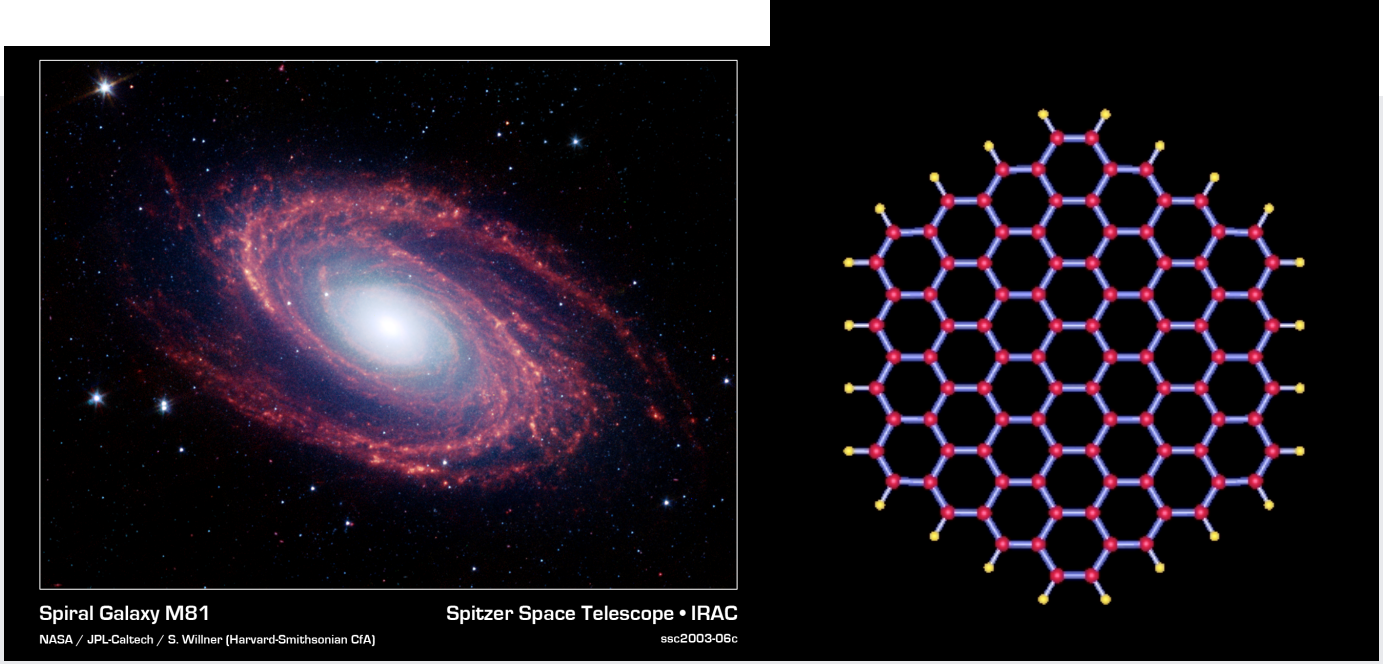


The PAH hypothesis after 25 years

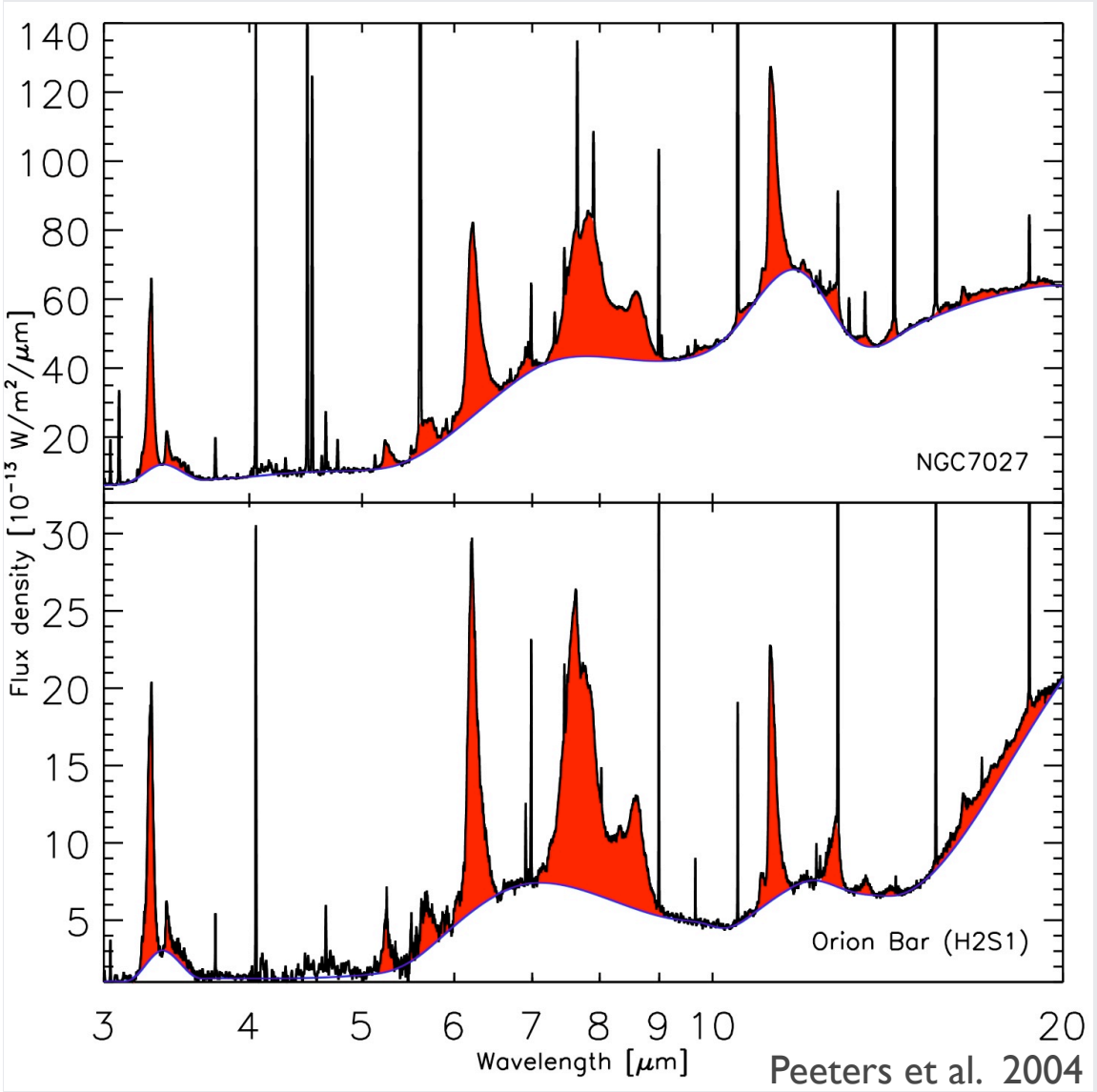
Els Peeters

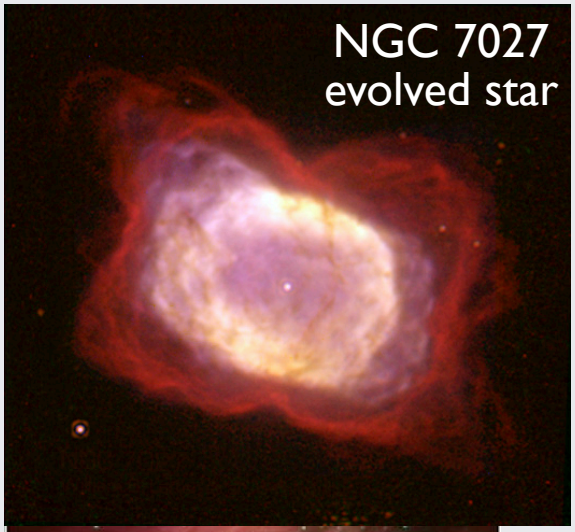
University of Western Ontario
& SETI Institute

Outline

- PAH hypothesis
- PAH emission reveals:
  - Ionization state
  - Interaction with environment
  - Molecular structure
  - Active modification of PAH population
- PAH toolbox
- PAH hypothesis

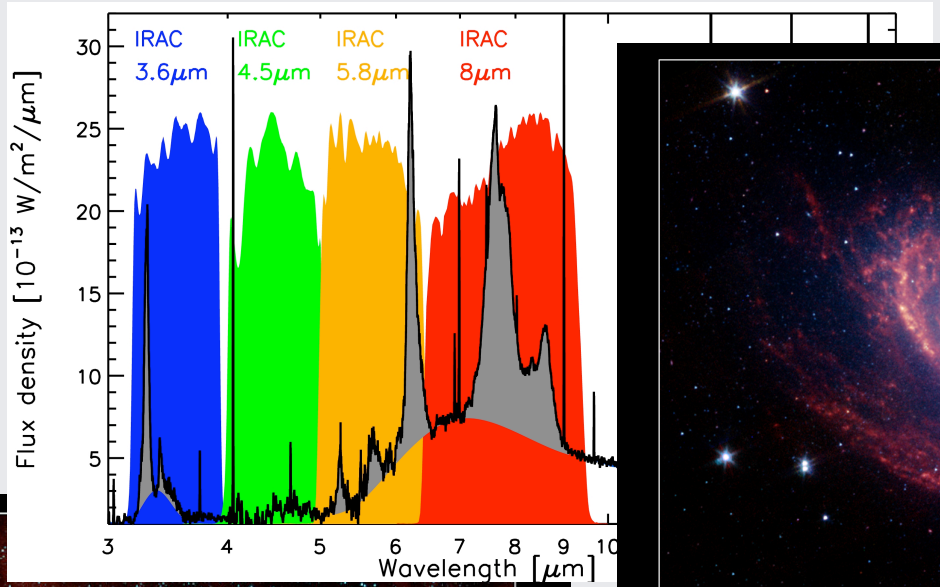
Unidentified IR emission bands

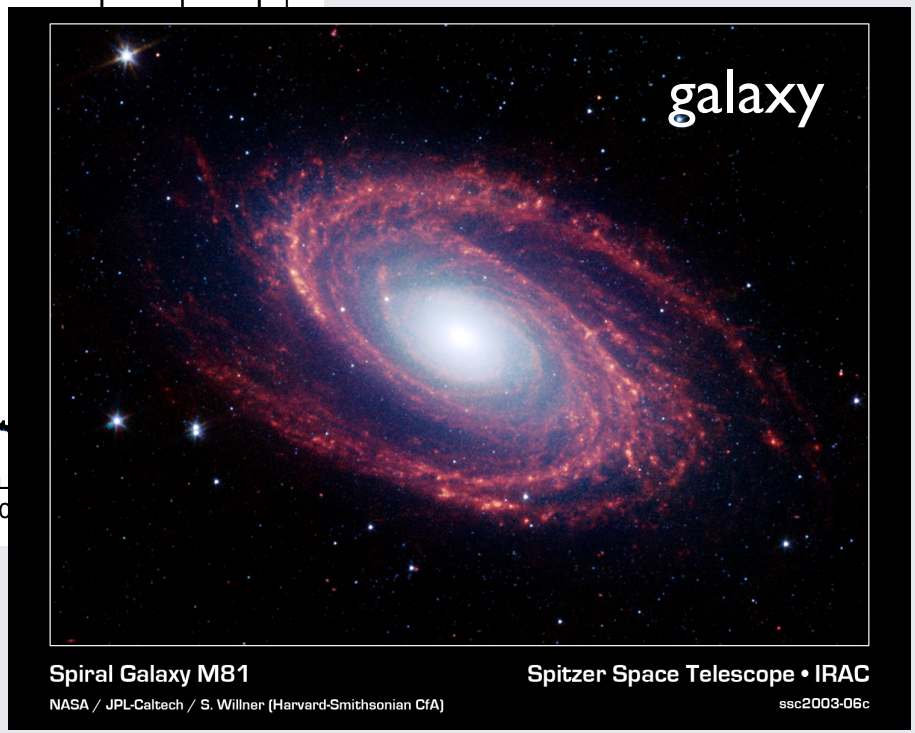


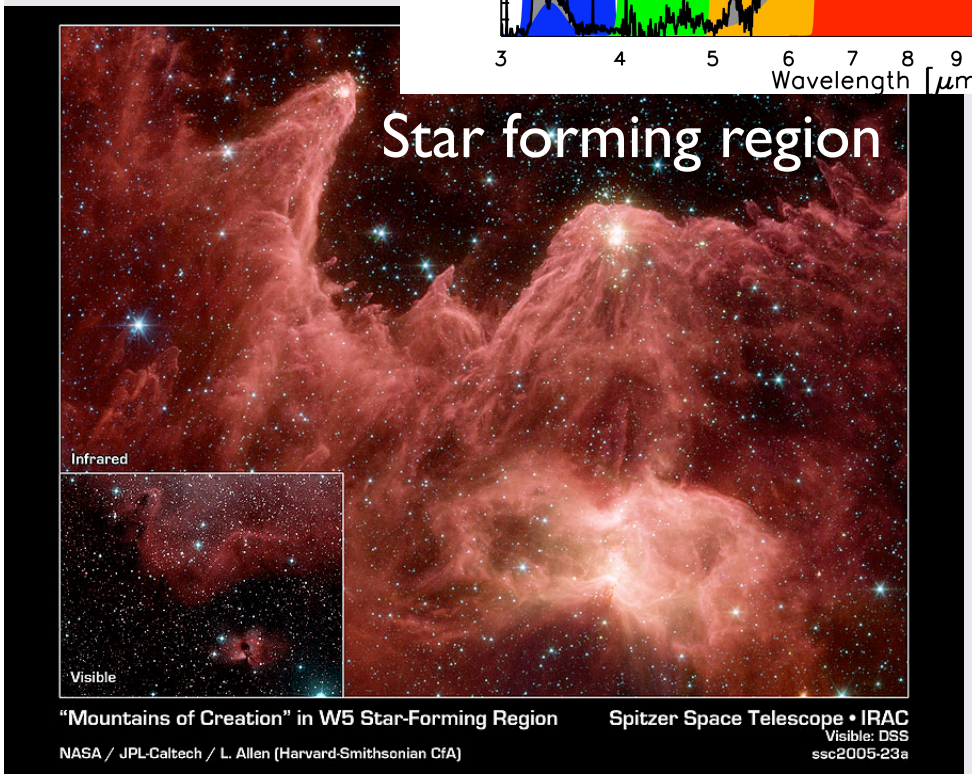




Unidentified IR emission bands







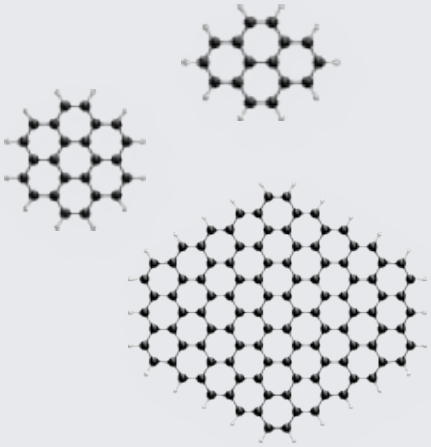
Unidentified IR bands

- Omnipresent
  - C-rich evolved stars
  - Interstellar medium (ISM)
  - Reflection nebulae
  - Star-forming regions
  - Galaxies

