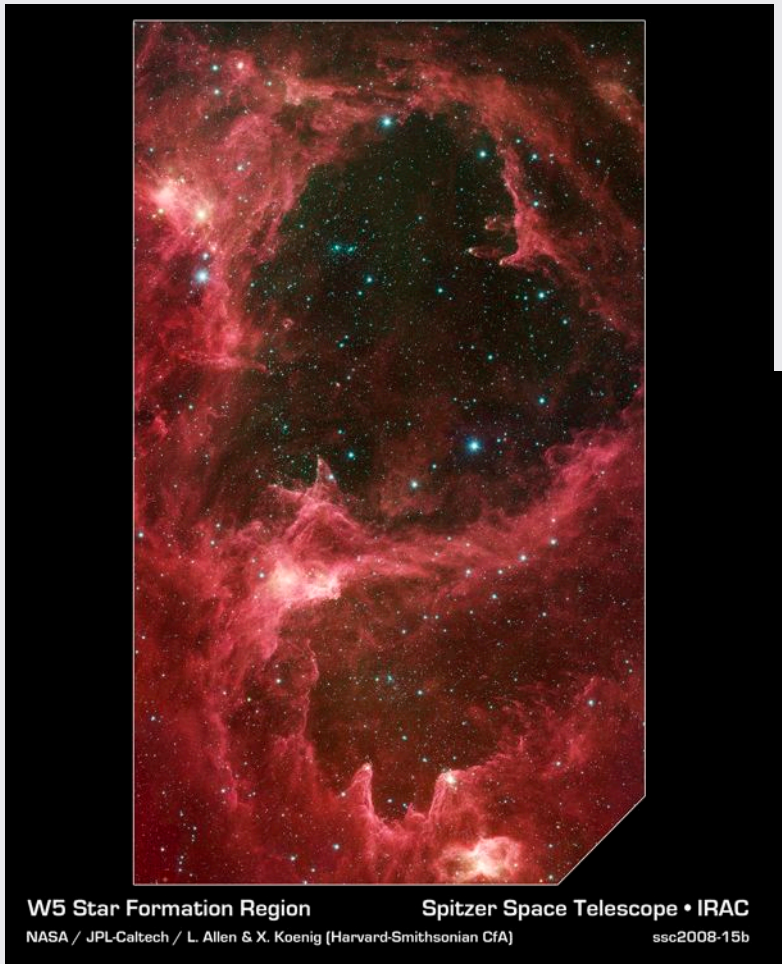
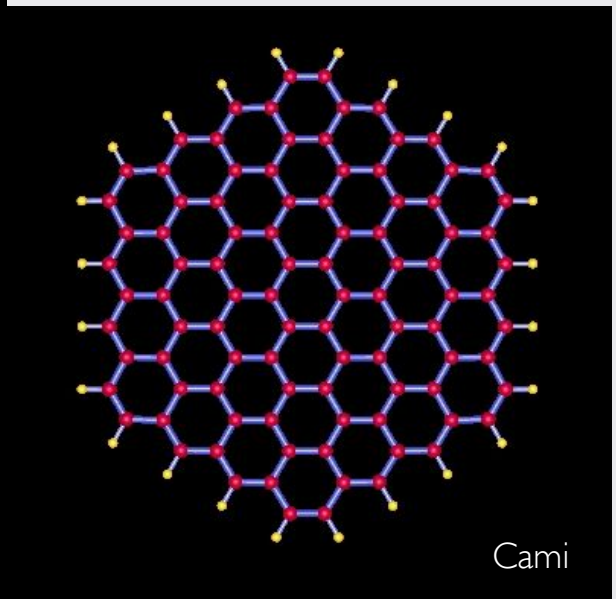
The spectral characteristics of the PAH emission features

Els Peeters*





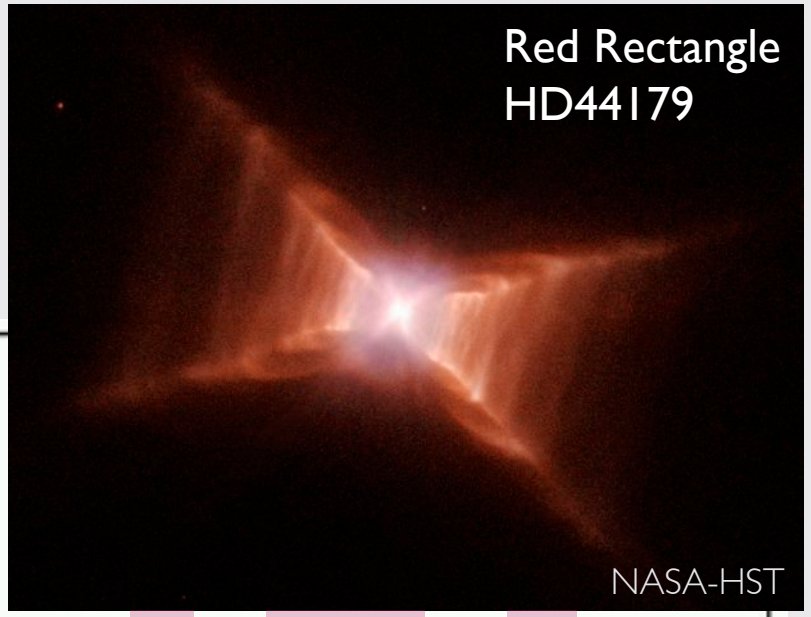
Collaborators: C. Bauschlicher, L. Allamandola, X. Tielens, A. Ricca, M. Wolfire

* University of Western Ontario & SETI Institute

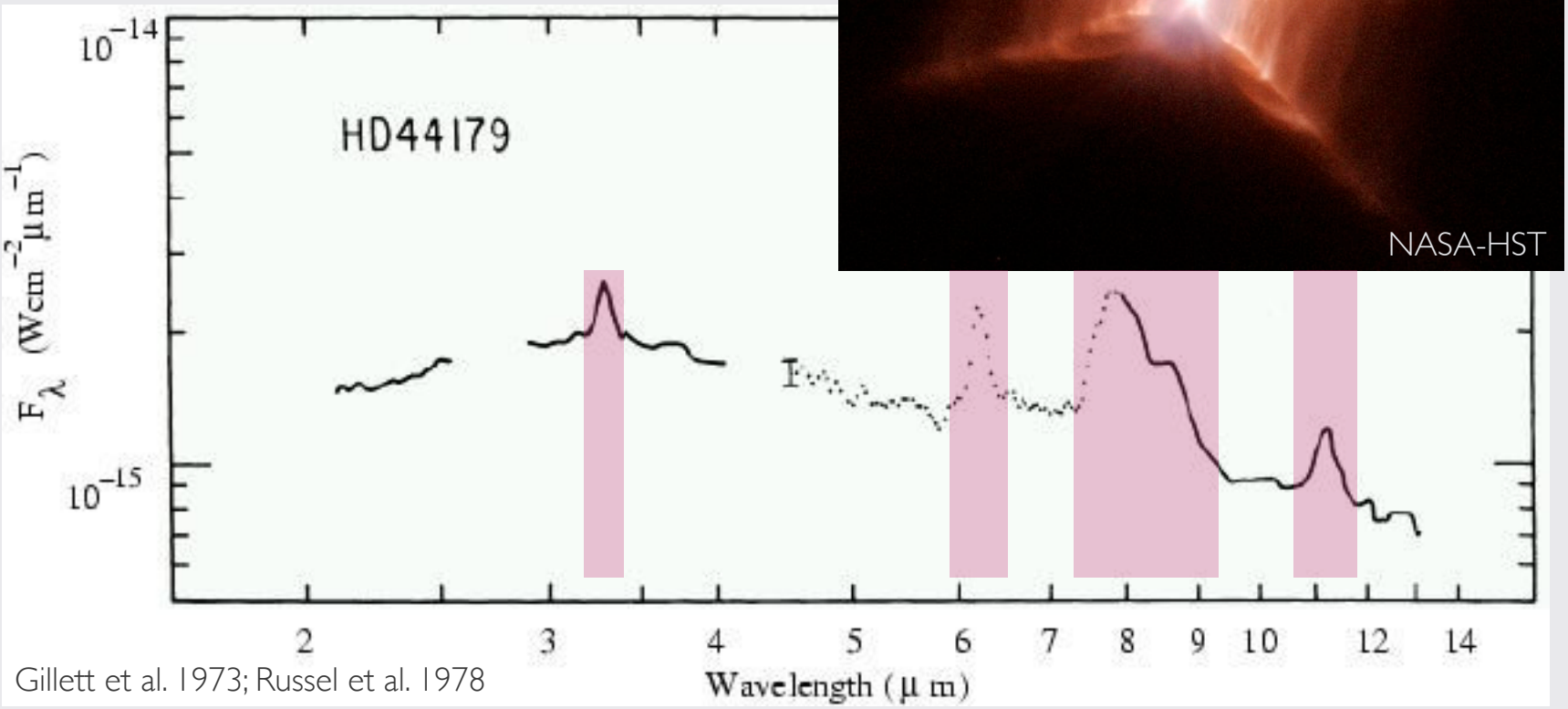
Outline

- Introduction
- PAH Intensities: 6.2, 7.7, 8.6
- Decomposition of the 7-9 μm region
- Spatial Sequence
- Comparison of observations with PAH database
- Summary
- SOFIA & PAHs

Discovery: IR emission bands

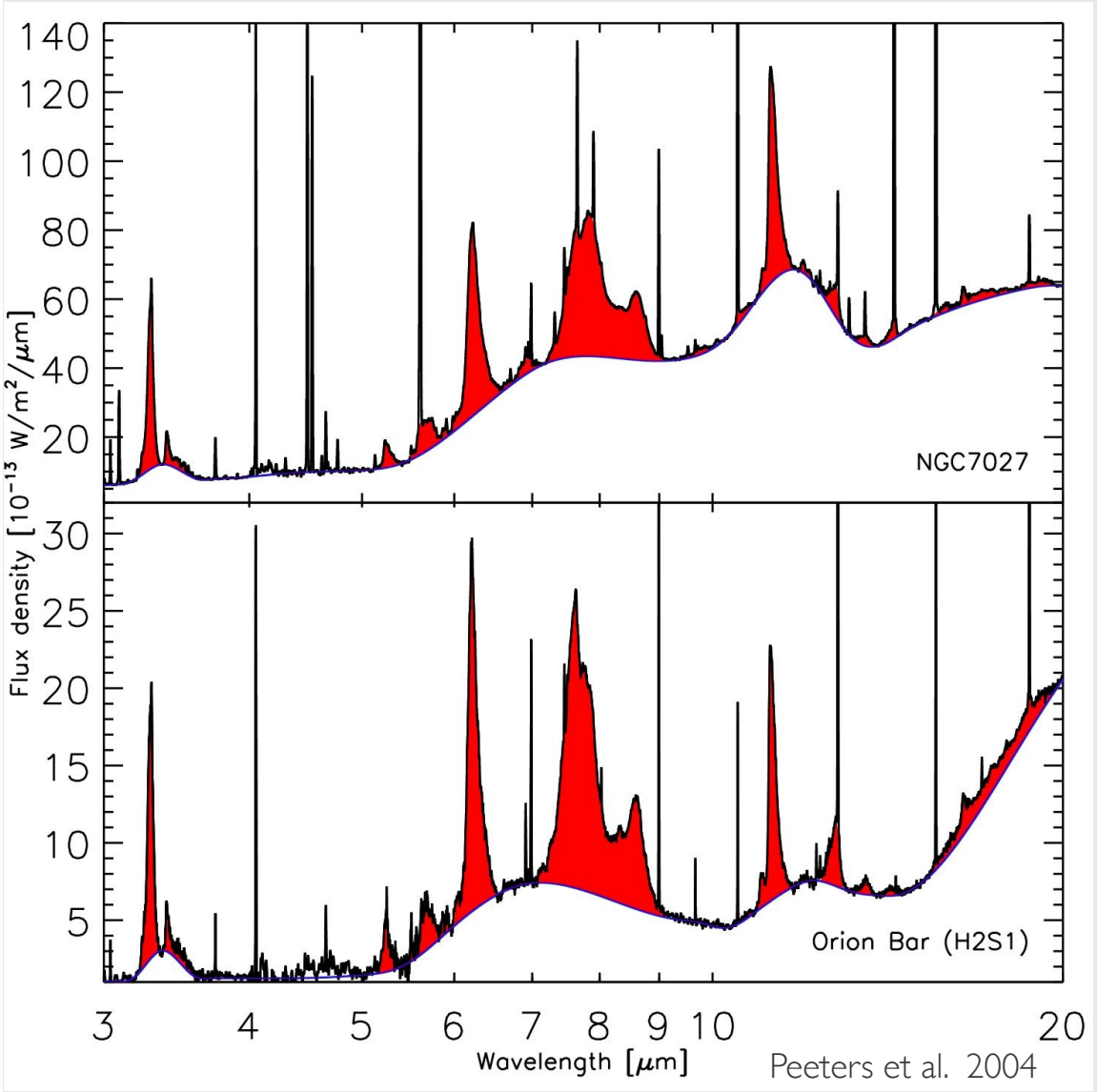


Evolved star



Gillett et al. 1973; Russel et al. 1978

Incredibly rich IR emission bands

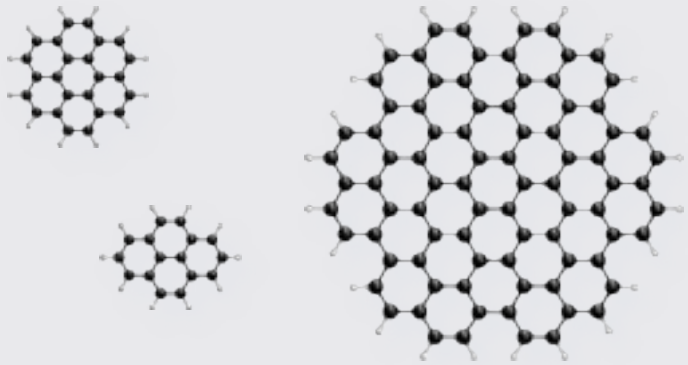


PAHs & the IR emission bands

- IR emission bands due to a population of Polycyclic Aromatic Hydrocarbon molecules (PAHs)

  → not strict chemical definition: side groups, impurities, clusters, ….

