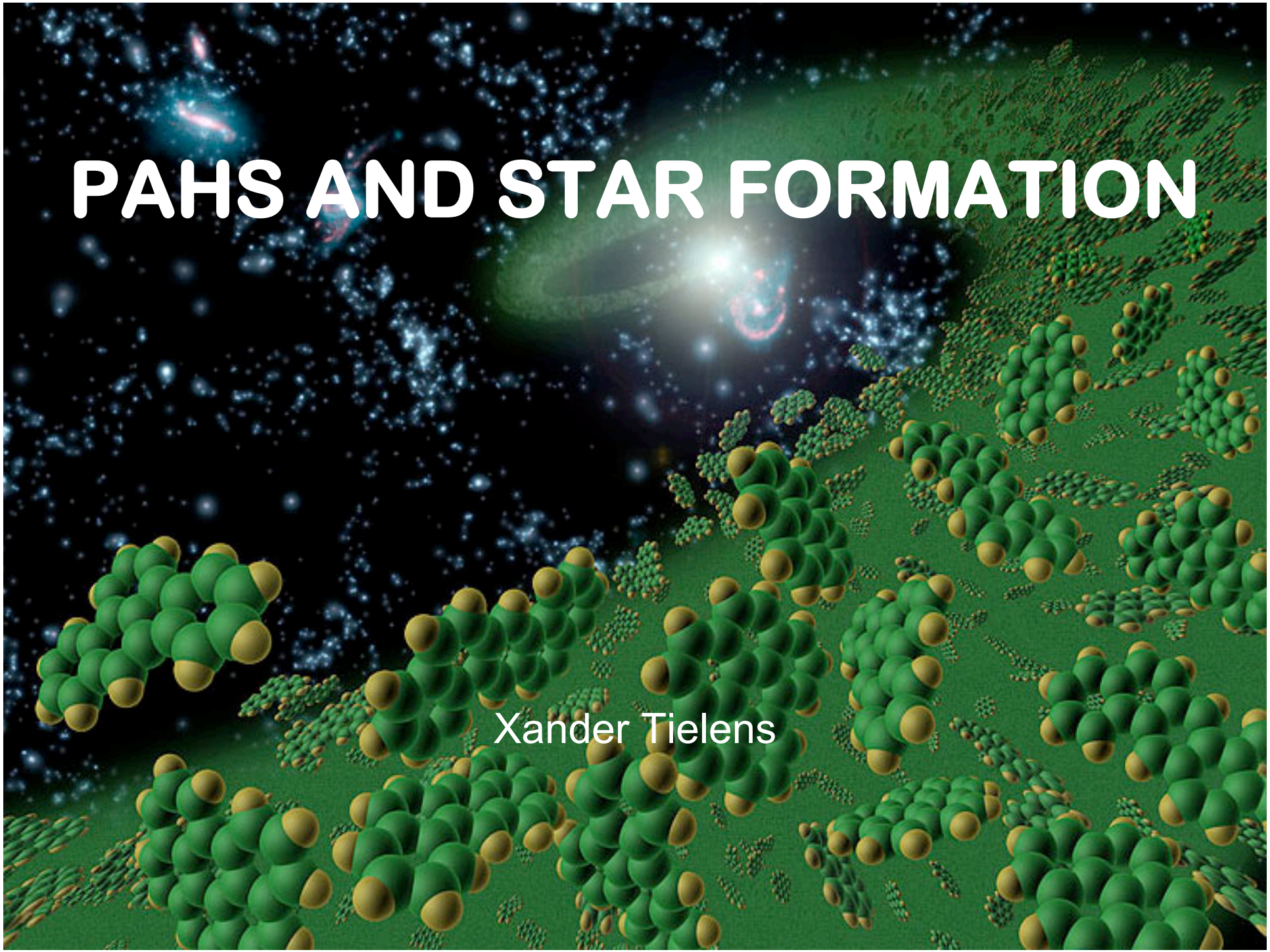
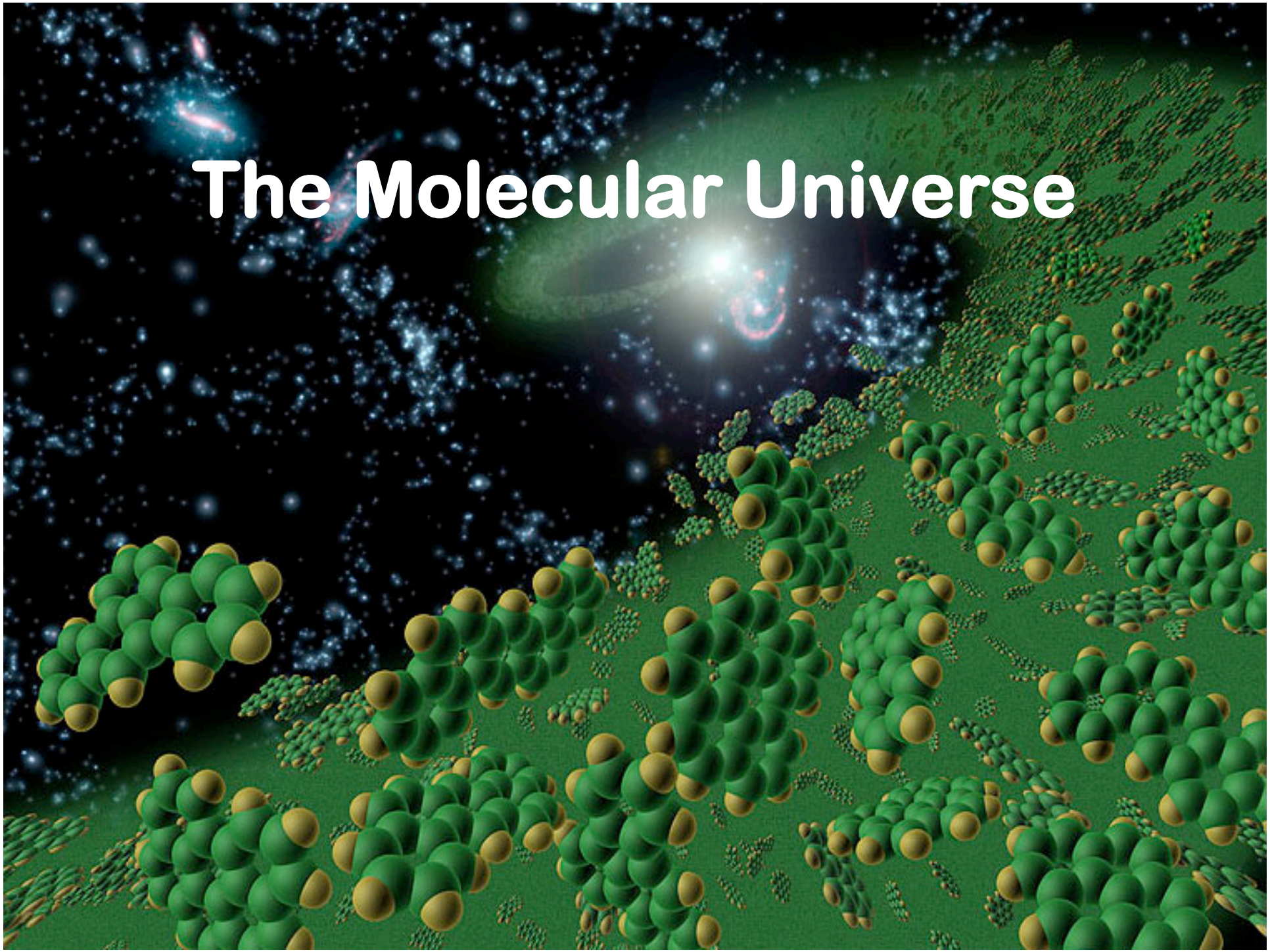
