Understanding the Physics and Chemistry of Photodissociation Regions: Insights from Spitzer, Herschel and SOFIA Observations of NGC 7023

Olivier Berné

Herschel OT1 program, PI C. Joblin, «Physics of gas evaporation at PDR edges»
A. Boulais, J. Pety, M. Gerin, J. R. Goicoechea, P. Gratier, V. Guzman, E. Habart, ,D. Teyssier, F. Le Petit, J. Le Bourlot, J. Montillaud, P. Pilleri, K. Sellgren, , A. Abergel

SOFIA cycle 2 program, PI O. Berné
C. Joblin, Xander Tielens, J. Montillaud, B. Orchsendorf + Support from Andrew Helton @ SOFIA

Outline

Prelude : A short presentation of the NGC 7023 reflection nebula

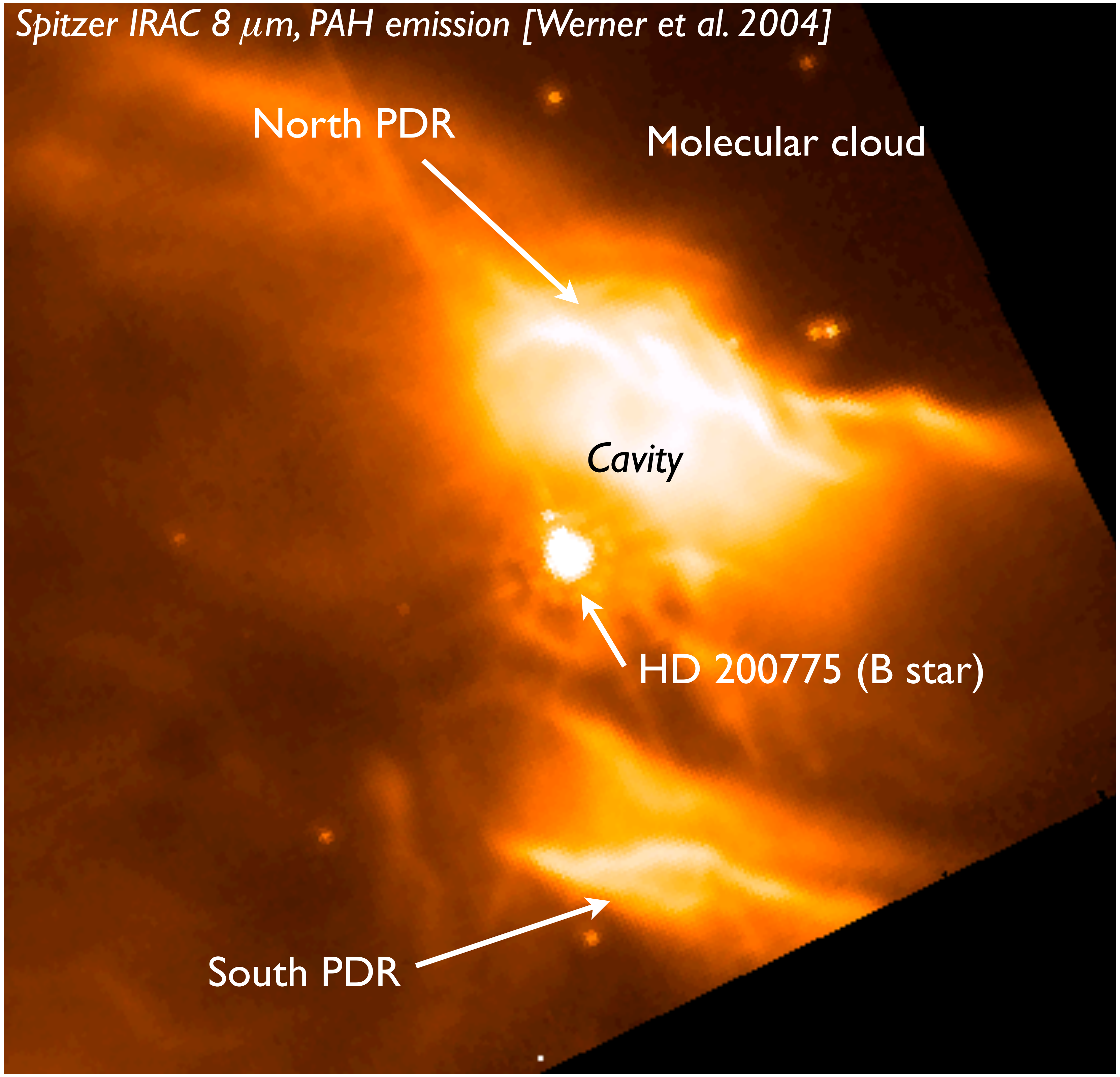
Part I : physics and chemistry of PAHs and fullerenes

- The discovery of PAHs and fullerenes
- The chemical evolution of large cabonaceous molecules in NGC 7023, from PAHs to C_{60}
- The size distribution of interstellar PAHs : SOFIA-FORCAST/FLITECAM

Part II : physics and chemistry of PDRs

- A short presentation of PDRs
- Evidence for intense dynamical activity in NGC 7023 seen with Herschel: photoevaporation
- Confirming this activity with SOFIA-EXES

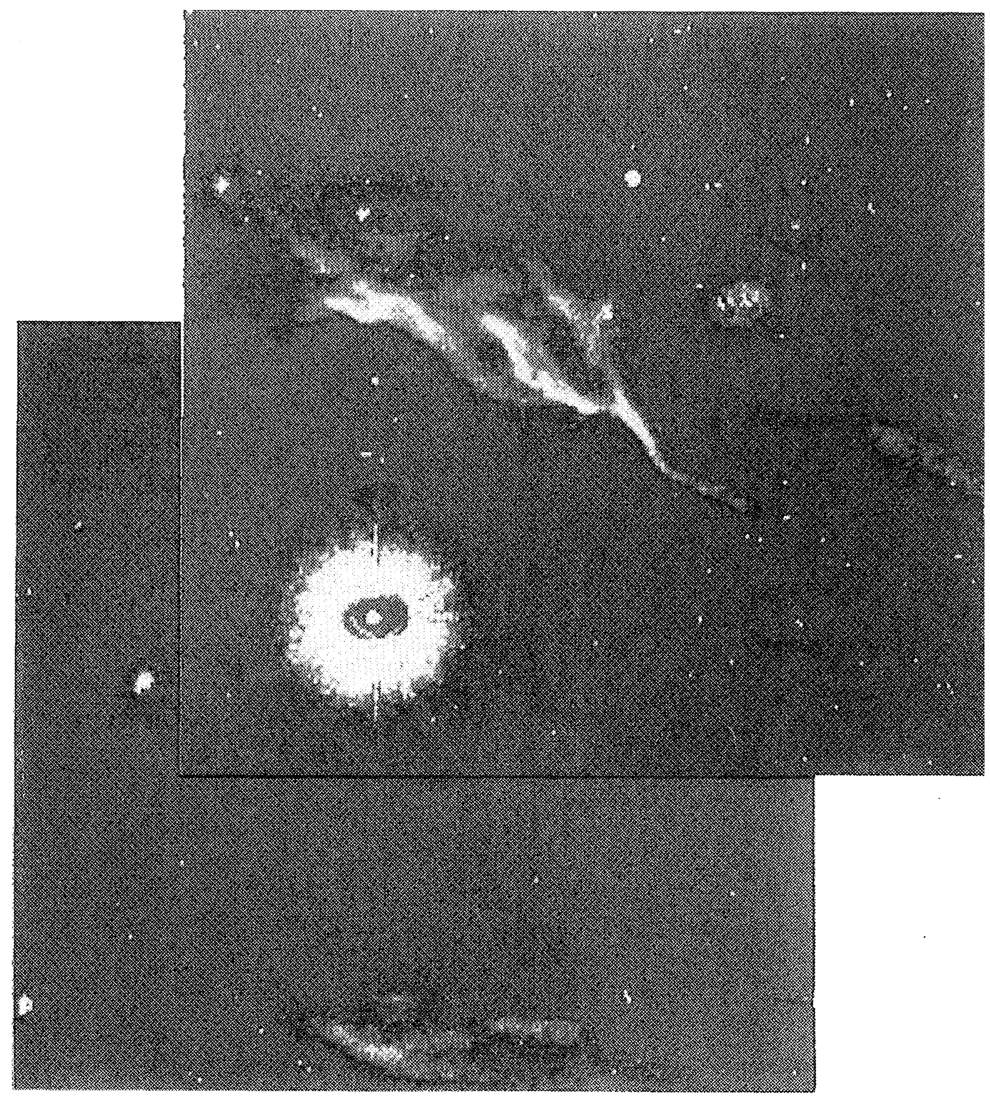
NGC 7023



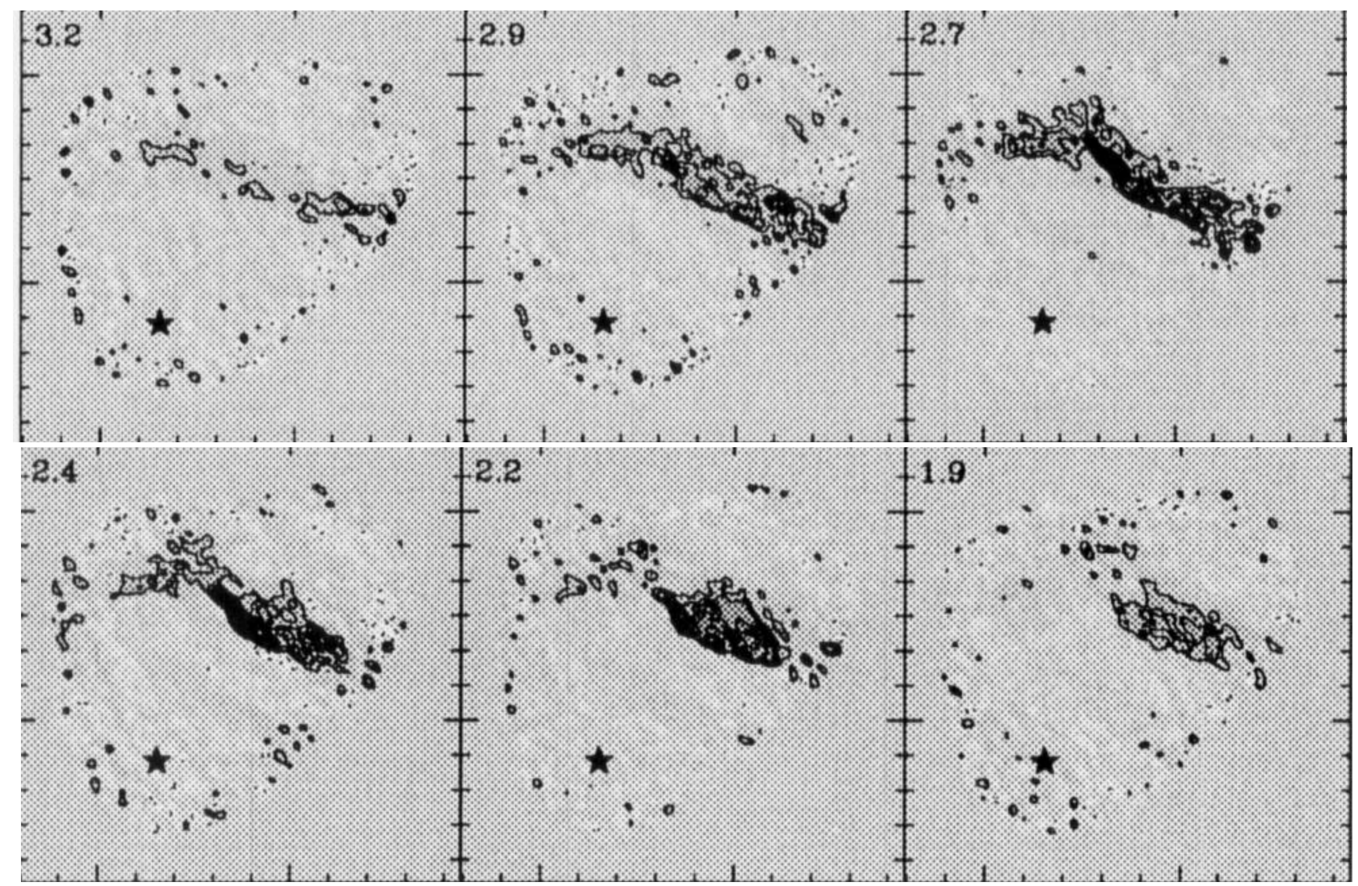
Spitzer IRAC 8 μm, PAH emission [Werner et al. 2004]
North PDR
Molecular cloud
Cavity
HD 200775 (B star)
South PDR

NGC 7023

Lemaire et al. 1996 (H_2 at 2.1 μm)



Fuente et al. 1996 (HCO+ 1-0)



Presence of bright and dense (above 10^5 cm^{-3}) «filaments» of 1” thickness at the molecular atomic interface

Outline

Prelude : A short presentation of the NGC 7023 reflection nebula

Part I : physics and chemistry of PAHs and fullerenes

- The discovery of PAHs and fullerenes
- The chemical evolution of large carbonaceous molecules in NGC 7023, from PAHs to C_{60}
- The size distribution of interstellar PAHs : SOFIA-FORCAST/FLITECAM

Part II : physics and chemistry of PDRs

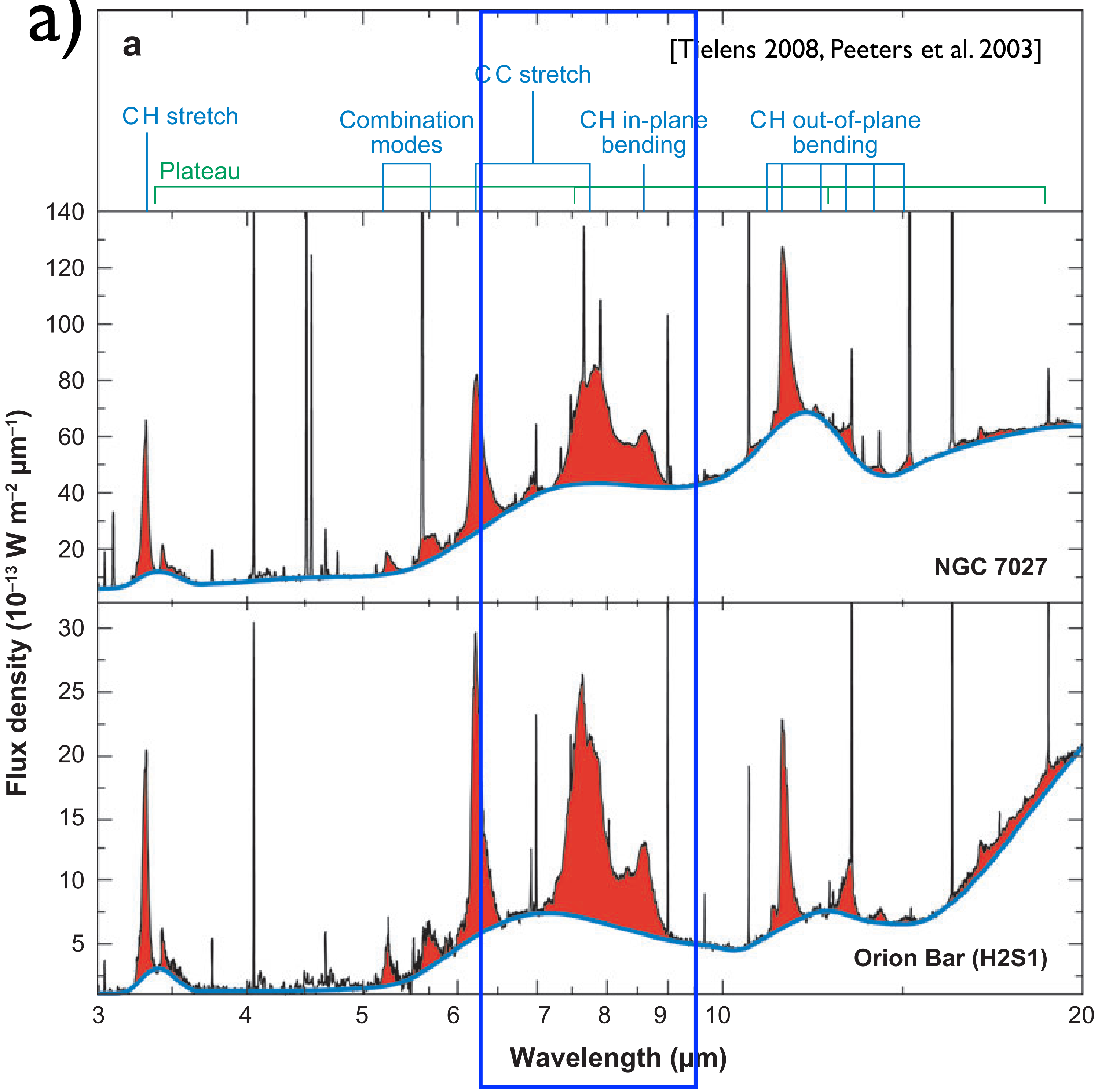
- A short presentation of PDRs
- Evidence for intense dynamical activity in NGC 7023 seen with Herschel: photoevaporation
- Confirming this activity with SOFIA-EXES

Polycyclic aromatic hydrocarbons (PAHs)

