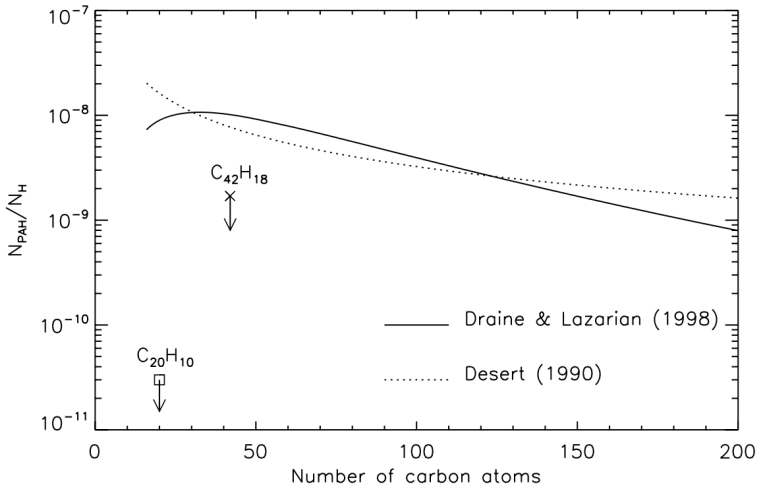
$k_{+H_2} = 0$



$k_{+H_2} = 5 \times 10^{-13}$ cm^3 s^{-1}

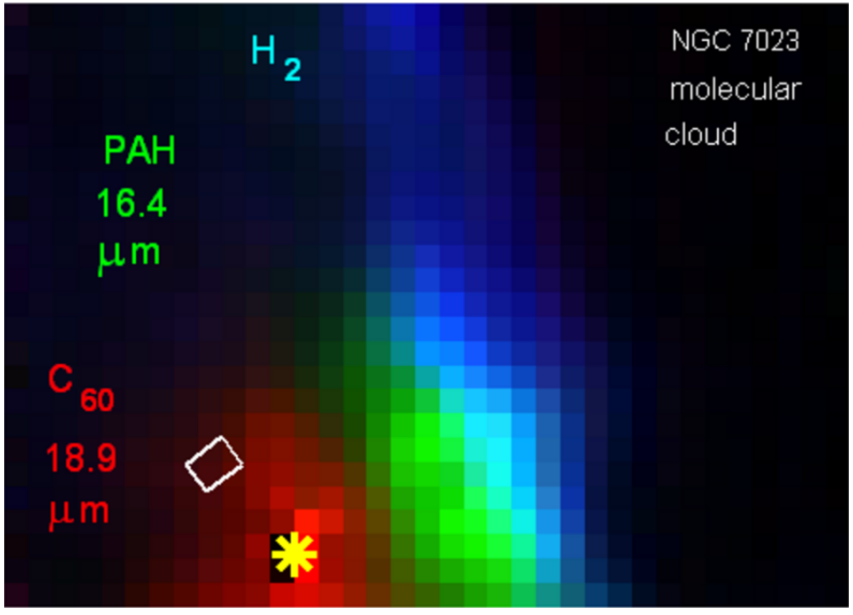


- 3 dominant populations:
  - superhydrogenated
  - normally hydrogenated
  - completely dehydrogenated (= carbon cluster)
- PAH: min. size $\sim$ 50 C
- Possible existence of carbon clusters
- + all species completely dehydrogenated in the cavity