- Dominate IR spectra
  - up to 10-15% of total power output of galaxies

(original) PAH hypothesis

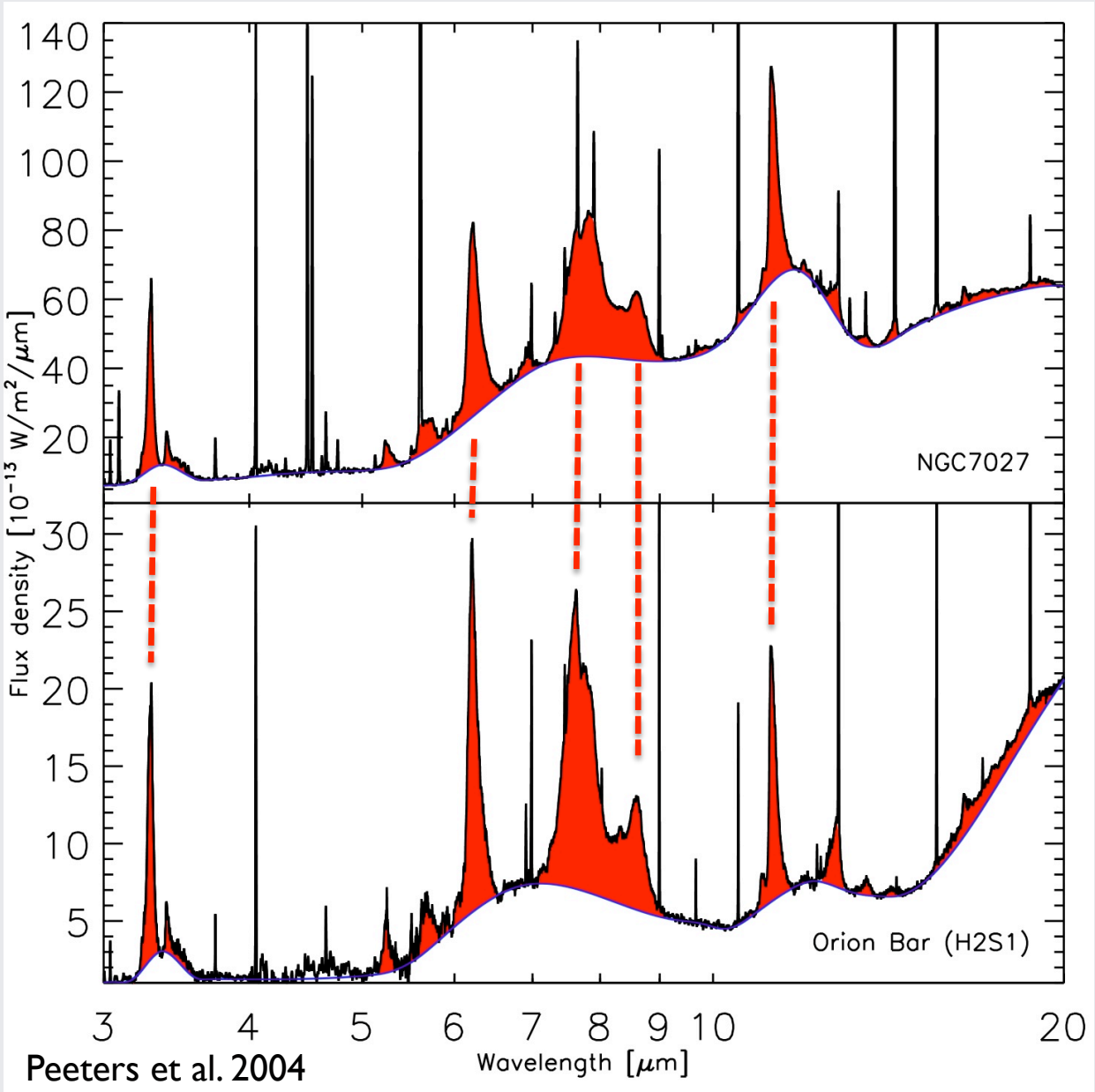
- UIR bands due to vibrational emission of Polycyclic Aromatic Hydrocarbons (PAHs) upon absorption of UV photons (~50 C-atoms)
- Large fraction of the available carbon in PAHs (~5%)
- Important in various physical and chemical processes





NASA Ames Astrochemistry Laboratory

Richness of the PAH spectrum



PAH IR Spectral Database

Ames Research Center

- 2.7 μm - 3.7 mm (mid - far IR)
- ~60 laboratory spectra (~200 measured)
- ~600 theoretical spectra
- $8 \leq N_{carbon} \leq 150$

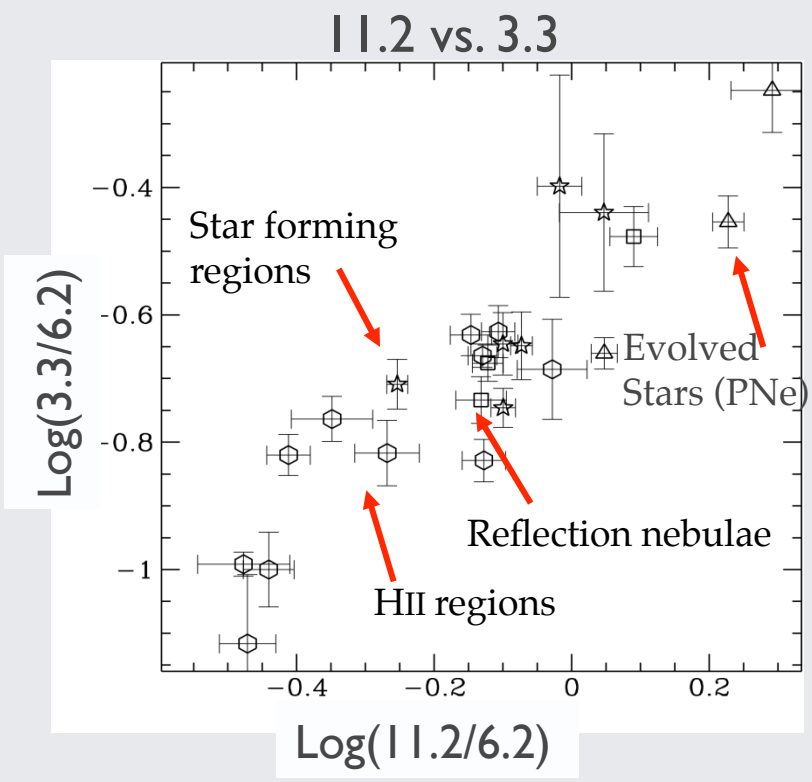
http://www.astrochem.org/pahdb/

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

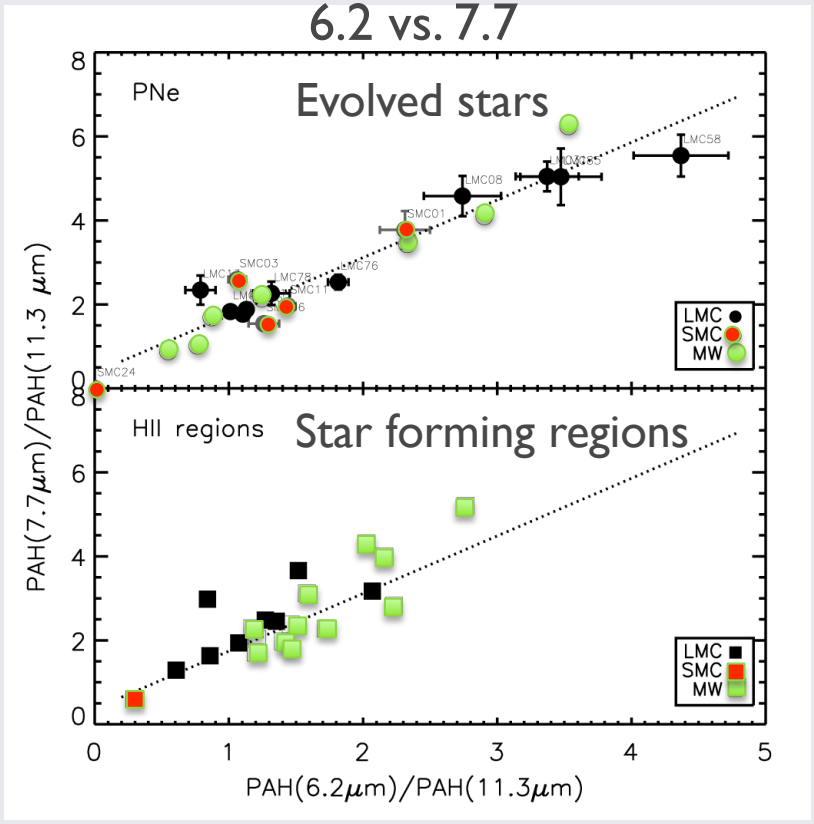


PAH intensities

- vary from object to object



Hony (Peeters) et al. 2001

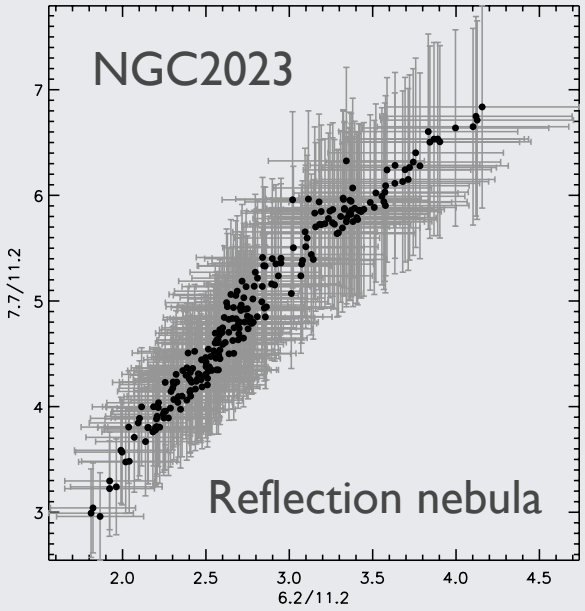


HII regions: Vermeij, Peeters et al. 2002
PNe: Bernard-Salas, Peeters et al. 2009

PAH intensities

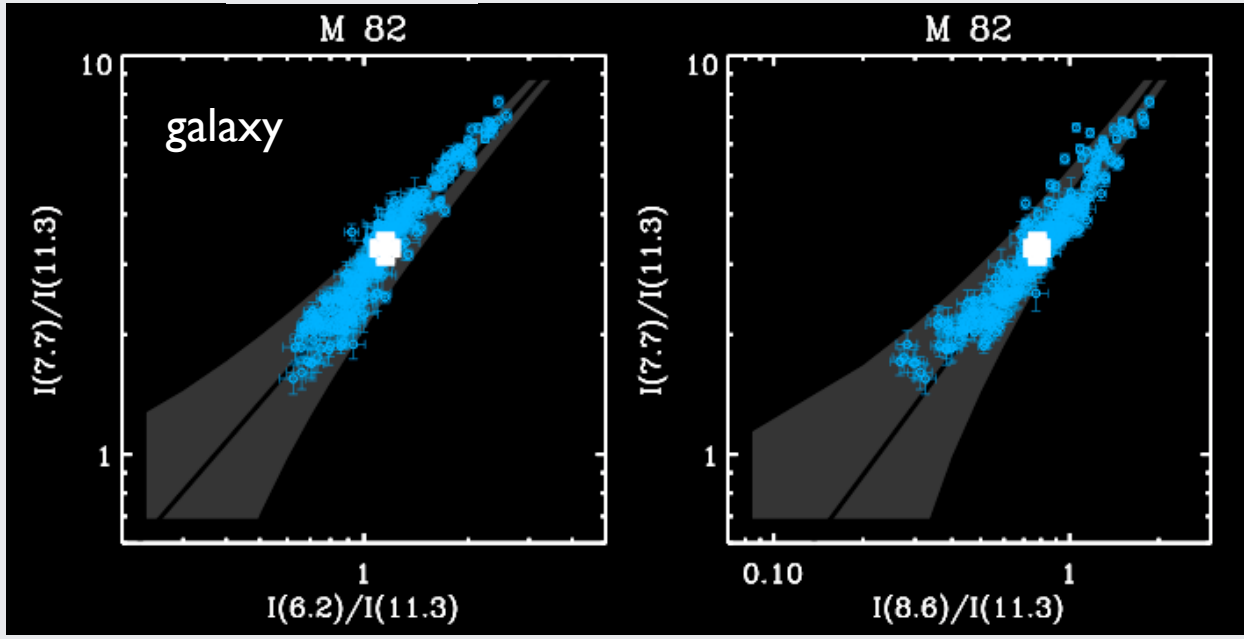
- vary within extended sources

6.2 vs. 7.7



Peeters et al., in prep.