1984/1985 proposal that mid-IR bands are due to gas phase PAHs

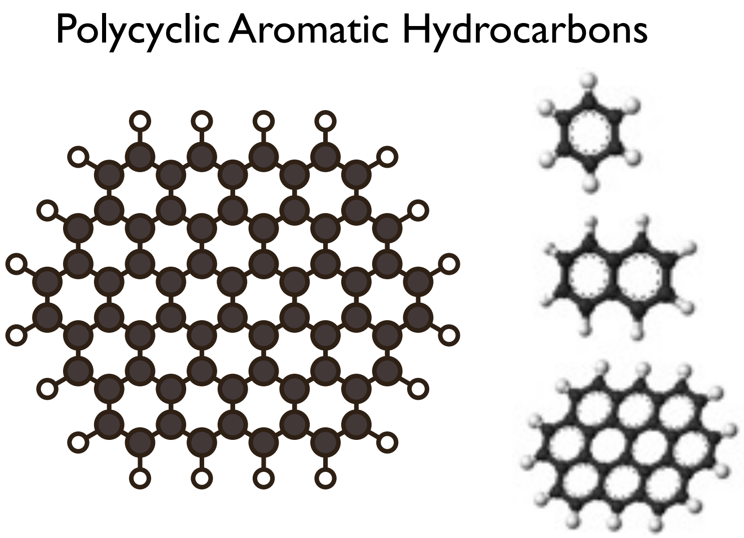
[Léger & Puget 1984] [Allamandola, Tielens, Barker 1985]

a)

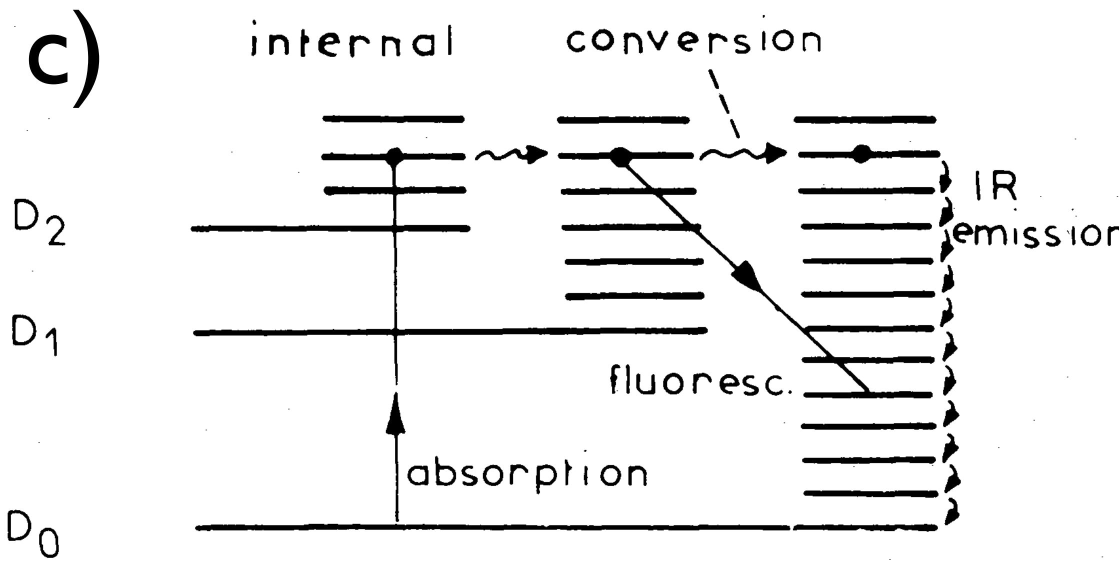


IRAC 8 filter

b)



c)



[Léger, d'Hendecourt, Défourneau, 1989]

No specific PAH molecule identified !

PAHs in space are expected to be large...

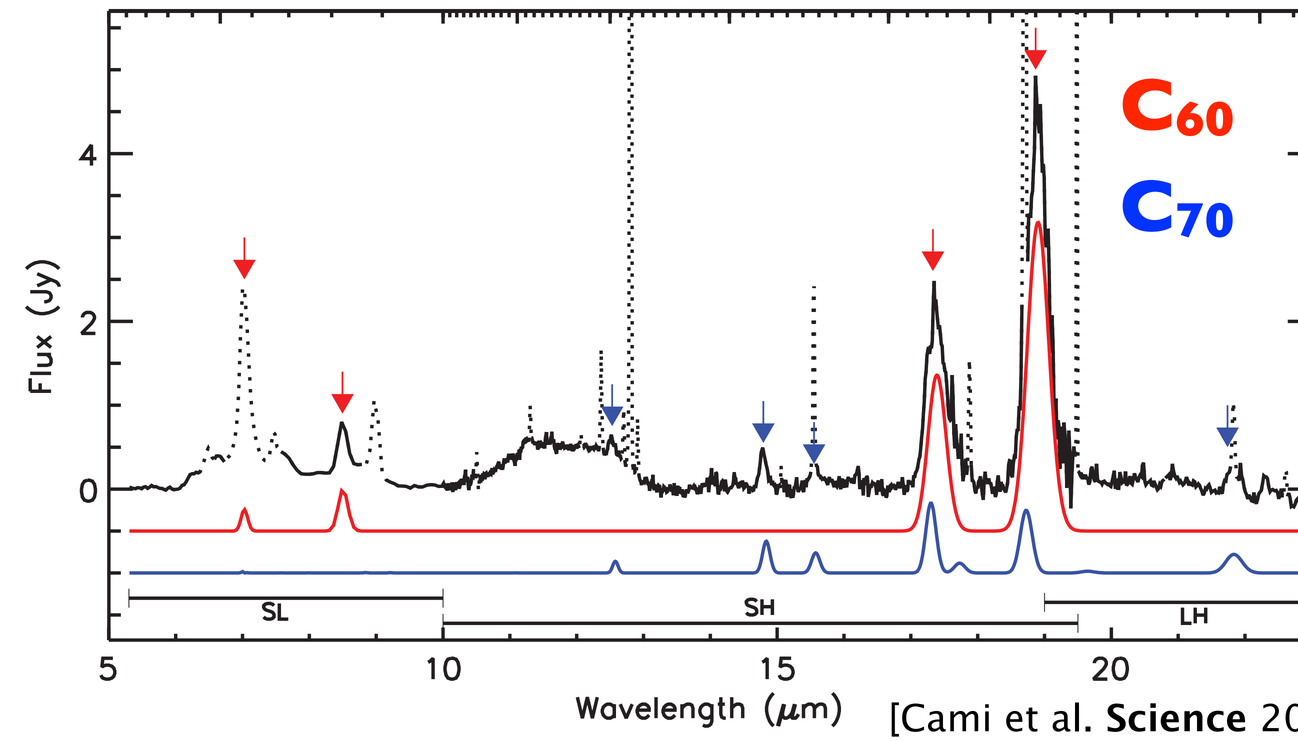
Fullerenes in space

1985 Discovery of the C_{60} molecule in the lab

[Kroto, Heath, Obrien, Curl, Smalley, 1985]

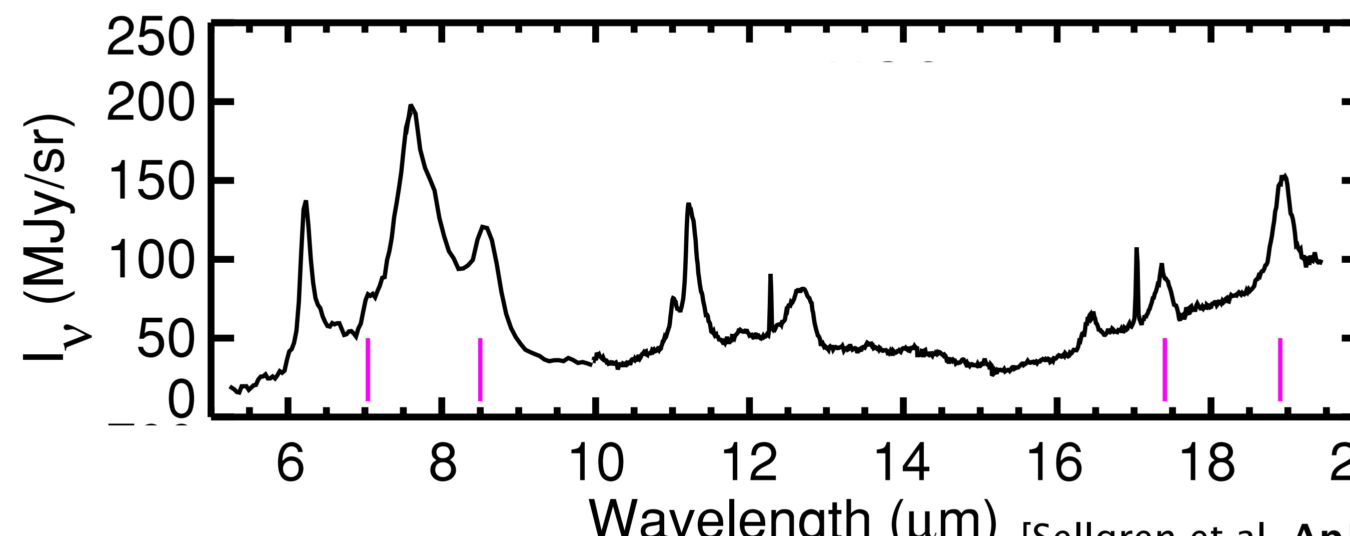
2010 Discovery of the C_{60} molecule in emission in space

Tc1 planetary nebula (evolved star)



[Cami et al. **Science** 2010]

NGC 7023 reflection nebula (interstellar medium)



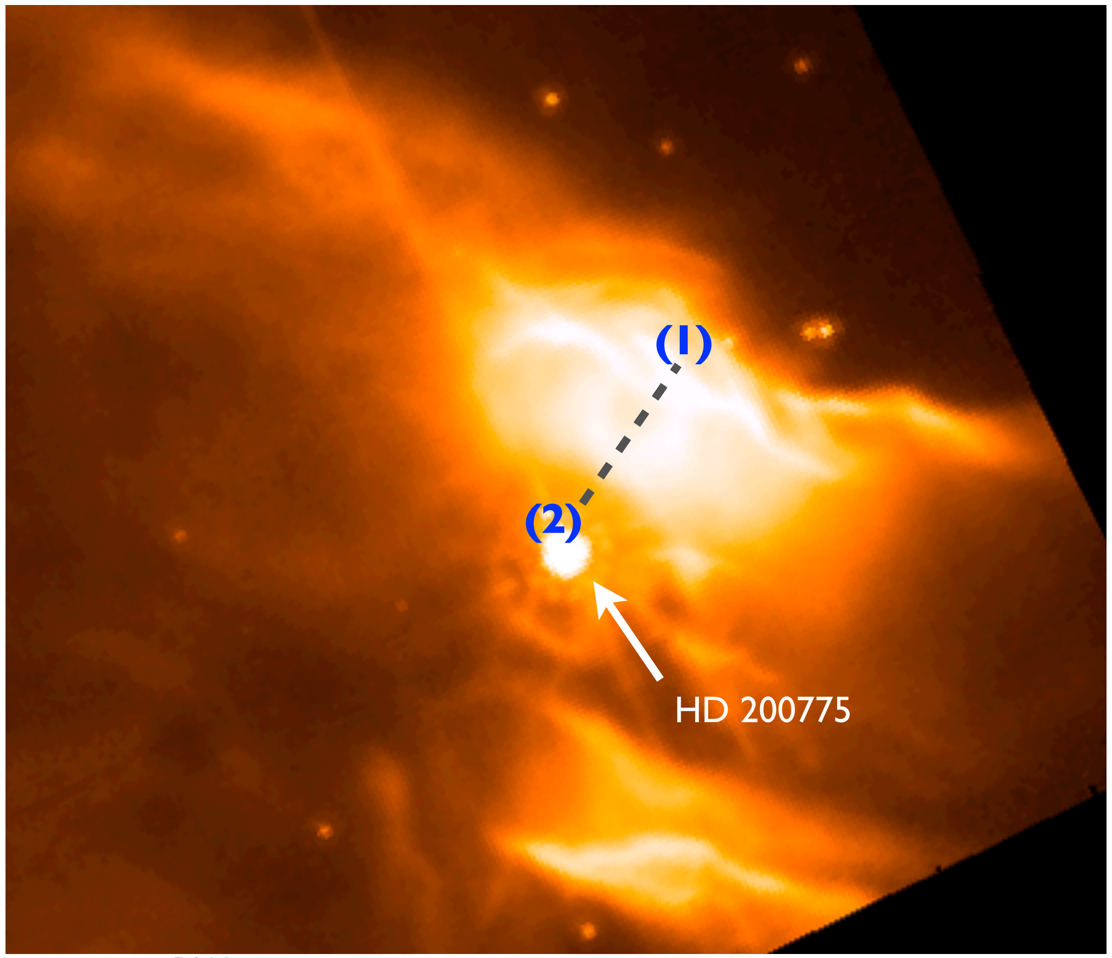
[Sellgren et al. **ApJ.** 2010]

The formation of C_{60} in space is not understood !

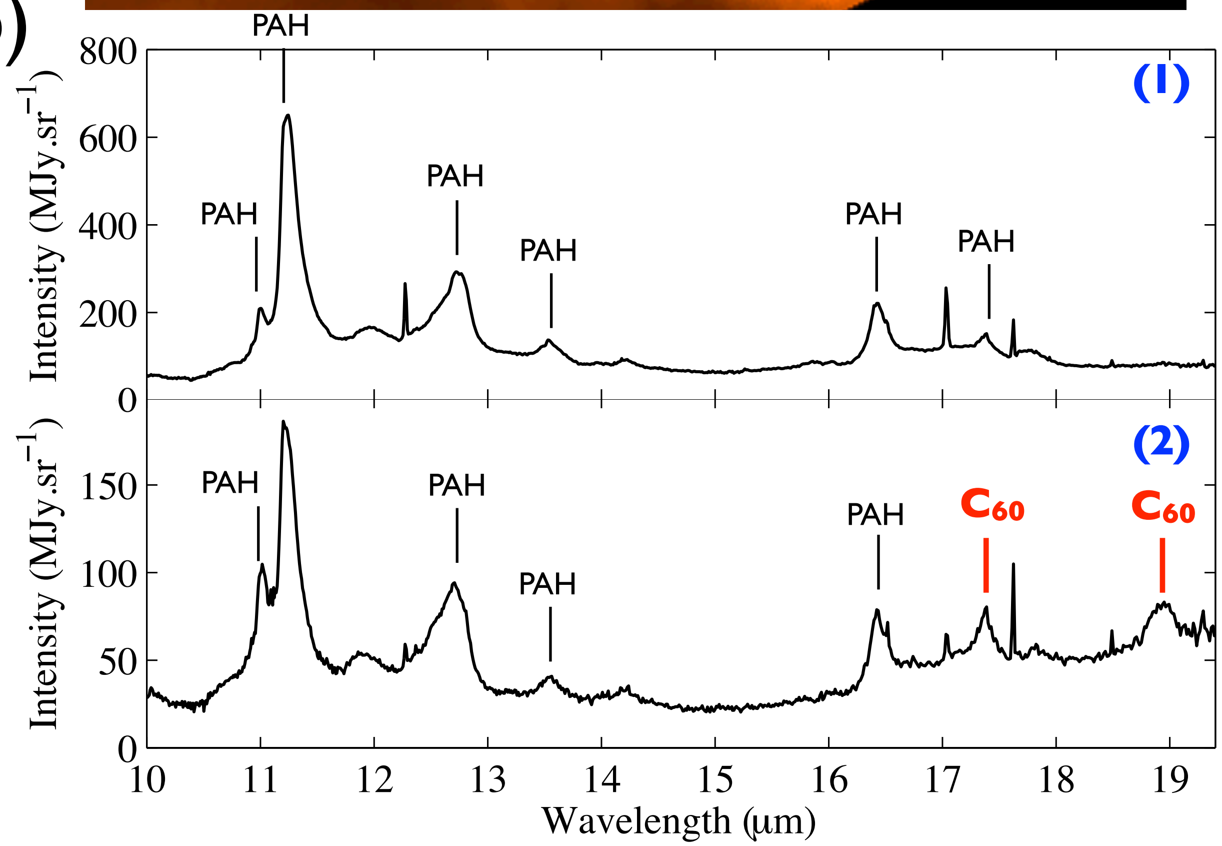
From PAHs to C_{60}

[Berné & Tielens **PNAS** 2012]

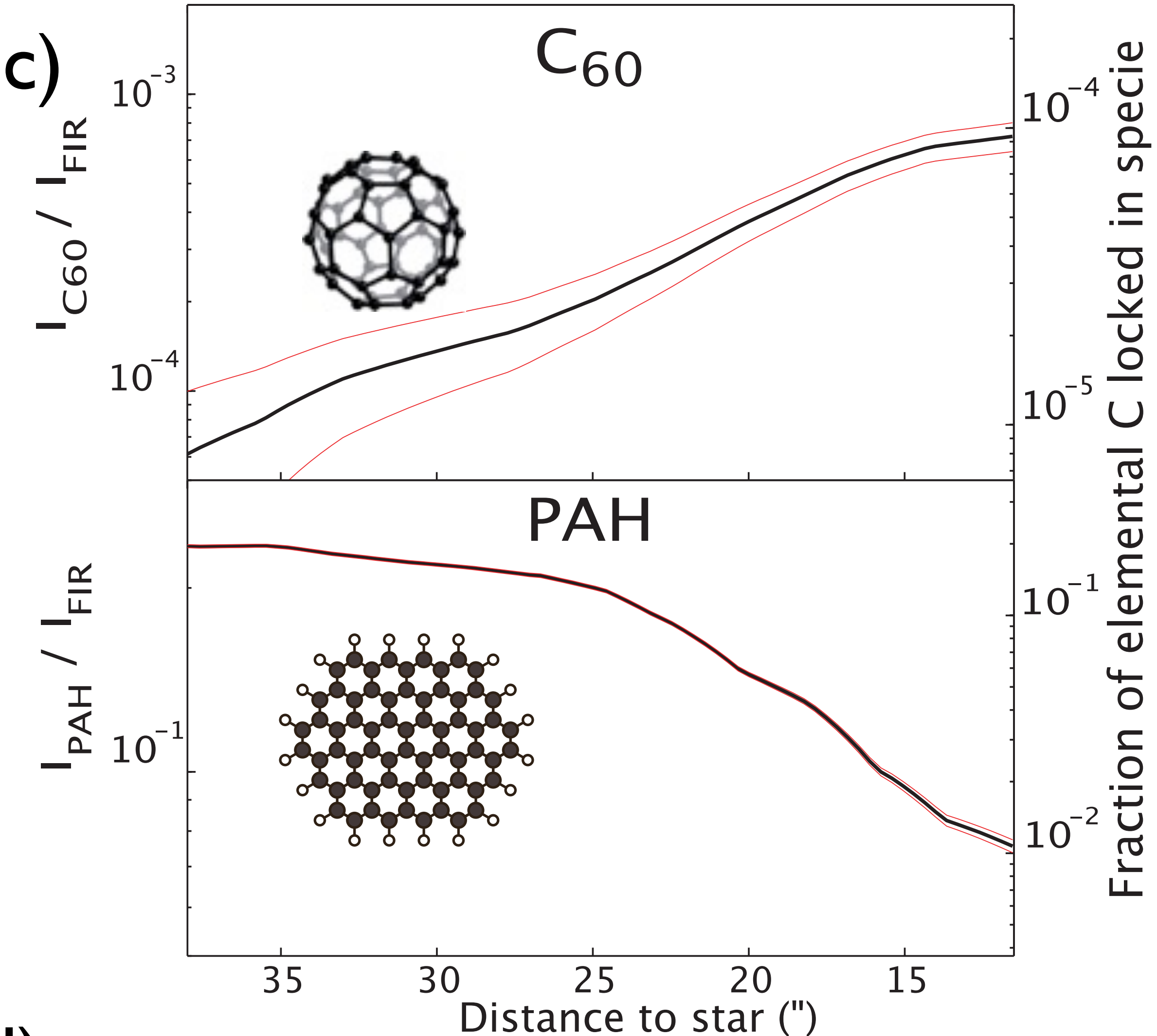
a)



b)



c)



d)

C_{60} is formed in the interstellar medium, at low density (n_H=100 cm^{-3}) !