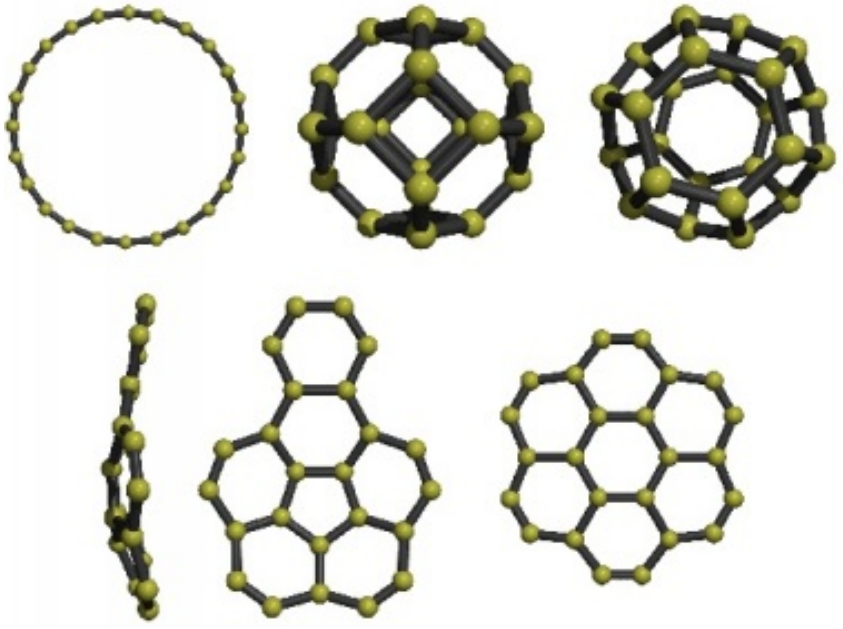


Pilleri et al., MNRAS, 2009

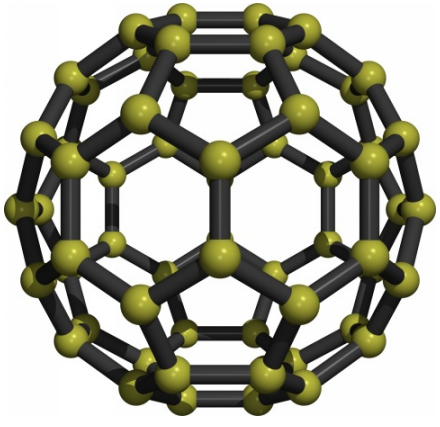
Carbon clusters



[Sellgren et al., ApJ, 2010]



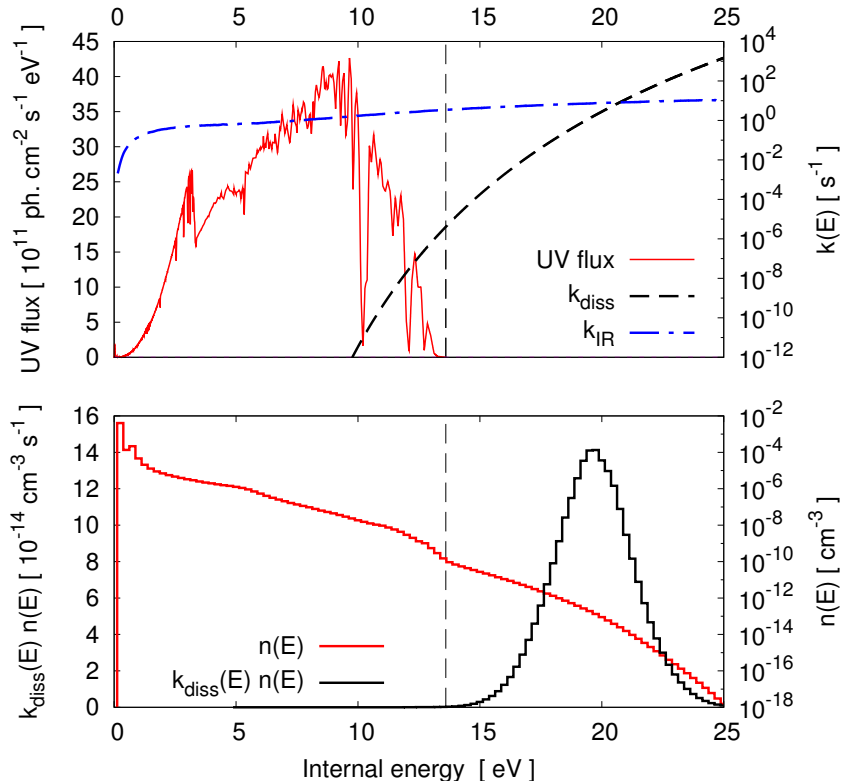
isomères de C_{24} [Kent et al., Phys. Rev. B, 2000]

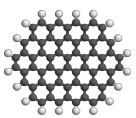


C_{60}

- Which isomers ?
- Which evolution of carbon clusters ?
- Which impact on the physics and chemistry of the medium ?