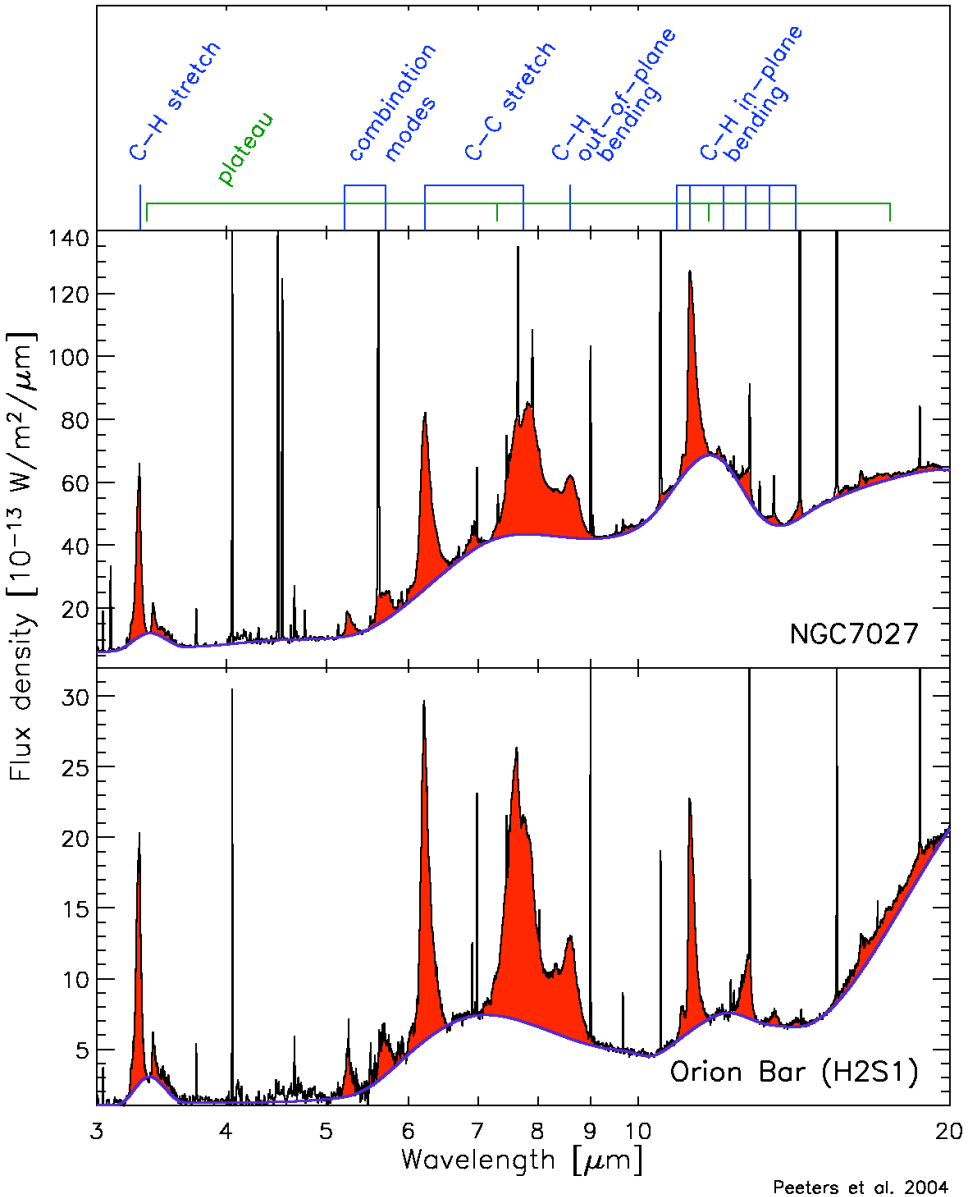