Aggregation (bottom up) process not possible !

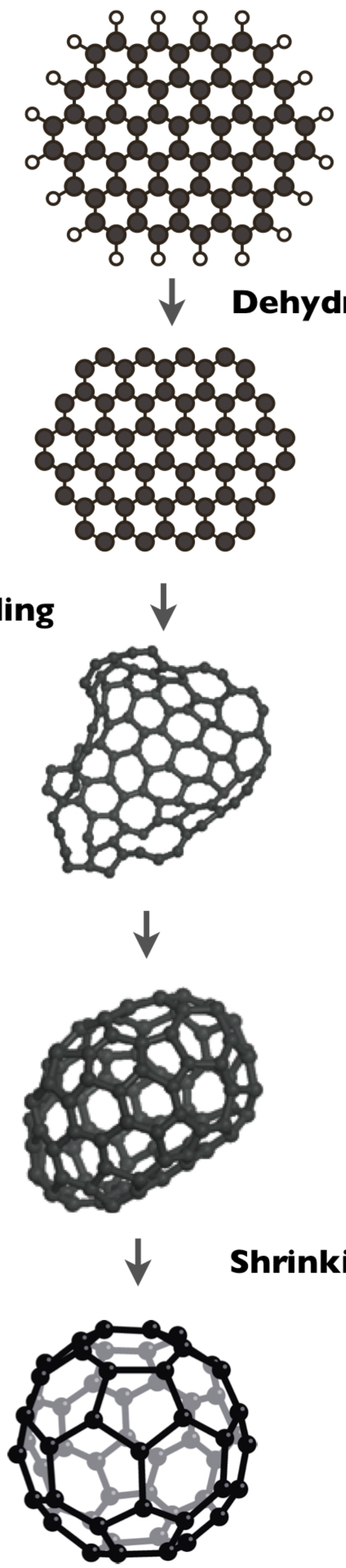
C_{60} formation from photochemical PAH processing ?

Conversion efficiency from PAHs to C_{60} ~0.1%
at 15'' from the star in 10^5 years (age of the nebula)

Proposed scenario

Theoretical studies
Experimental studies

Increasing UV radiation field



Dehydrogenation

[Le Page et al. 2001]
[Montillaud et al. 2013]
[Lifshitz and co-workers, 199x]
[Jochims et al. 1994]
[Ekern et al. 1998]
[Szczepanski et al. 2001] ...

Folding

[Lebedeva et al. 2012]
[Chuvilin et al. 2010]

Shrinking

[Irle et al. 2006]
[Zheng et al. 2007]
[Huang et al. 2007]

[Berné, Montillaud Joblin in Prep.]

Photochemical model for $C_{66}H_{20}$ to C_{60} in NGC 7023

Photochemical Model

[Montillaud, Joblin, Toublanc, 2013, A&A 552, A15]

- Time evolution of PAHs in fixed physical conditions
- Rate equation formalism
- UV photon absorption explicitly described including multiple photon absorptions
- Description of the internal energy of the molecules
- Cooling by infrared emission and visible emission for cages
- Dissociation using state of the art rate constants for the dehydrogenation, folding and shrinking steps
- Reactions with e-, H and C^+

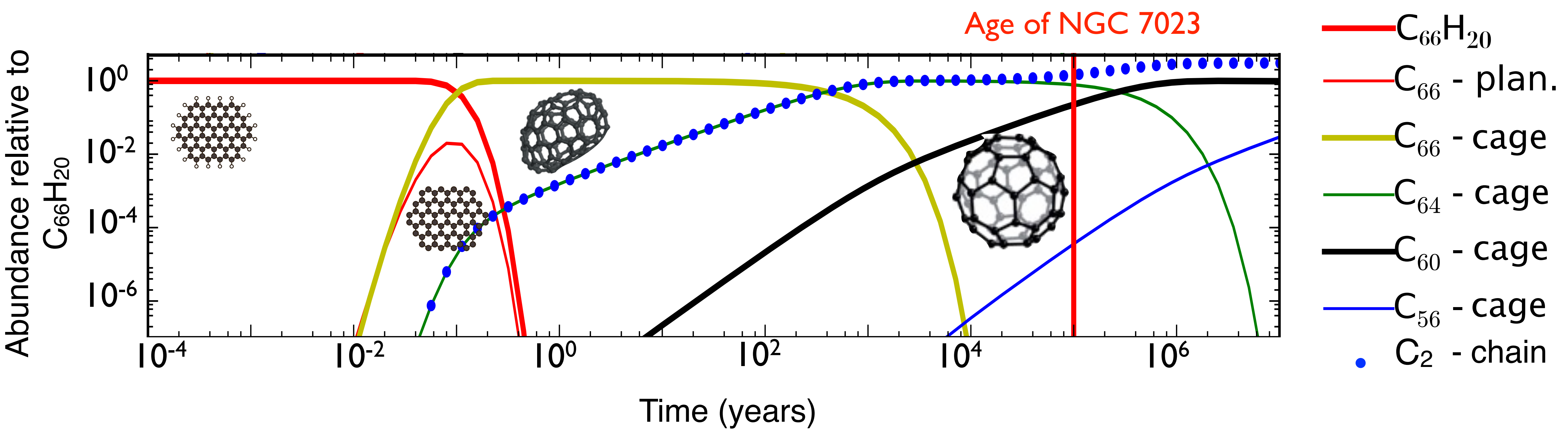
Physical conditions in NGC 7023

- Density profile derived from far-IR emission of dust with Herschel
- Radiation field : derived from the star spectral type
- Gas temperature, H/H2 abundance etc. derived using Meudon PDR code [Le Petit et al. 2006]

Work in progress ! (Berné, Montillaud Joblin in Prep.)

Photochemical model for $C_{66}H_{20}$ to C_{60} in NGC 7023

Results for C66H20 at 10" from the star

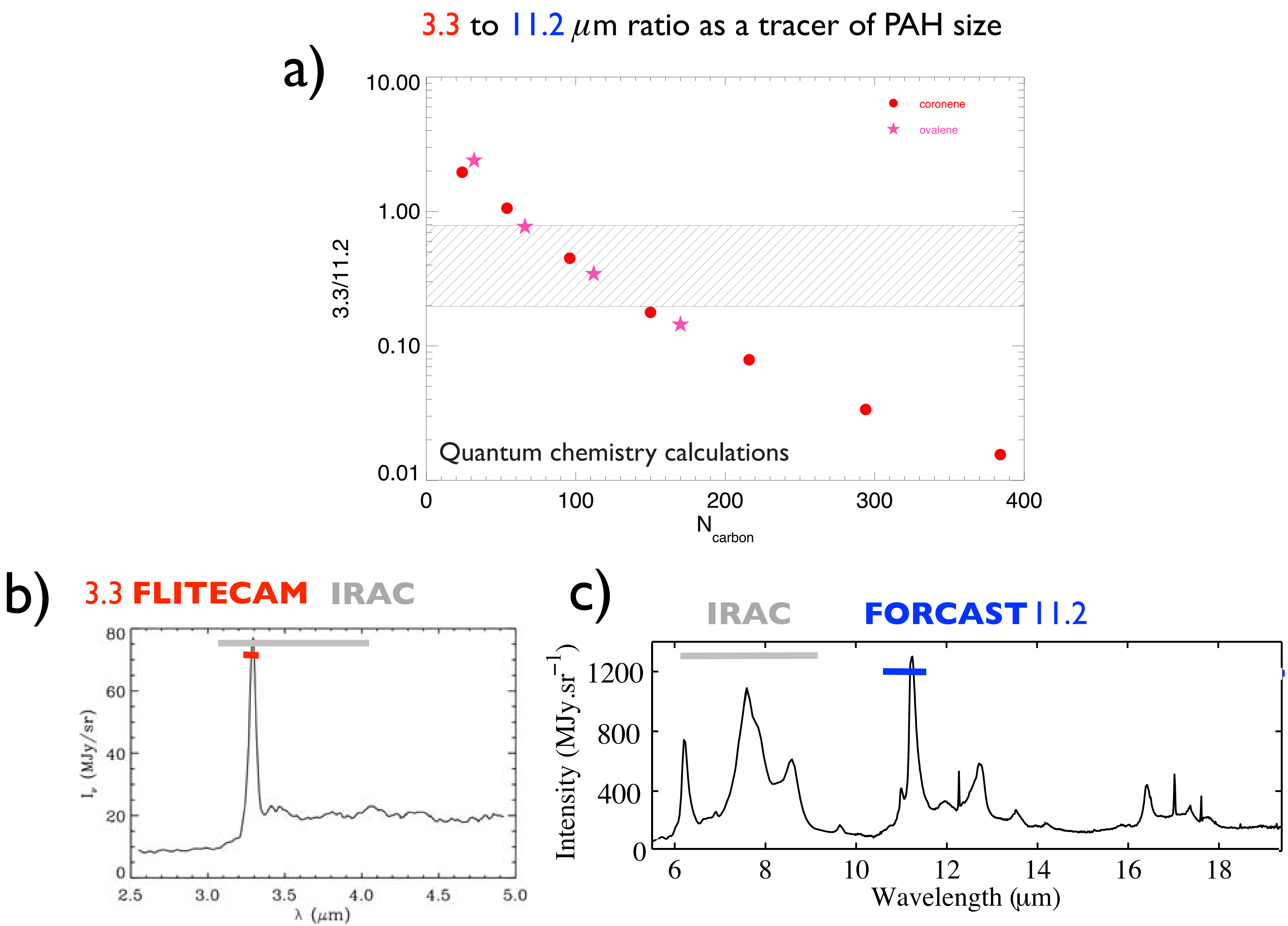


- PAHs of 66 C atoms are quickly destroyed near the star (larger PAHs may survive)
- Graphene flakes (dehydrogenated PAHs) are unstable, we will not detect them (e.g. Kokkin et al. 2008)
- Shrinking is the process limiting C_{60} formation efficiency
- C_{60} is almost never destroyed, that's why we see it
- The conversion efficiency of $C_{66}H_{20}$ is ~60% in 10^5 yrs at 10" from the star,
- This means only a few 10th of a percent of the PAHs need to be of size ~ 66 C atoms to reproduce observations...

...but in reality, we don't now anything about the size distribution of PAHs !!!!

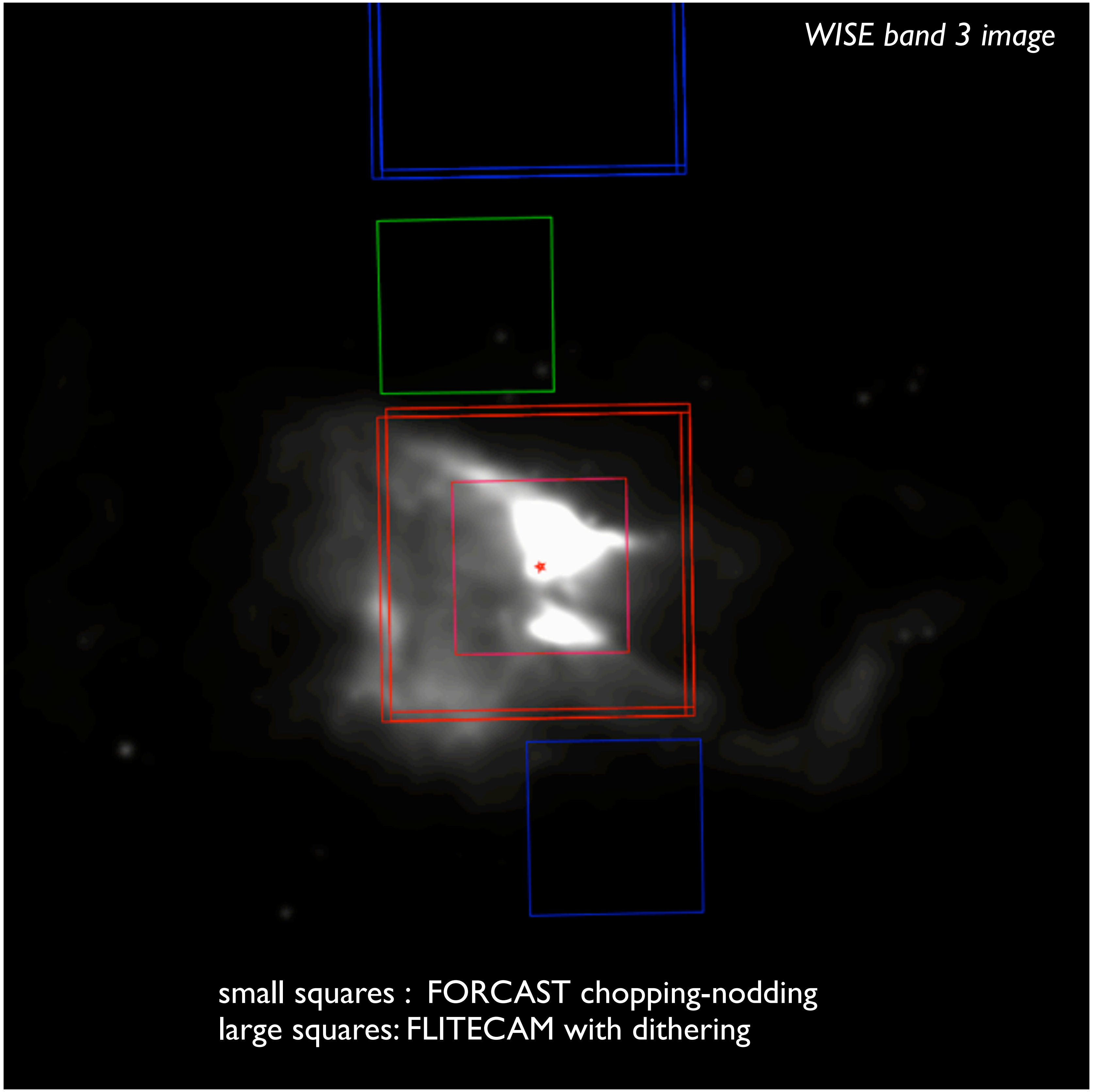
Work in progress ! (Berné, Montillaud Joblin in Prep.)