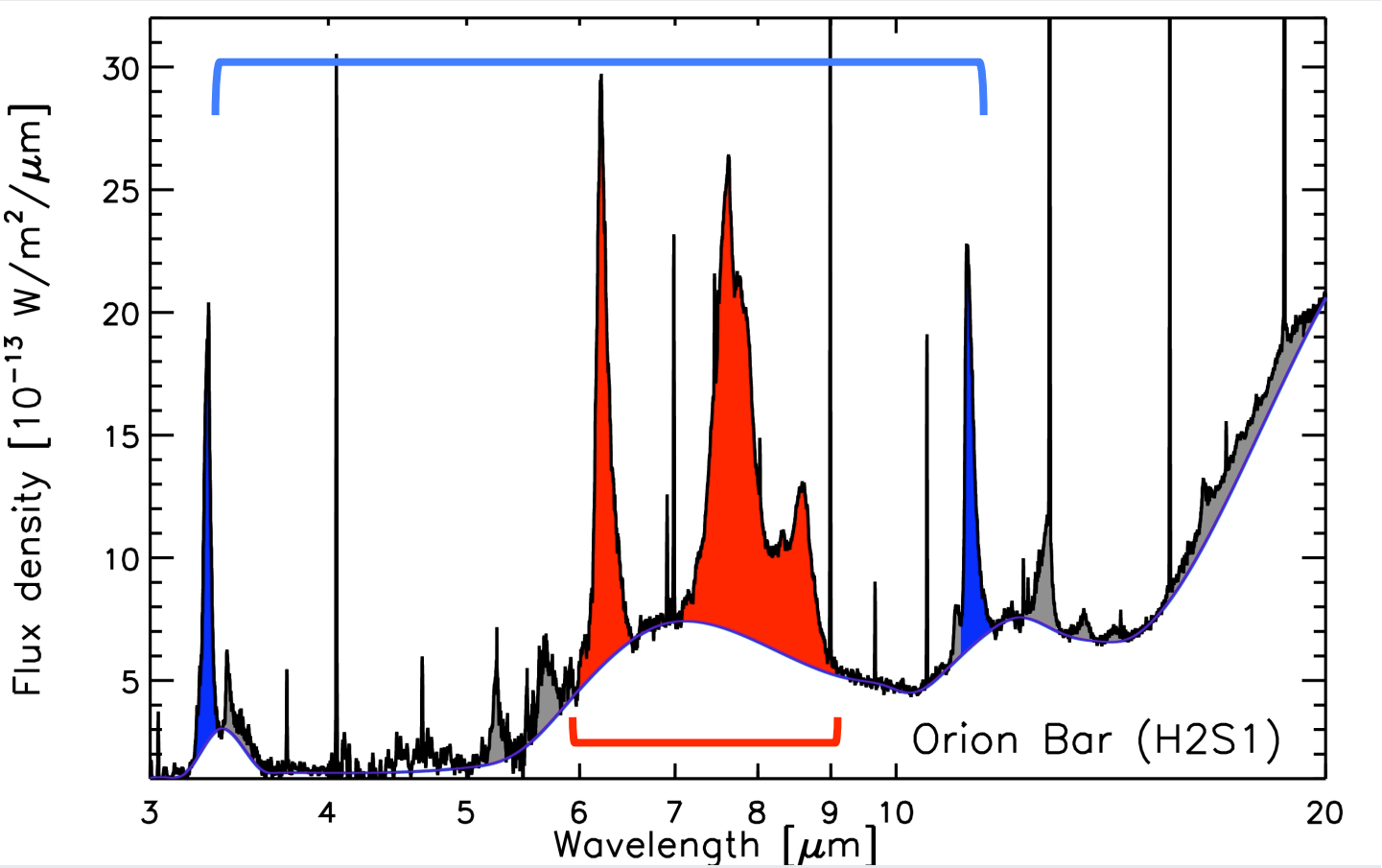
6.2 vs. 7.7 8.6 vs. 7.7



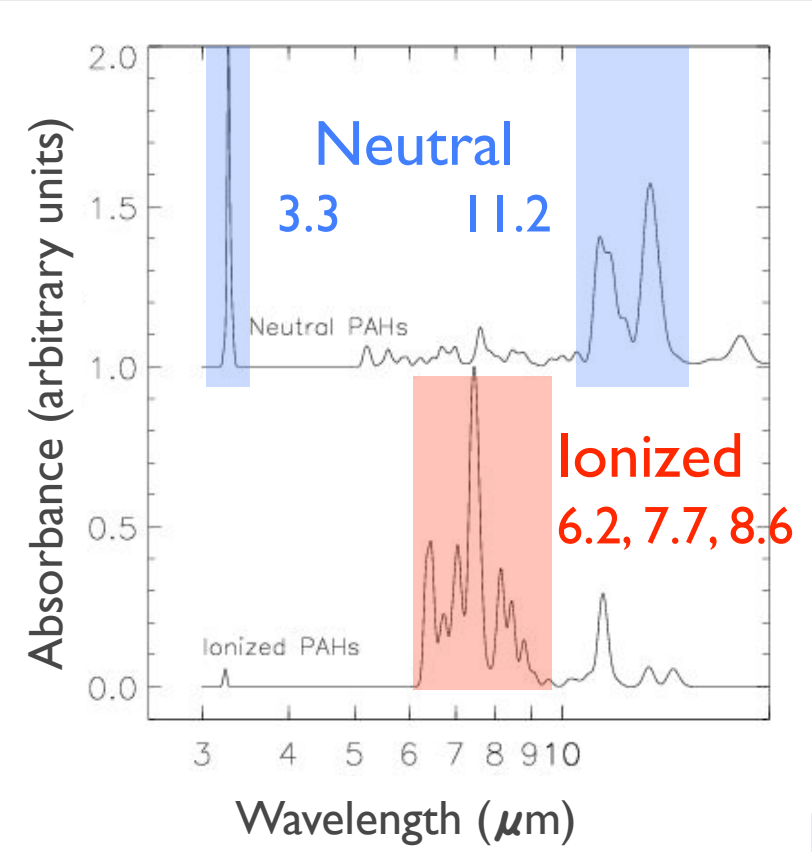
Galliano (Peeters) et al. 2008

PAH intensities

- families:
  - 3.3, 11.2
  - 6.2, 7.7, 8.6



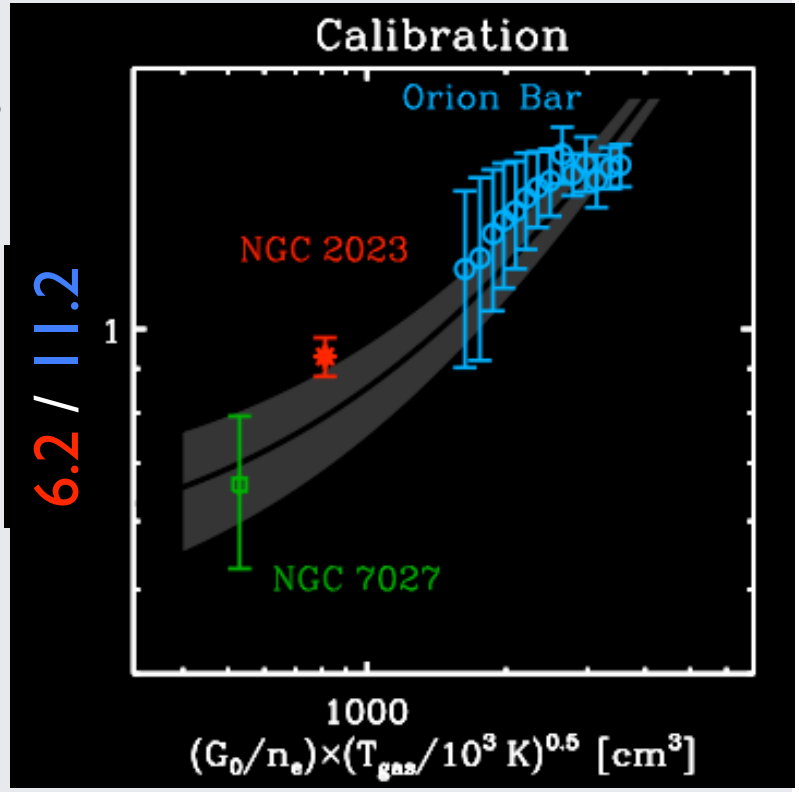
PAH intensities: charge



Allamandola et al. 1999

PAH toolbox?

- Empirical calibration of PAH bands
- Charge of PAHs:
  - Rate of ionization & recombination
  - Determine with other diagnostics
- Goal: PAHs as diagnostic tool for the local physical conditions