PAHS AND STAR FORMATION
Xander Tielens


The Molecular Universe

Key Questions

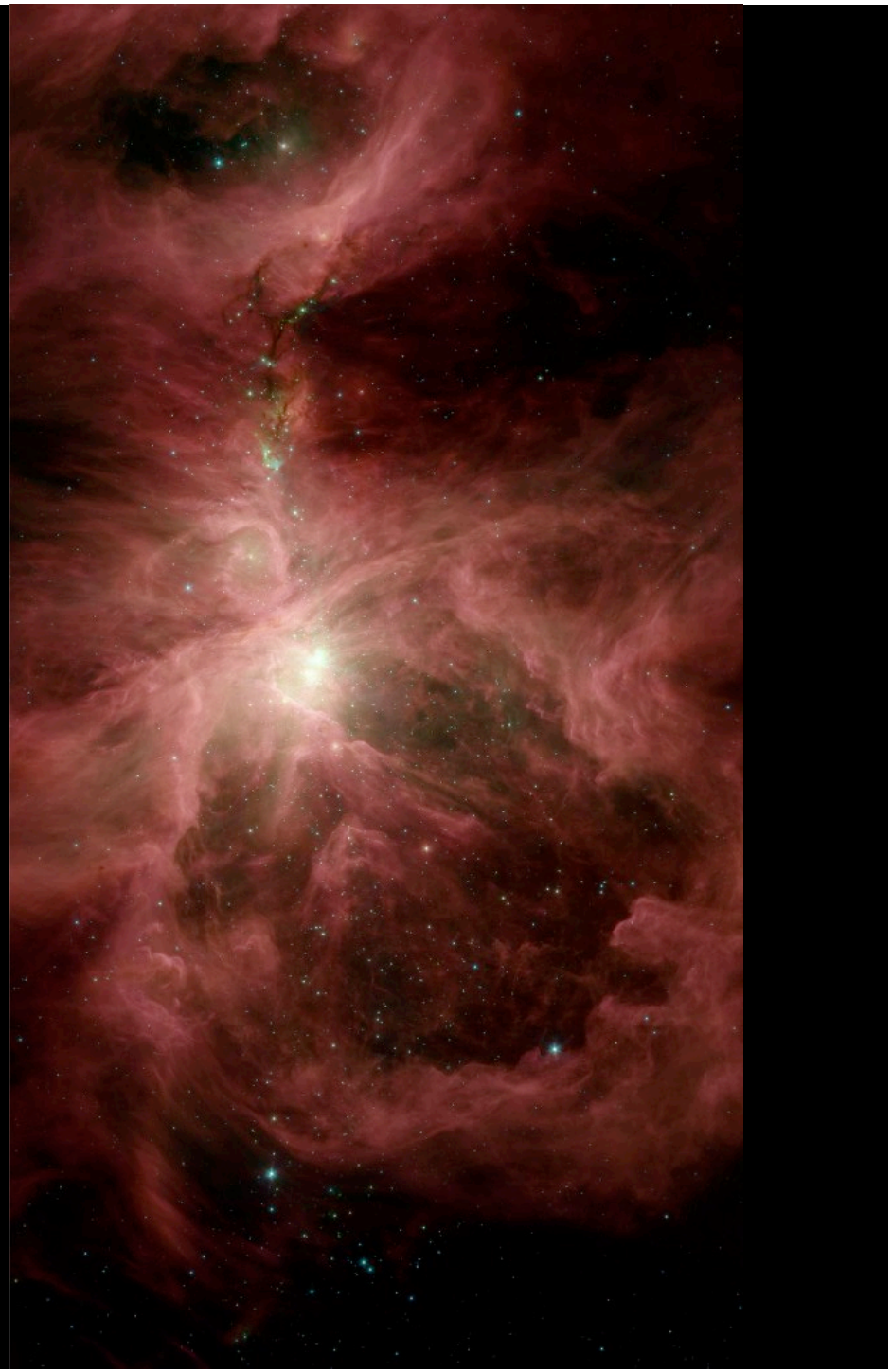
- What is the molecular inventory of the universe ?
- What processes play a role in the origin and evolution of molecules in the interstellar medium ?
- What kind of molecules entered the Solar Nebula and other planetary systems ?
- What processes played a role in their evolution in the planetary systems ?
- How are molecules affected near black holes and in starburst environments ?
- How did the molecular universe evolve with time ?
- How did this molecular evolution affect the evolution of galaxies, stars and planets ?

The incredibly rich spectrum of interstellar PAHs



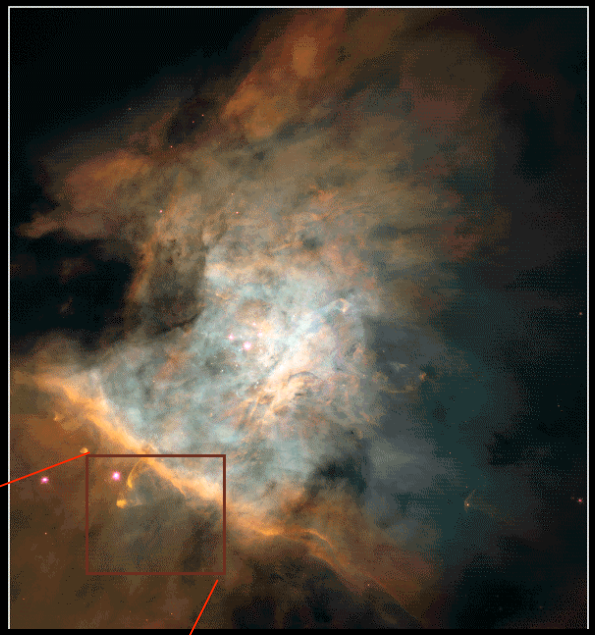
Peeters et al. 2004
proceedings Astrophysics of Dust