Constraining the size distribution of PAHs with SOFIA



Constraining the size distribution of PAHs with SOFIA

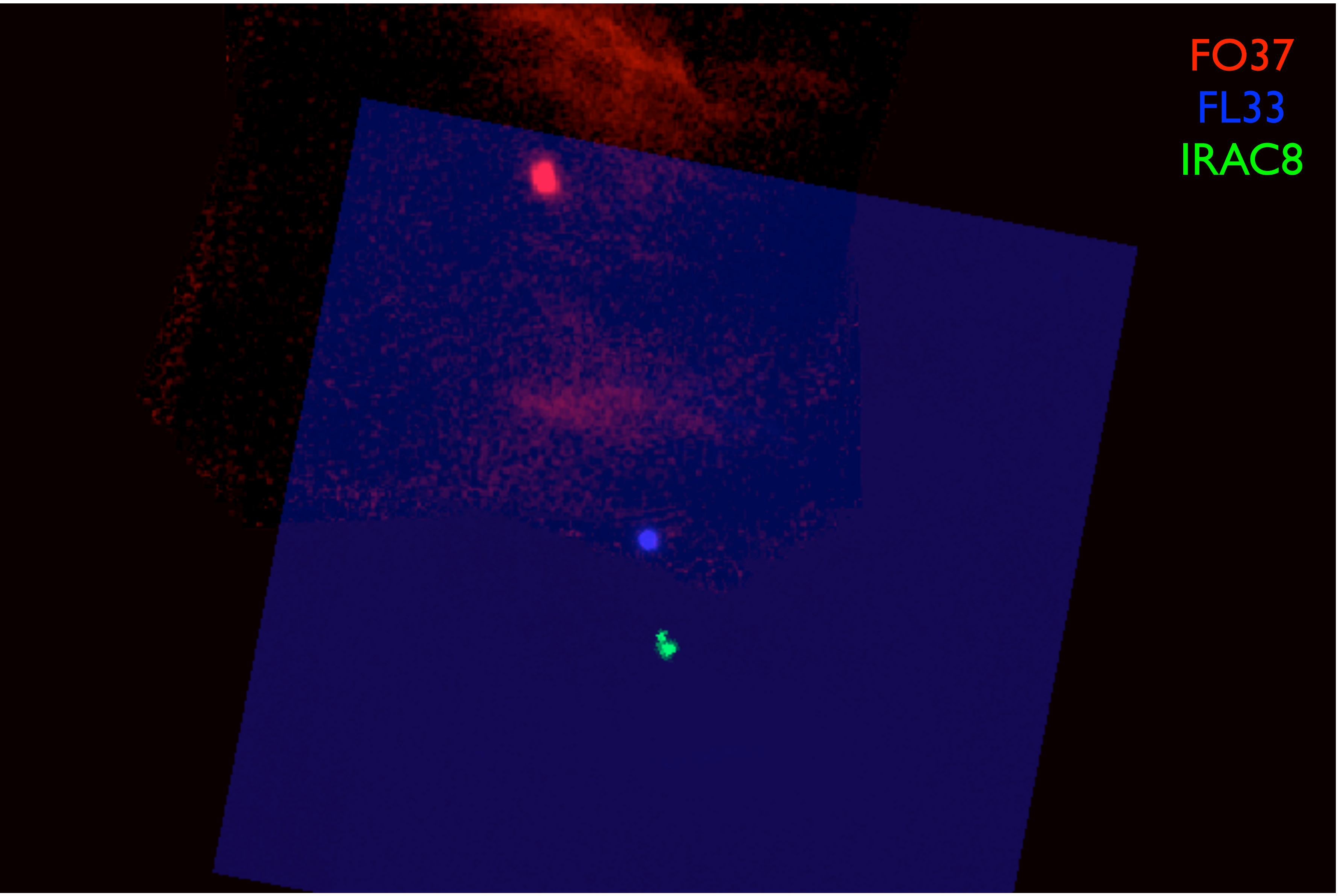
Observing strategy



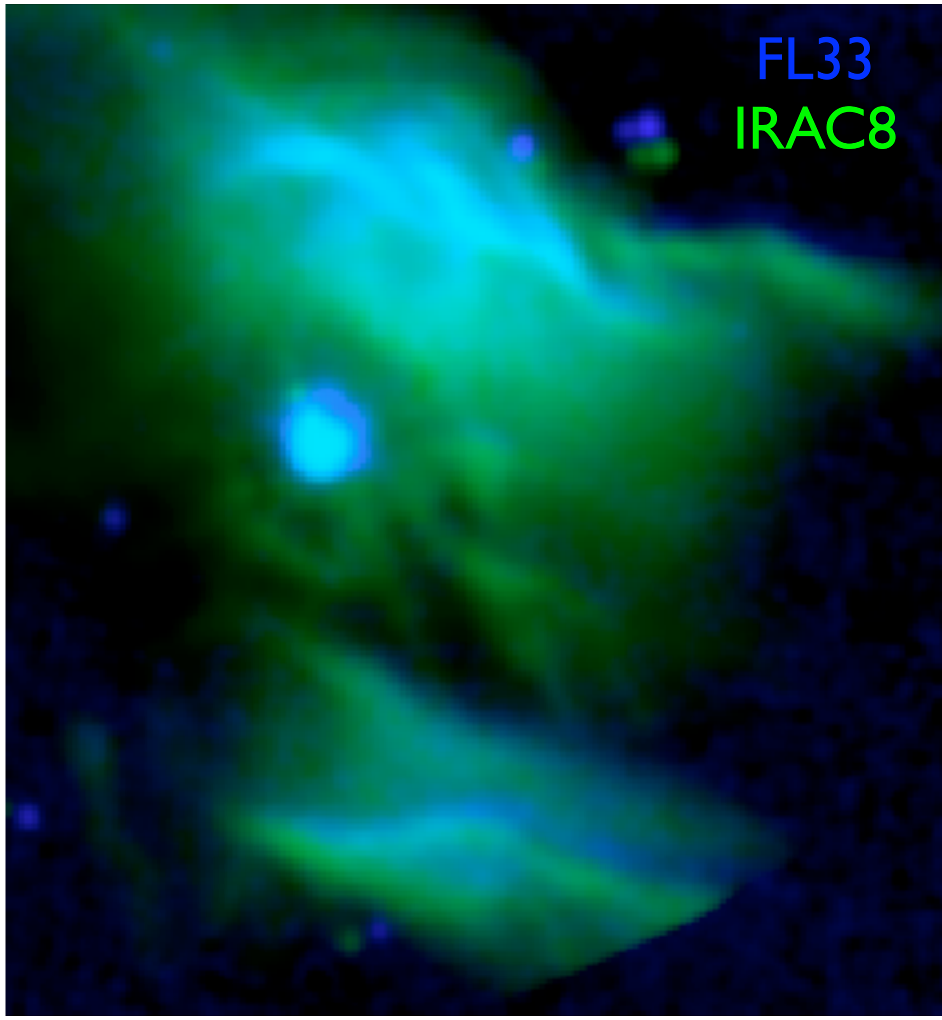
Constraining the size distribution of PAHs with SOFIA

Data reduction

Misalignment

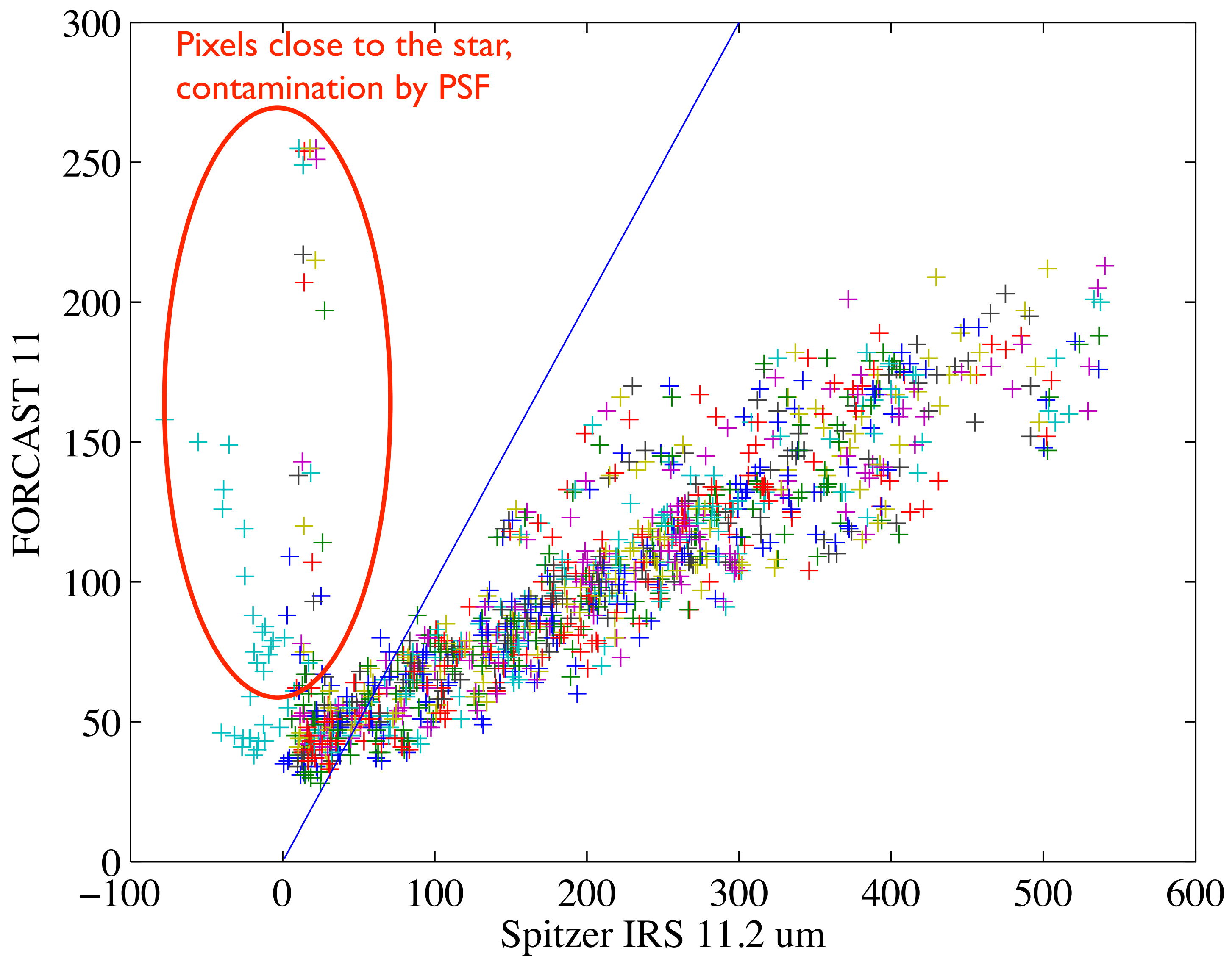


Rotation on the sky



Constraining the size distribution of PAHs with SOFIA

Cross calibration



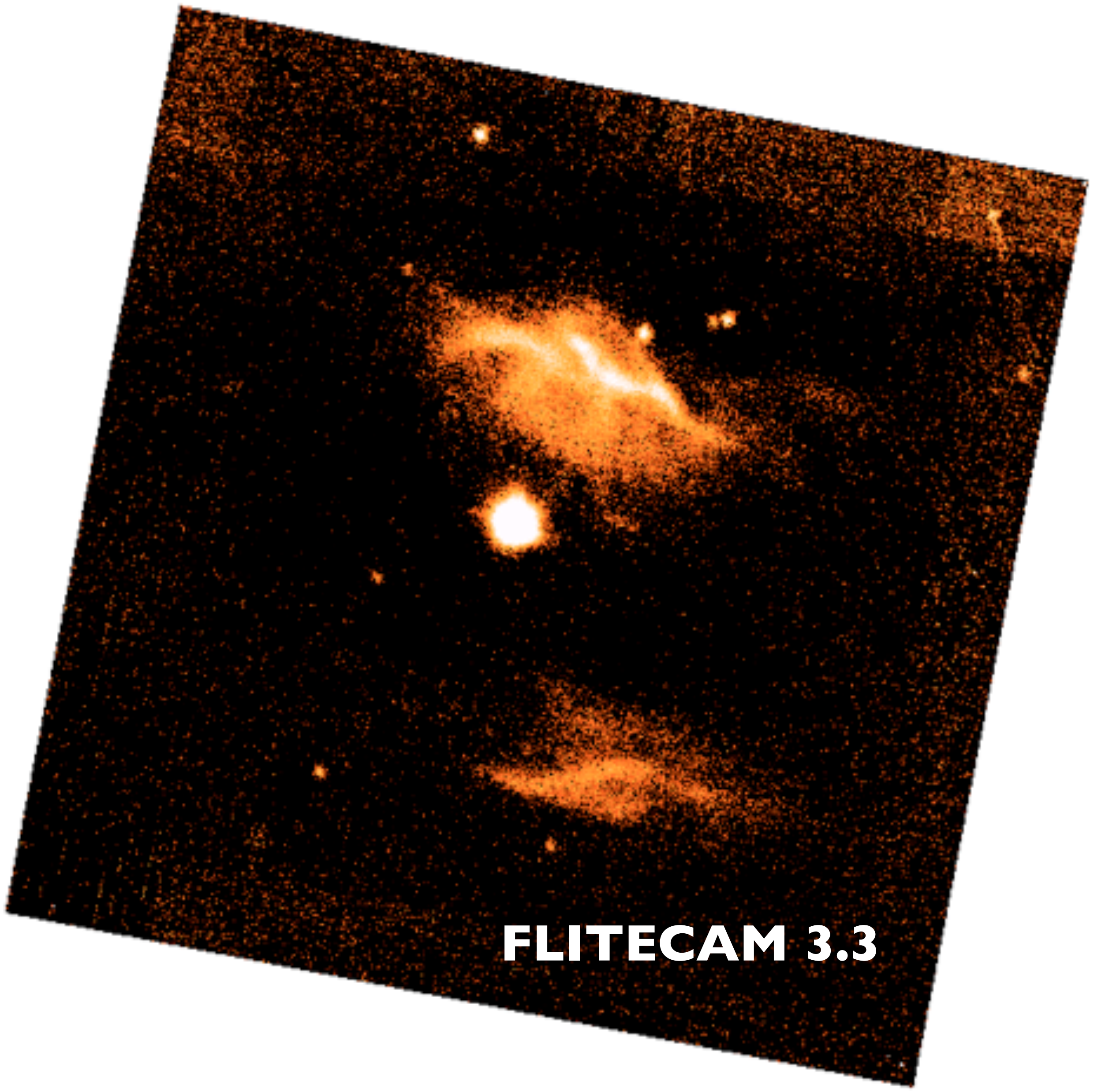
- FORCAST11 map convolved and reprojected in the Spitzer IRS pixels at same wavelength

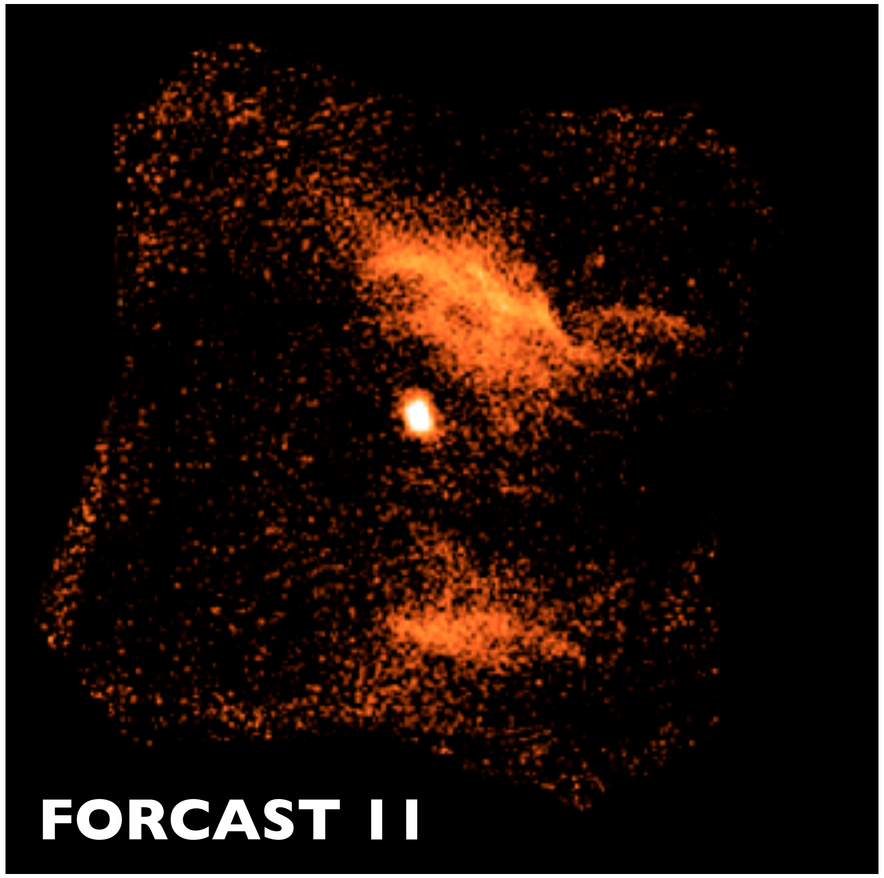
- Linear proportionality between the two maps

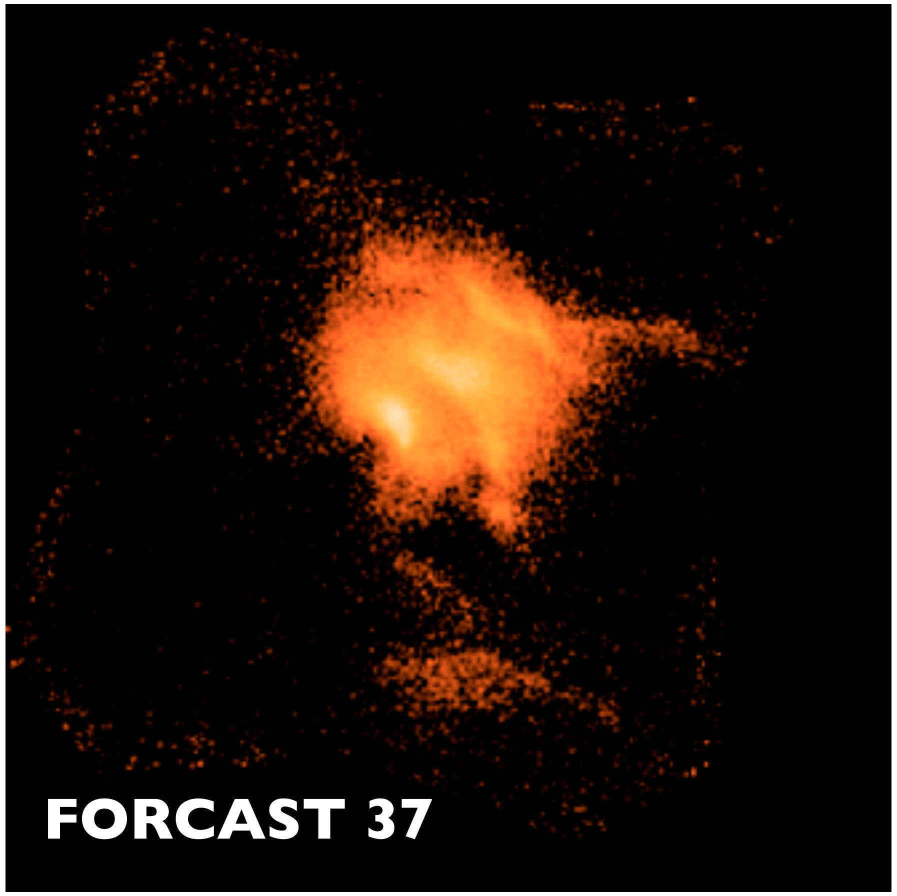
- But FORCAST intensities are lower than the Spitzer-IRS intensities by a factor ~3