- Typical size: ~50 C-atoms

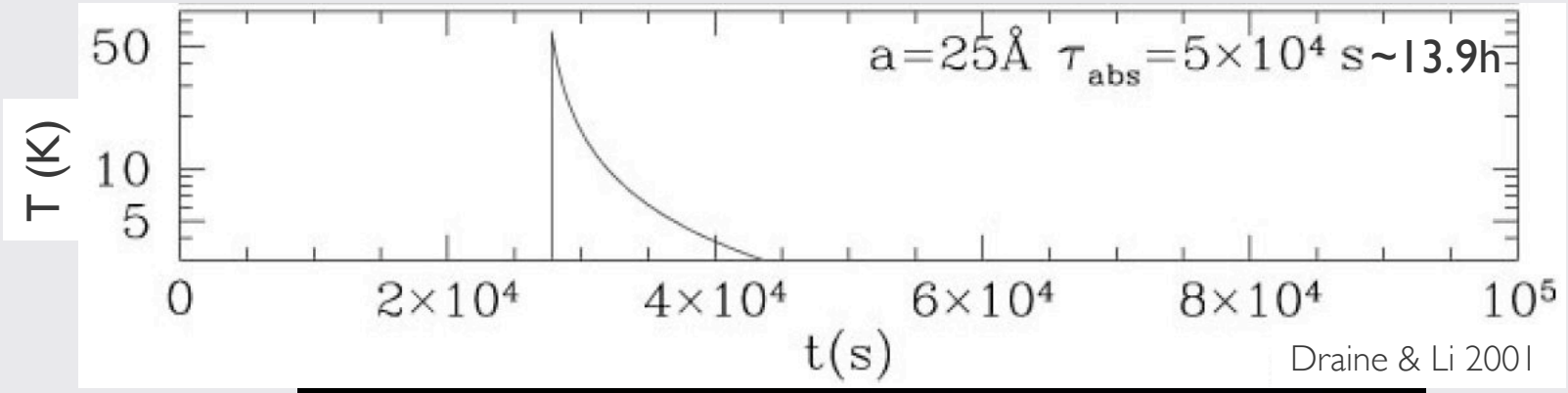


Boersma

NASA Ames Astrochemistry Laboratory

PAH excitation & relaxation

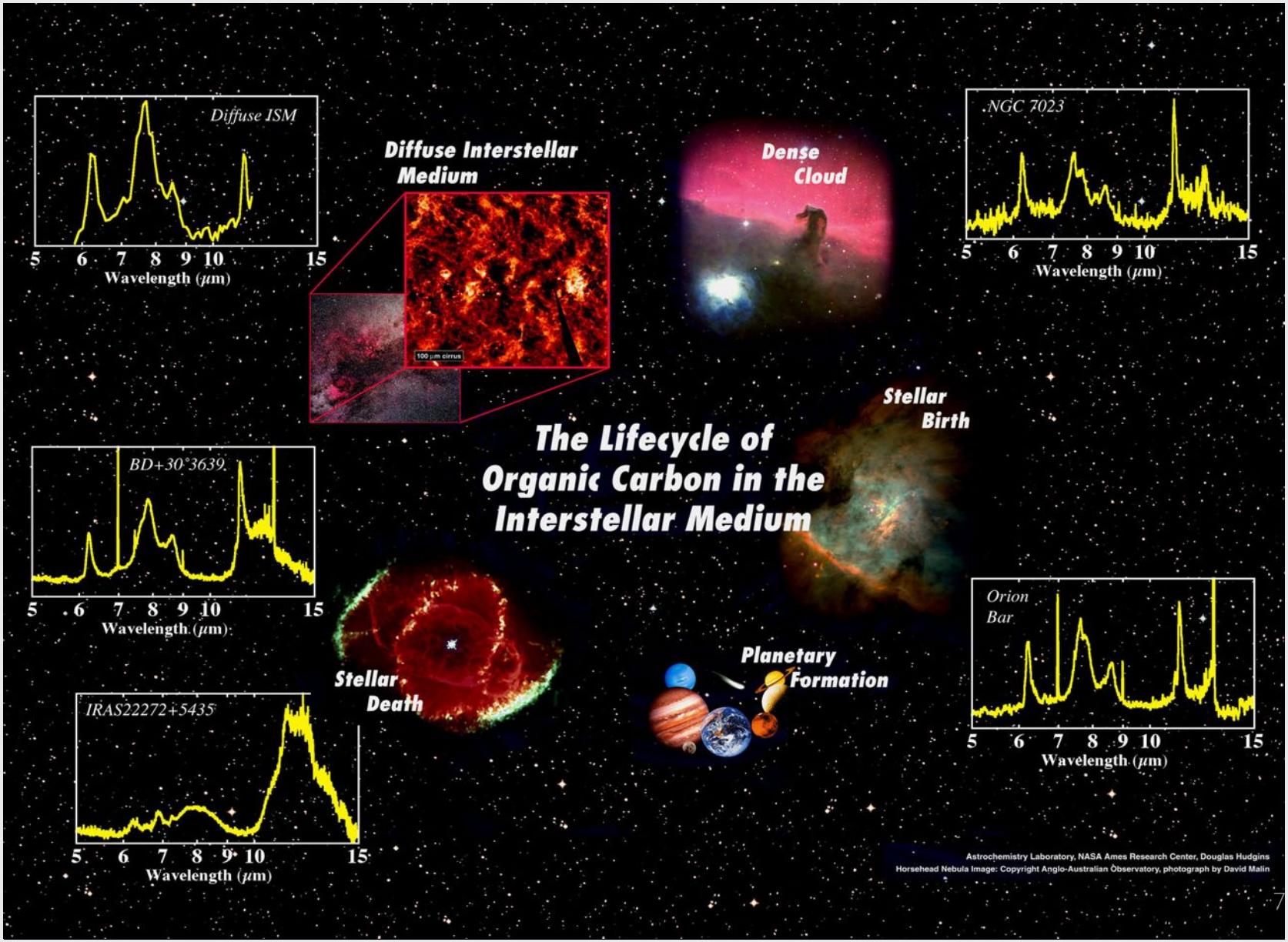
- Excited by photon absorption, relax through IR vibrational modes
- not molecule specific ….. → no single molecule identified



Draine & Li 2001


NASA Ames Astrochemistry Laboratory

Life cycle


Diffuse ISM
5 6 7 8 9 10 15
Wavelength (μm)
Diffuse Interstellar Medium
100 μm cirrus
Dense Cloud
NGC 7023
5 6 7 8 9 10 15
Wavelength (μm)
The Lifecycle of Organic Carbon in the Interstellar Medium
Stellar Birth
BD+30°3639
5 6 7 8 9 10 15
Wavelength (μm)
Stellar Death
Planetary Formation
Orion Bar
5 6 7 8 9 10 15
Wavelength (μm)
IRAS22272+5435
5 6 7 8 9 10 15
Wavelength (μm)
Astrochemistry Laboratory, NASA Ames Research Center, Douglas Hudgins
Horsehead Nebula Image: Copyright Anglo-Australian Observatory, photograph by David Malin

Importance

- large complex carbonaceous molecules
- up to 30% of the IR emission is carried by PAHs
- some 5-20% of the elemental carbon in space
- PAHs play an important role in the energetics and chemical processes in the ISM:
  - Photo-electric heating
  - Charge balance → gas-phase abundances
  - Surface chemistry
- PAHs are used as a tracer for star

PAH questions

- What is the molecular composition of the PAH family?
- How does the PAH family relate to the carbonaceous inventory of the Universe?
- How do the characteristics of PAHs interact with and reflect the physical conditions of their environment?
- How can we use the UIR bands as a probe of the physical conditions in regions near and far?

Lab & Theory

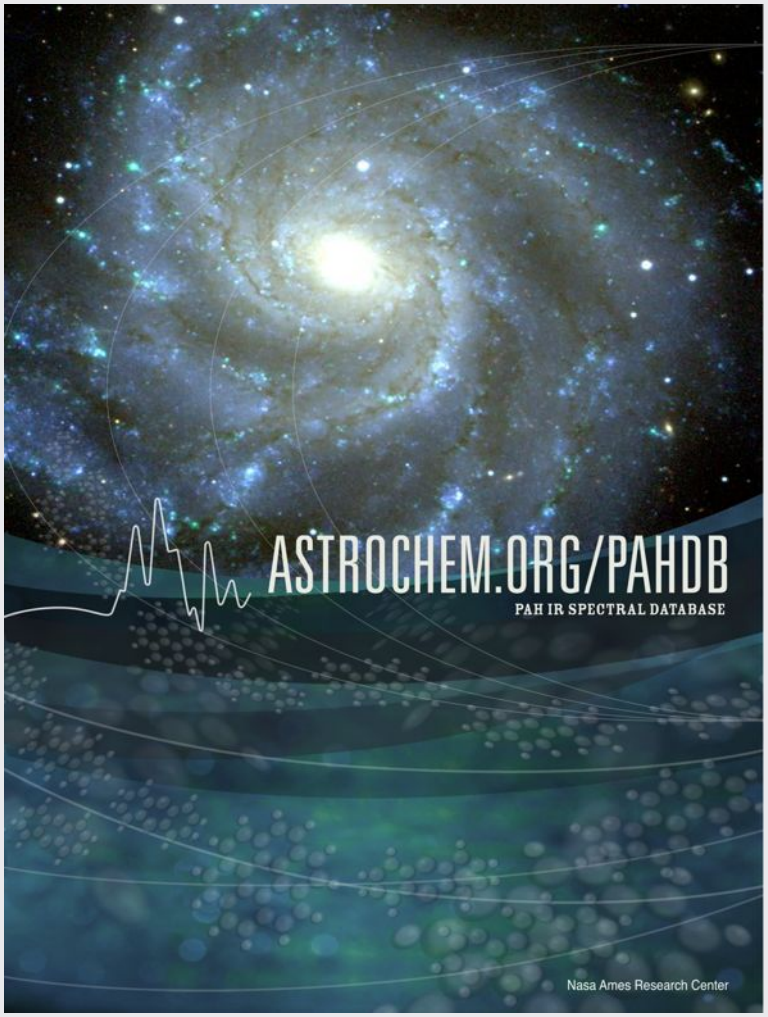
PAH IR Spectral Database
Ames Research Center

- 2.7 μm - 3.7 mm (mid - far IR)
- ~75 laboratory spectra (~200 measured)
- ~700 theoretical spectra
- $8 \leq N_{carbon} \leq 400$

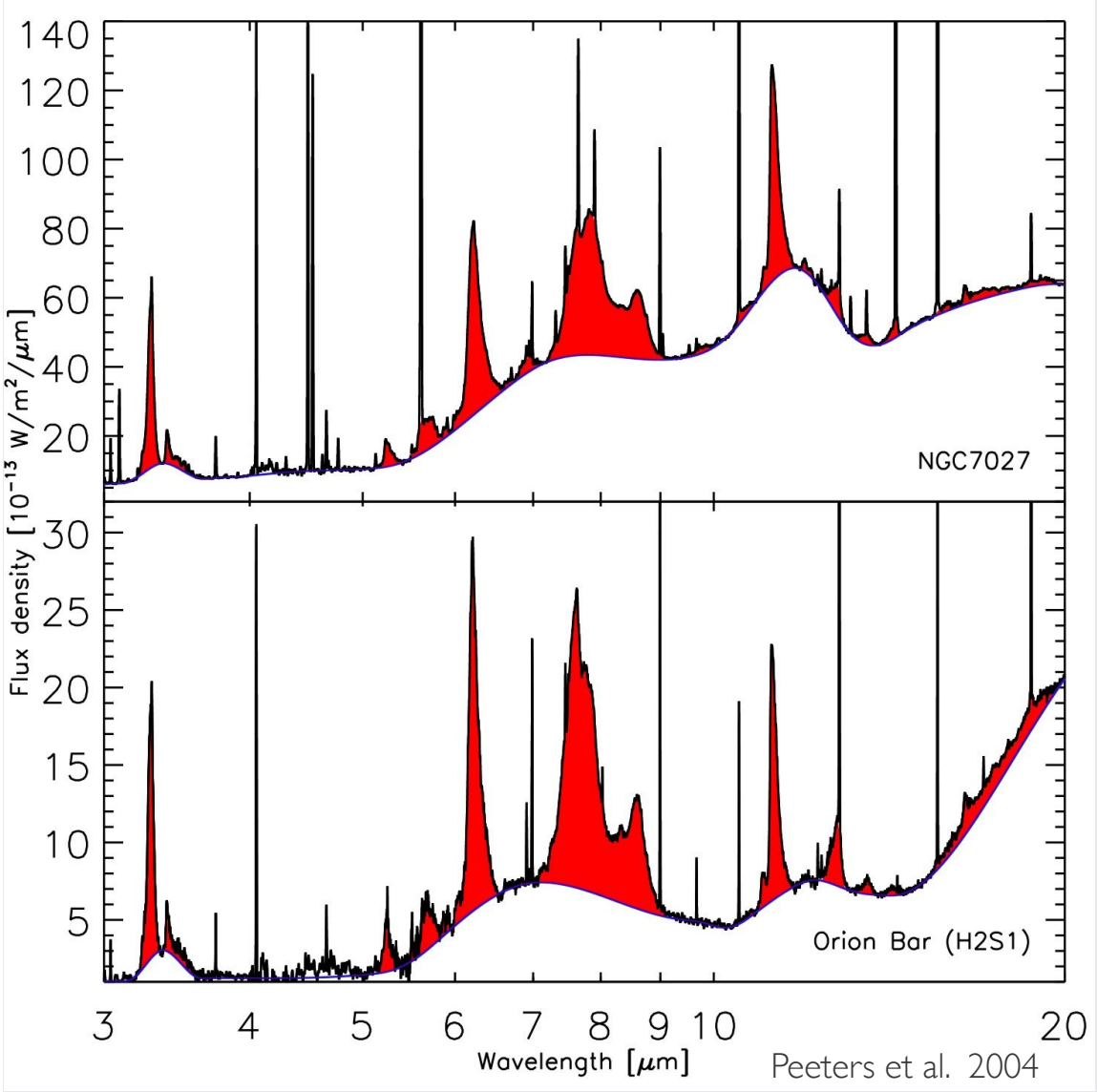
Bauschlicher (Peeters) et al. 2010
Boersma (Peeters) et al. 2014
Mattioda et al., in prep.

Experimental data from carbonaceous species

Duley et al., Pino et al. ,Jager et al.