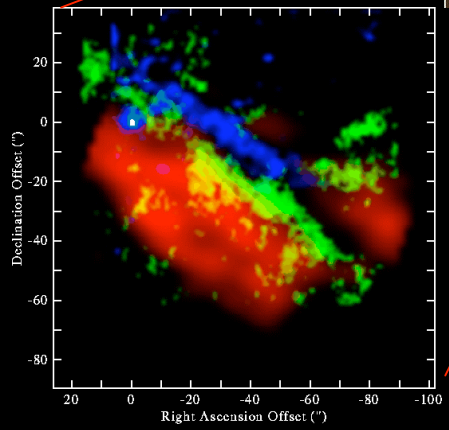
PAHs and PDRs in Orion



PAHs as Tracers of PDRs

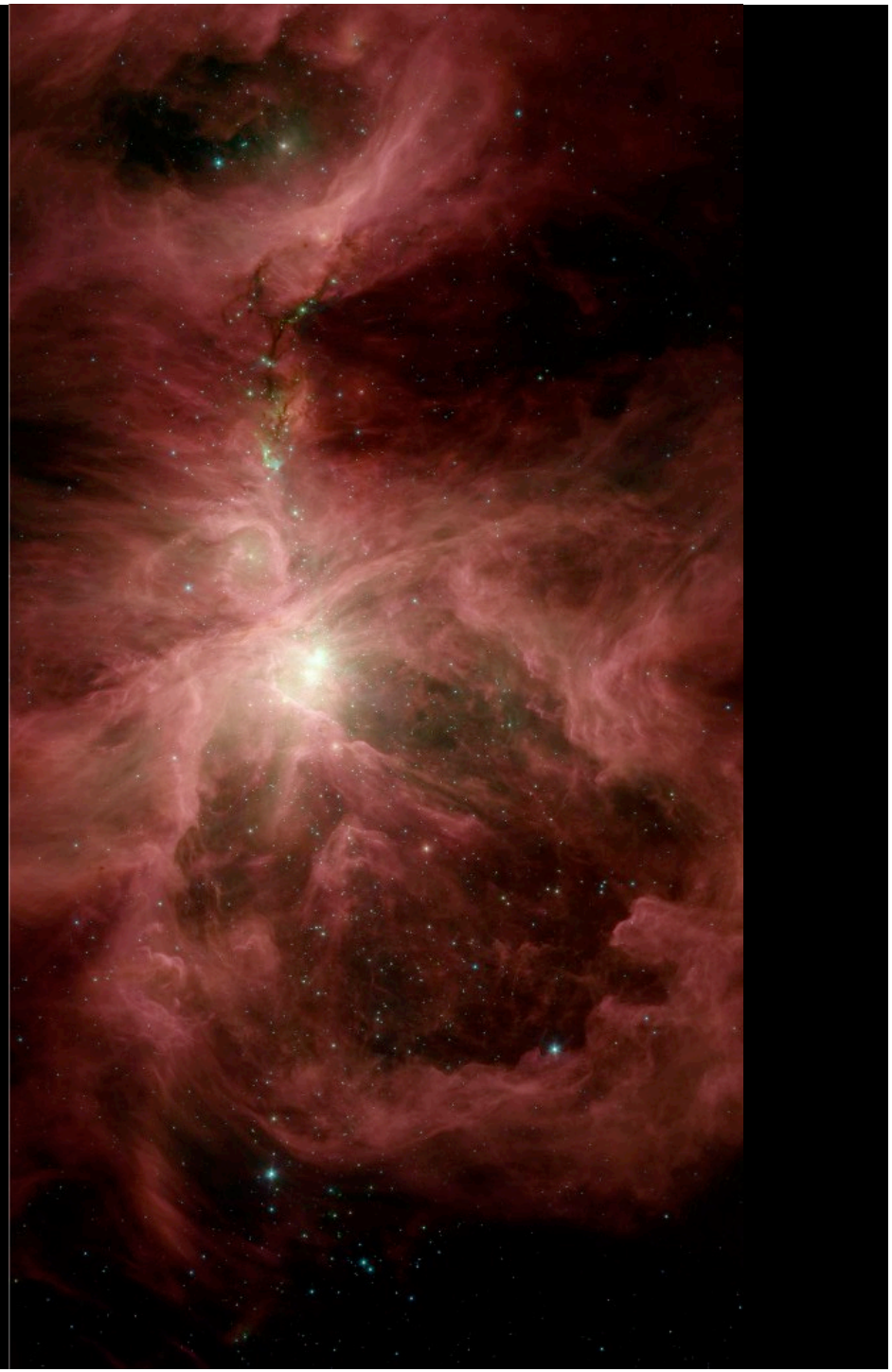
- PAH emission originates from PhotoDissociation Regions (neutral atomic layer irradiated by ultraviolet stellar radiation)
- PAHs destroyed in ionized gas