Constraining the size distribution of PAHs with SOFIA

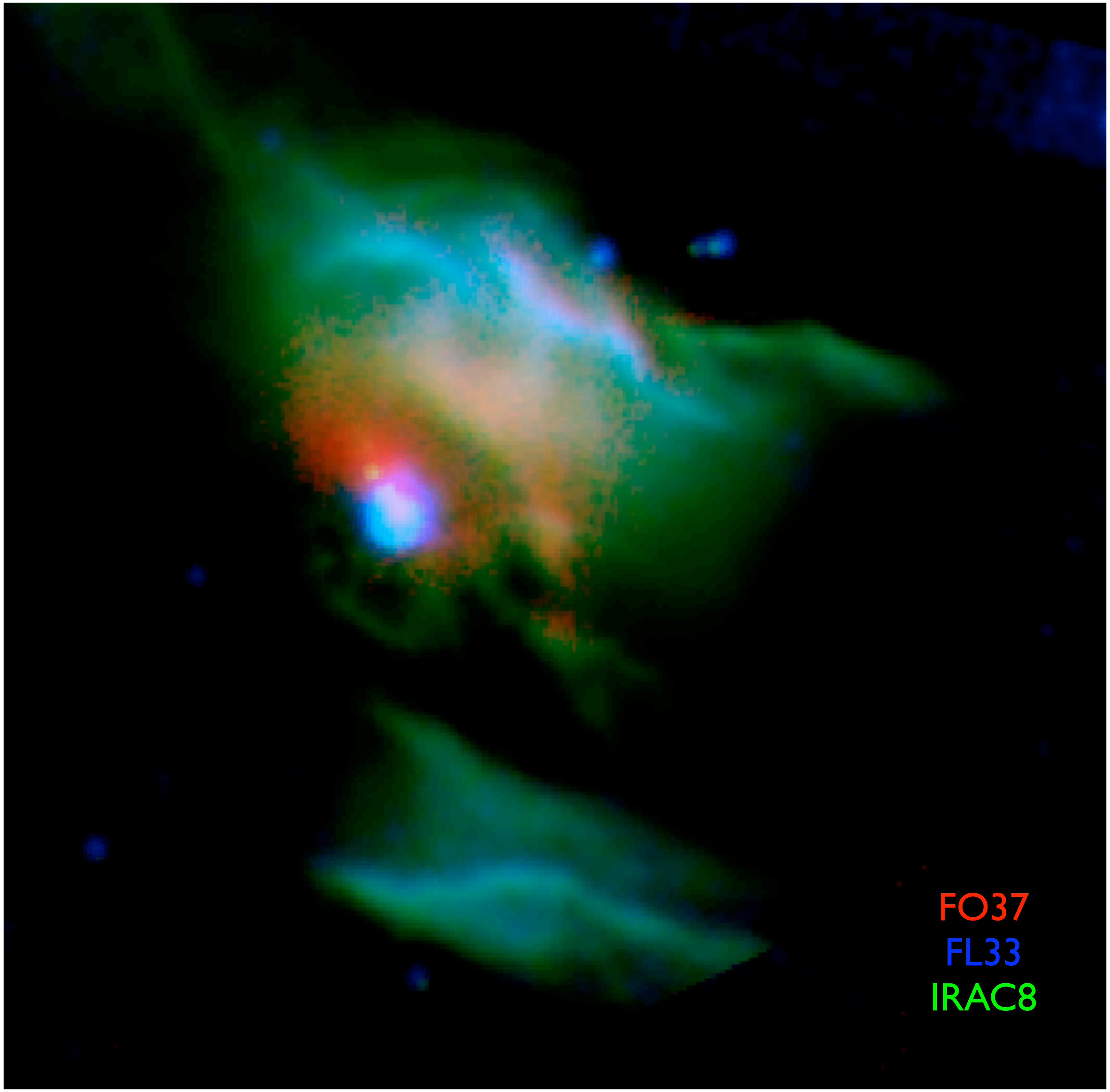
Final images





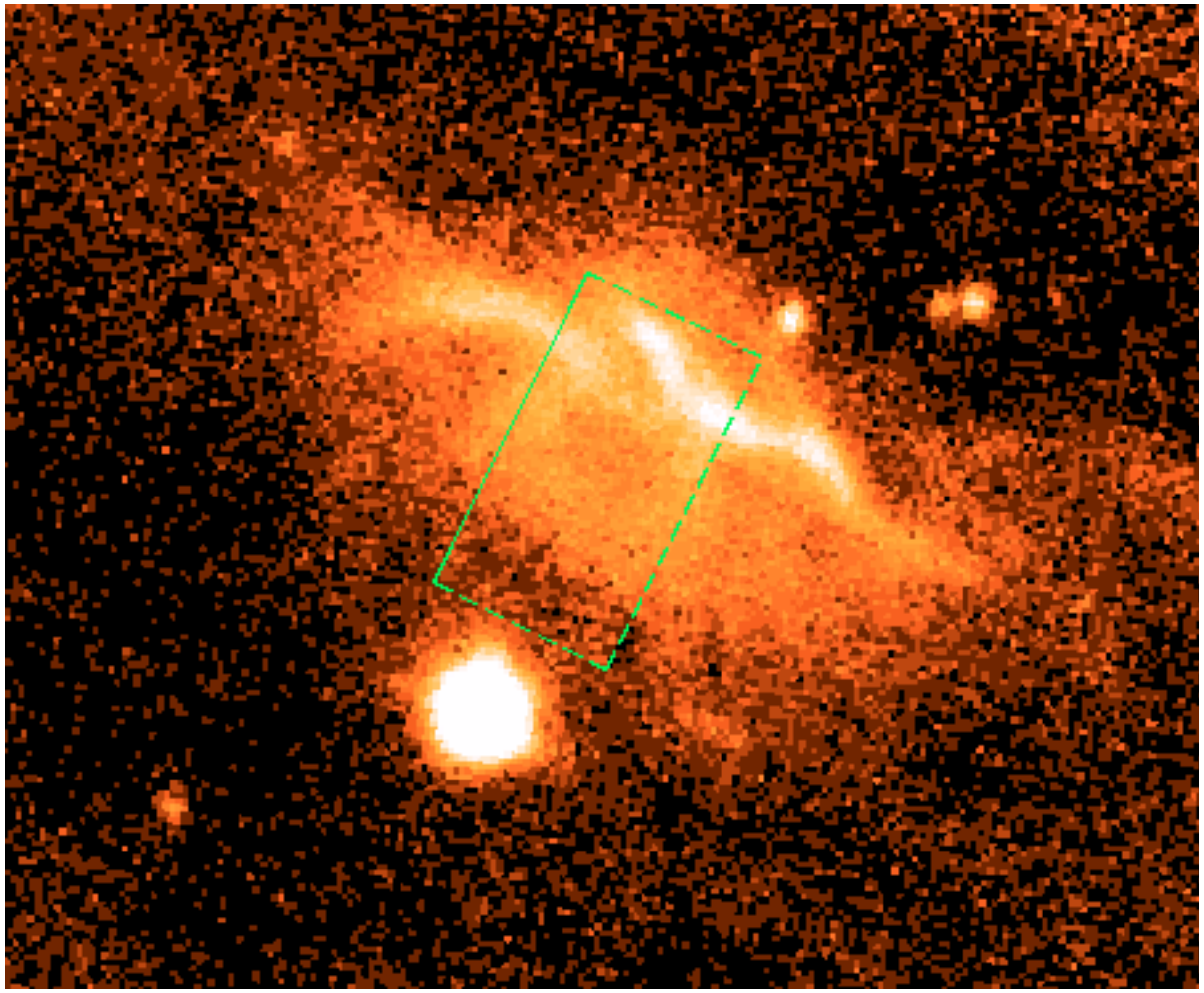


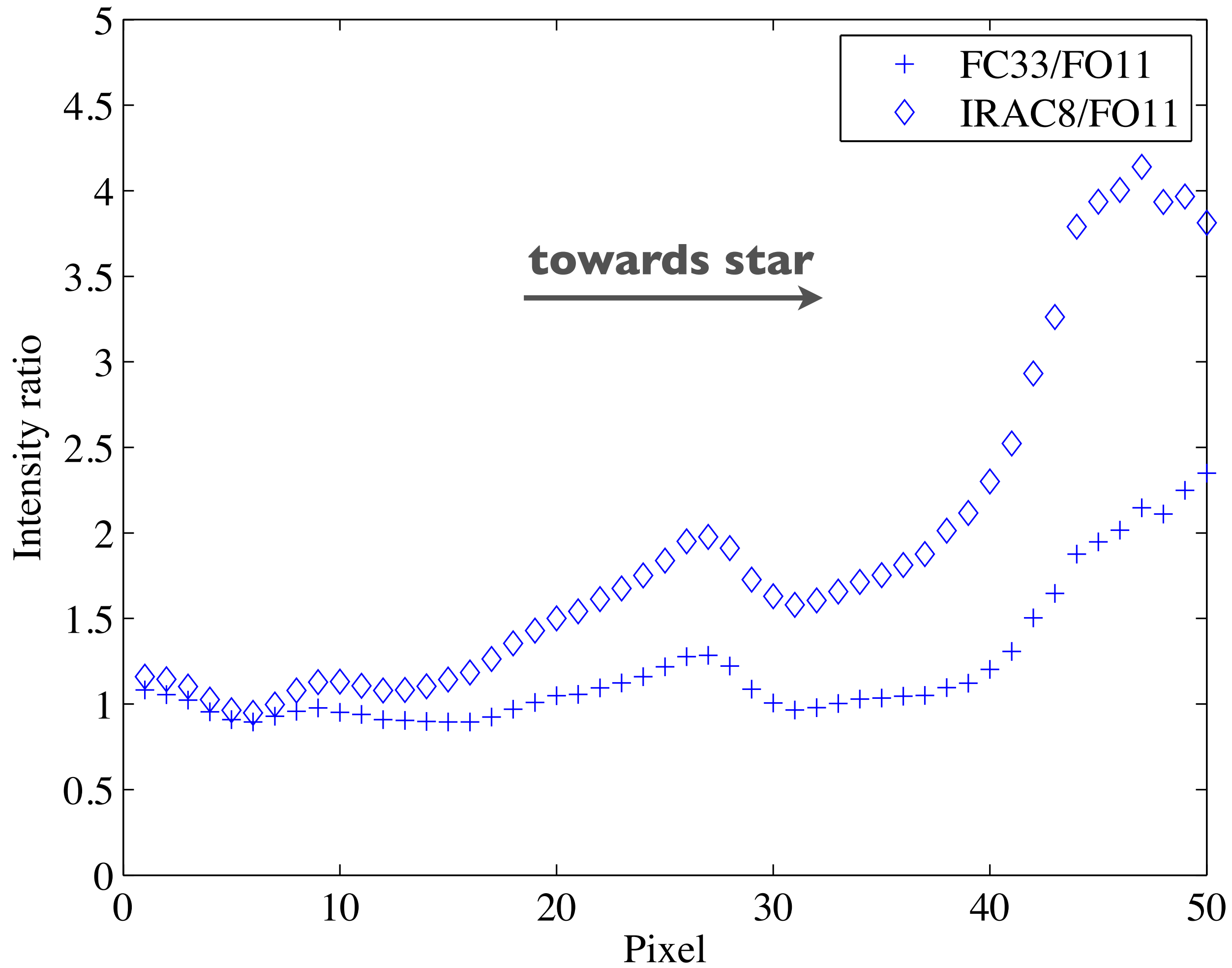
Constraining the size distribution of PAHs with SOFIA



Constraining the size distribution of PAHs with SOFIA

Basic «Science»





- 8 to 11 μm ratio increasing towards star, suggesting PAHs are more ionized towards the star

- 3.3 over 11.1 μm ratio increases towards star, suggesting smaller PAHs close to the star (?!??)

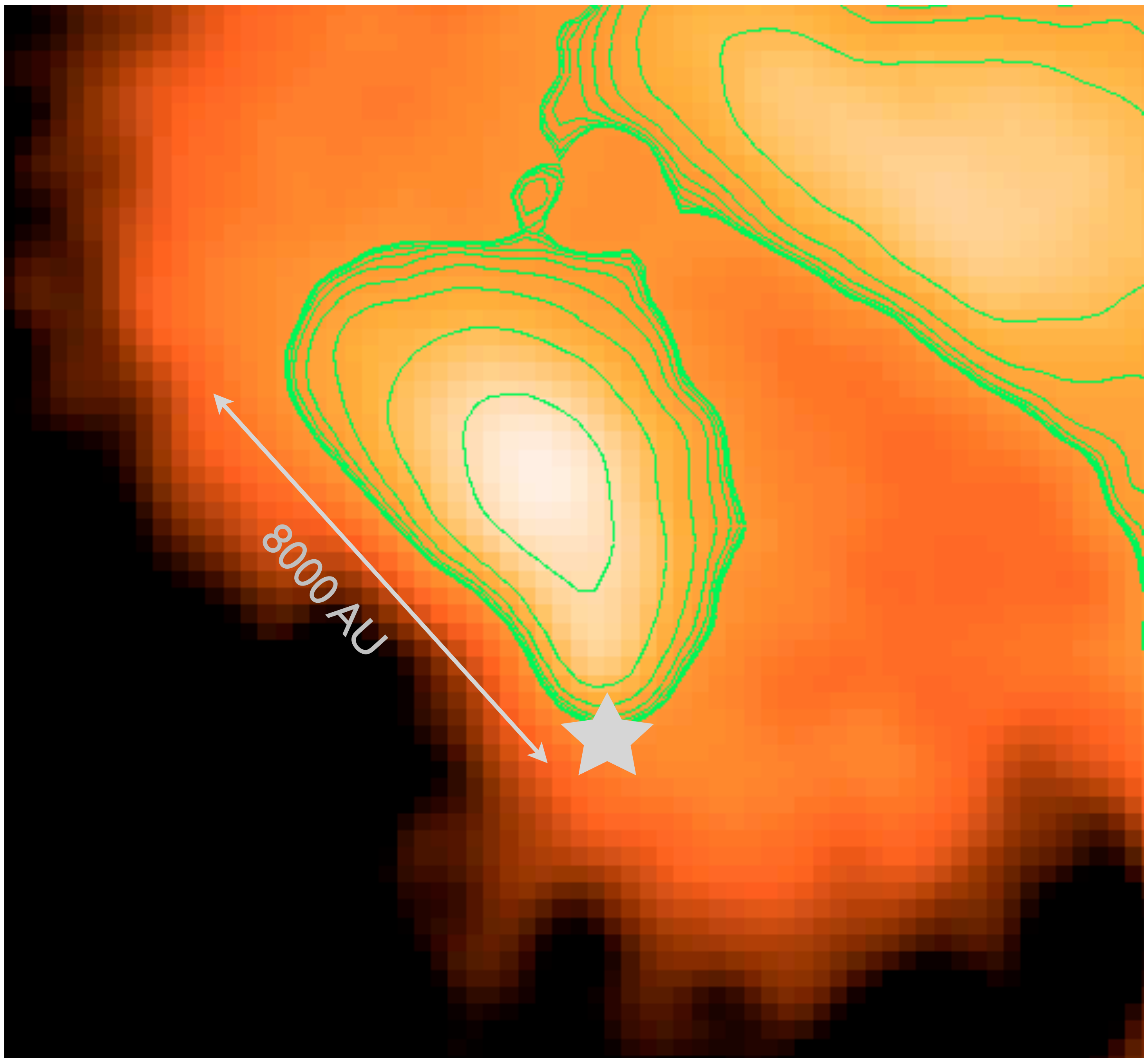
- 3.3 over 11.1 μm ratio ratio of the order of 2, i.e. corresponding to small PAHs ~20 C atoms or smaller... (?!??)