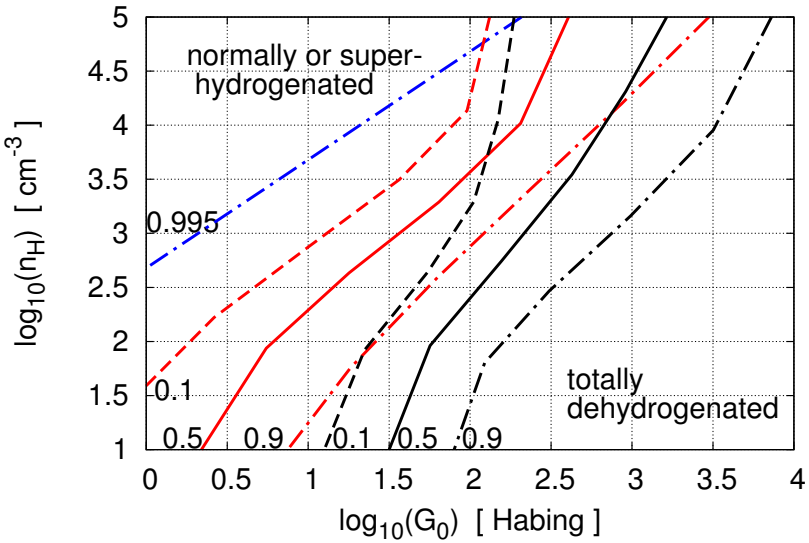
Importance of multiphoton events

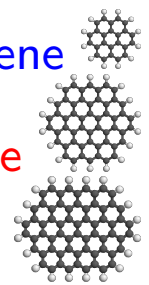




in NGC 7023 NW

Calculation for the diffuse ISM



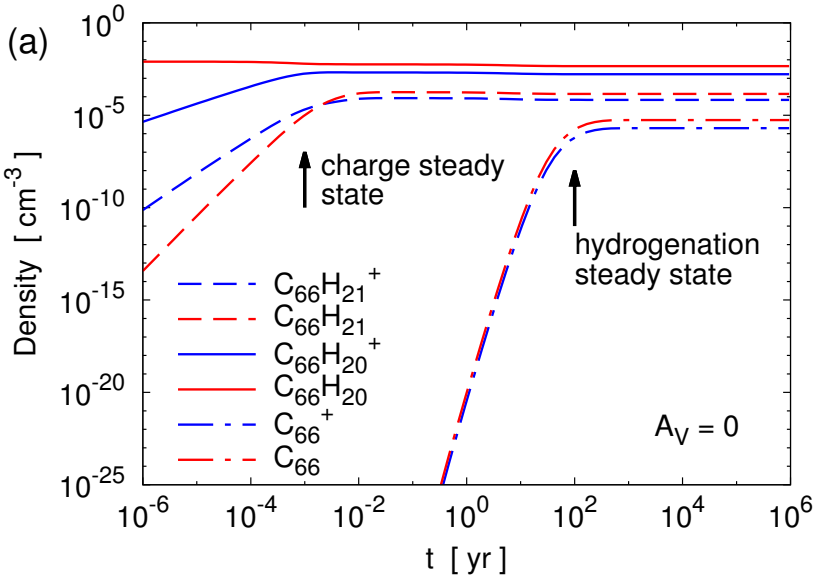


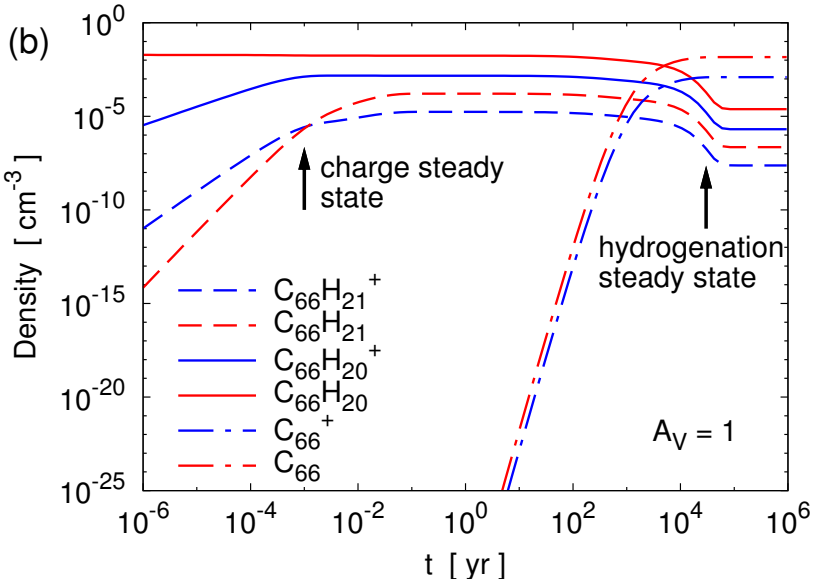
coronene

circumcoronene

circumovalene

Surprising timescales





Plan

Conclusion

- multiphoton events are not negligible
- need for new molecular data:
  - recombination with electrons
  - PAH^+ with H_2
  - reactivity and photodissociation of superhydrogenated PAHs
  - **large PAHs !**
- guideline for spectroscopic identification of an individual PAH:
  - normally hydrogenated
  - **large PAHs !**
- carbon clusters could be abundant

Thank you for your attention !