Observational characteristics



Peeters et al. 2004

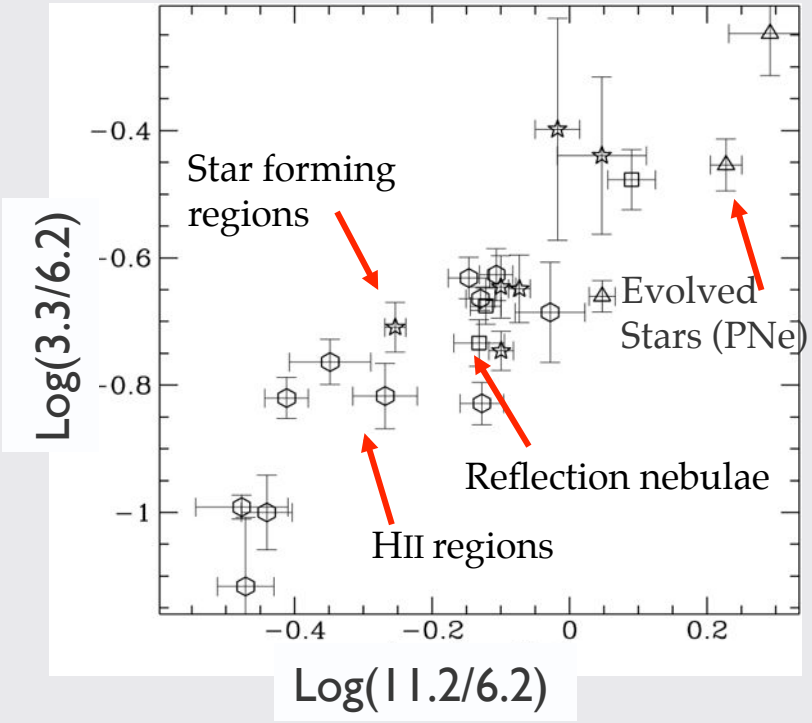
PAH emission:

- is variable:
  - (relative) intensity
  - peak position & profile
- depends on environment, physical conditions

Well-known PAH intensity correlations

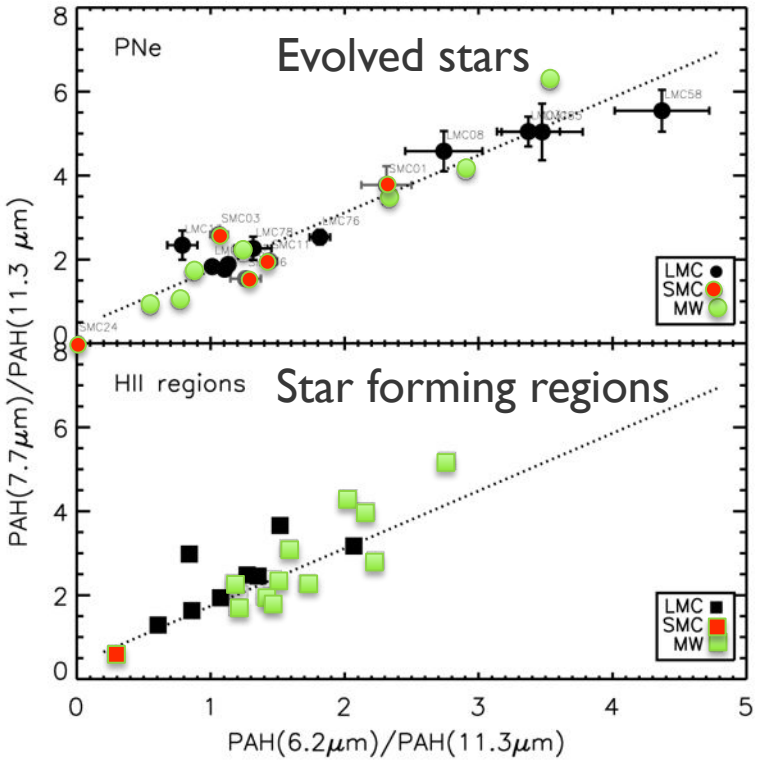
- from source to source

11.2 vs. 3.3



Hony (Peeters) et al. 2001

6.2 vs. 7.7

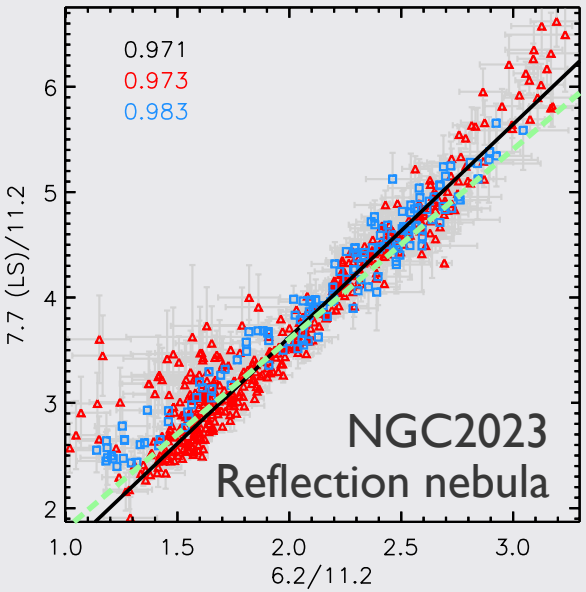


HII regions: Vermeij, Peeters et al. 2002
PNe: Bernard-Salas, Peeters et al. 2009

Well-known PAH intensity correlations

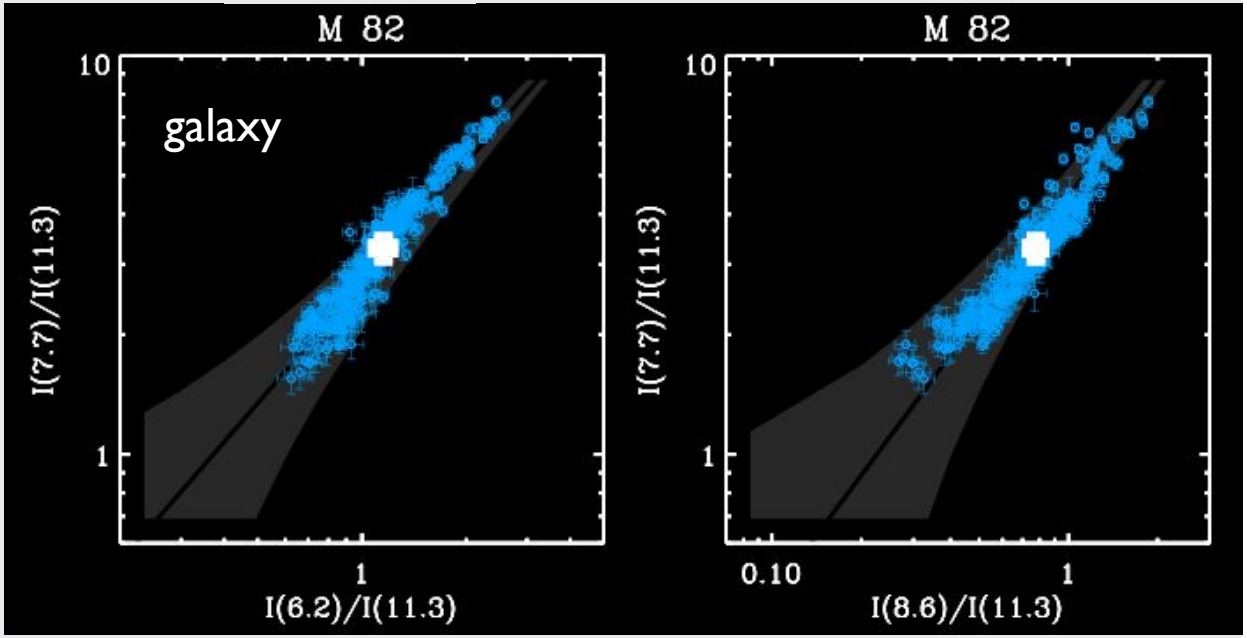
- within extended sources

6.2 vs. 7.7



Peeters et al., 2015

6.2 vs. 7.7 8.6 vs. 7.7



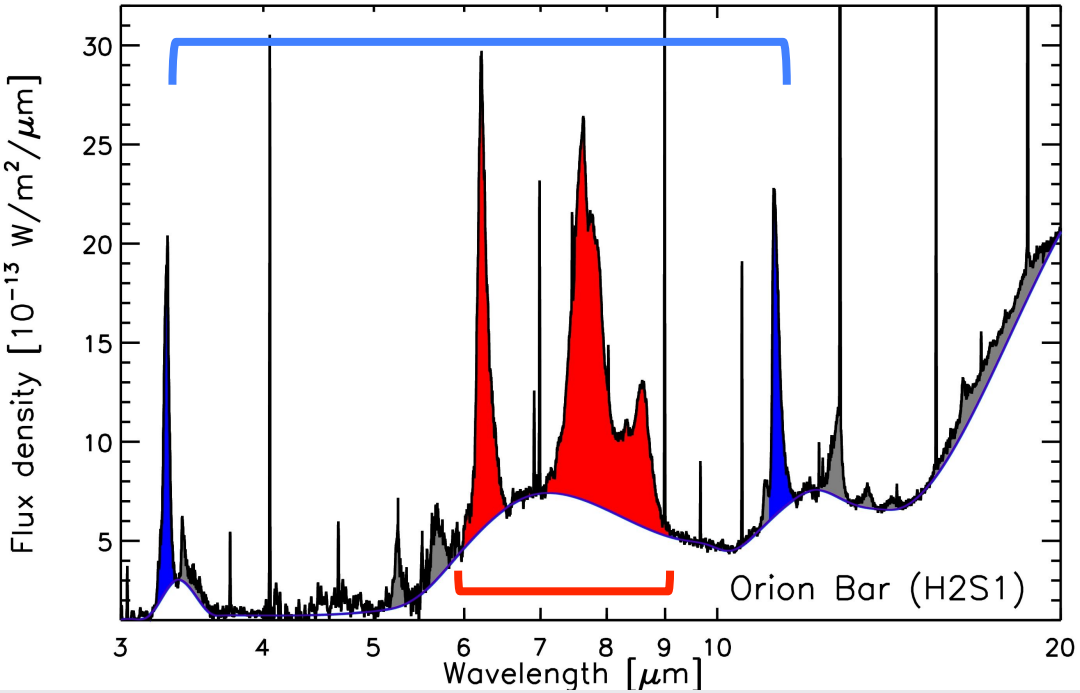
Galliano (Peeters) et al. 2008

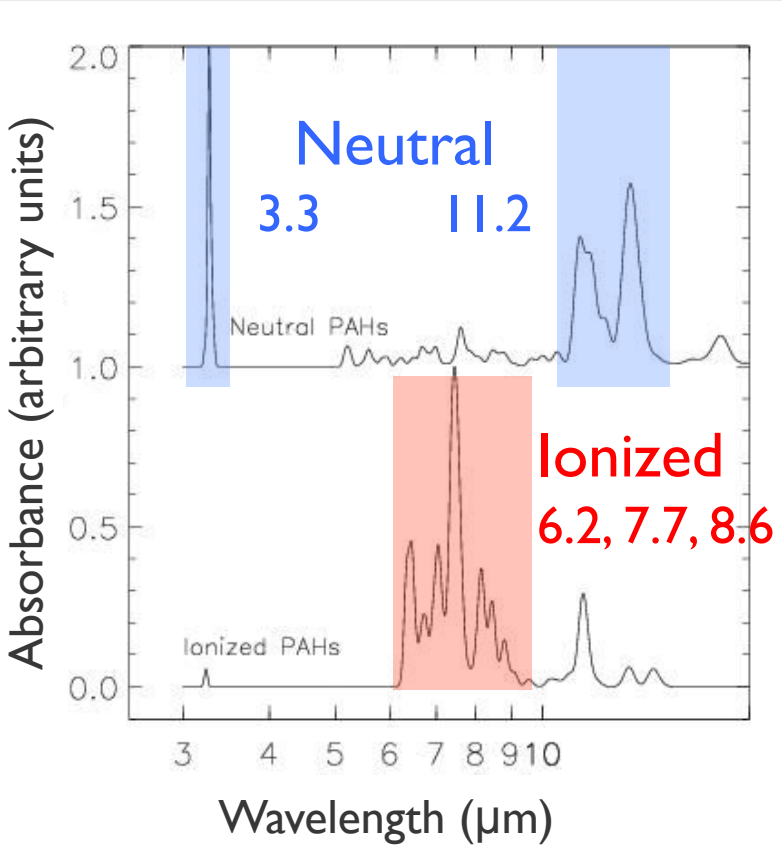
Observations vs. Lab/theory: charge

well-known intensity correlations: → PAH charge

3.3, 11.2

6.2, 7.7, 8.6

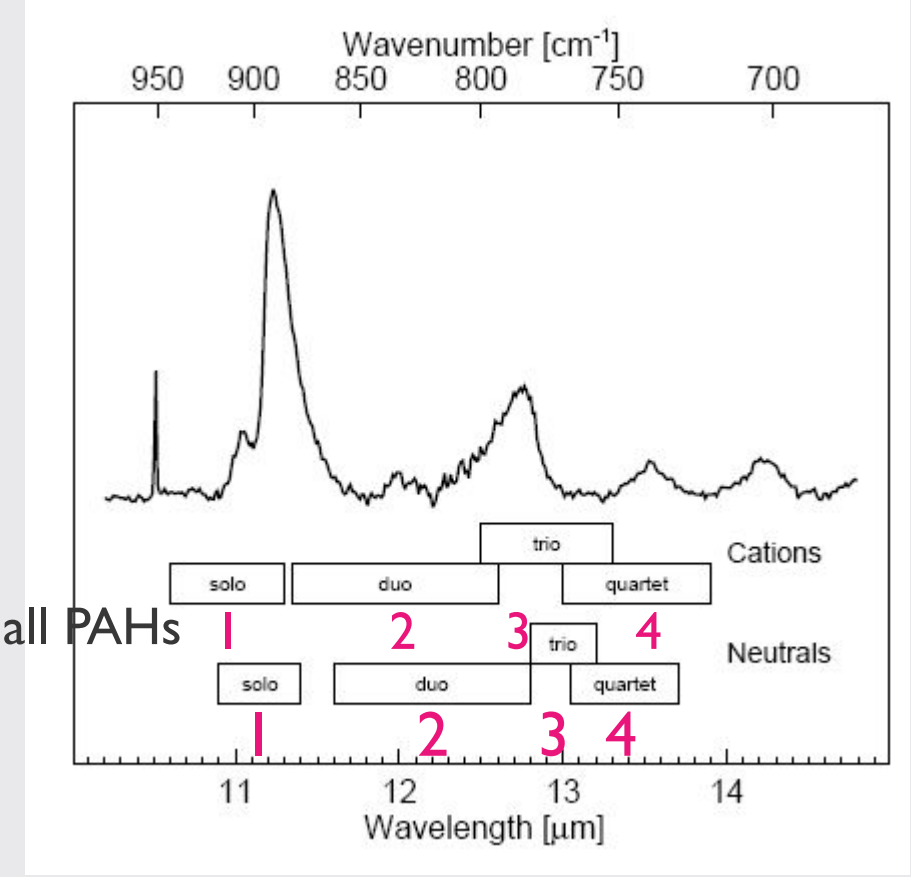




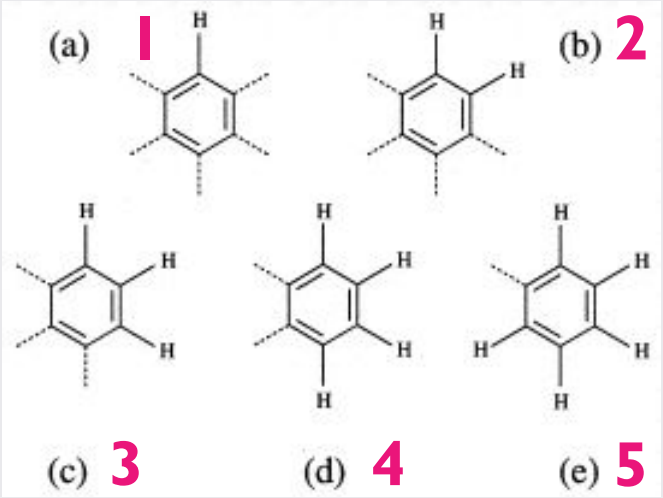
Allamandola et al. 1999

Observations vs. Lab/theory: molecular structure

Spectral pattern is sensitive to "H-adjacency"