If the FORCAST image has higher flux by a factor 3, then the sizes are more of the order of 50-60 C atoms

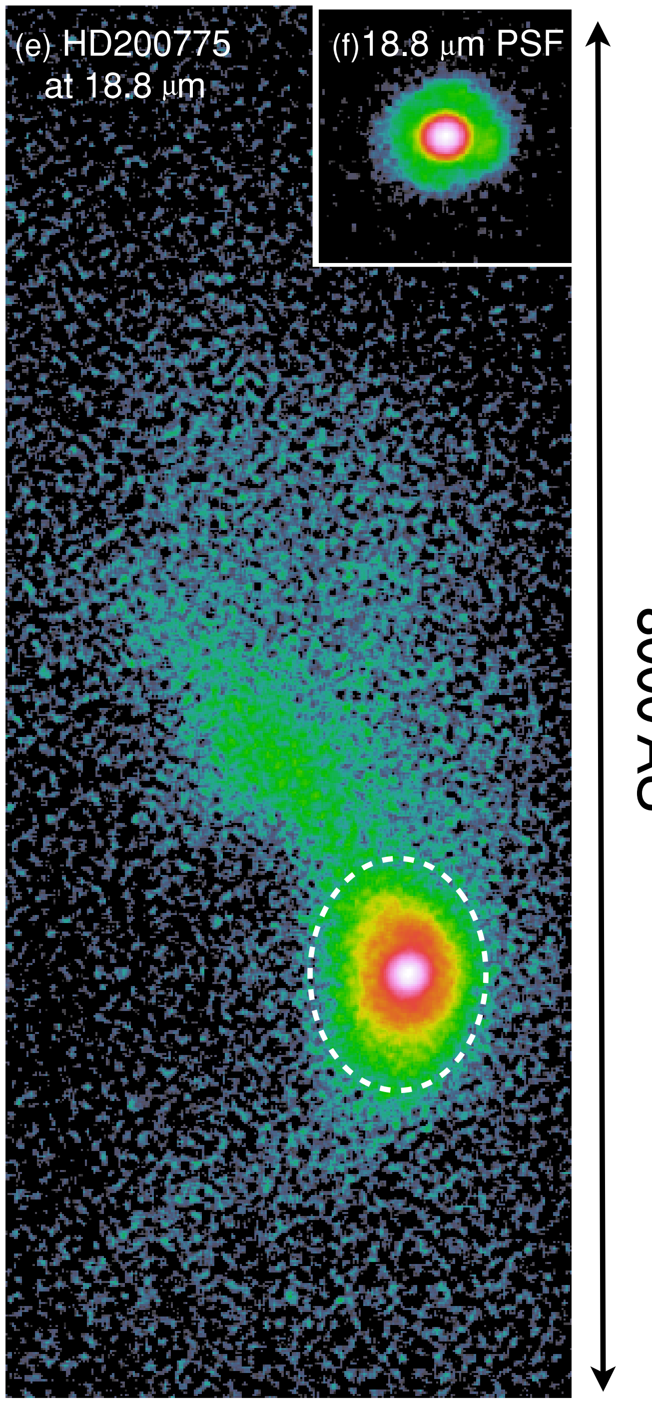
Constraining the size distribution of PAHs with SOFIA

A puzzling structure

FORCAST 37



SUBARU
(Okamoto et al. 2009)



Outline

Prelude : A short presentation of the NGC 7023 reflection nebula

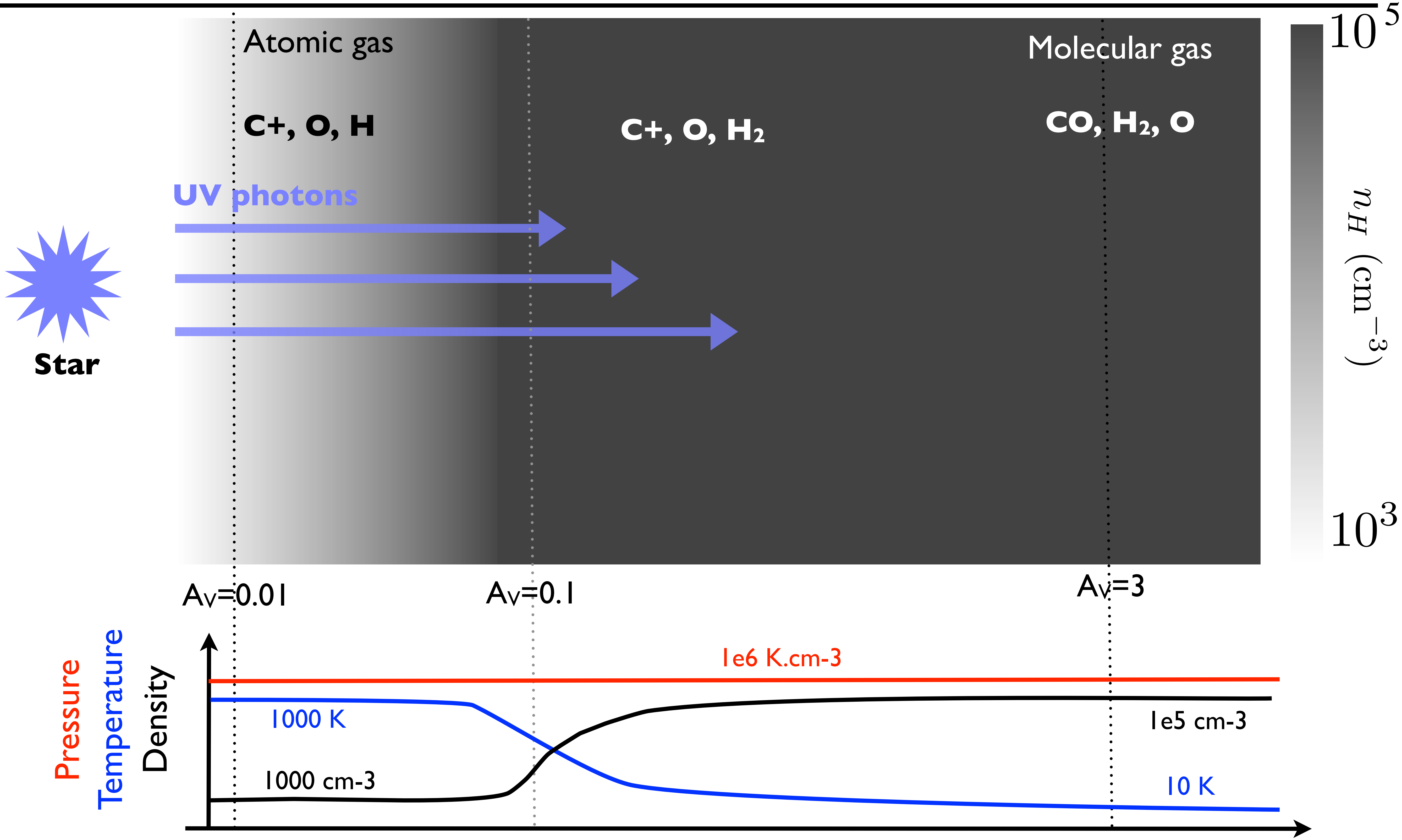
Part 1 : physics and chemistry of PAHs and fullerenes

- The discovery of PAHs and fullerenes
- The chemical evolution of large cabonaceous molecules in NGC 7023, from PAHs to C_{60}
- The size distribution of interstellar PAHs : SOFIA-FORCAST/FLITECAM

Part II : physics and chemistry of PDRs

- A short presentation of PDRs
- Evidence for intense dynamical activity in NGC 7023 seen with Herschel: photoevaporation
- Confirming this activity with SOFIA-EXES

The physical structure of irradiated gas



Detailed PDR models generally consider either pressure equilibrium or constant density.
They do not include the dynamical evolution of the PDR.

The concept of PDR

why focus on PDRs ?

The concept of PDR

why focus on PDRs ?

Akari (JAXA) all sky
mid-infrared PAH emission

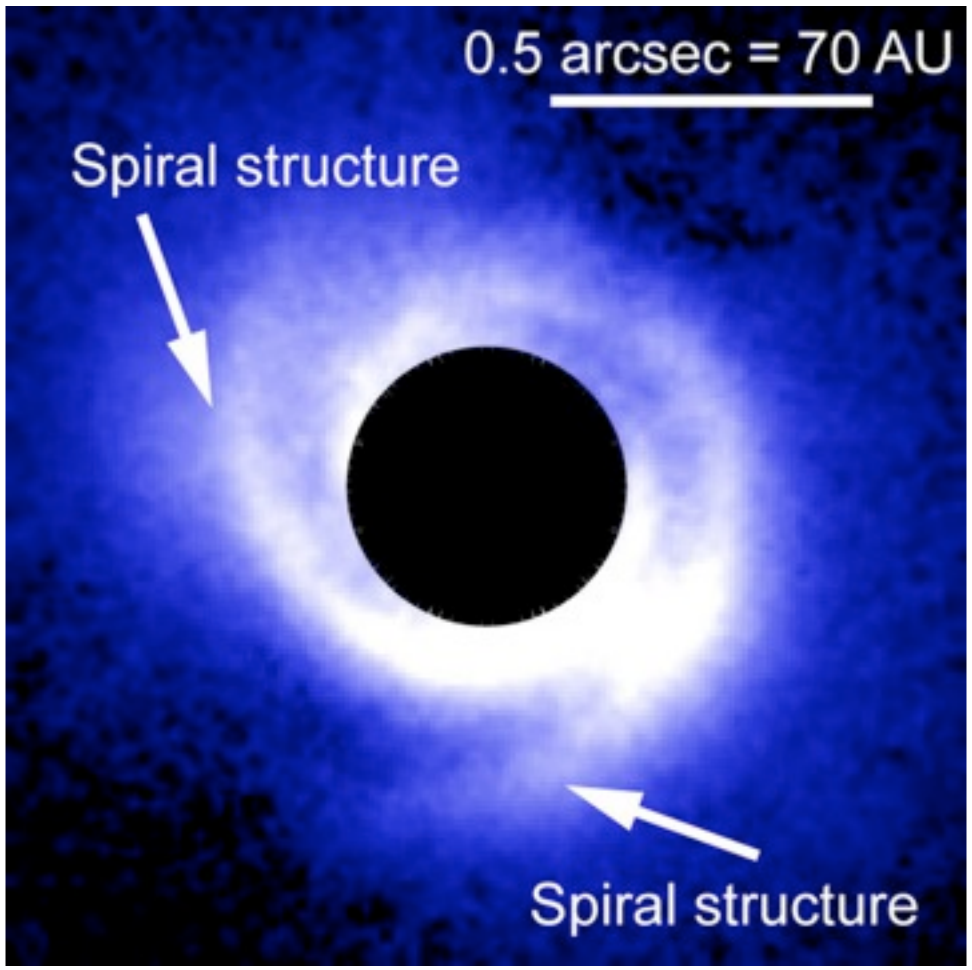
Ishihara, Onaka, Kataza et al. A&A 2010

The concept of PDR

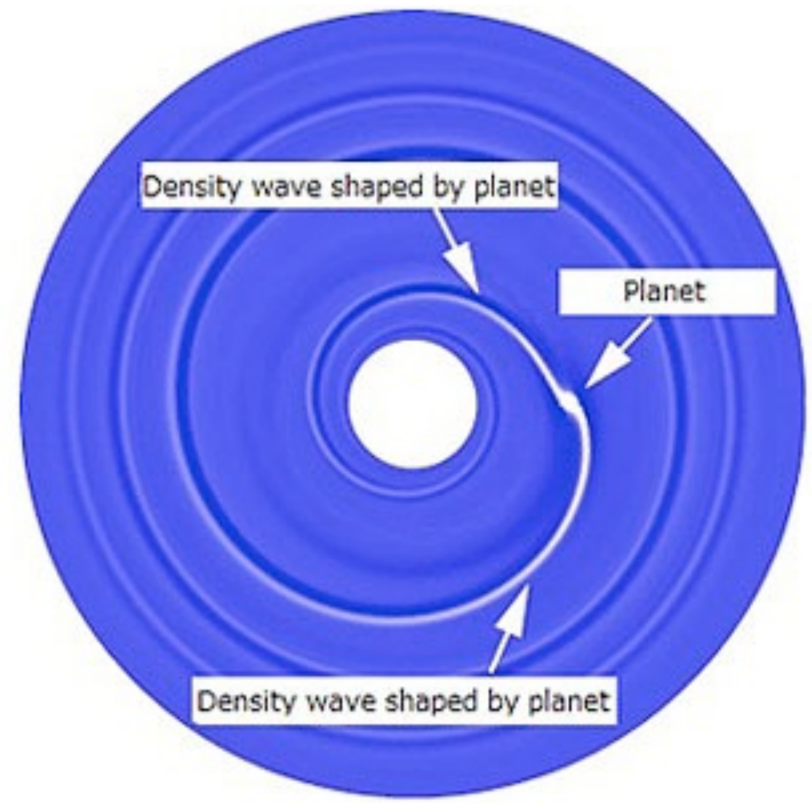
why focus on PDRs ?

The concept of PDR

Emission from the PDR at the surface of a planet-forming disk around a young star

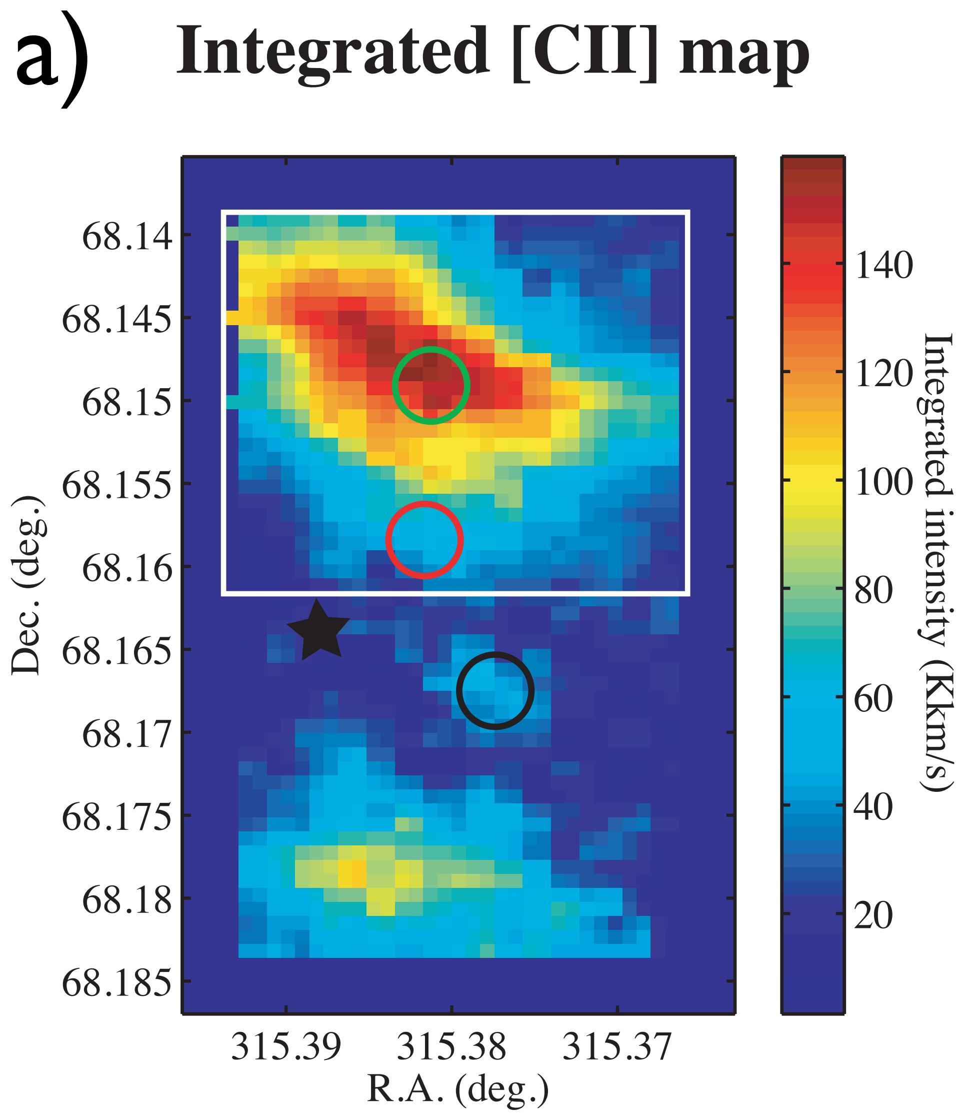


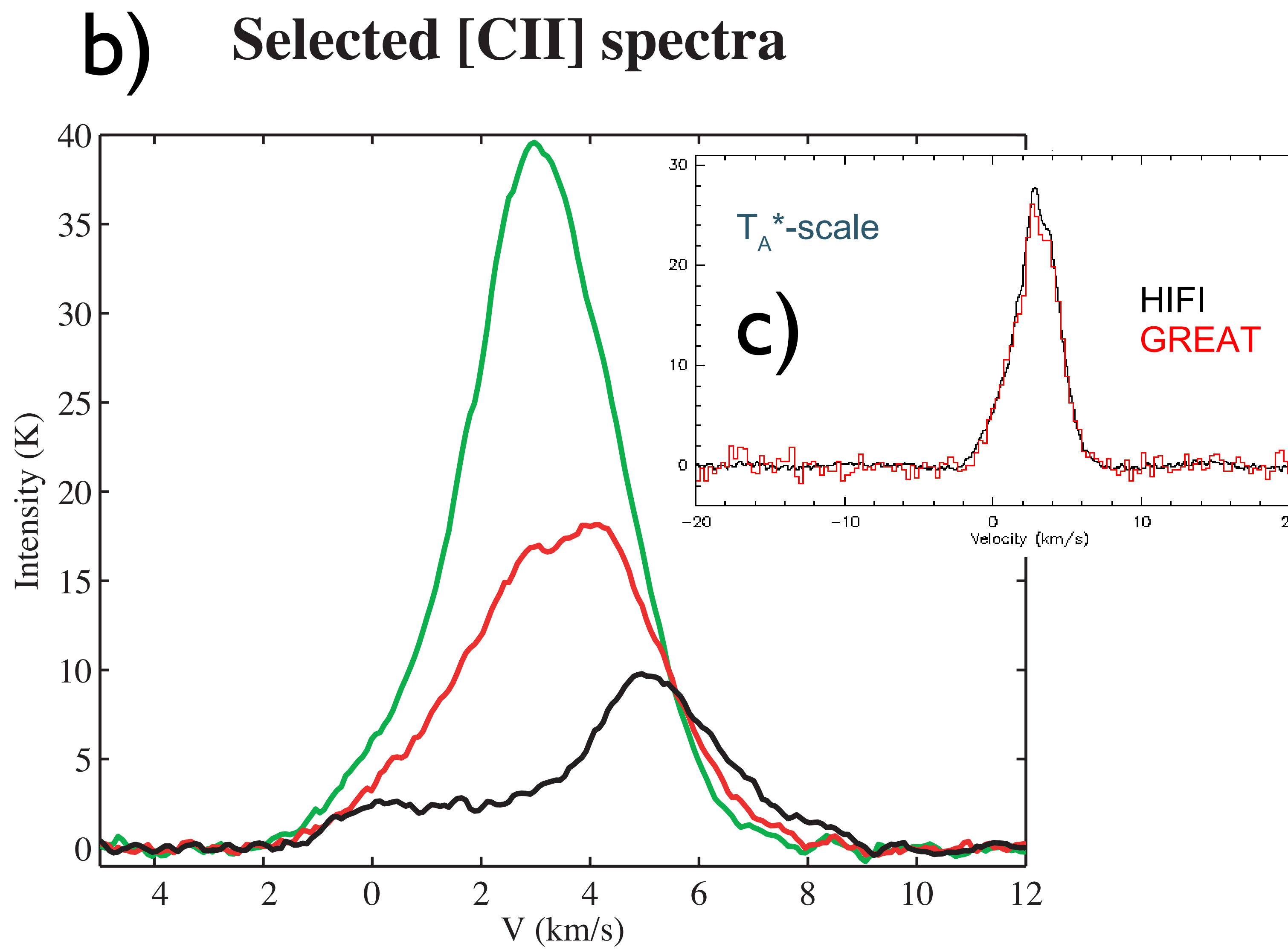
Subaru telescope (NAOJ)
Muto et al. 2012 ApJL