Low → High

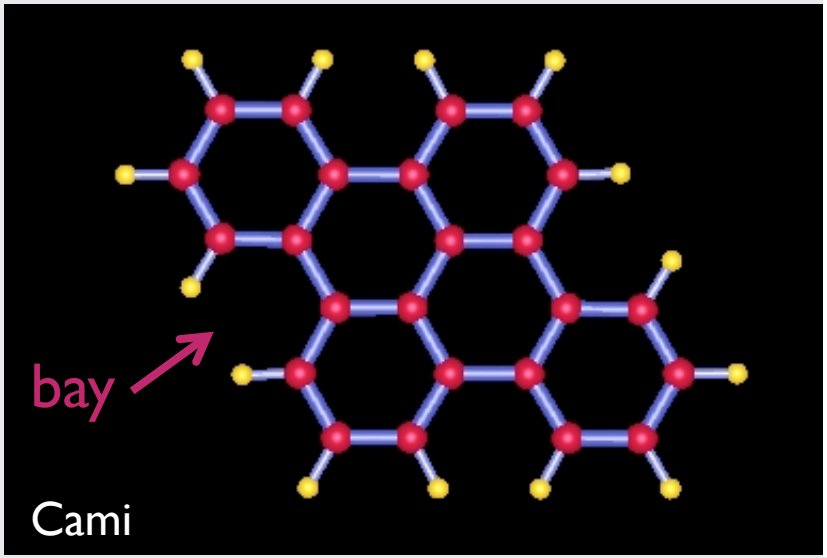
Ionization

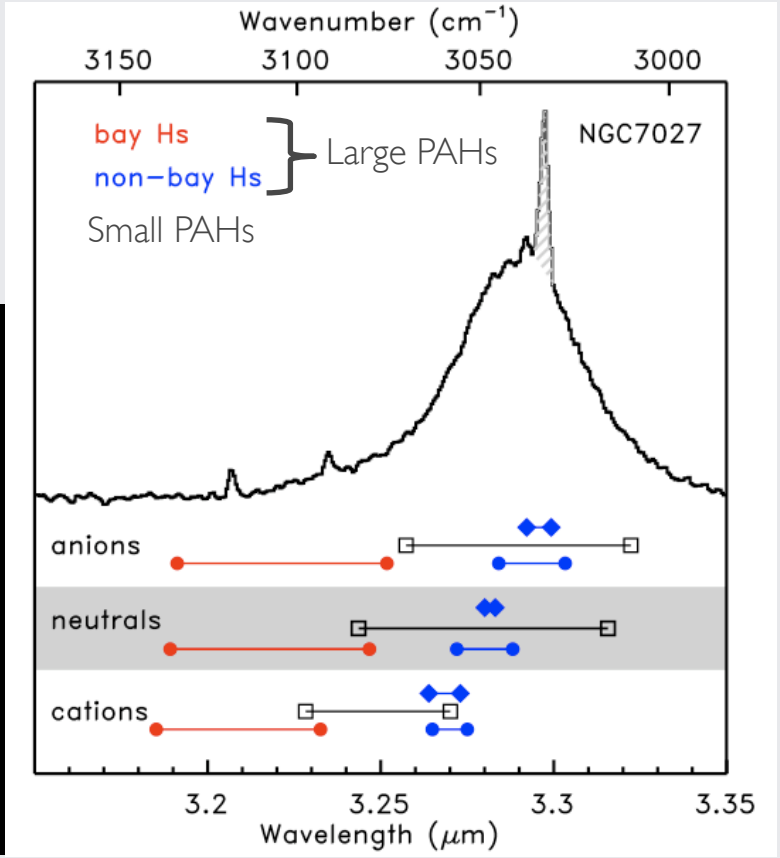
Galliano (Peeters) et al. 2008

PAH intensities: structure

- majority of emission at 3.3 μm due to non-bay Hs

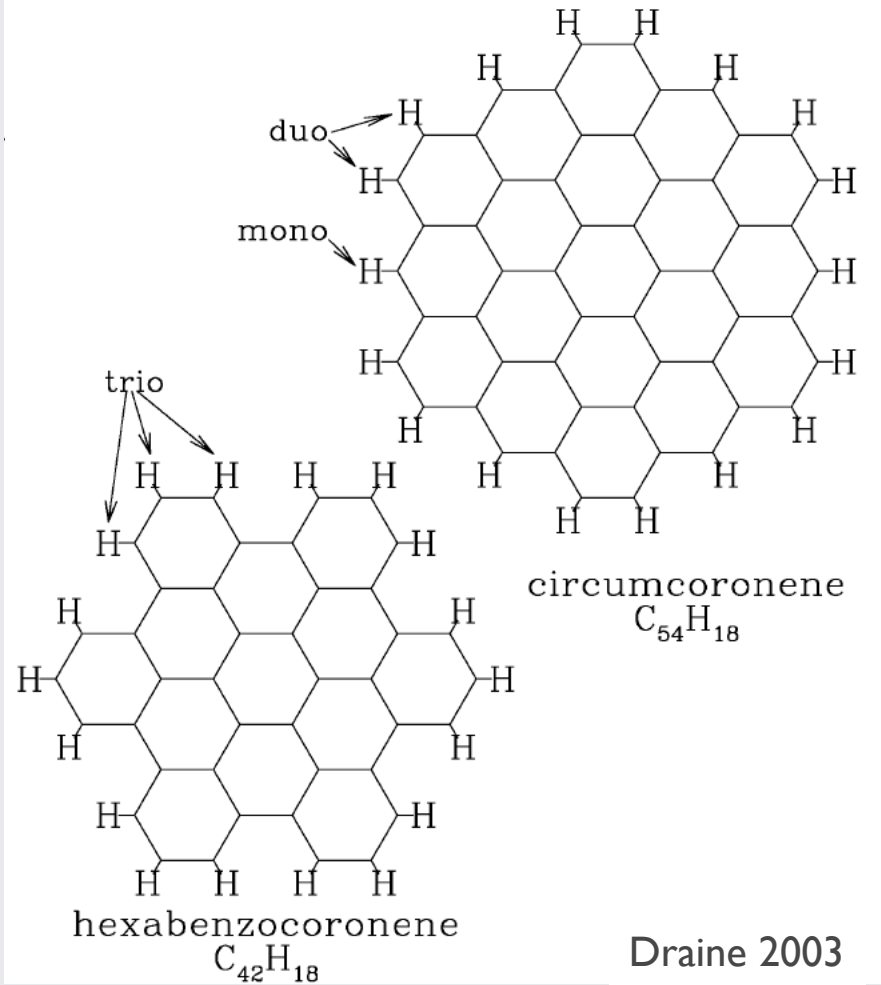
smooth edge structure



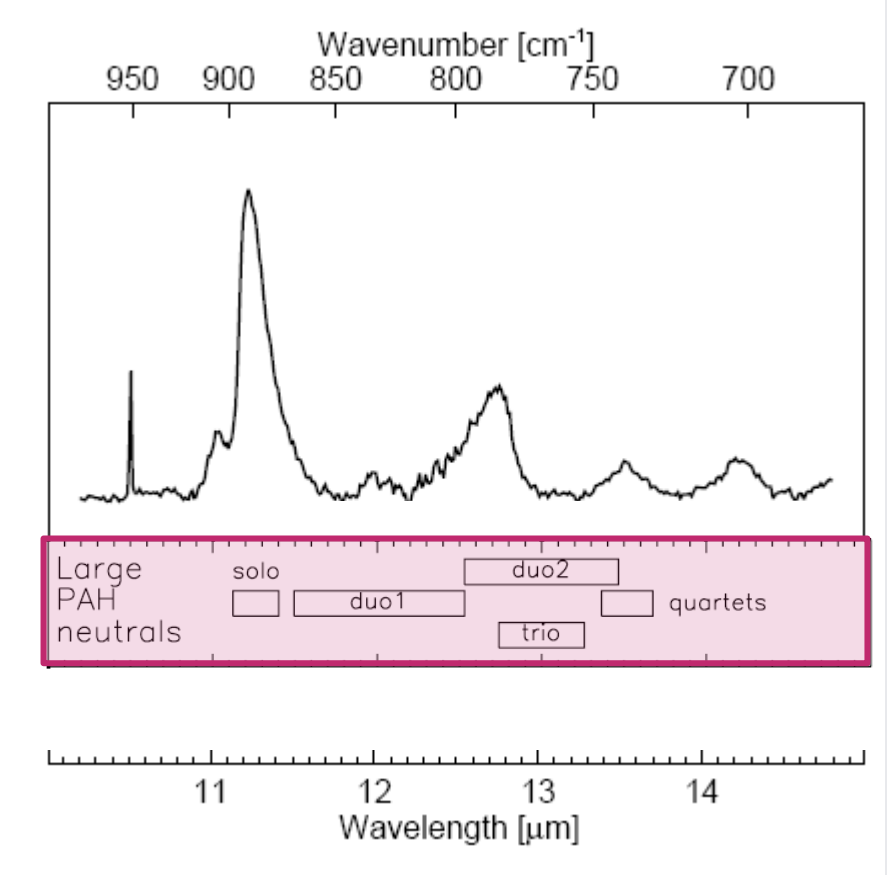


van Diedenhoven, Peeters et al. 2004
Bauschlicher, Peeters, Allamandola 2009

PAH intensities: structures



Draine 2003

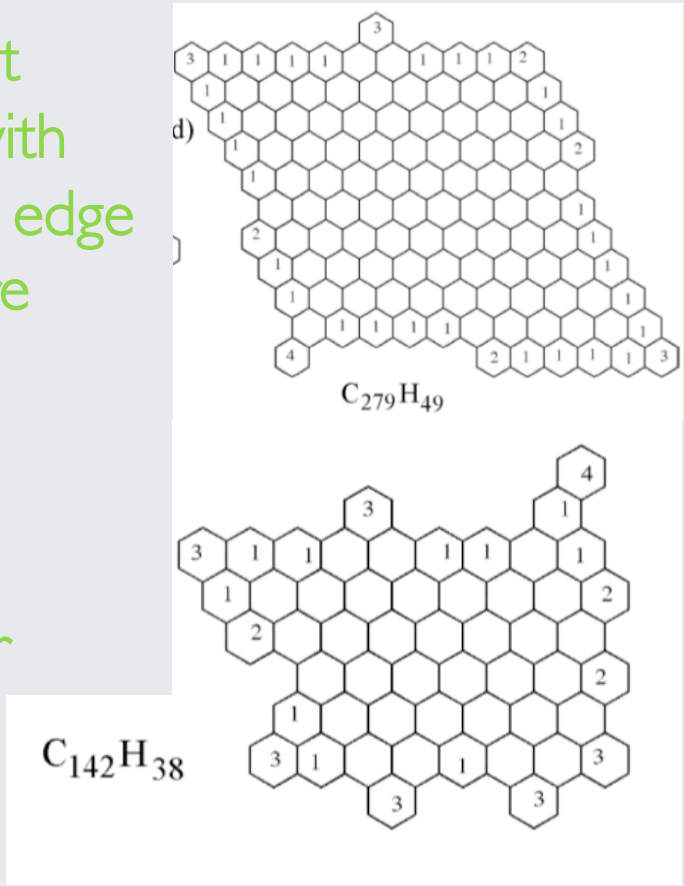


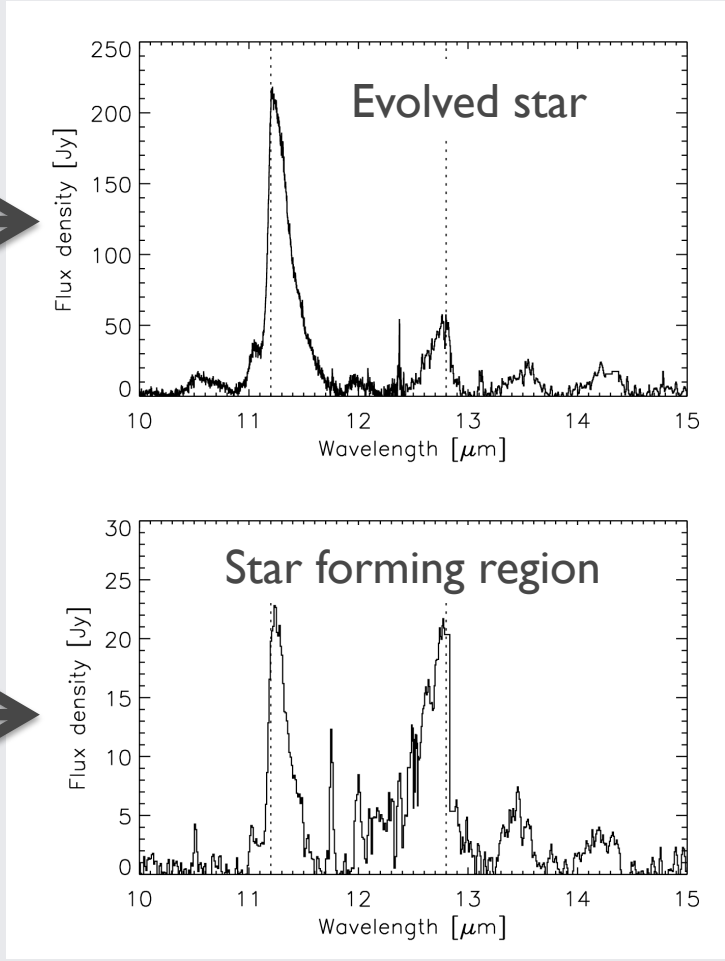
Hony (Peeters) et al. 2001
Bauschlicher, Peeters, Allamandola 2009

PAH intensities: structures

compact PAHs with smooth edge structure

more irregular

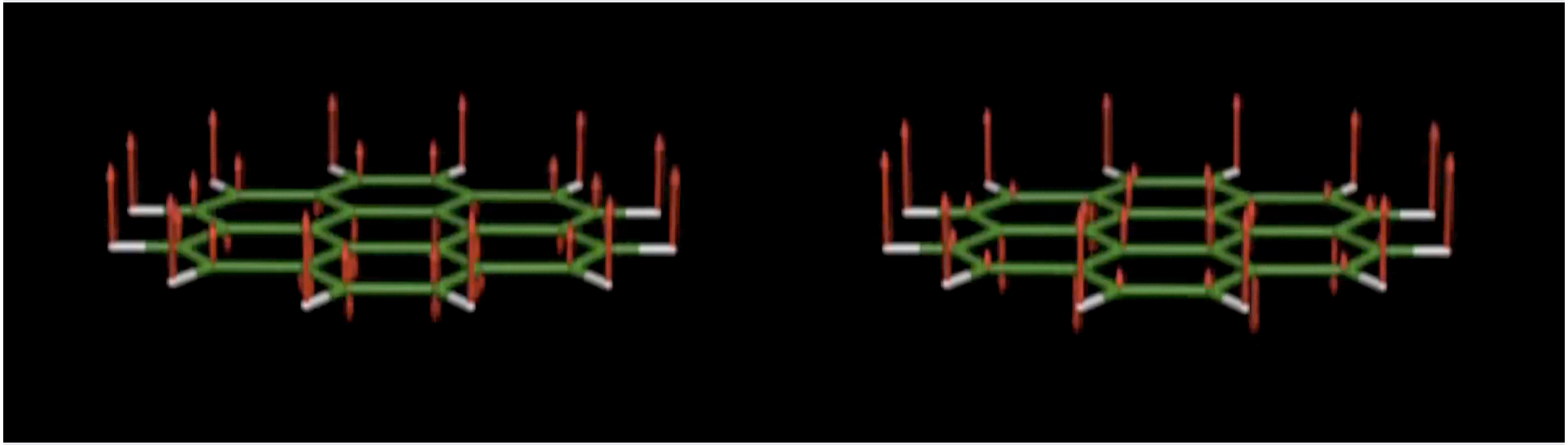




Hony (Peeters) et al. 2001
Bauschlicher, Peeters, Allamandola 2008, 2009

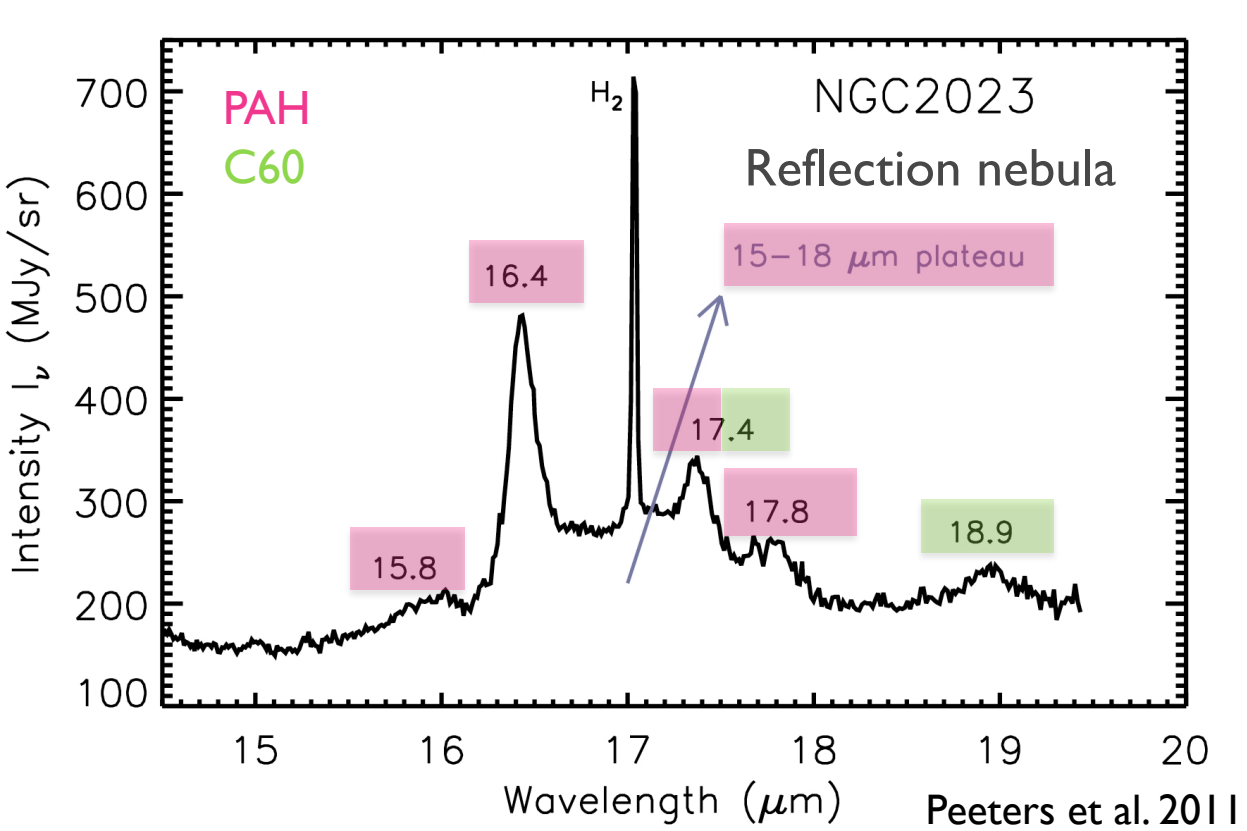
PAH intensities: structures

- PAH bands at longer wavelengths ($\lambda > 15$ μm) due to vibrations of entire PAH skeleton
  ---- more sensitive to molecular structure