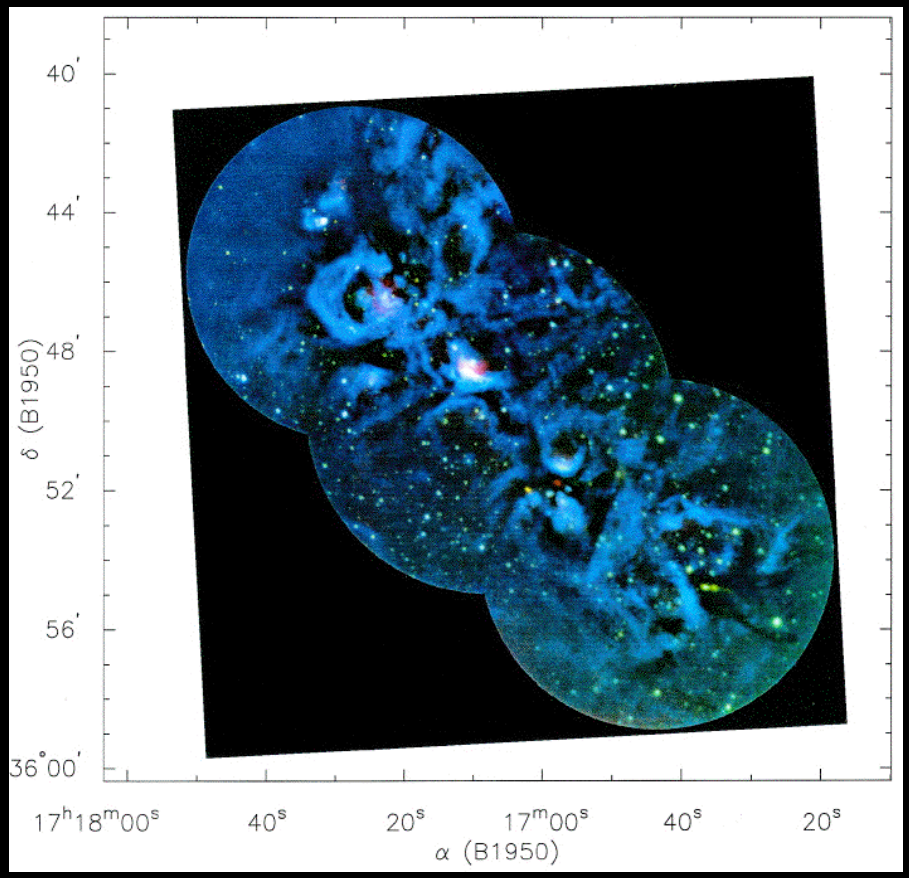


Tielens et al, 1993, Sci, 262, 86

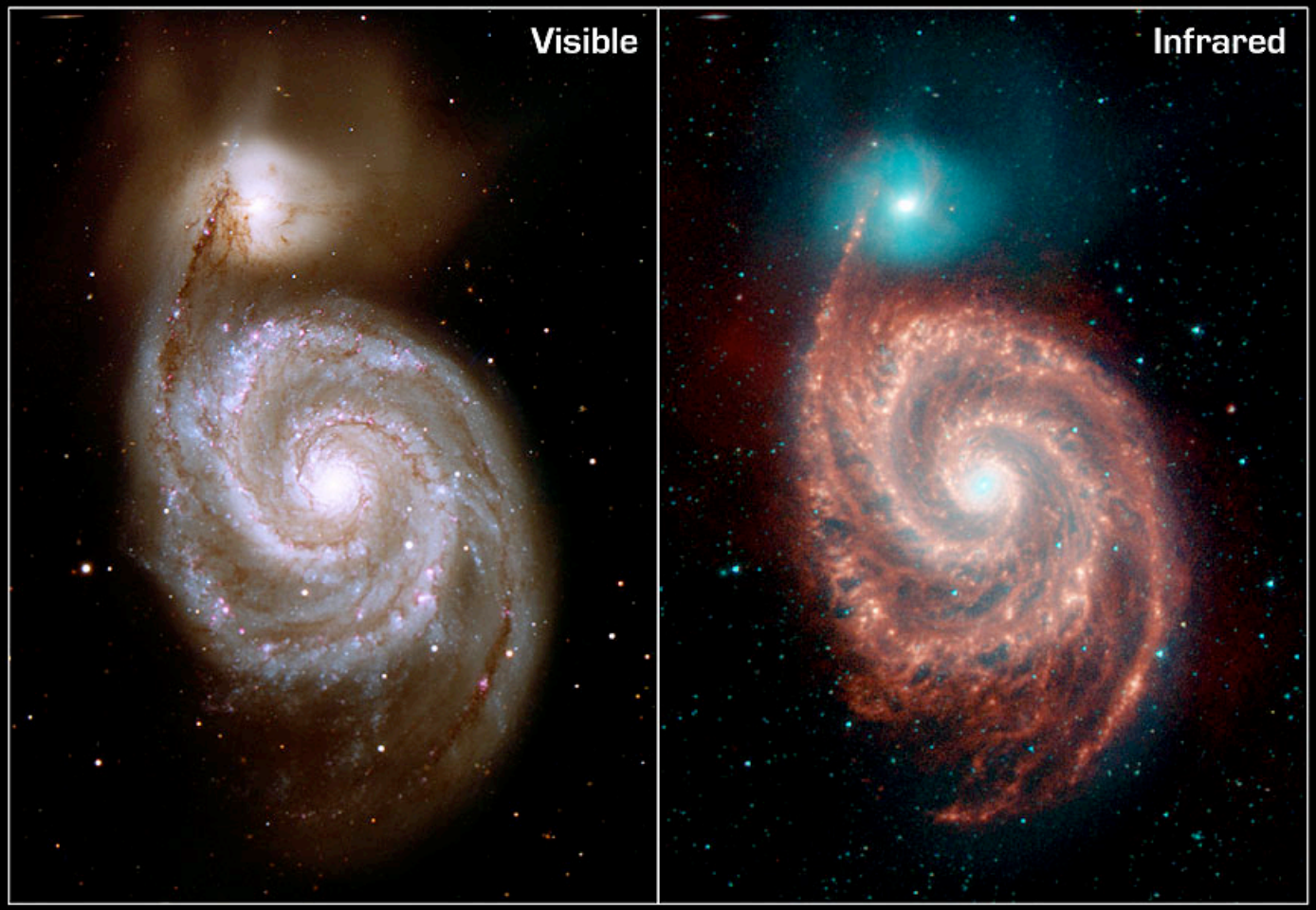
PAHs and PDRs in Orion



PAHs as tracer of Molecular Clouds



NGC 6334: Burton et al, 2000, ApJ, 542, 359



Spiral Galaxy M51 ("Whirlpool Galaxy")