HIFI [CII] cube

data reduction J. Pety & D. Teyssier





Hypothesis

- Each observed spectrum is a linear combination of elementary spectra
- We observe different mixtures of the same elementary spectra

The evolution of spectral shape seen as a linear combination of a limited number of spectra

Linear instantaneous model (optically thin)

a) $$x(p_x, p_y, v) = \sum_{i=1}^{r} a^i(p_x, p_y) s^i(v)$$

b) $$\begin{pmatrix} x_i(v) \\ \vdots \\ x_m(v) \end{pmatrix} = \begin{pmatrix} a_{1,1} & \dots & a_{1,r} \\ \vdots & & \vdots \\ a_{m,1} & \dots & a_{m,r} \end{pmatrix} \times \begin{pmatrix} S_1(v) \\ \vdots \\ S_m(v) \end{pmatrix}$$

Observation matrix

Mixing matrix

Matrix of «source» spectra

c) $$X = A \times S$$

Goal identifying A *and* S, from X

Non-Negative Matrix Factorization
NMF

The problem

a) $X = A \times S$

Approach:

b) $X \approx W \times H$

The criteria, Euclidian distance

c) $$\|X - WH\|^2 = \sum_{ij} (X_{ij} - (WH)_{ij})^2$$

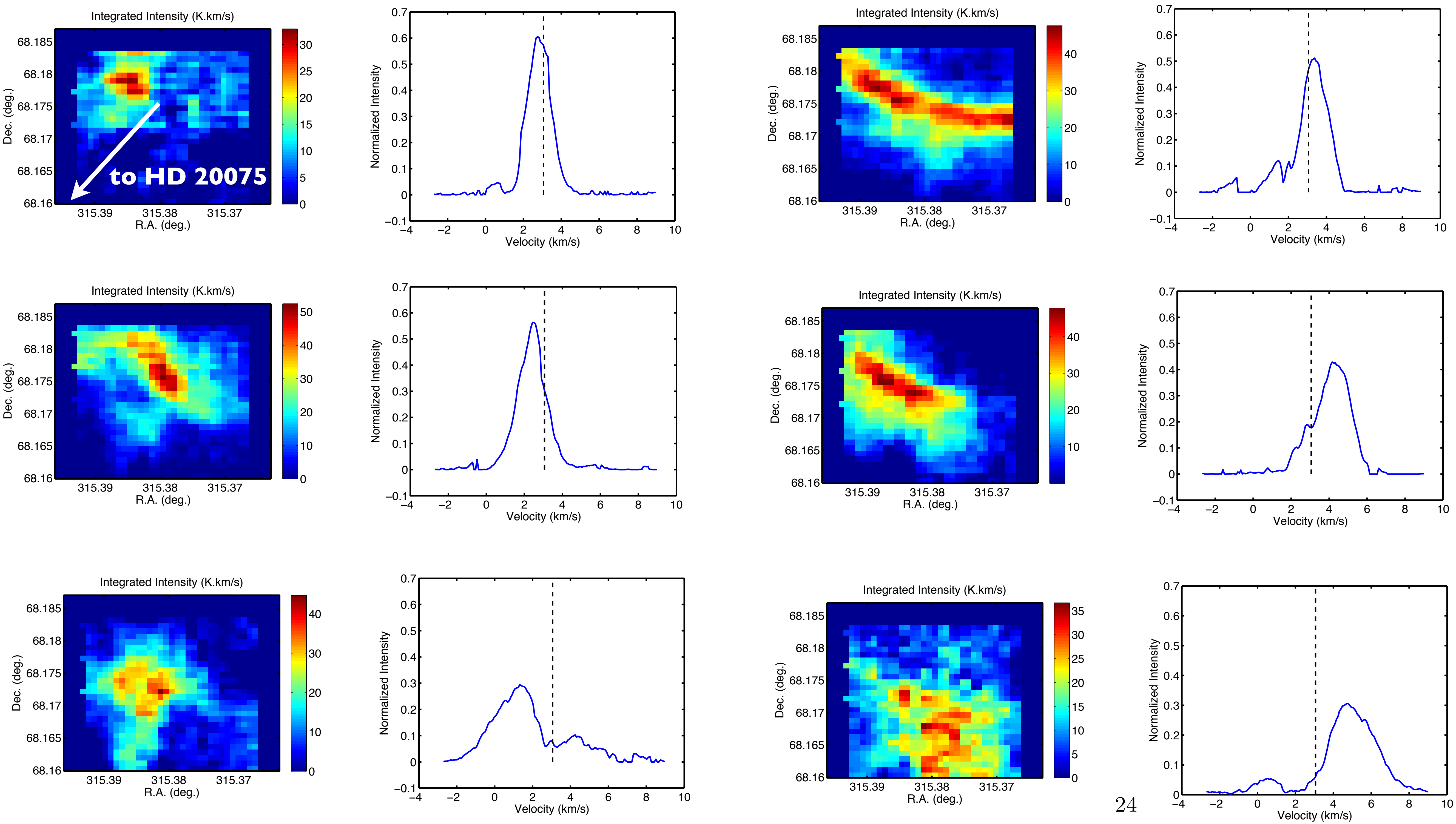
The algorithm

d) $$H_{a\mu} \leftarrow H_{a\mu} \frac{\sum_i W_{ia} X_{i\mu}/(WH)_{i\mu}}{\sum_k W_{ka}}, W_{ia} \leftarrow W_{ia} \frac{\sum_\mu H_{a\mu} X_{i\mu}/(WH)_{i\mu}}{\sum_\nu H_{a\nu}}$$

- We "set" the number of rows of **H**
- **W** and **H** must be positive
- We start iteration with random **W** and **H**
- Monte-carlo estimation of errors with 100 initialization

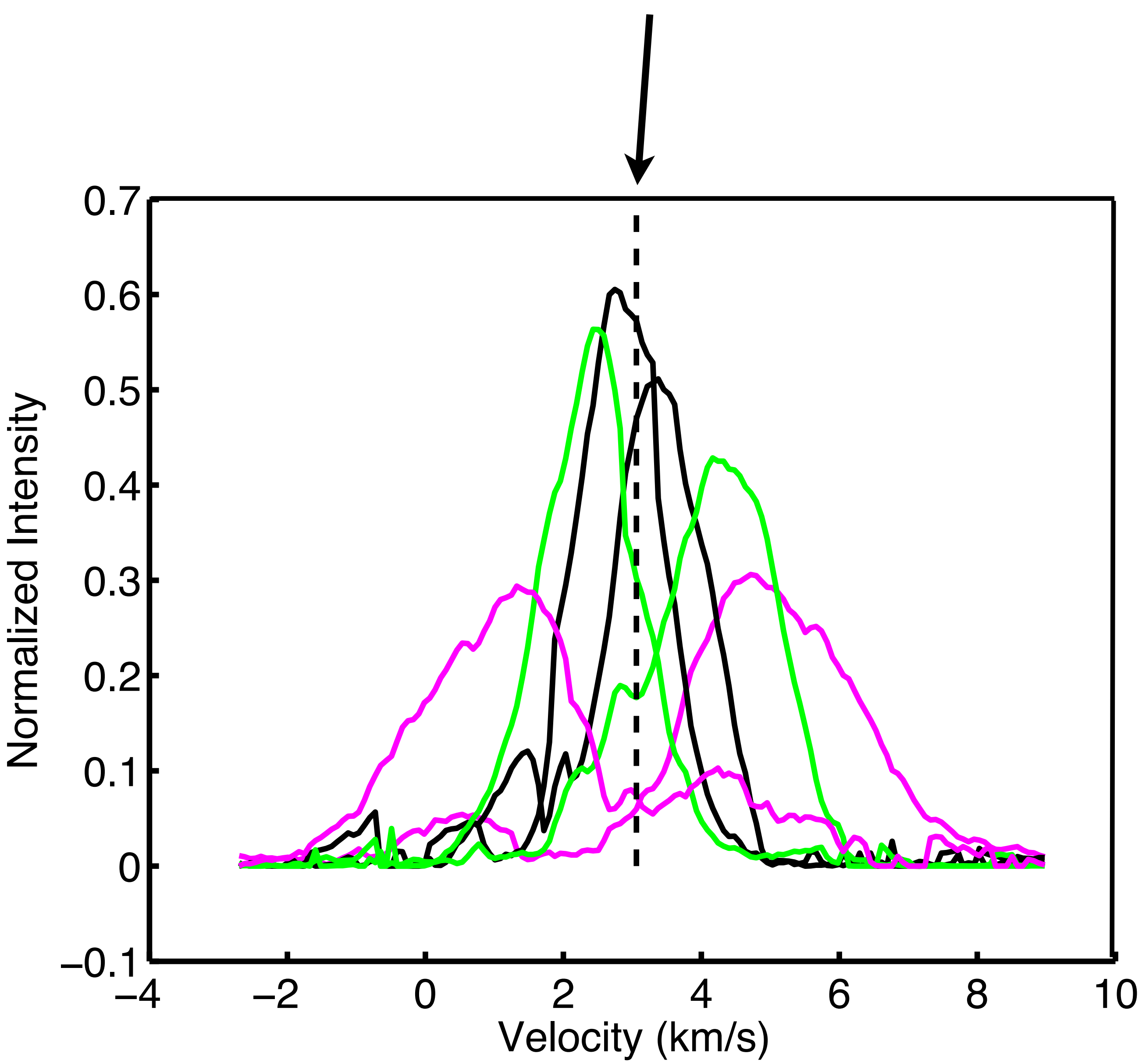
[Lee and Seung, Nature, 2001]

Decomposition results for NGC 7023

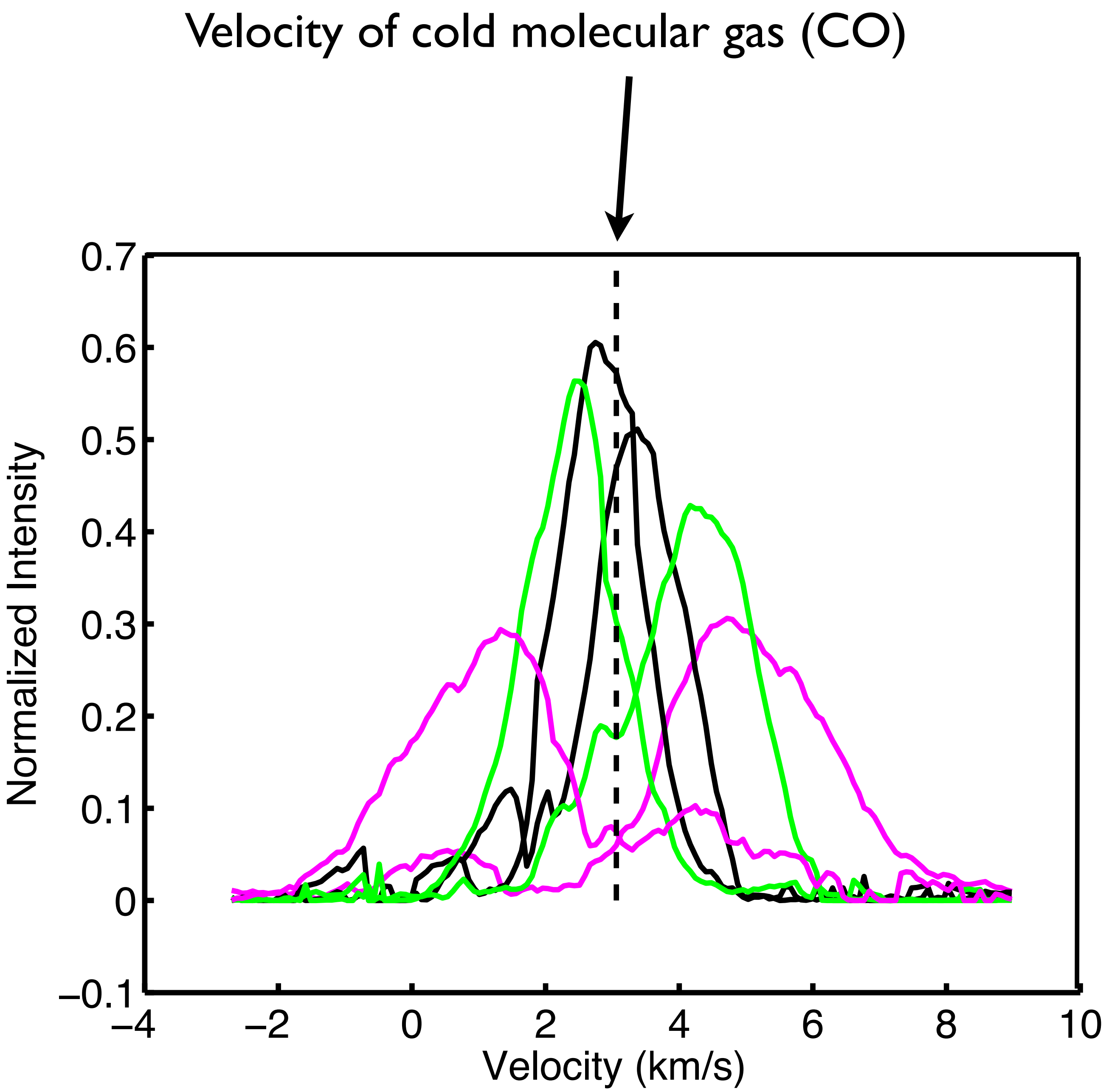


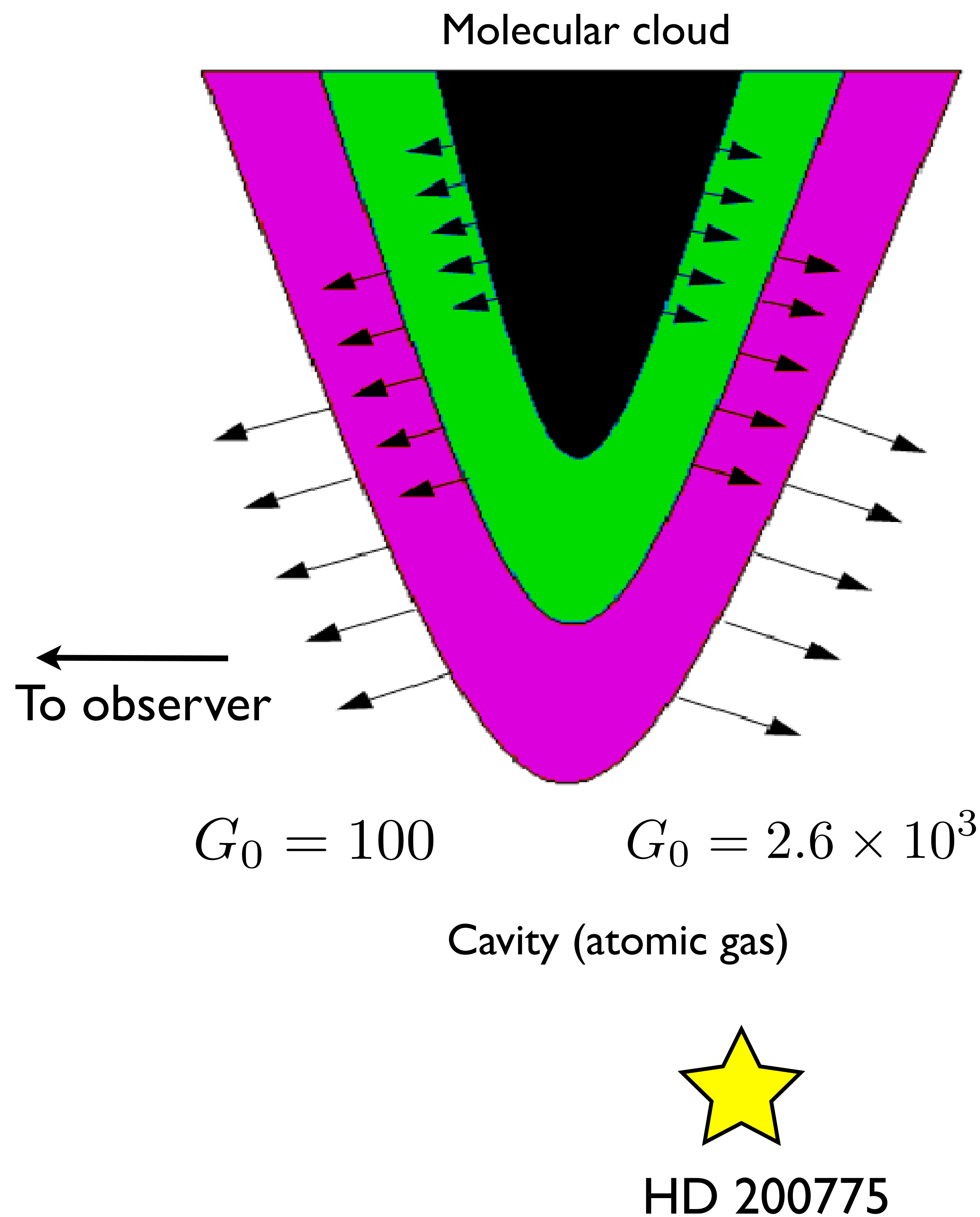
Proposed kinematic structure

Velocity of cold molecular gas (CO)