NASA Ames Astrochemistry Lab

PAH intensities: 15-20μm



Observations vs. lab/theory

- Charge:
  - no influence on peak position
  - little influence on relative intensities
- Structure:
  - 16.4 band: PAHs with pendant ring or pointy edges
  - large compact PAHs show emission near 17.4
  - no systematic behaviour for other bands

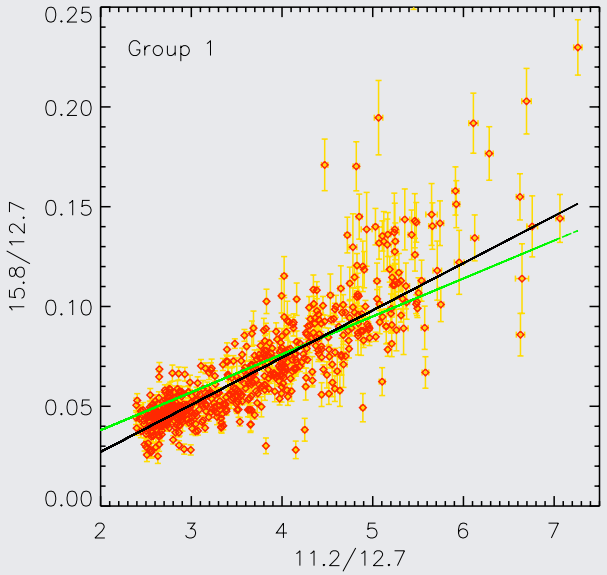
Boersma (Peeters) et al. 2010

Database is highly biased

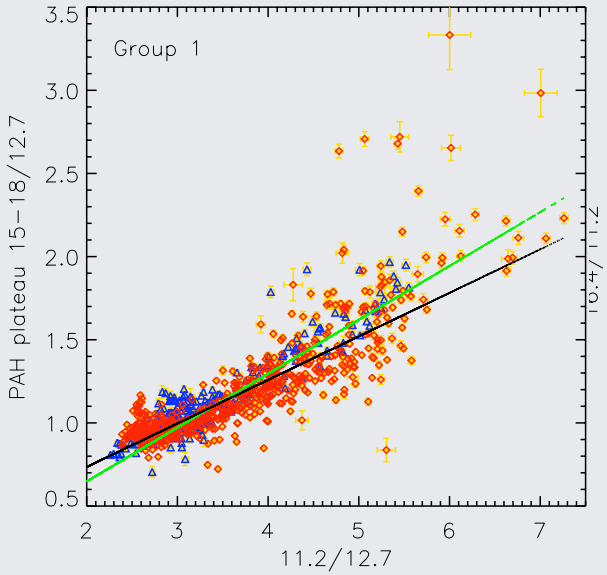
PAH intensities: 15-20μm

Reflection Nebula NGC2023

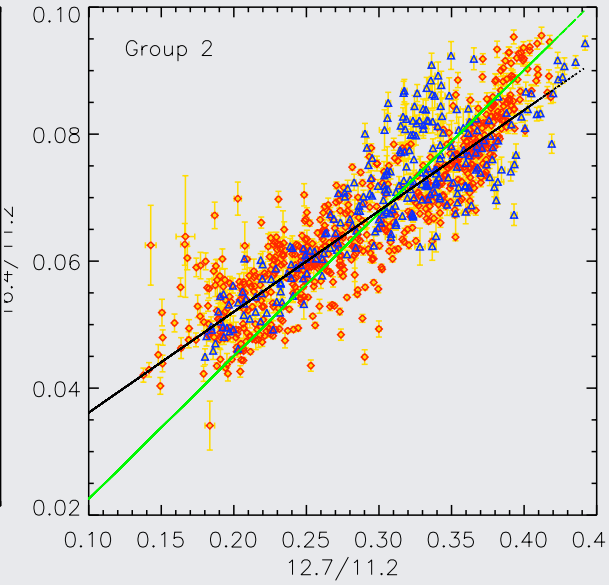
11.2 vs. 15.8



11.2 vs plateau

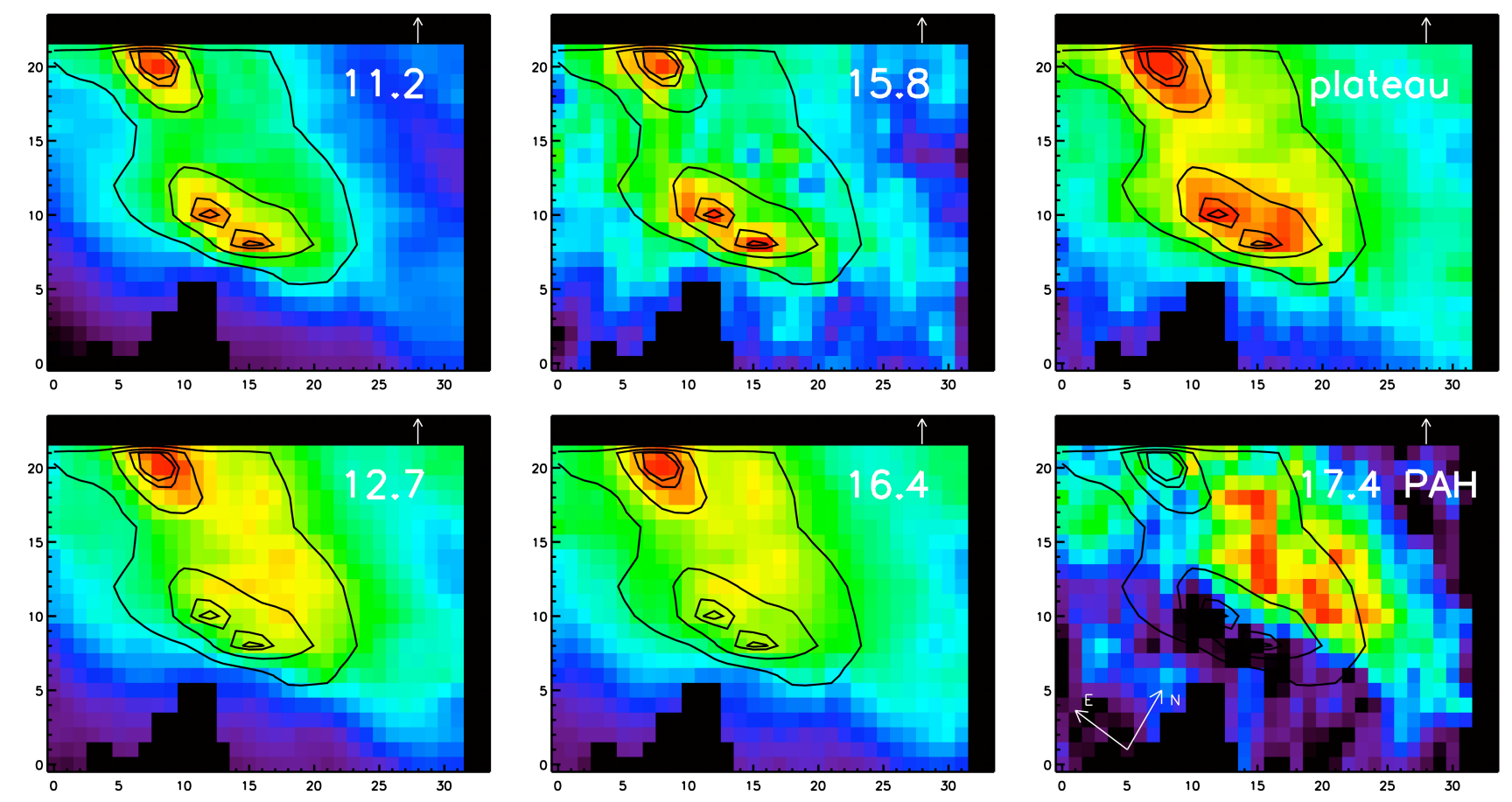


12.7 vs 16.4



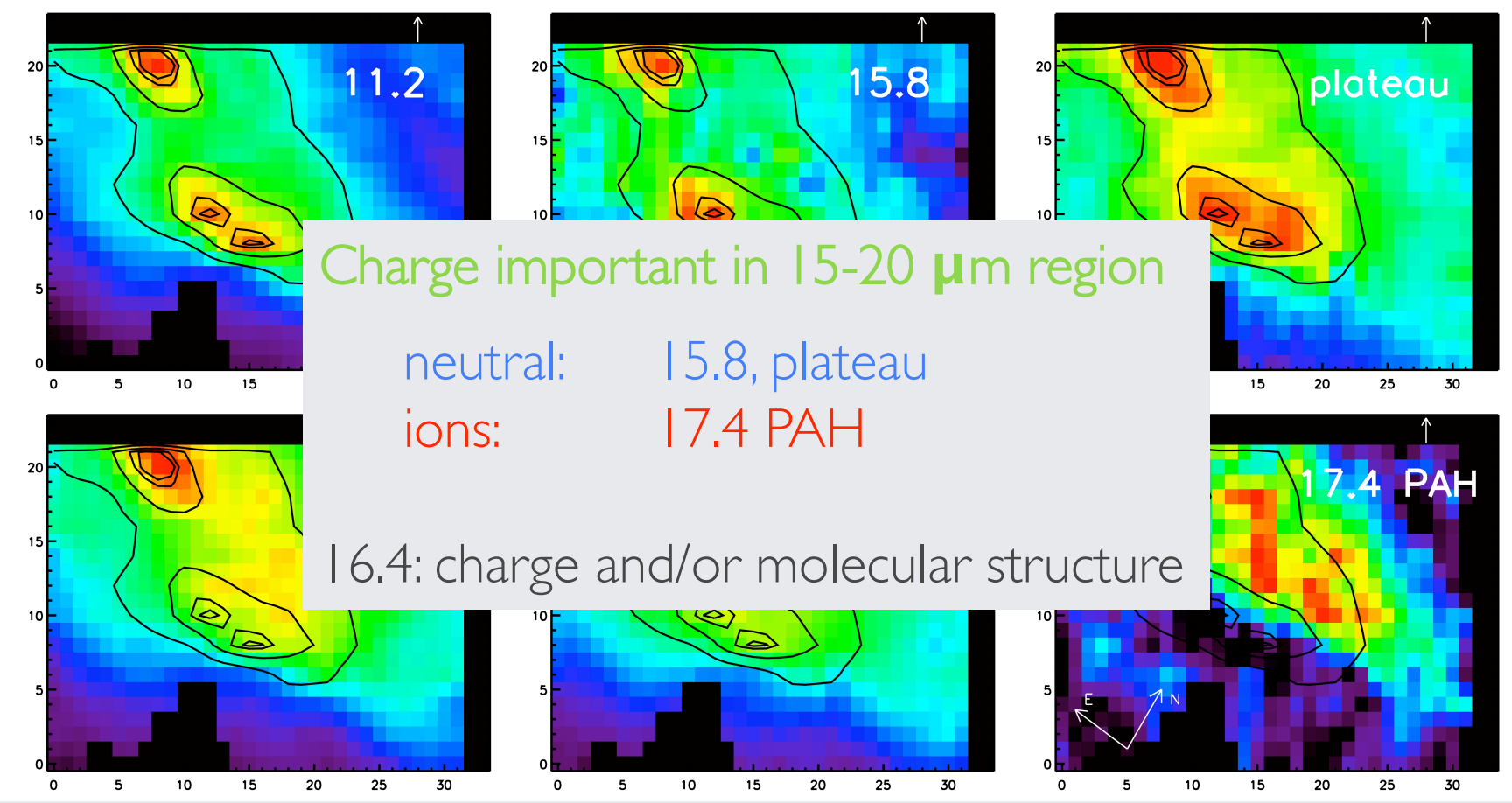
Peeters et al. 2011

PAH intensities: 15-20μm



Peeters et al. 2011

PAH intensities: 15-20μm



Charge important in 15-20 μm region

neutral: 15.8, plateau