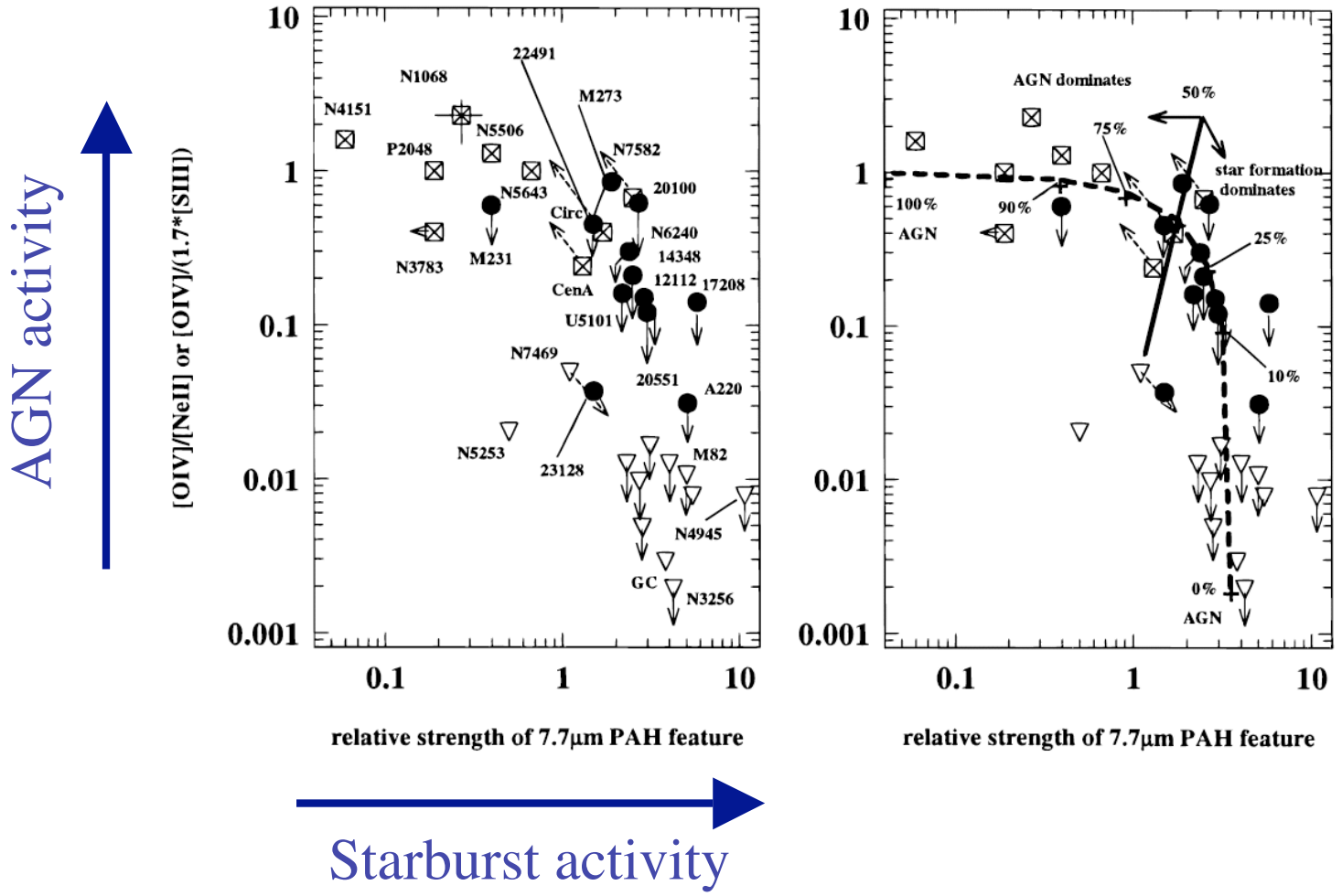
Spitzer Space Telescope • IRAC

NASA / JPL-Caltech / R. Kennicutt (Univ. of Arizona)

ssc2004-19a


M82 Galactic Wind

PAHs as a Measure of Starburst Activity



Genzel et al., 1999, ApJ, 498, 579

PAHs and the Universe

- PAHs as tracers of the universe
  - FUV photons, PDRs, massive stars & star formation
  - Molecular/diffuse clouds: Structure in the ISM
  - Entrainment: PAHs as a dye
- PAHs and their role in the universe
  - Energy balance of interstellar gas
  - Ionization balance of interstellar gas
  - Chemistry & molecular inventory