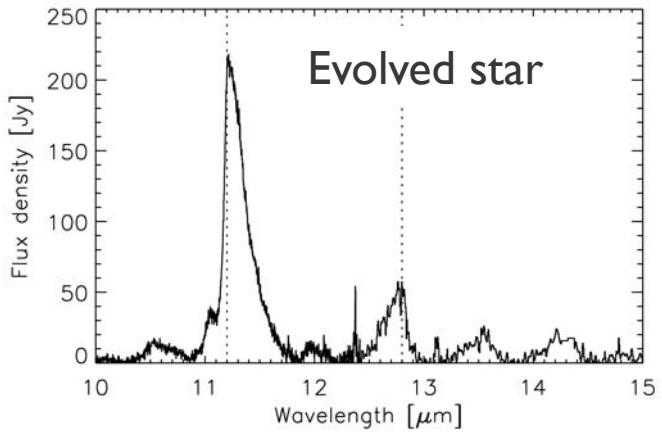
Small PAHs

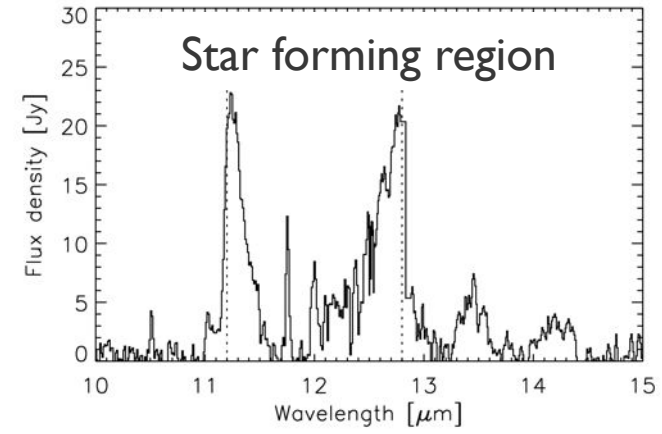


Hony (Peeters) et al. 2001
Bauschlicher, Peeters et al. 2008, 2009

Observations vs. Lab/theory: molecular structure

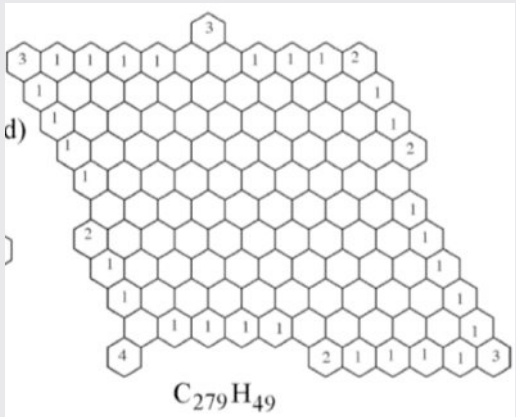
Spectral pattern is sensitive to "H-adjacency"

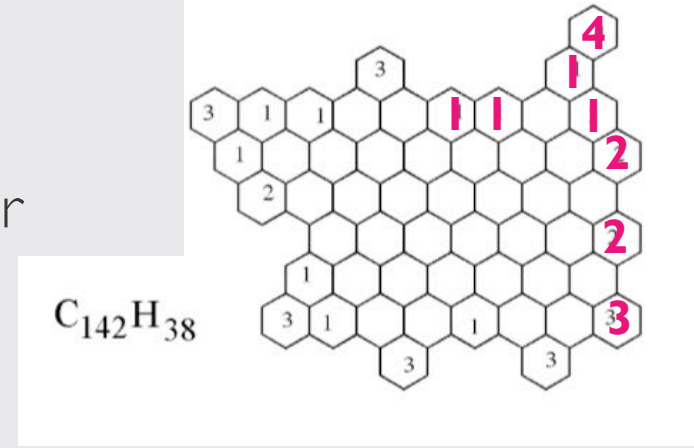




compact PAHs with smooth edge structure

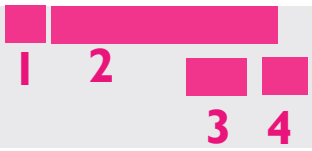
more irregular



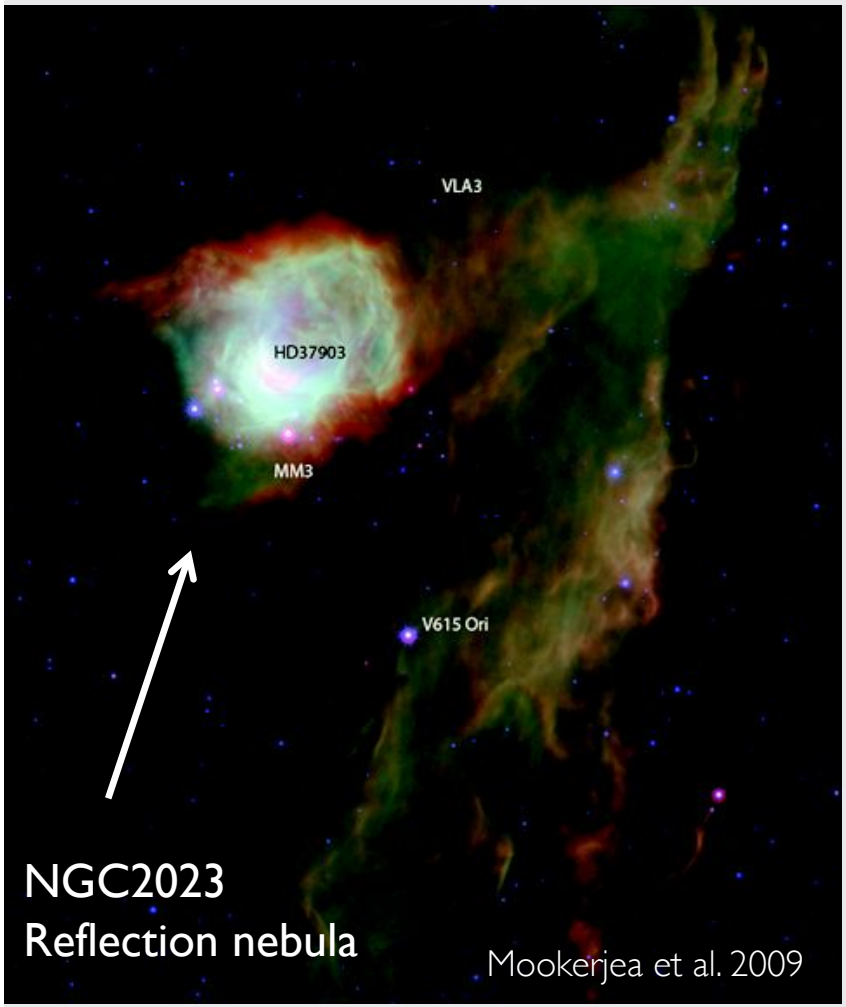


Hony (Peeters) et al. 2001
Bauschlicher, Peeters et al. 2008, 2009

Large neutral PAHs



NGC 2023

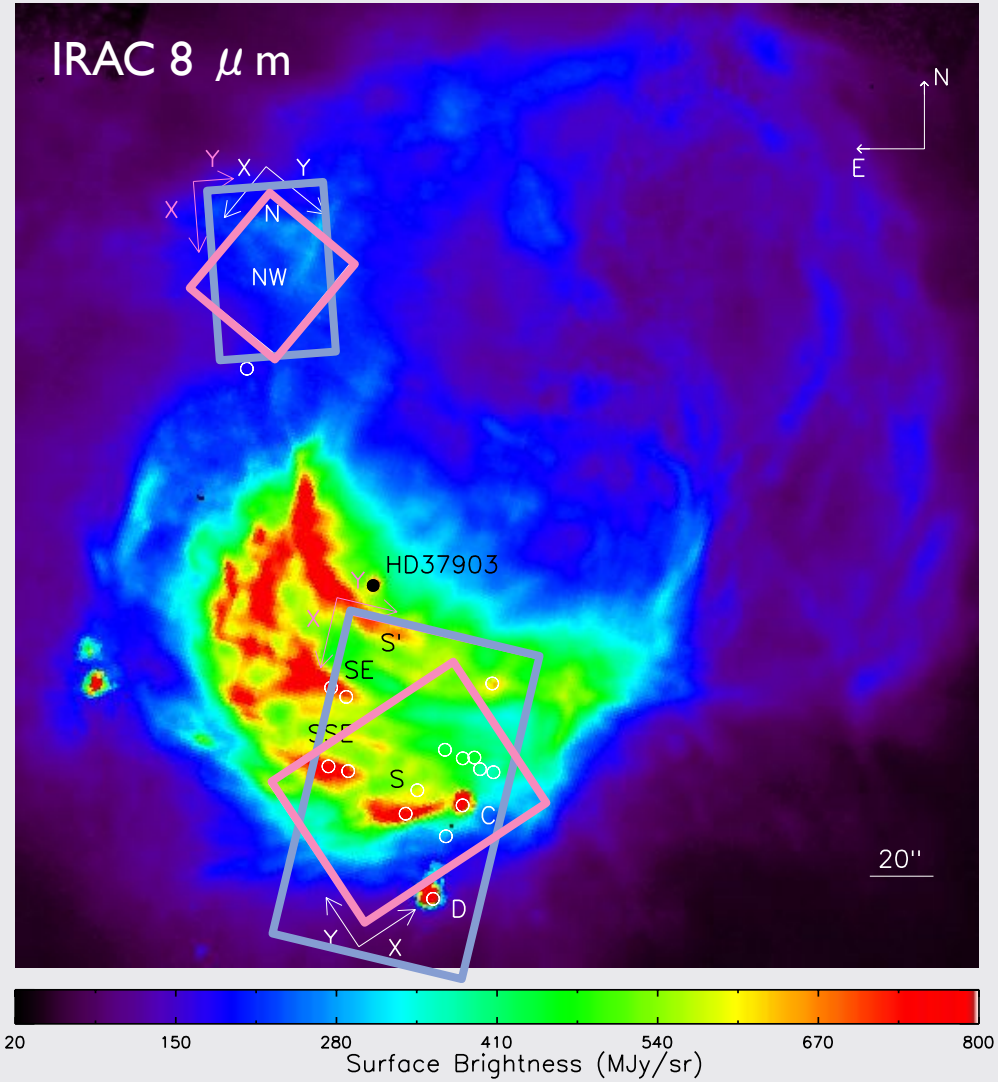


- Reflection Nebula
- illuminating star: B1.5V star HD 37903
- distance of 350 pc

- a FUV radiation field of ~500 to 10^4 G_0 incident on a clumpy molecular cloud
- densities: varying from 10^3 to $>10^5$ cm^{-3} , depending on location.

NGC2023

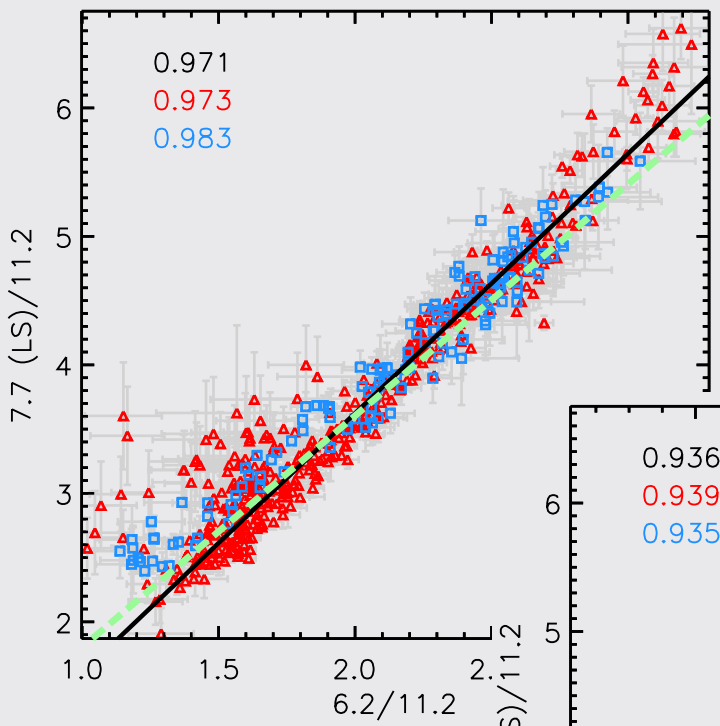
- Spitzer-IRS spectral maps
- SL:
  - 5-15 μm
  - R=~60-128
- SH:
  - 10-20 μm
  - R=~600