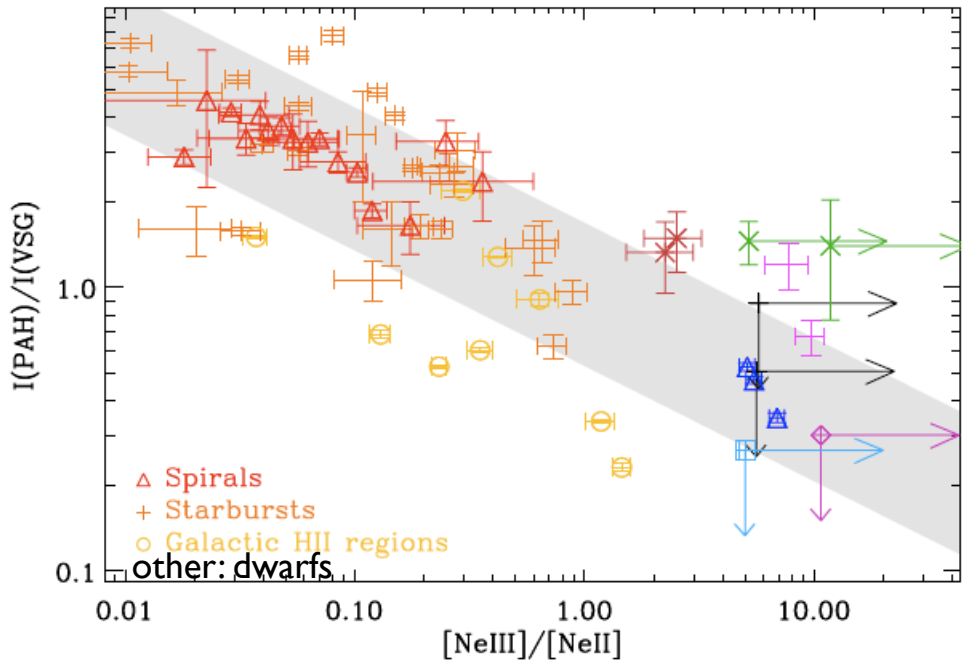
ions: 17.4 PAH

16.4: charge and/or molecular structure

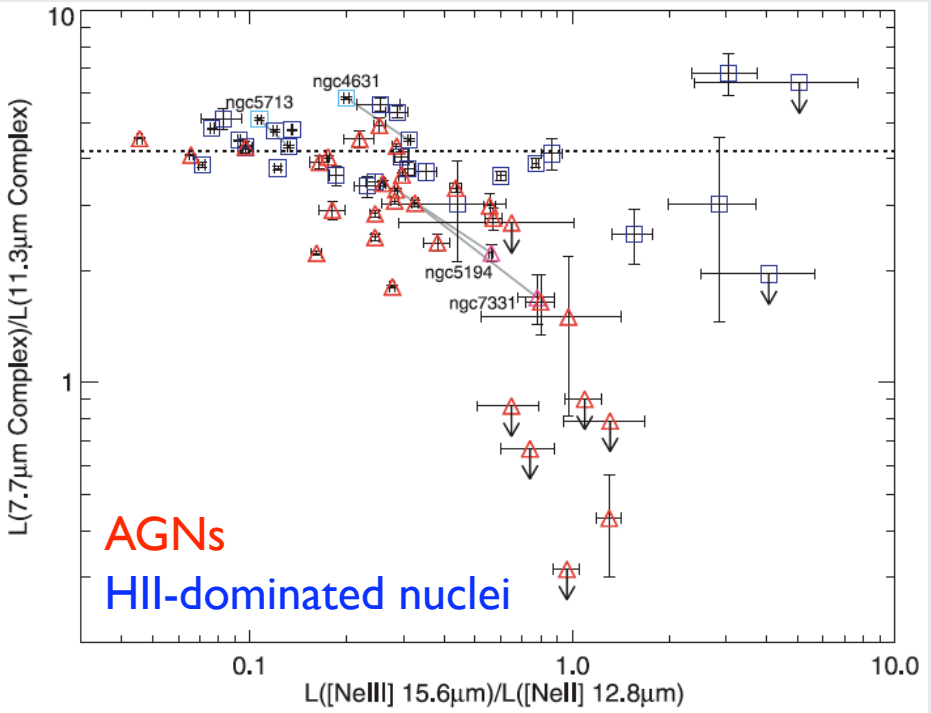
Peeters et al. 2011

PAH intensities

- Dependence on:
  - Hardness of radiation field
  - Metallicity



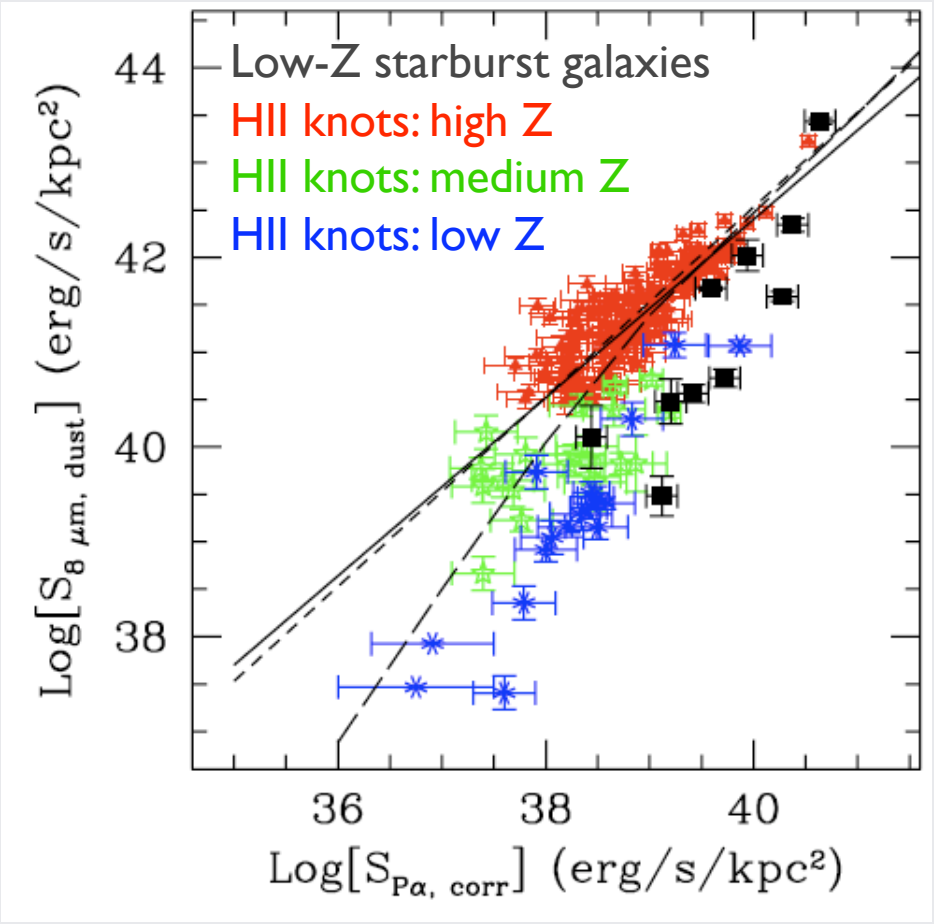
Madden et al. 2006



Smith et al. 2007

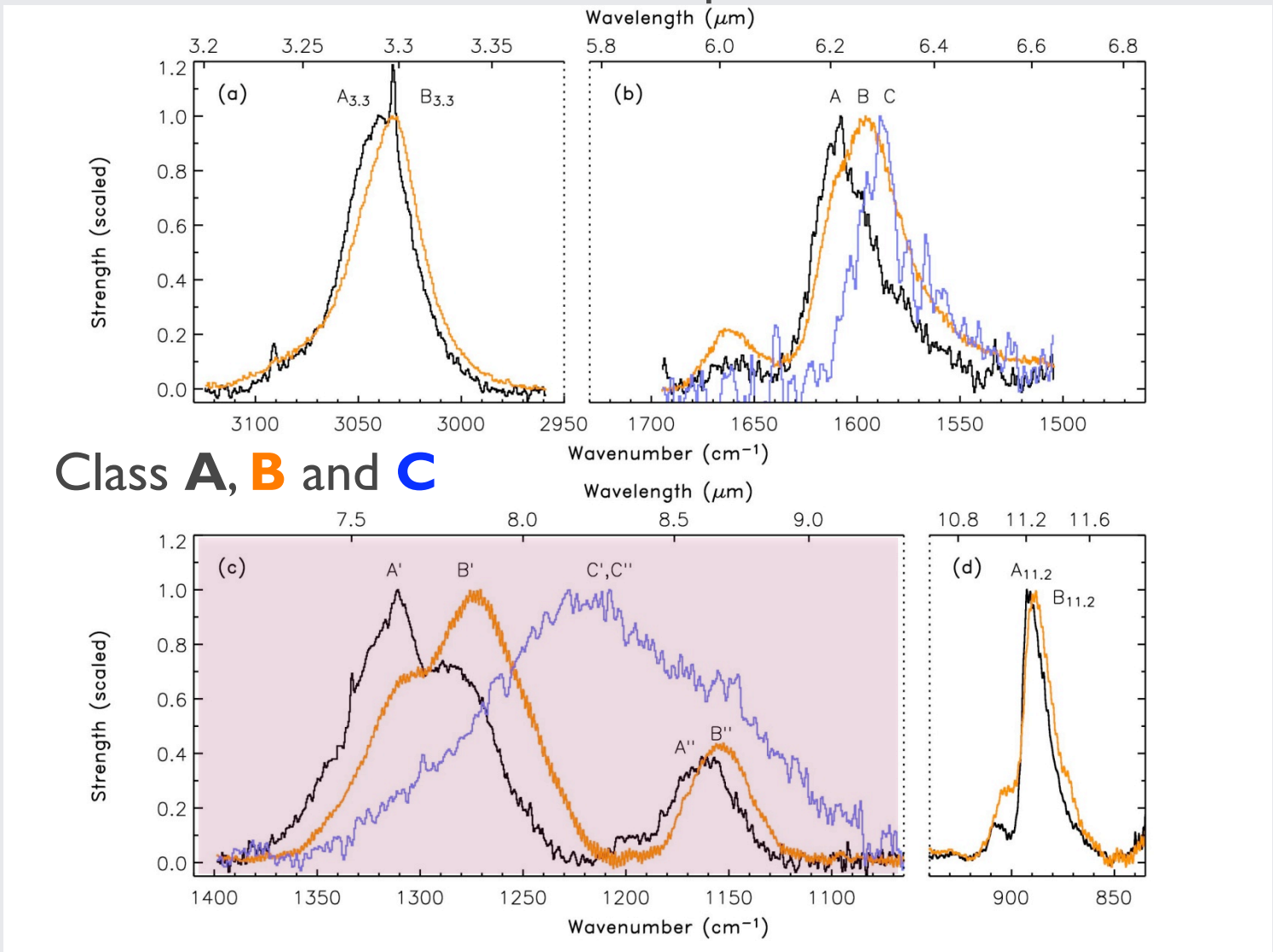
PAH toolbox

- Tracer of star formation
- Tool to distinguish between AGN vs. starburst



Calzetti et al. 2007

PAH band profiles

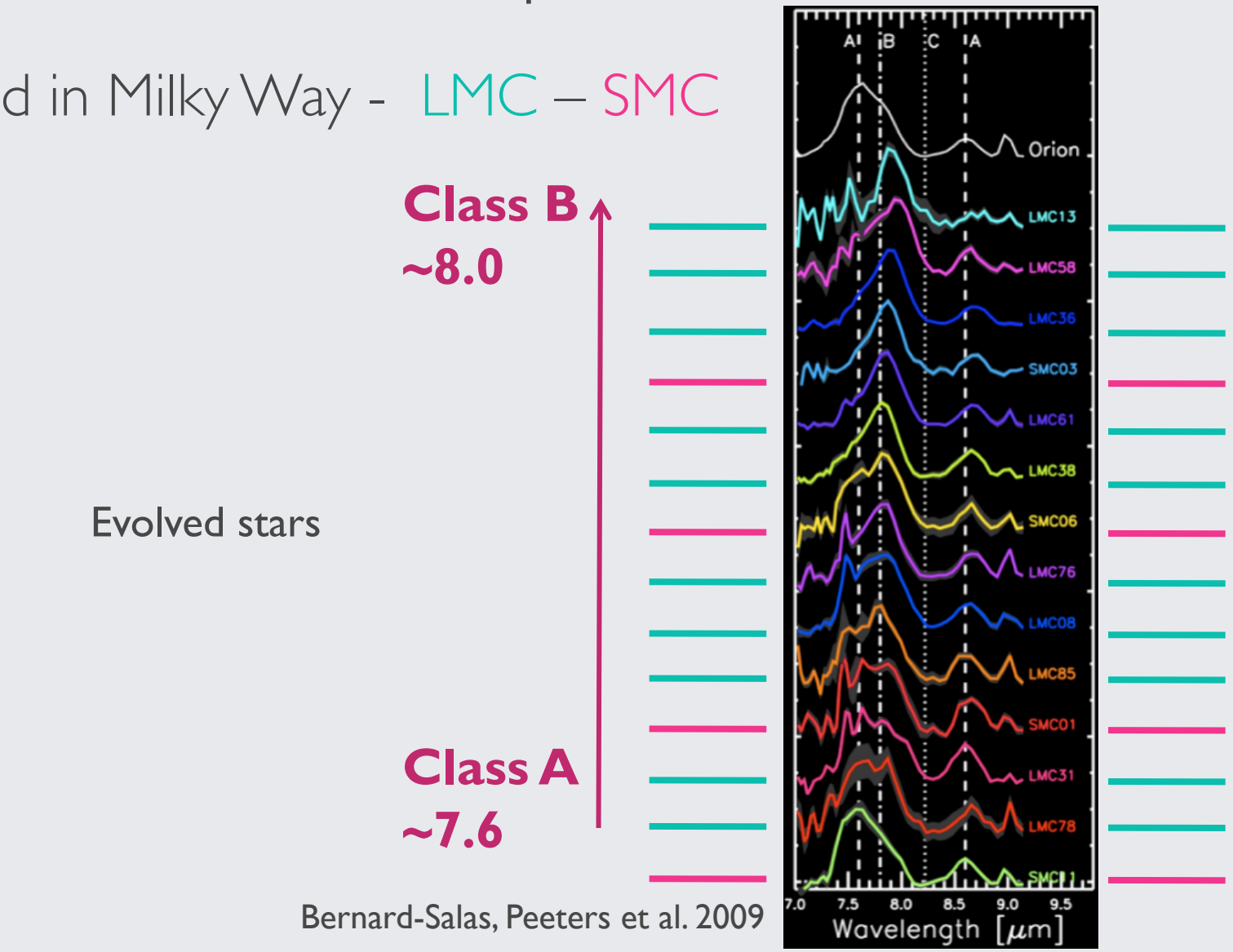


Class **A**, **B** and **C**

Peeters et al. 2002, van Diedenhoven, Peeters et al. 2004

PAH band profiles

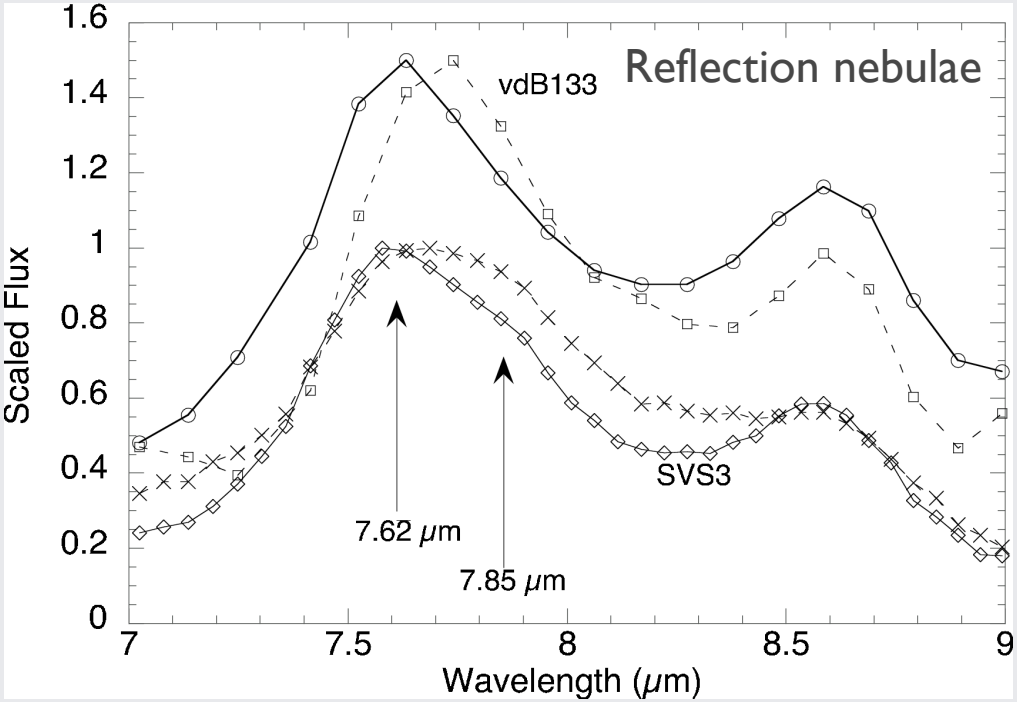
- Observed in Milky Way - LMC – SMC



Bernard-Salas, Peeters et al. 2009

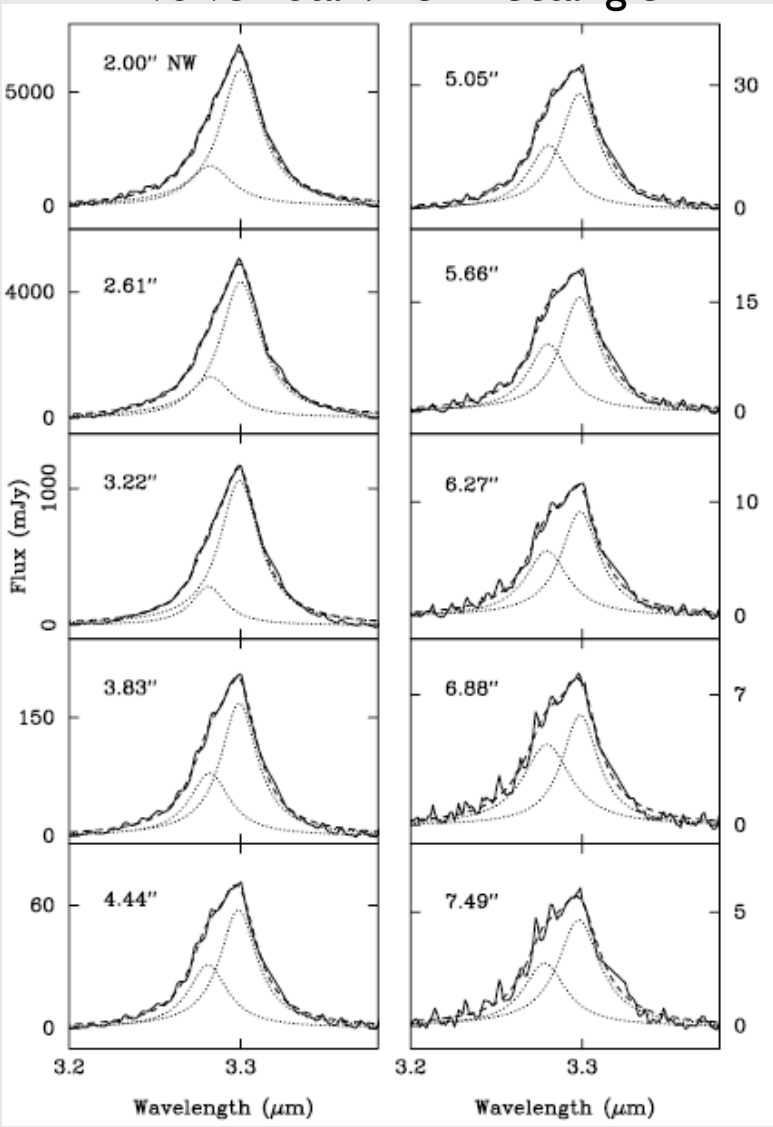
PAH band profiles

- Variation within extended sources