Proposed kinematic structure



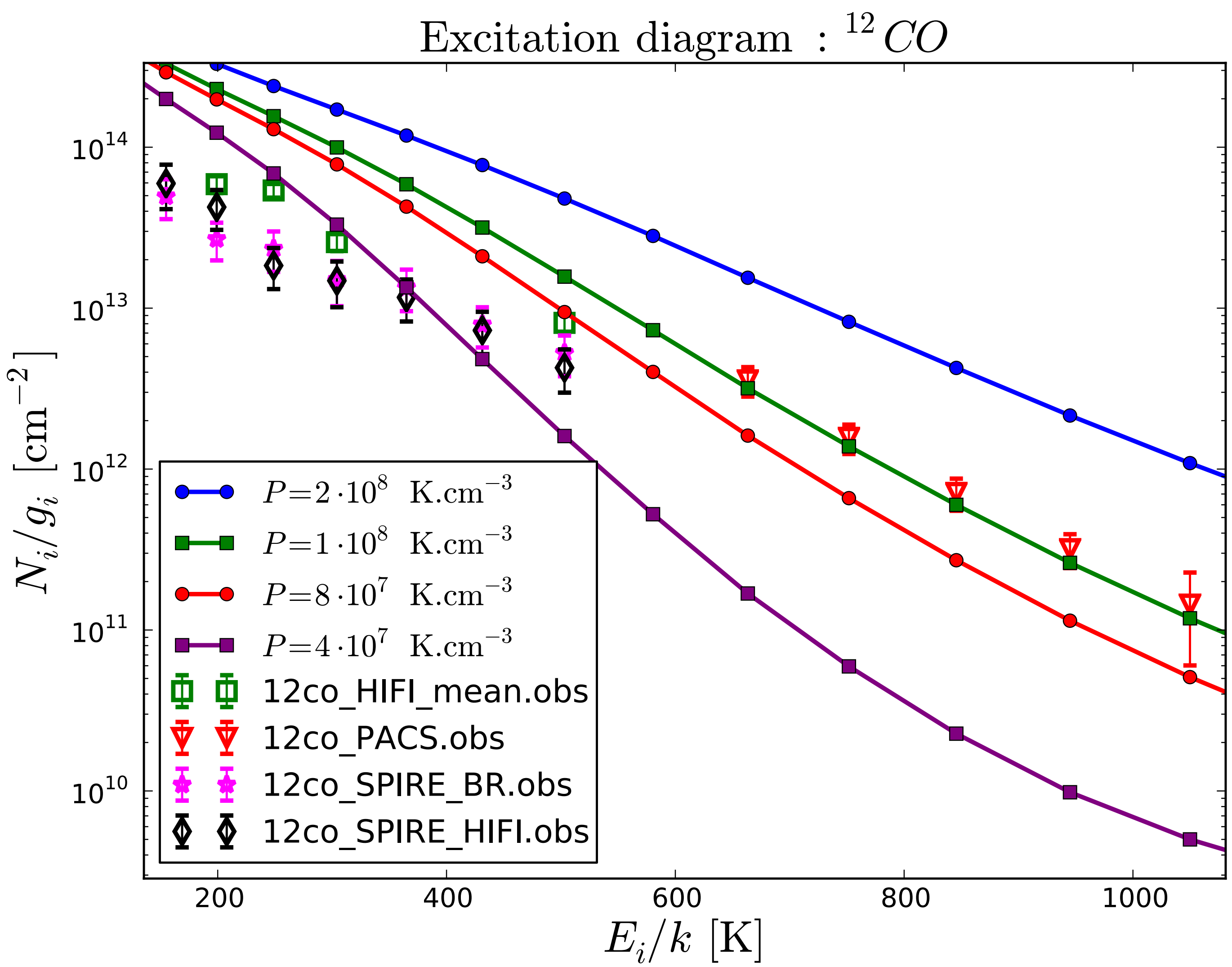


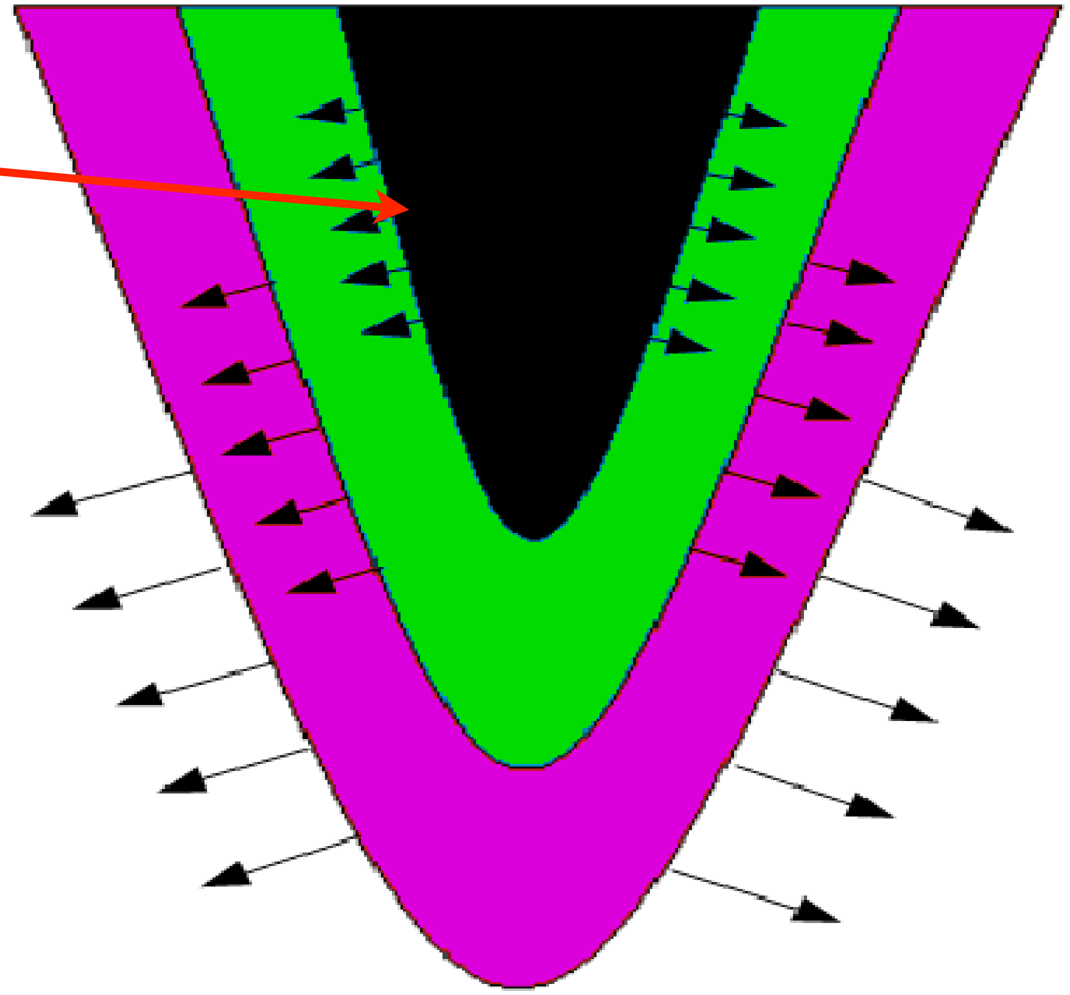
Proposed kinematic structure

P~10⁸ K.cm⁻³

To reproduce High-J CO lines

(Joblin et al. in prep, Koehler et al. subm.)





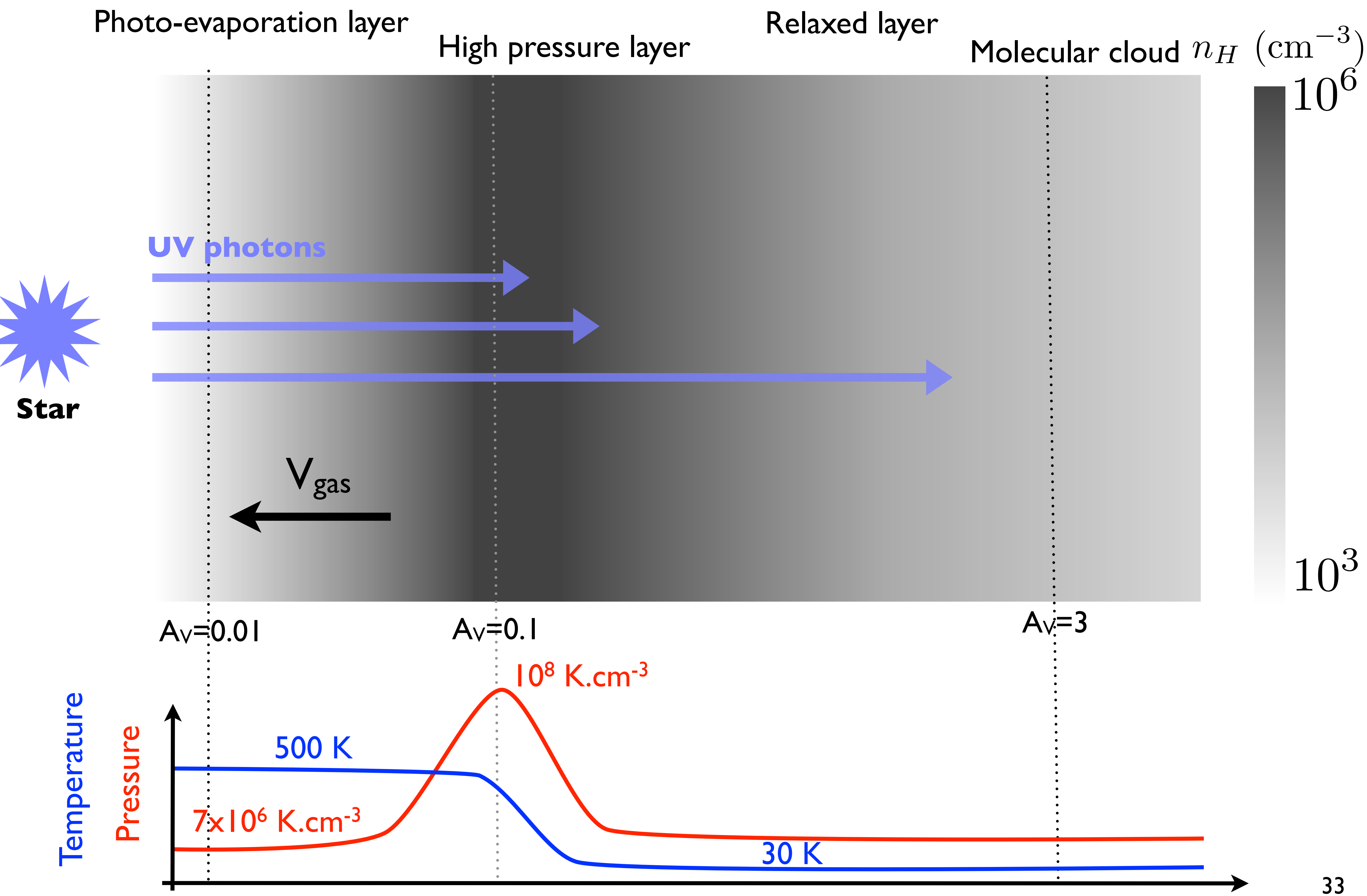
According to several tracers:

$n_H < 10^4$ cm^{-3}, $T < 10^3$ K

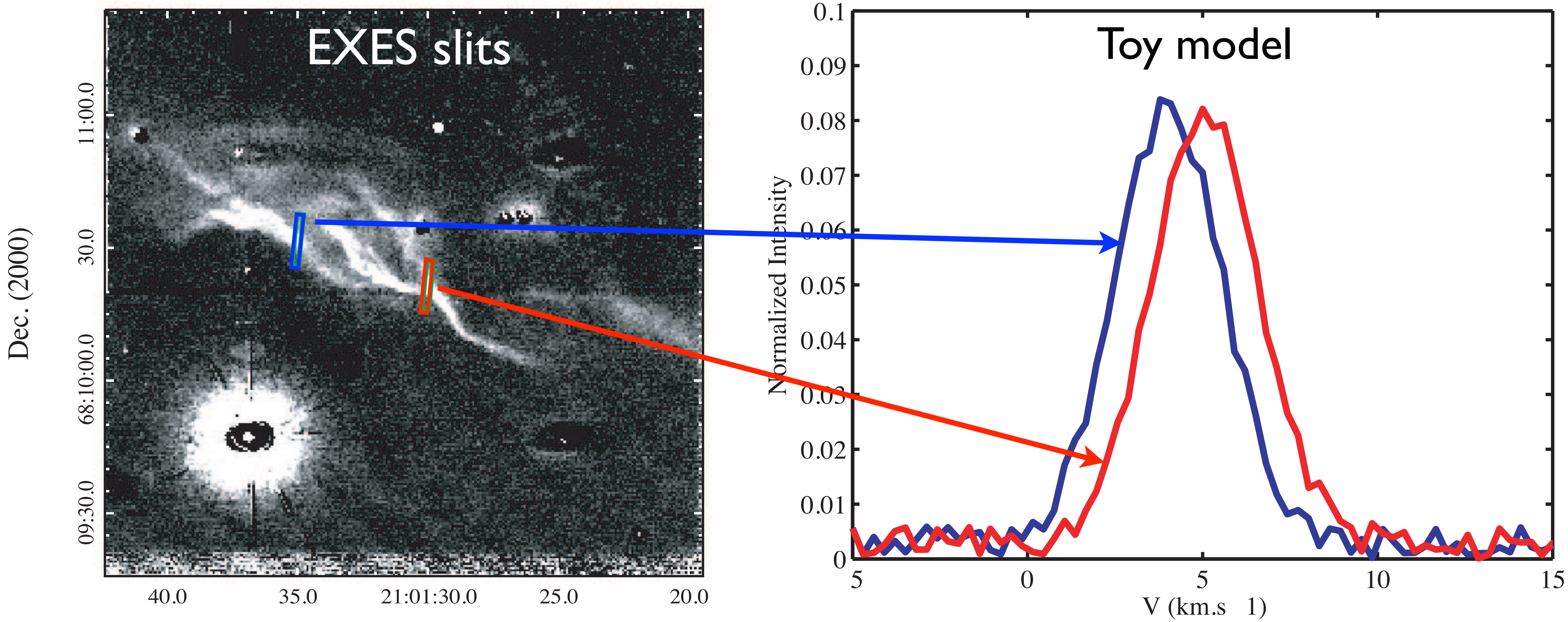
P<10⁷ K.cm⁻³

HD 200775

Pressure and velocity gradients: Photo-evaporation



Testing this scenario with EXES



- If our scenario is correct, the velocity shift between the two components should be seen in H_2 emission

- Target the H_2 S(5) pure rotational line at 6.91 μm (SOFIA only!)

- Resolution with EXES ~ 2.7 km/s

- SNR=10 per resolution element => 45 seconds per slit !

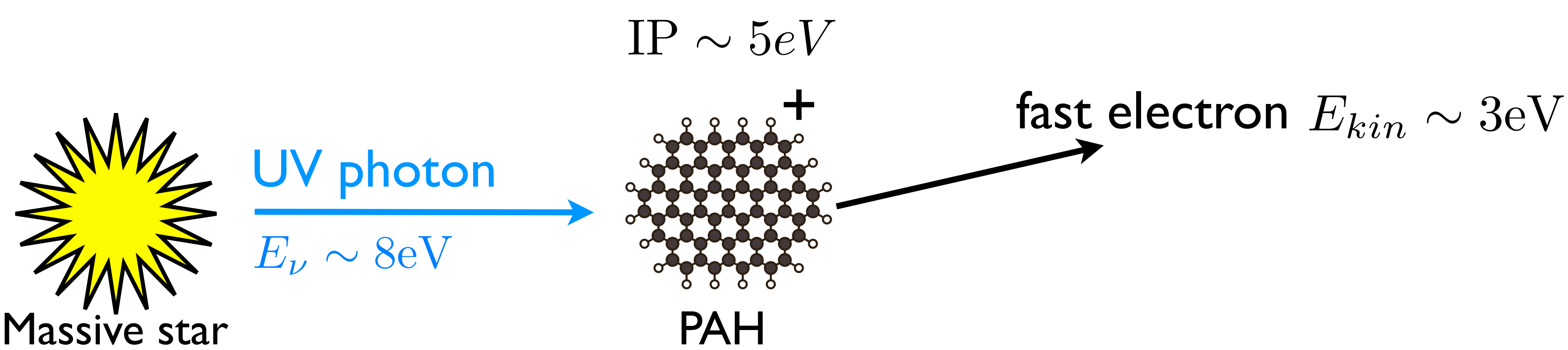
Thanks for you attention

Please let me fly with SOFIA !

Gas heating mechanisms

FUV photo-electric heating

see recent review in [Verstraete et al. 2010] in «PAHs and the universe»



Heating efficiency depends mostly on the availability of neutral PAHs which can provide electrons, so on the recombination rate of PAHs with slow electrons which depends on :

- number of C atoms in PAH (higher recombination rate for small PAHs)
- the ionization parameter:

$$\gamma = \frac{G_0\sqrt{T}}{n_e}$$

In PDRs, when all carbon is ionized

$n_e \sim 1.6 \times 10^{-4} n$