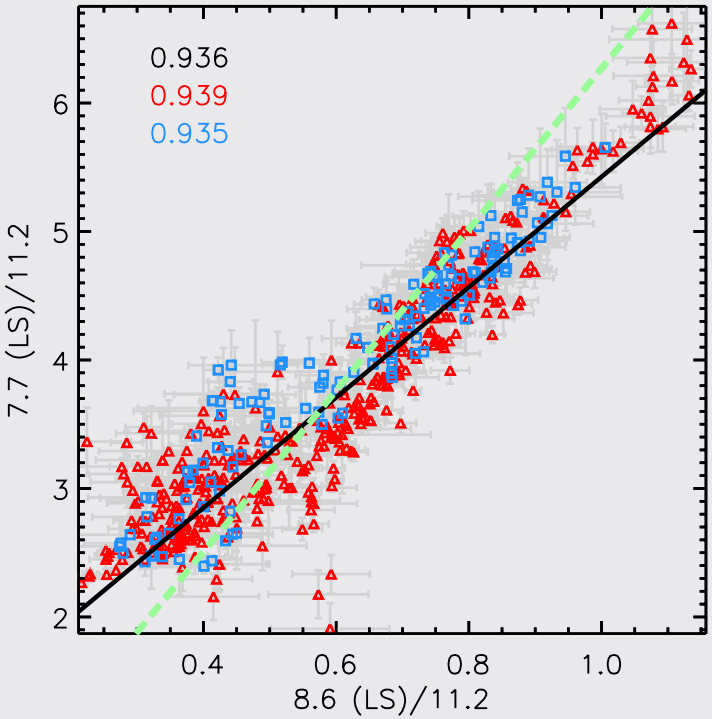


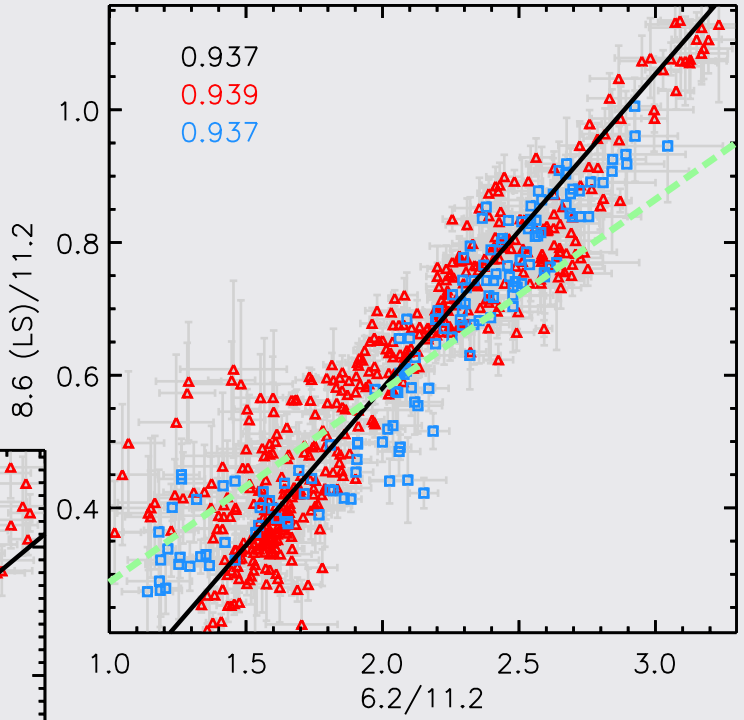
Peeters et al. 2012 & 2015

Well-known correlation of 6.2, 7.7, 8.6

Consistent with previous studies





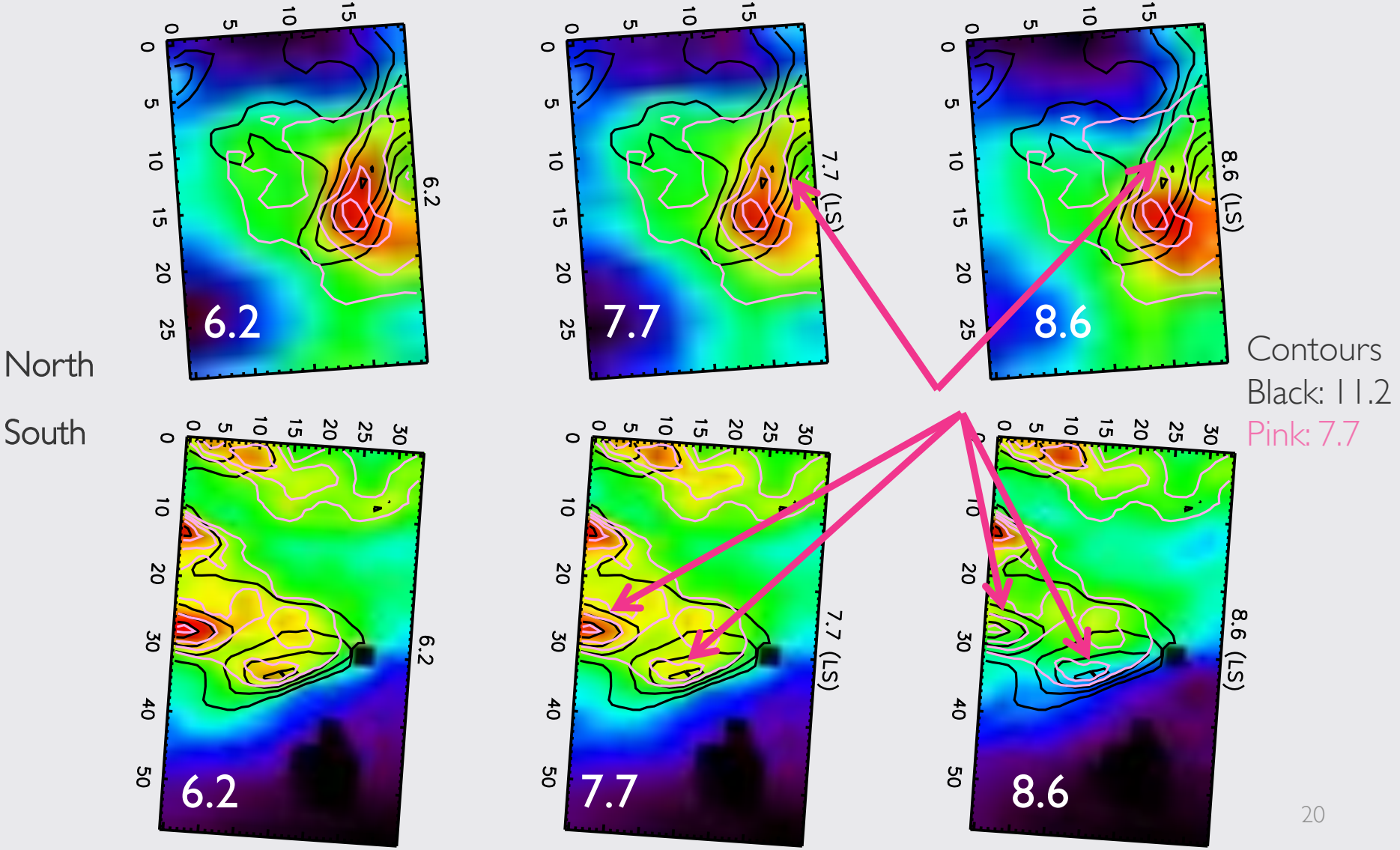


North

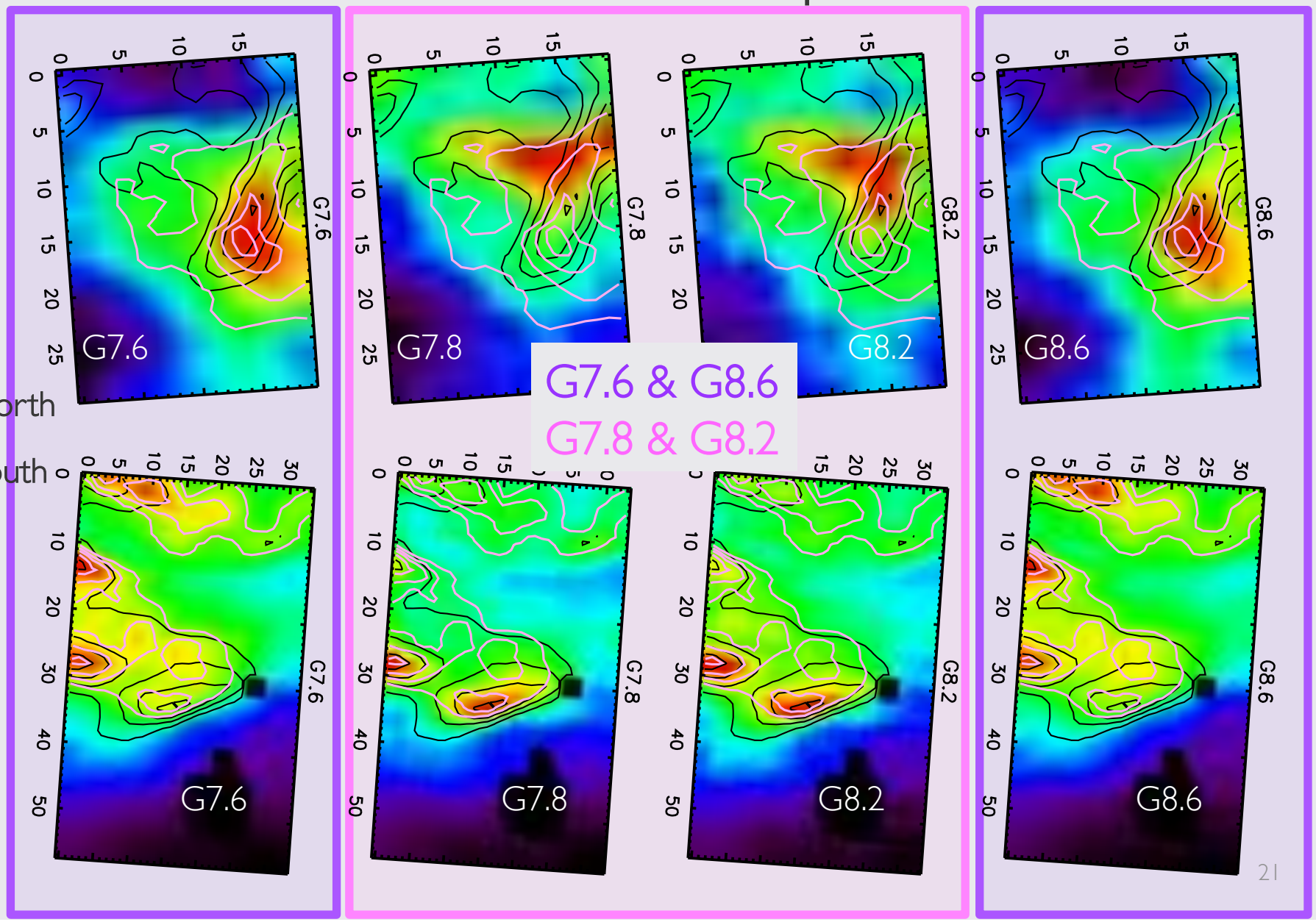
South

Distinct morphology of 6.2, 7.7, 8.6

BUT subtle differences between bands that correlate with each other



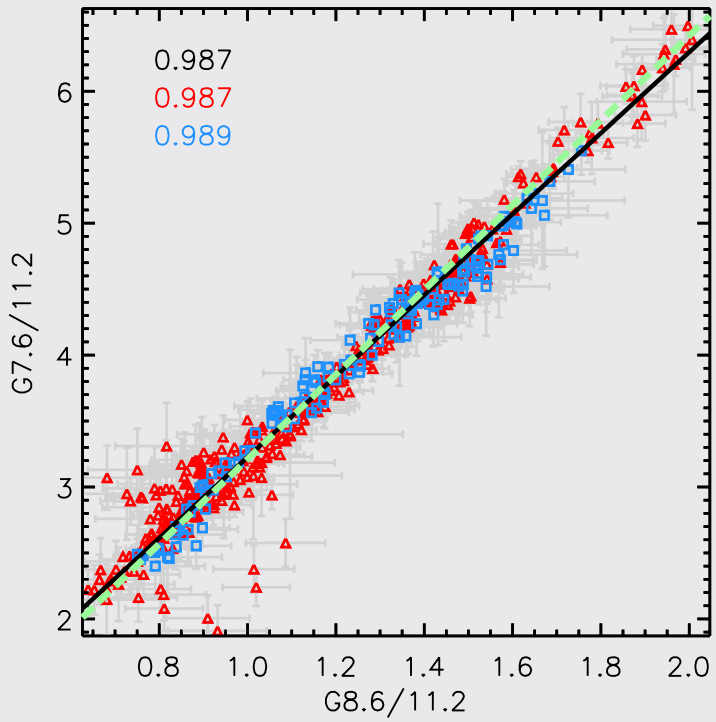
7-9 μm decomposition



7-9 μm decomposition

best correlation:

G7.6 & G8.6

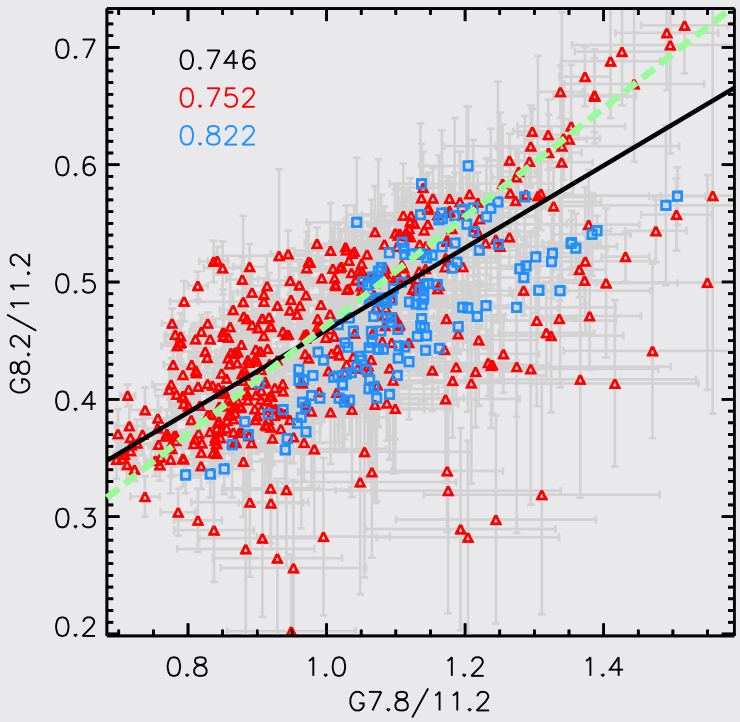


North

South

weaker correlation:

G7.8 & G8.2



7-9 μm decomposition

- Well established that 7.7 complex consists of 7.6 and 7.8 subcomponents

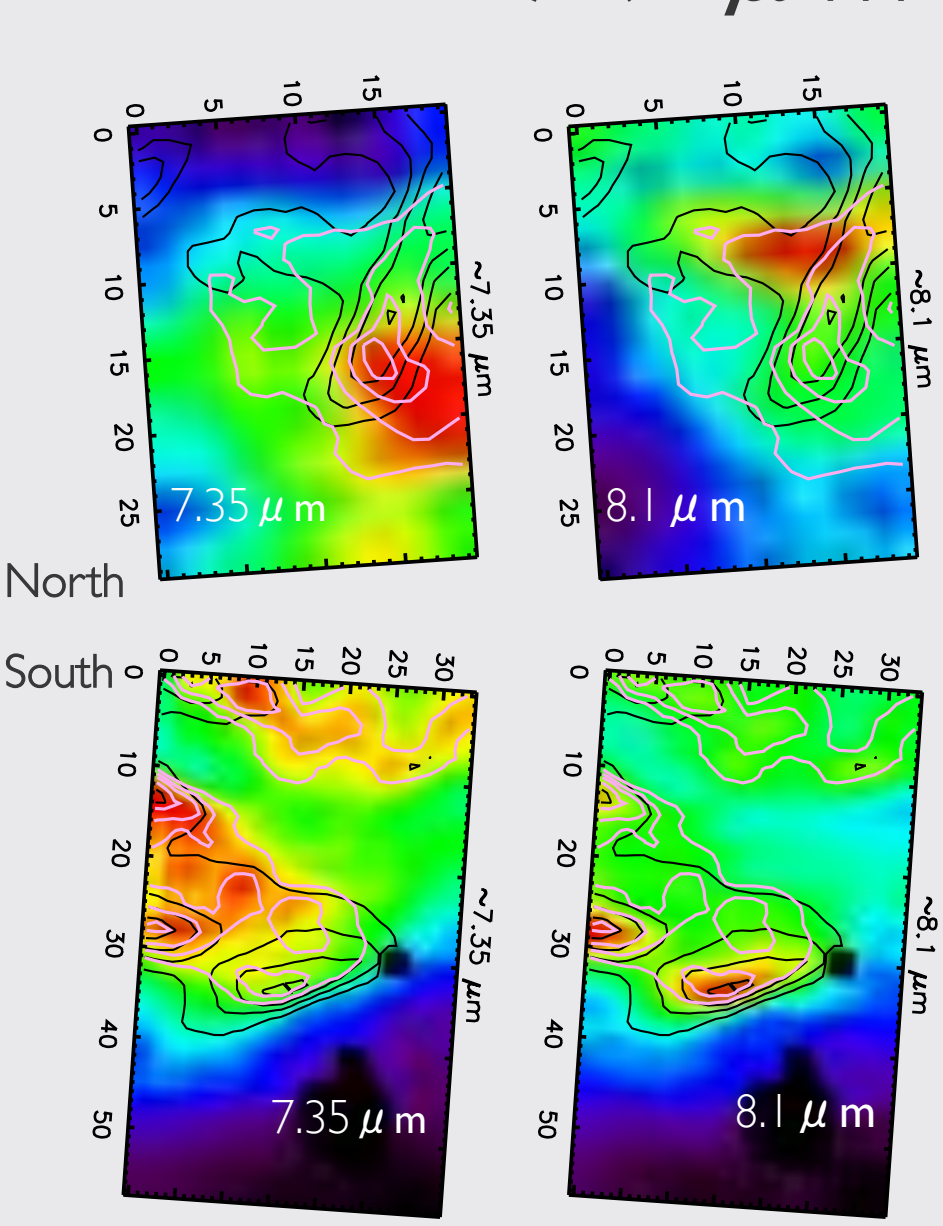
e.g. Bregman 1989; Cohen et al. 1989; Beintema et al. 1996; Molster et al. 1996; Roelfsema et al. 1996