PAHs & the Universe II

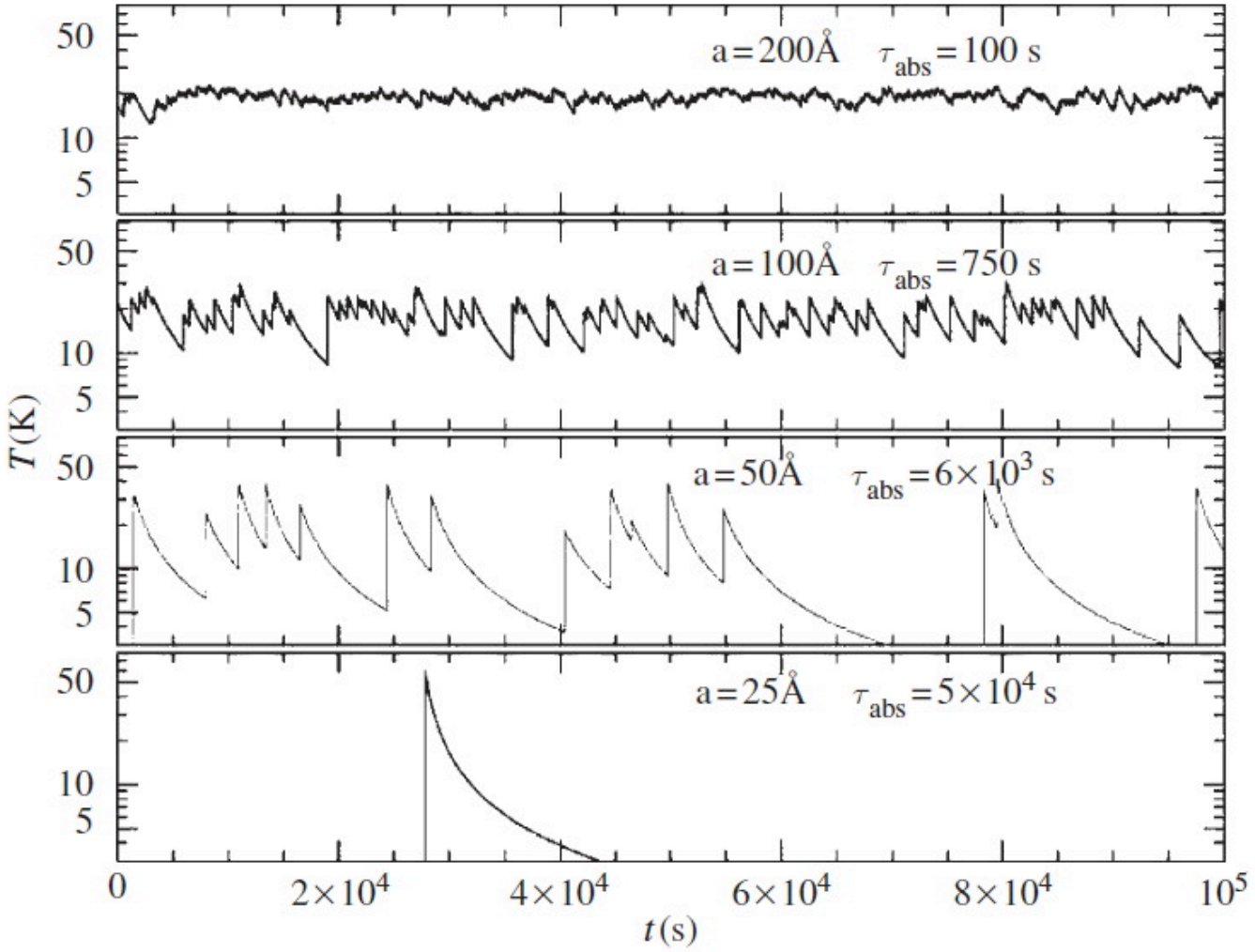
- In order to use PAHs as astronomical tools:
  - Understand PAHs from first principles
  - Characterize PAH tools empirically
- Goal of this talk is to overview the status of these two different aspects of interstellar PAHs
- Current understanding of interstellar PAHs
  - PAH spectroscopy: properties, sizes
  - Molecular structure of PAHs
- PAHs as star formation diagnostics
- The future

Interstellar PAHs

PAHs & IR Emission Features

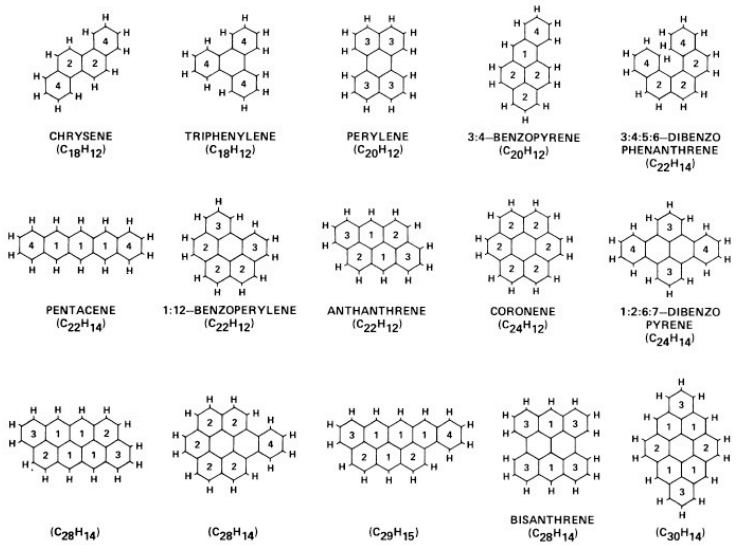
- Properties IR Emission Features
  - Exceedingly rich spectrum
  - Widespread
  - Spectral family
  - Variations in intensity ratios
  - Variations in peak position
- Evidence for molecular emission
  - Energetics (Sellgren 1984)
  - Feature-to-continuum ratio
  - Anharmonic profile

A day in the life .....