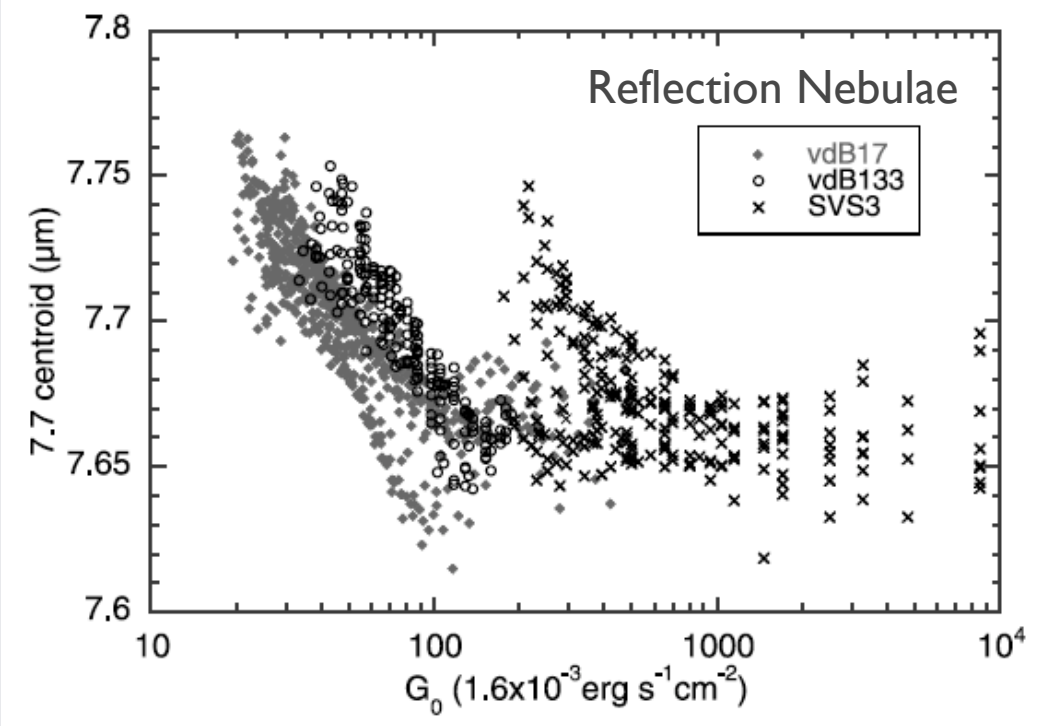
Bregman et al. 2005

Evolved Star: Red Rectangle



Song et al. 2007

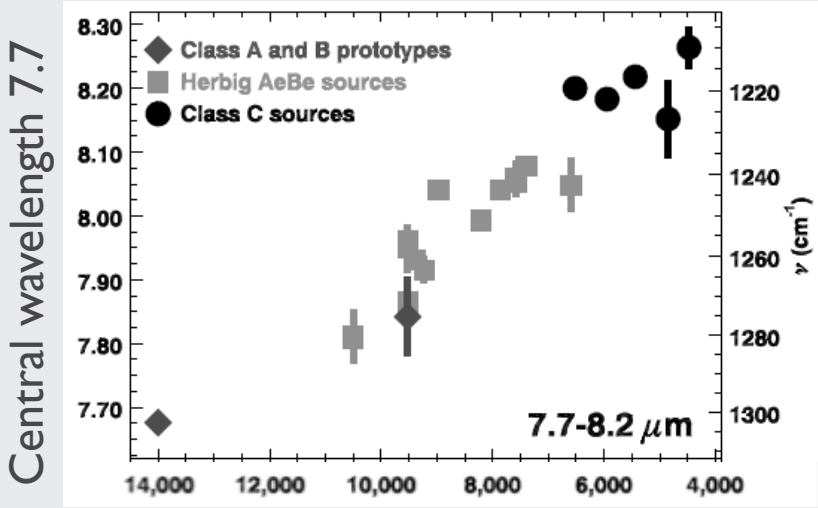
PAH band profiles



Bregman & Temi 2005

PAH band profiles

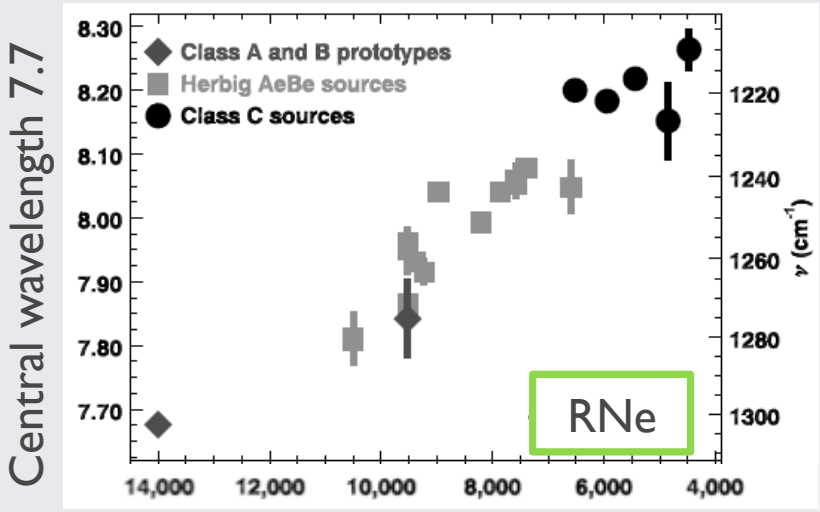
UV processing of PAHs



Sloan et al. 2007, Keller et al. 2008

PAH band profiles

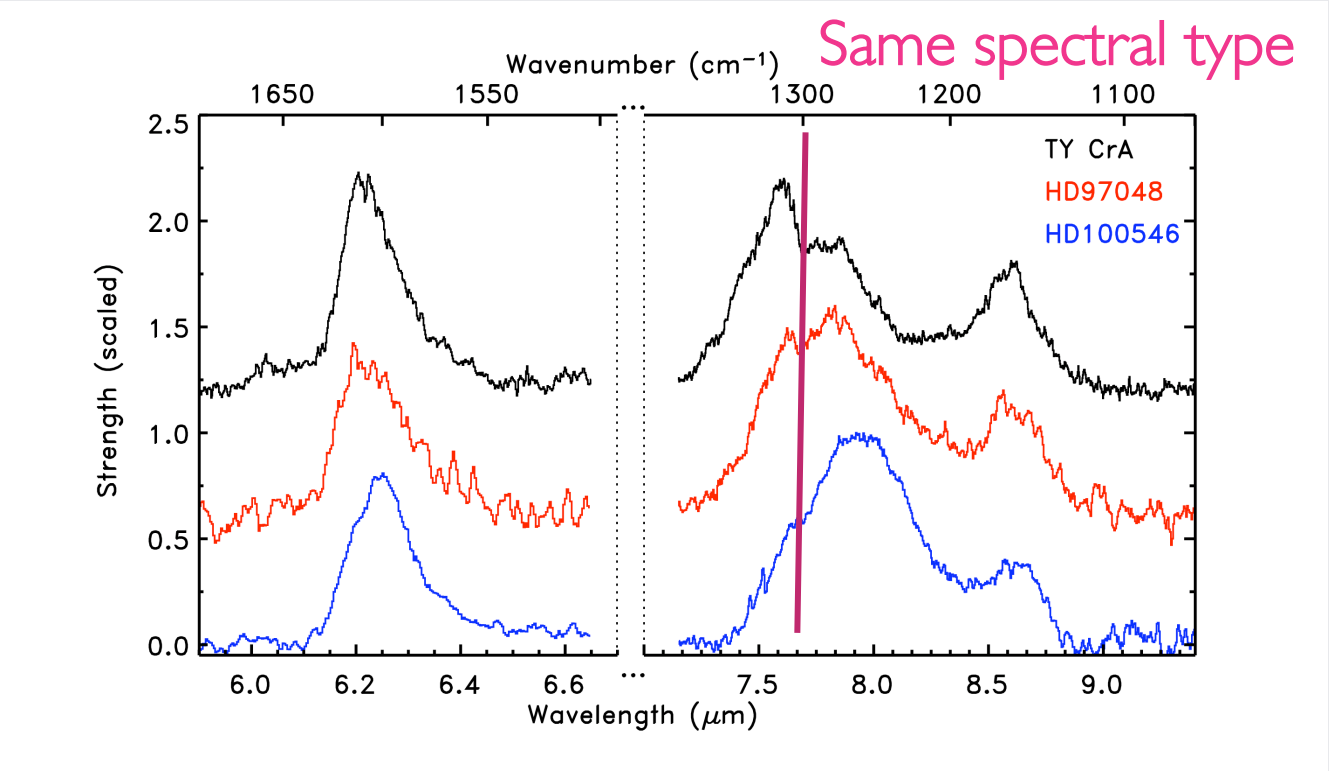
PNe



Sloan et al. 2007, Keller et al. 2008

PAH band profiles

- Circumstellar (HD100546) versus interstellar (TY Cra)



Van Kerckhoven 2002, Peeters et al. 2002, Boersma et al. 2008

PAH band profiles

Circumstellar material vs. interstellar material

UV processing

chemical modification of the PAH population

PAH band profiles

proposed interpretations:

- hetero-atom substituted PAHs

(e.g. Peeters et al. 2002, Hudgins et al. 2005, Bauschlicher, Peeters et al. 2009)