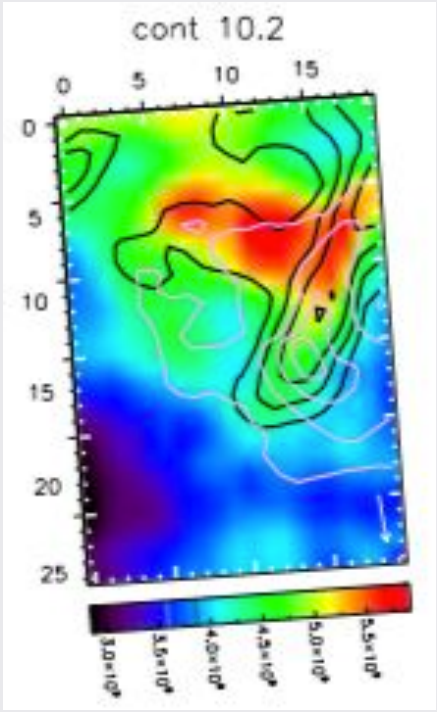
- 7.6 is related to 8.6

7.8 is related to 8.2

- **They arise from at least two PAH subpopulations with spatially distinct morphologies**

7-9 μm extremes





Spatial distribution varies:

- with λ across bands
- between 2 extremes at 7.35 and 8.1 μm
- 8.1 μm ~ continuum

Morphology of PAH emission changes

7.35 extreme

8.6, G7.6, G8.6

6.2, 7.7

G7.8, G8.2

8.1 extreme

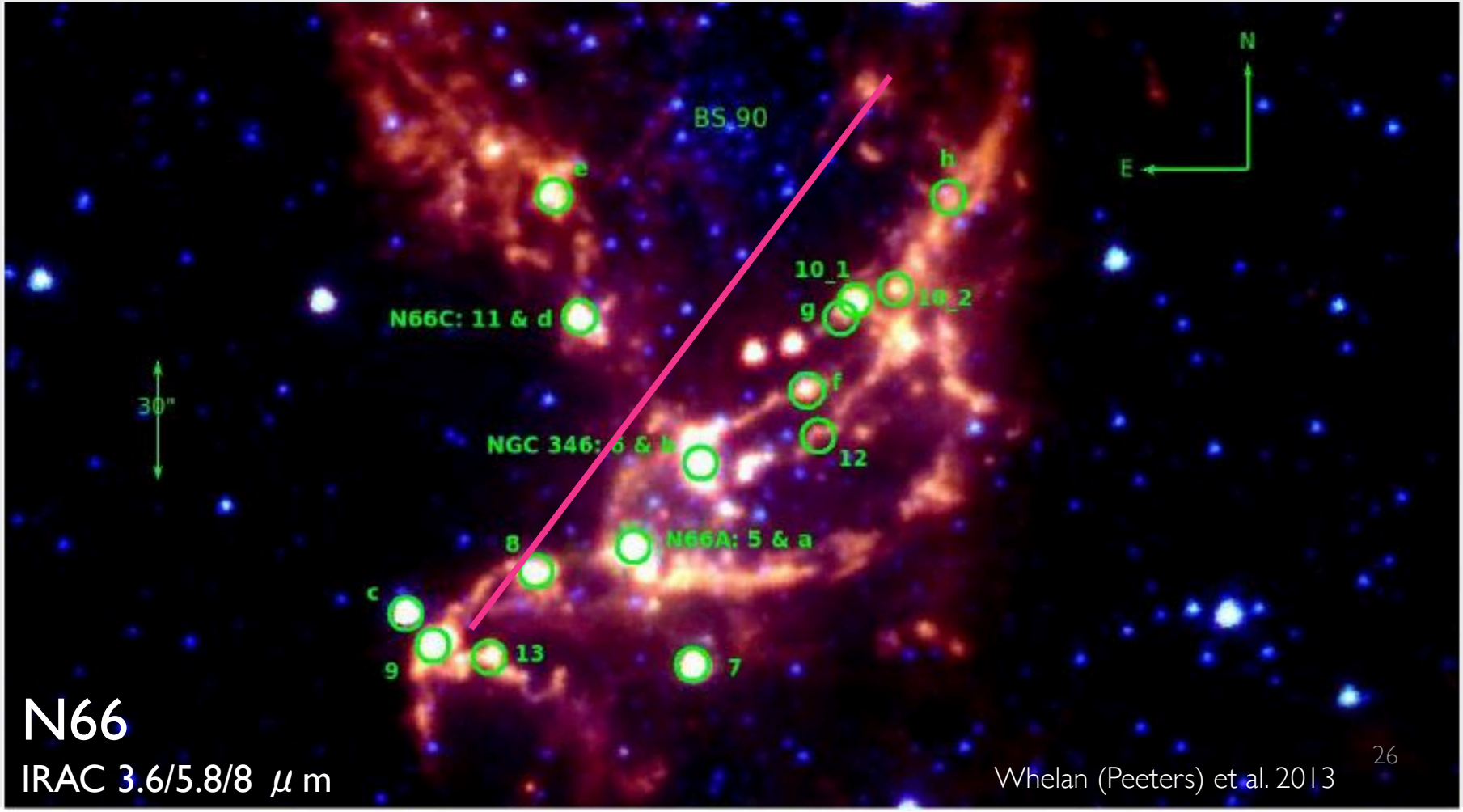
Increasing distance from the star

2 extremes in 7-9 μm PAH emission

4 Gaussian decomposition

Break-down between 6.2 & 7.7?

- Giant star forming regions W49 (Milky Way) and N66 (SMC) suggest disconnection between 6.2 and 7.7



Break-down between 6.2 & 7.7?

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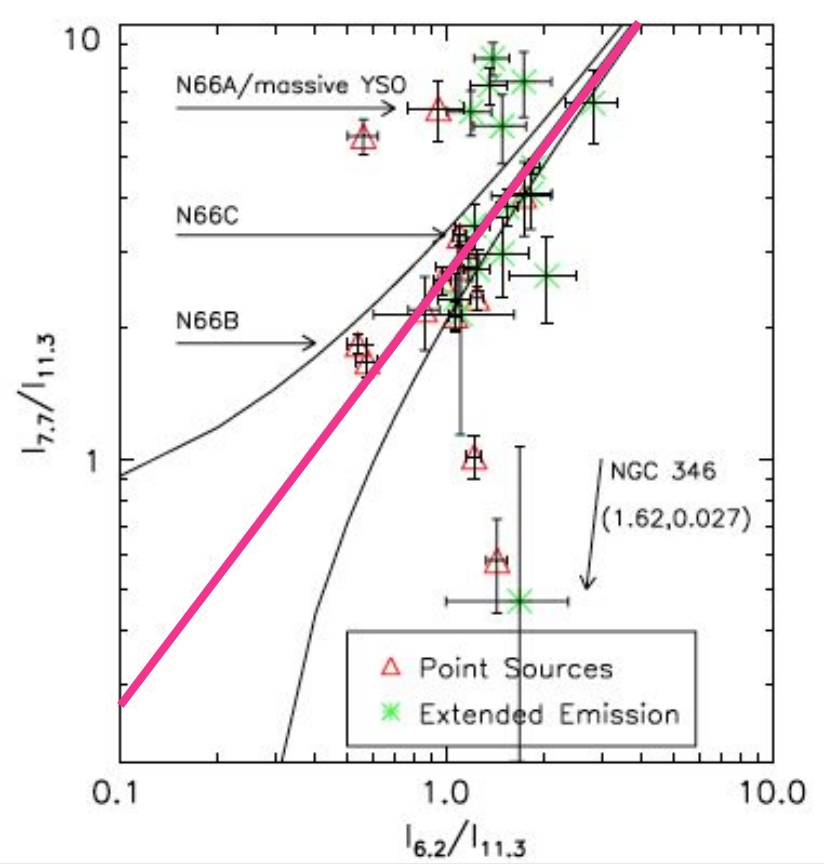

Whelan (Peeters) et al. 2013

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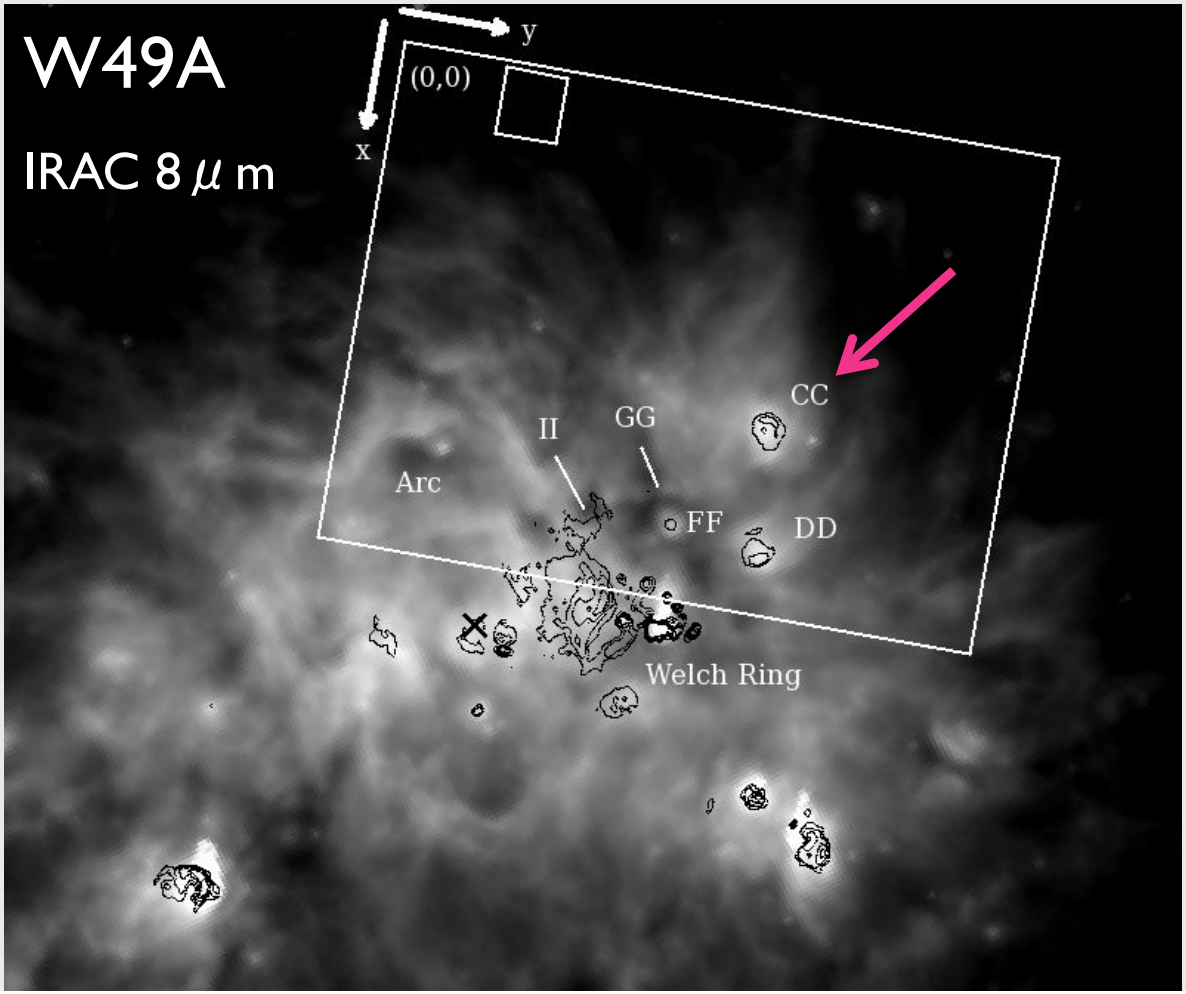

Stock, Peeters et al. 2013

Break-down between 6.2 & 7.7?

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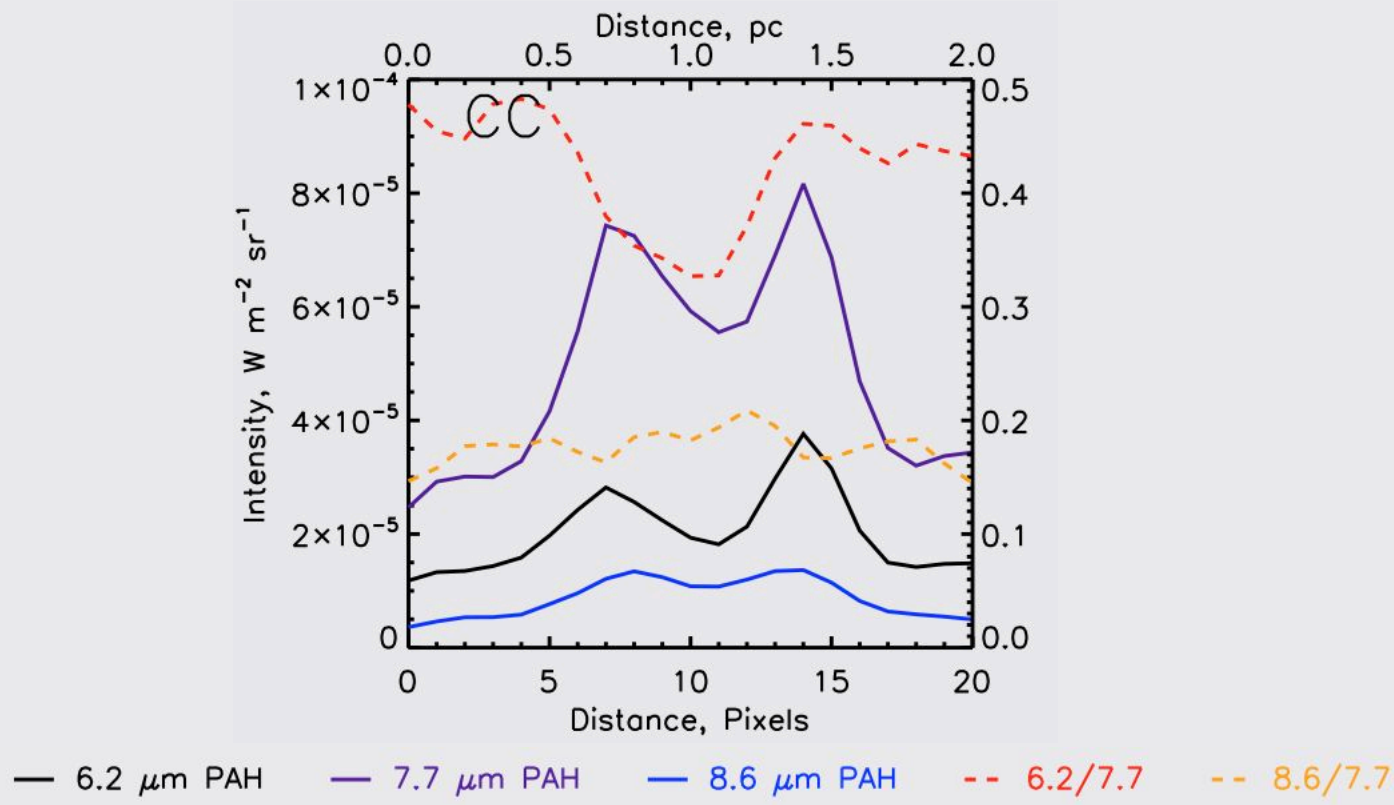