- PAH-metal complexes

(e.g. Hudgins et al. 2005, Bauschlicher, Peeters et al. 2009, Simon & Joblin 2007, Joalland et al. 2009)

- PAH clusters

(e.g. Peeters et al. 2002, Rapacioli et al. 2005, Simon & Joblin 2009)

- aliphatic vs aromatic

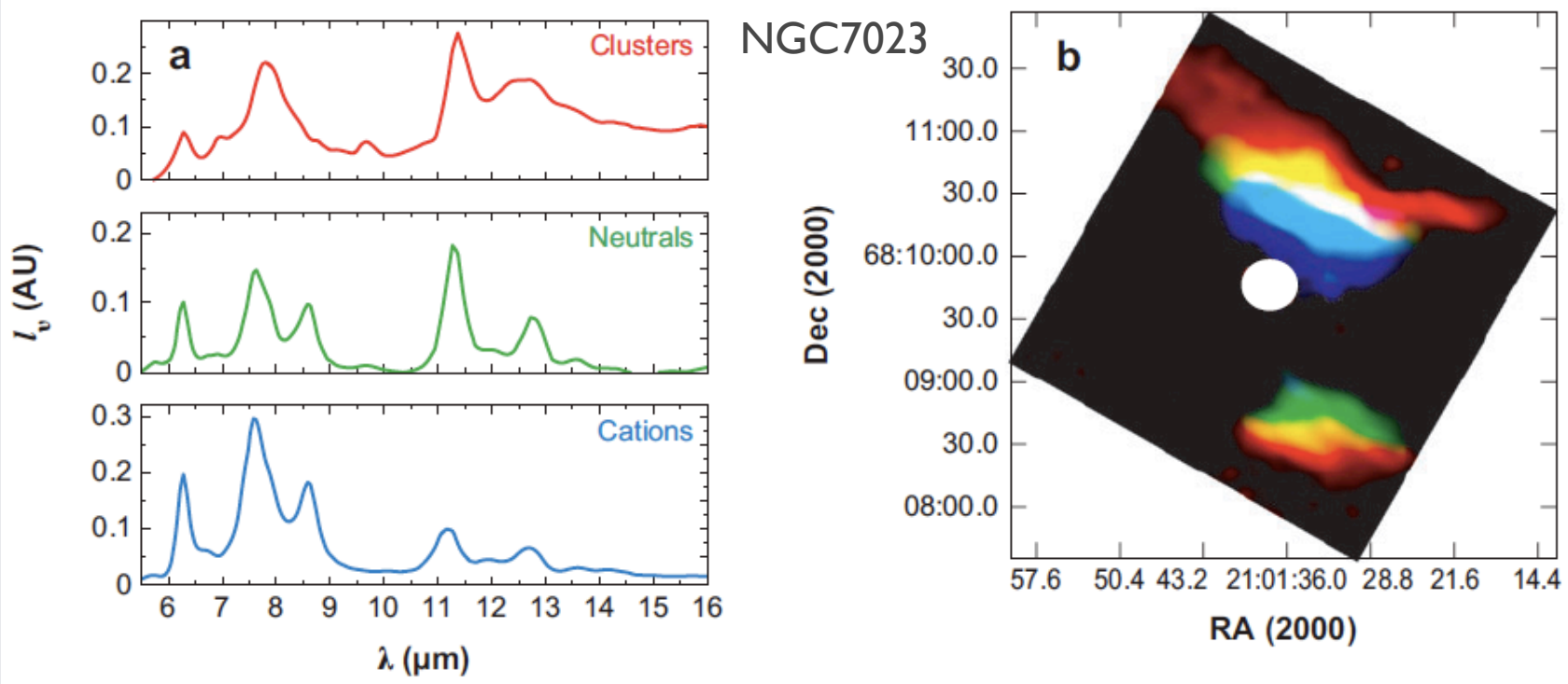
(e.g. Sloan et al. 2007, Pino et al. 2008, Kwok & Zhang 2011)

- PAH size

(e.g. Bauschlicher, Peeters et al. 2008, 2009, Cami 2011, Cami, (Peeters) et al. 2011.)

Spectral decomposition

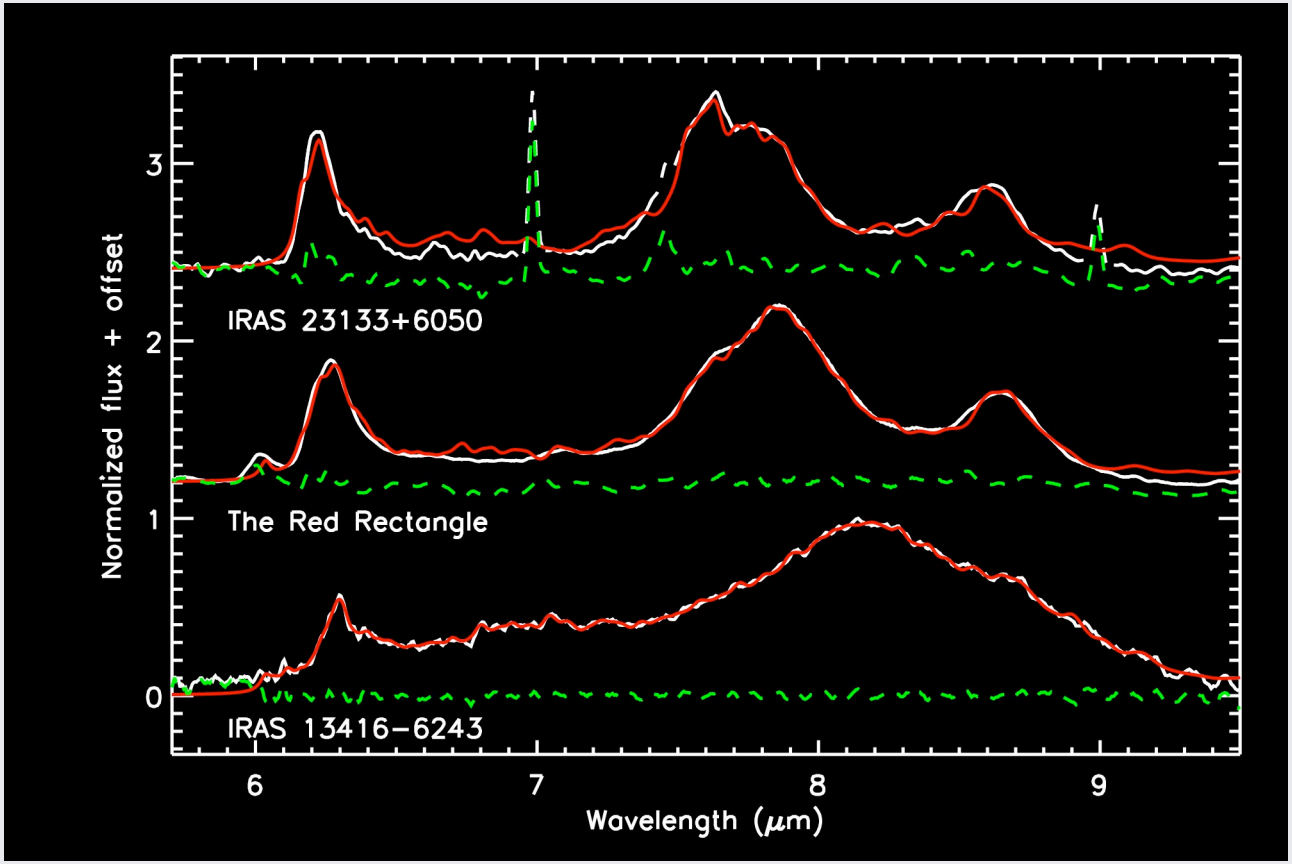
- Singular value decomposition: separate components with different spatial distributions
- PAH^0, PAH^+, VSGs (i.e. clusters), BF8, BF12, PAH^x, dBF
- destruction of VSGs by UV to form PAHs



Rapacioli et al. '05, Berné et al. '07, '08, '09, Joblin et al. '08, Rosenberg et al. '11

Spectral fitting

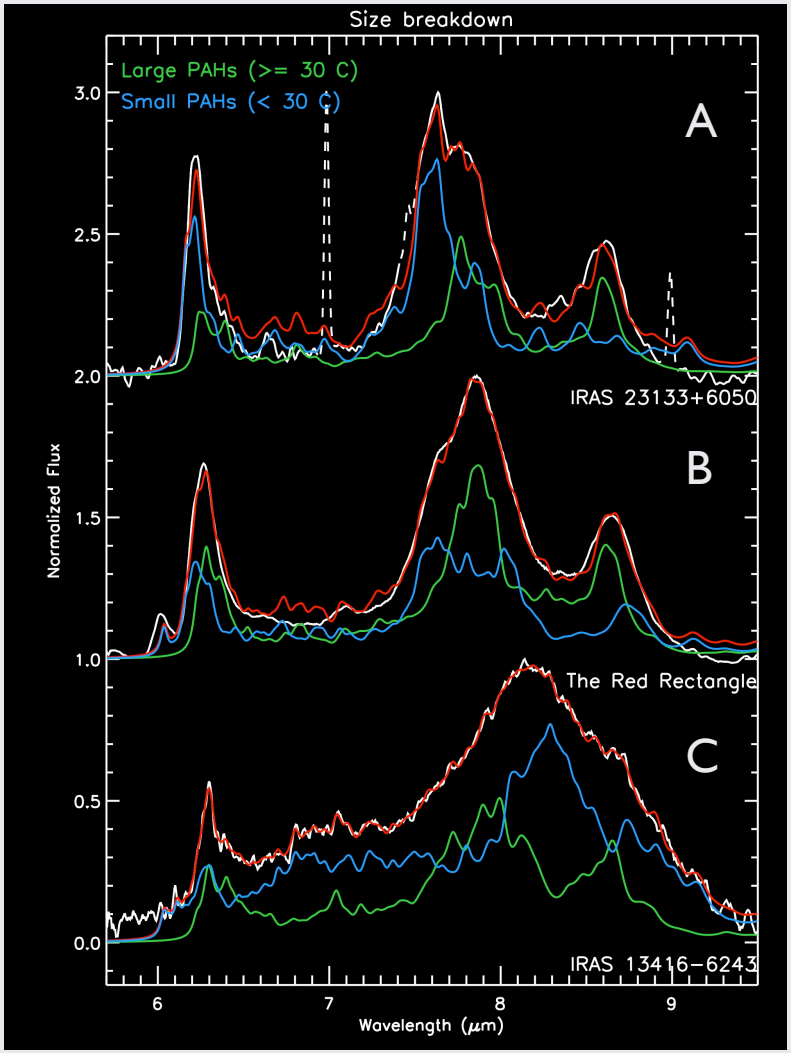
- Fit with NASA Ames PAH Database

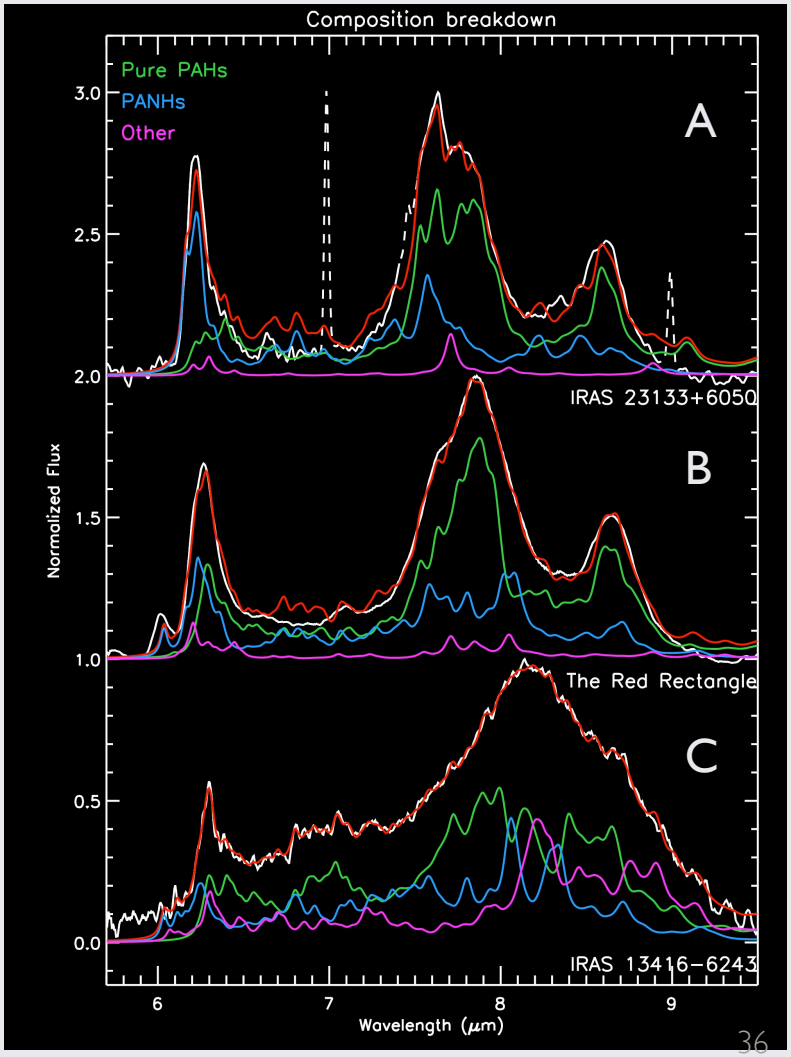


Cami 2011, Cami (Peeters) et al., 2011

Spectral fitting

- Fit with NASA Ames PAH Database





Cami 2011, Cami (Peeters) et al., 2011

(refined) PAH hypothesis

- Still alive and kicking
- PAHs: not strict chemical definition
  - Impurities
  - Clusters
  - …

Summary

Proceedings conference: "PAHs and the Universe"

EAS Publications Series, Vol. 46, 2011

- PAH emission reveals:
  - Ionization state
  - Interaction with environment
  - Molecular structure
  - Active modification of PAH population
- PAH toolbox