Stock, Peeters et al. 2013

Morphology of PAH emission changes

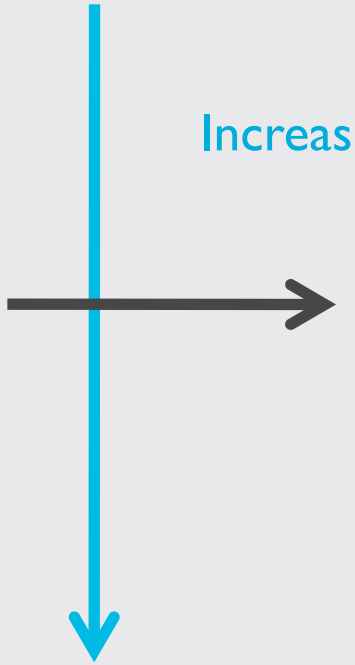
7.35 extreme,

8.6, G7.6, G8.6

6.2, 7.7

G7.8, G8.2

8.1 extreme



Increasing distance from the star

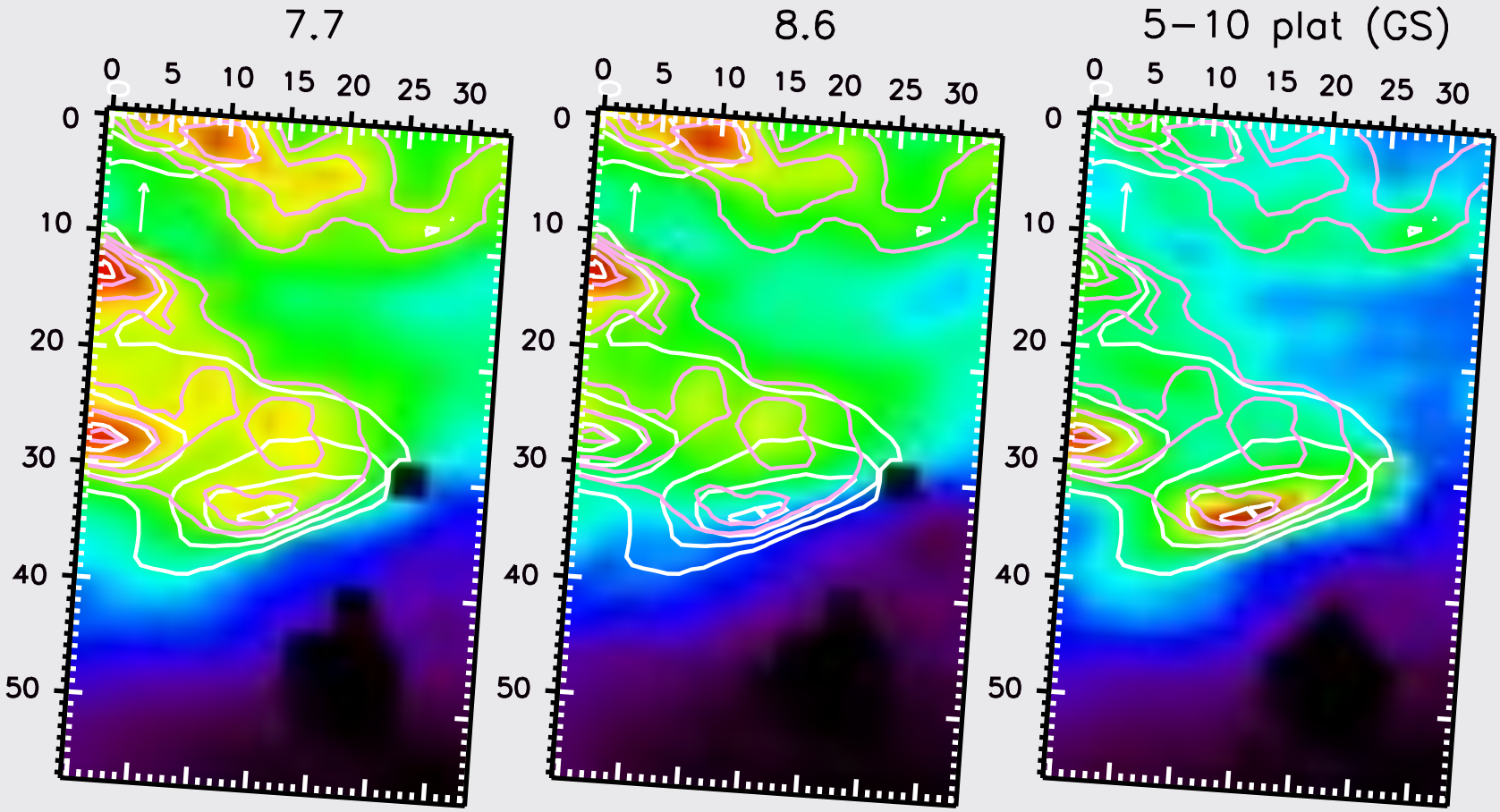
BUT 6.2 – 7.7 breakdown inside some star-forming regions

2 extremes in 7-9 μm PAH emission

4 Gaussian decomposition

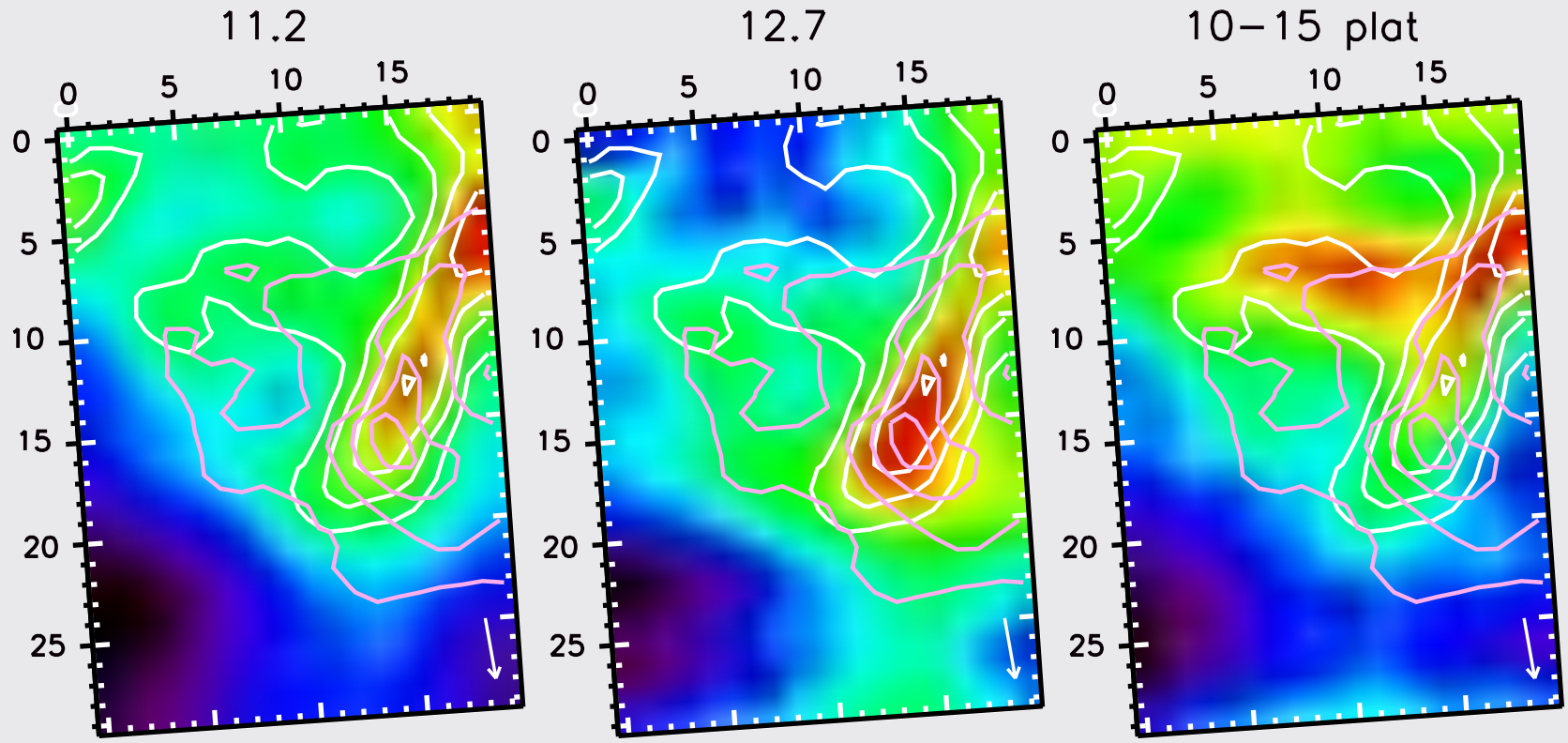
PAH plateaux vs. features: 5-10μm

- Plateau is distinct from PAH features



PAH plateaux vs. features: 10-15μm

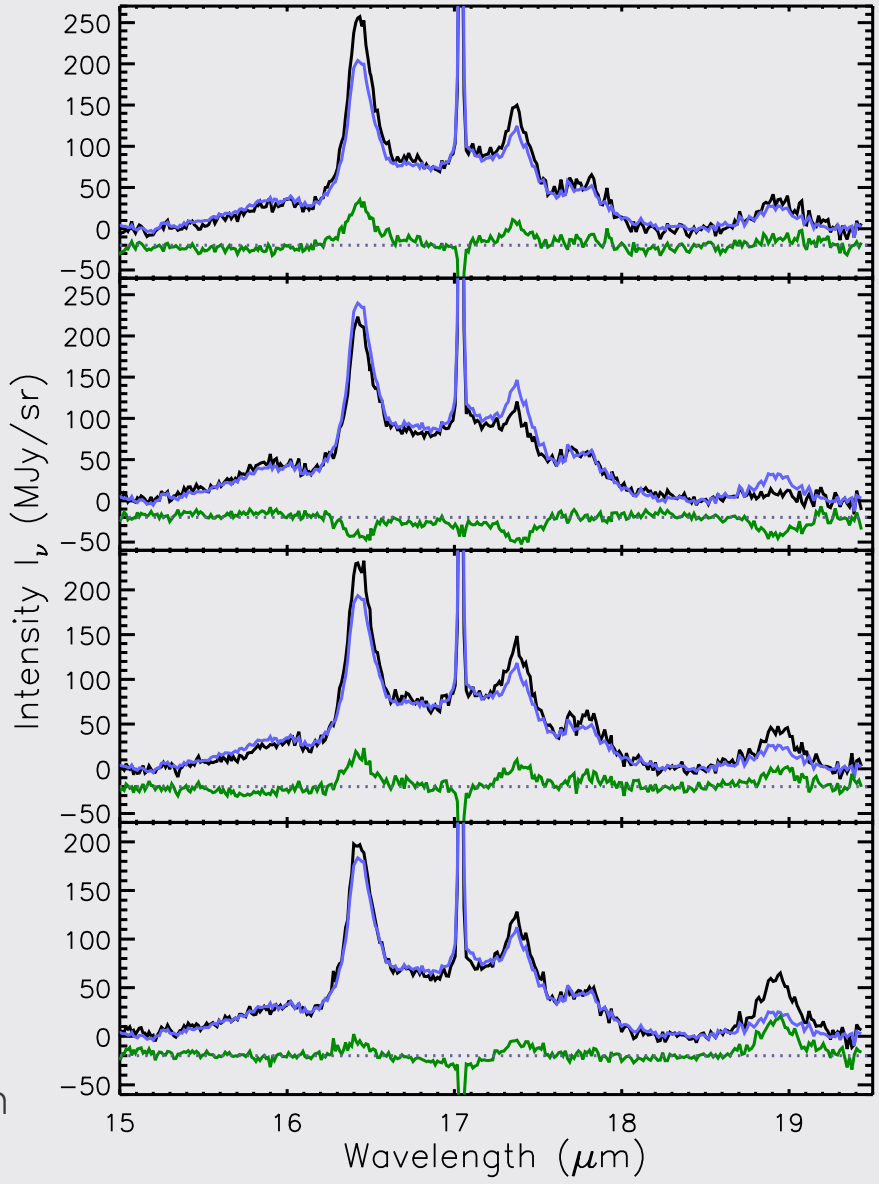
- Plateau is distinct from PAH features



PAH plateaux vs. features: 15-20μm

- features vary independent of plateau
- plateau profile invariable

→ **Need to be treated independently**



Black: spectra at given position
Blue: scaled averaged spectrum
Green: residuals

Morphology of PAH emission

- Morphology of integrated PAH bands changes:

Increasing distance from the star

7.35 extreme,

11.0, 17.4 PAH

8.6, G7.6, G8.6

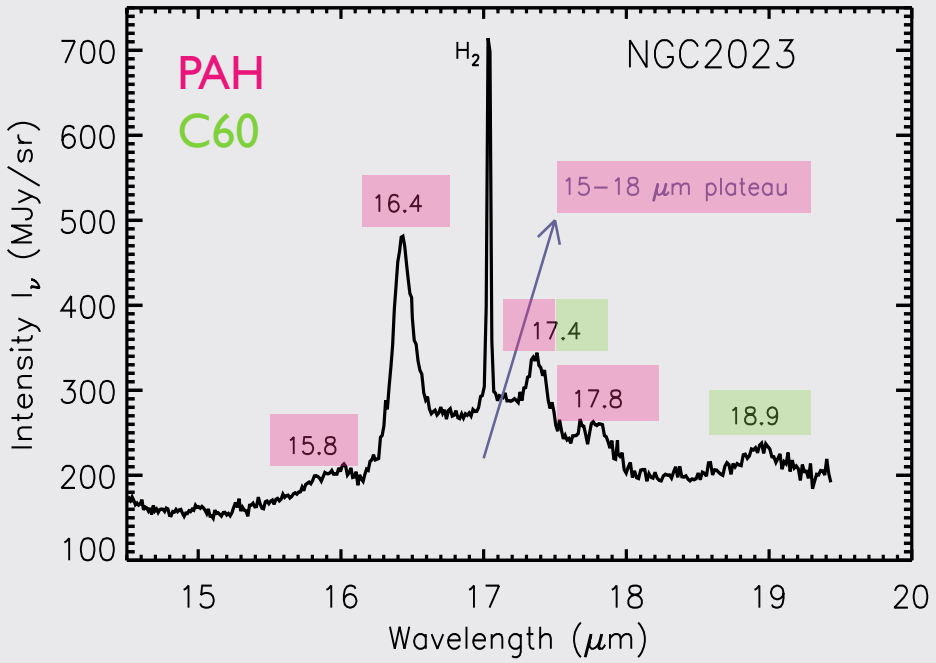
6.2, 7.7, **16.4**

12.7, 17.8

11.2, 15.8, 15-20 plateau

G7.8, G8.2, **plateaux**

8.1 extreme



2 extremes in 7-9 μm PAH emission

4 Gaussian decomposition

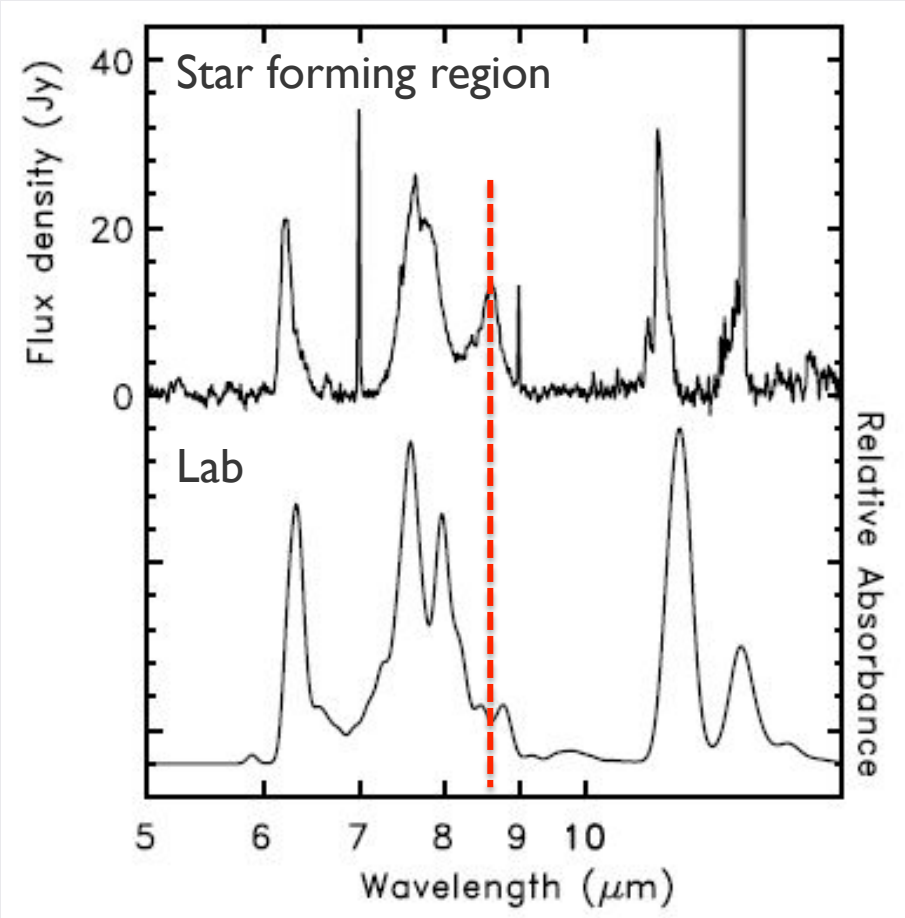
Morphology of PAH emission

- Reveals variation beyond charge state (neutrals - ions):

6.2-7.7-8.6: lab/theory

Different vibrational assignments:

- 6.2: C-C stretch
- 7.7: coupled C-C stretch and C-H in-plane bending
- 8.6: C-H in-plane bending



Peeters et al. 2002

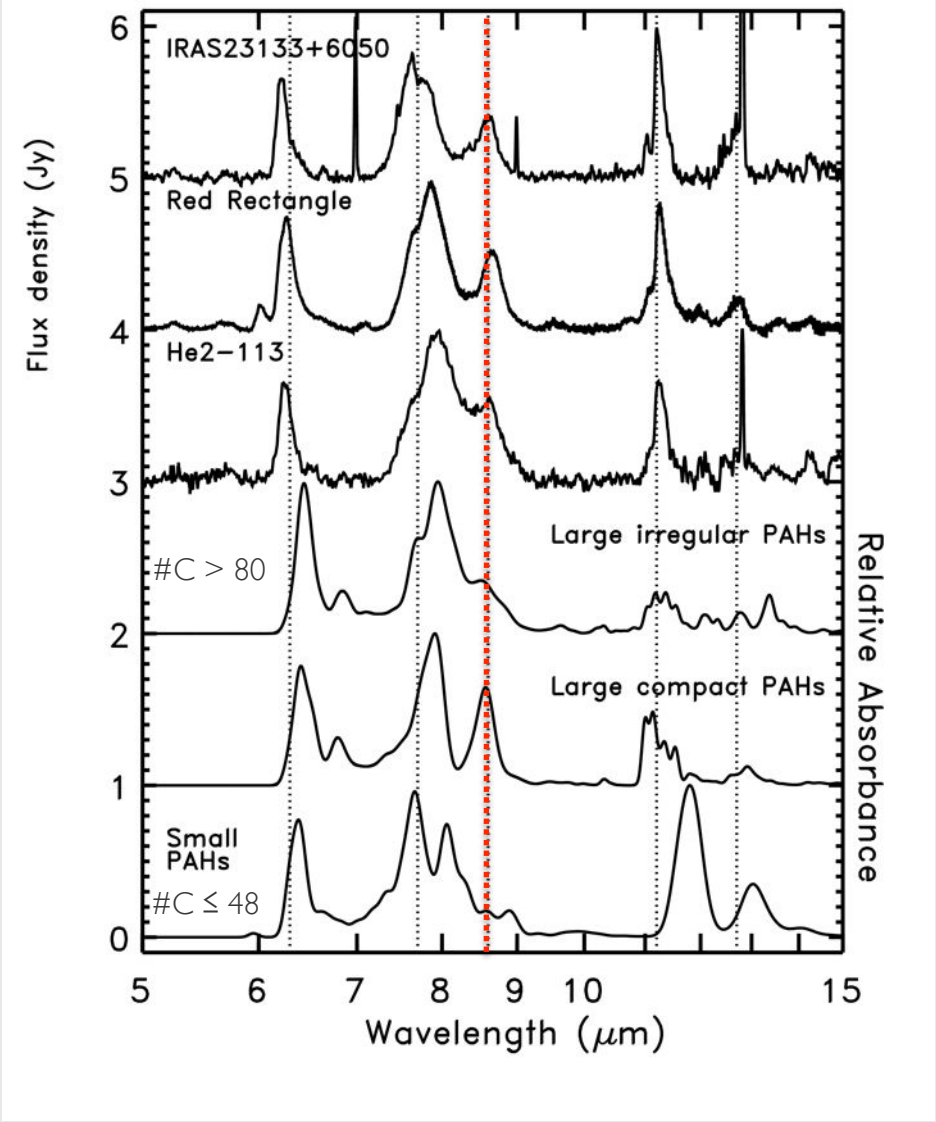
6.2-7.7-8.6: lab/theory

Different vibrational assignments:

- 6.2: C-C stretch
- 7.7: coupled C-C stretch and C-H in-plane bending
- 8.6: C-H in-plane bending

Different sub-populations:

- 8.6 μm PAH band: large compact PAHs



Star forming region

Evolved star

Evolved star

Theory

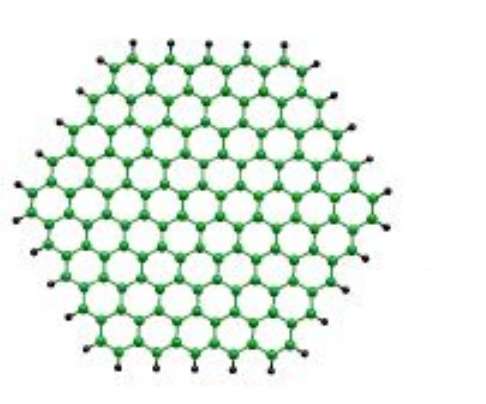
Theory

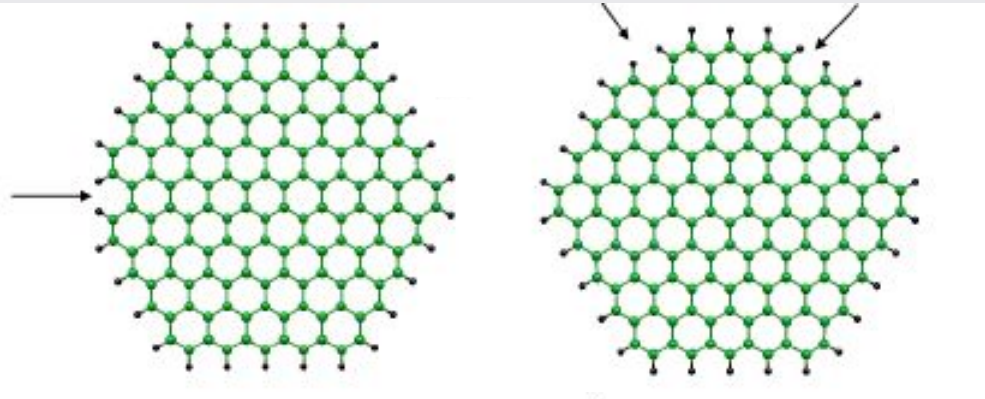
Lab

Bauschlicher, Peeters et al. 2008, 2009

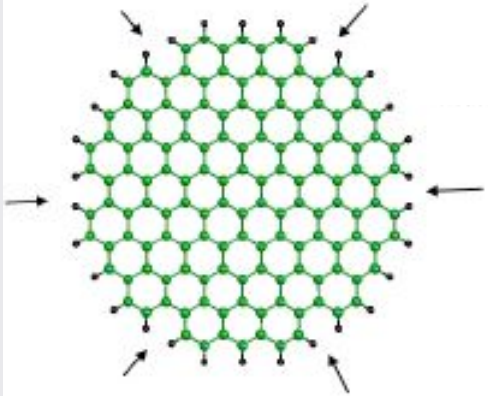
7.6-7.8-8.2-8.6: Theory

- **8.6:** C-H in-plane bending modes in large compact symmetric PAHs
  - almost any change reduces the size of the 8.6 μm emission
- **8.2:**



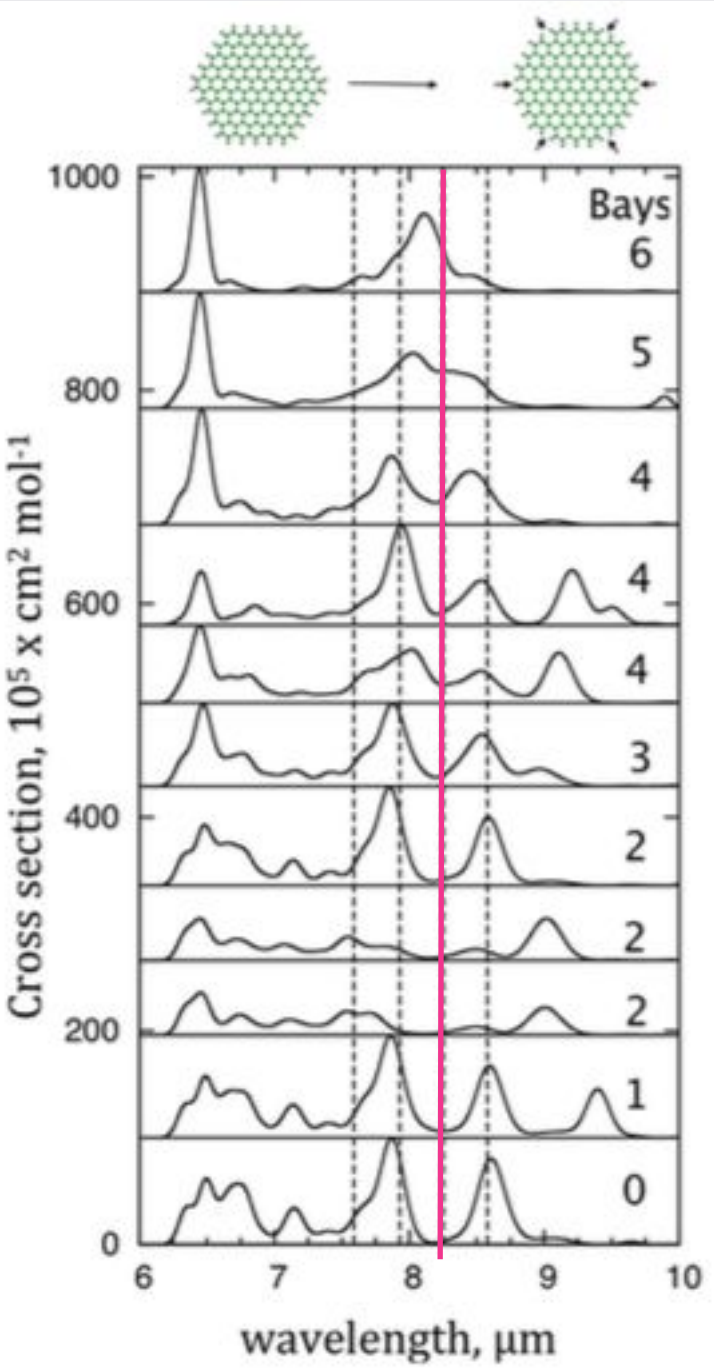


  - Increase number of bay regions



7.6-7.8-8.2-8.6: Theory

- **8.6:** C-H in-plane bending modes in large compact symmetric PAHs
  - almost any change reduces the size of the 8.6 μm emission
- **8.2:** C-H in-plane bending modes in PAHs with multiple bay regions
- **7.6 vs 7.8:** band positions influenced by
  - size (Bauschlicher, Peeters et al. 2008, 2009)
  - **molecular edge structure**



8.6-11.0-17.4: lab/theory

Different vibrational assignments:

- 8.6: C-H in-plane bending
- 11.0: C-H out-of-plane bending
- 17.4: C-C-C bending

Different sub-populations:

- 8.6: large symmetric, compact PAH cations
- 11.0: solo CH groups in any large PAH cation
- 17.4: large compact PAHs of all charge

➔ 17.4 due to cations & all three bands dominated by a few PAHs

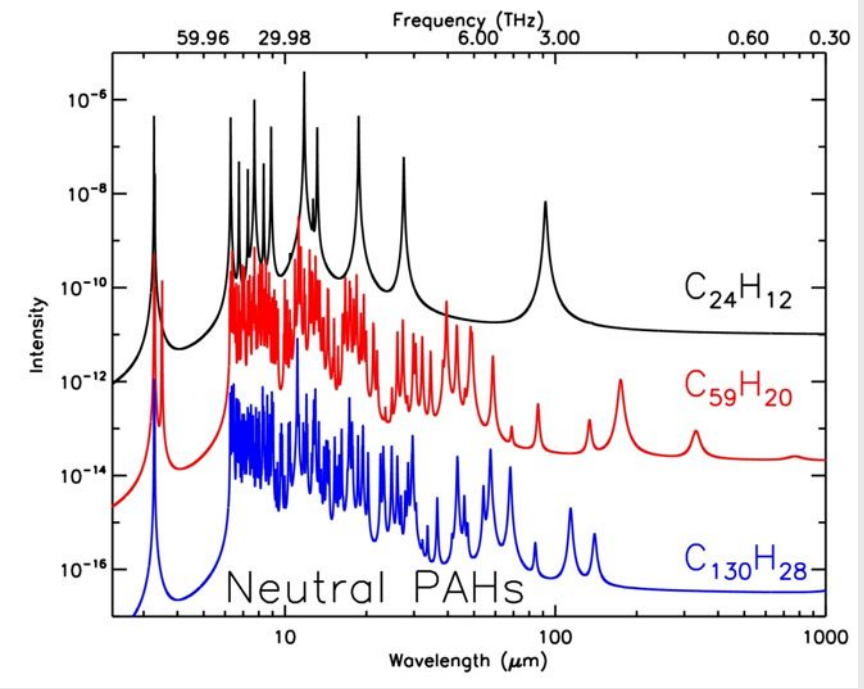
Implication for 7.6?

Summary

- Spectral maps reveal subtleties missed by correlation plots
  - Plateaux are independent of features
  - Spatial sequence with distance from the star
- Morphology varies with λ across PAH bands
- 7-9 μm PAH emission:
  - varies between 2 extremes
  - 8.6 & 7.6 --- 7.8 & 8.2
  - from at least two PAH subpopulations
- Sensitive to both charge and molecular structure

SOFIA & PAHs

- Identification of PAHs through their FIR modes
  - due to low-lying vibrational states
  - are molecule specific



Bauschlicher et al.
Mulas et al. 2006, Boersma et al. 2010, Ricca et al. 2012

SOFIA & PAHs

- Study the behavior of PAHs relative to other diagnostics (e.g. H_2, PDR lines etc.)
- 3.3 PAH
  - not observed with Spitzer
  - traces small neutral PAHs
  - trace size distribution of PAHs (combined with 11.2 PAH)