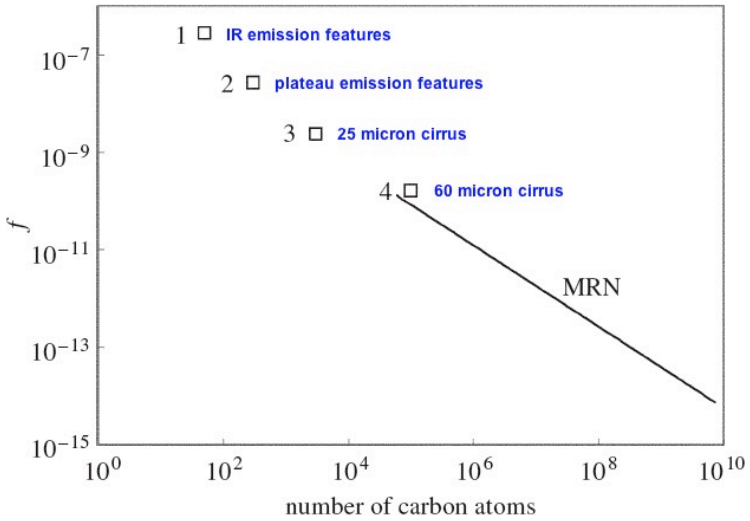


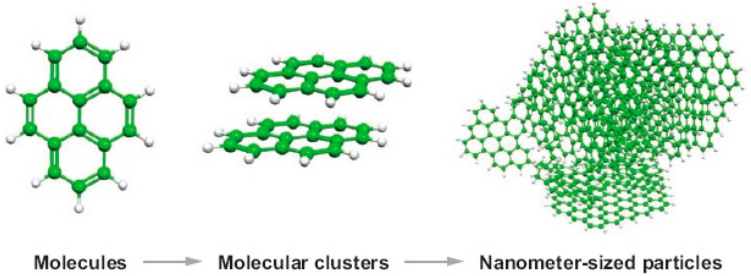
Interstellar PAHs

- Aromatic hydrocarbon structure
- PAHs contain ~50 C-atoms
- 14 ppm with respect to H or 5% of the elemental C
- PAHs are an important and ubiquitous component of the ISM



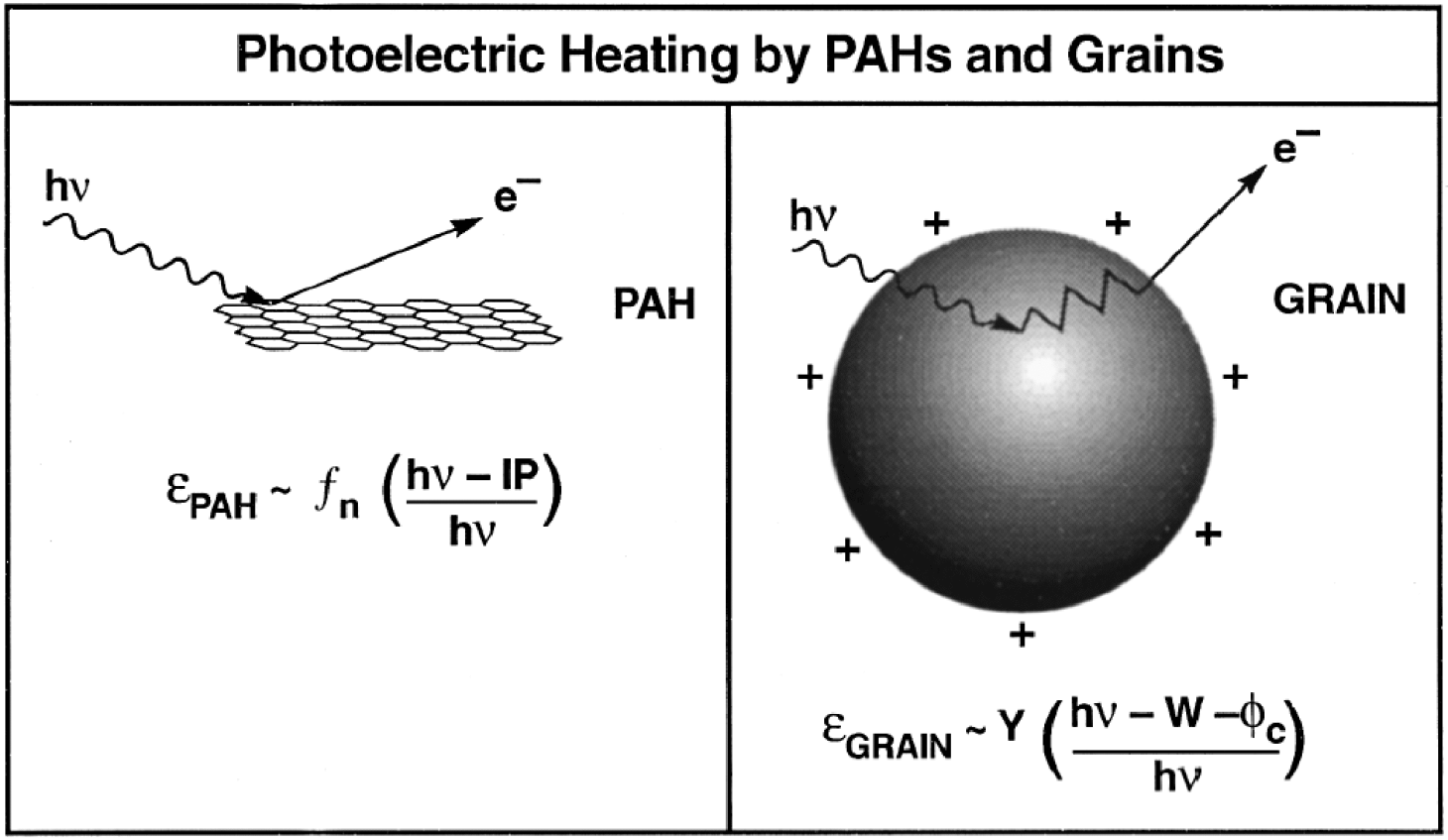
The Relationship of PAHs & Dust





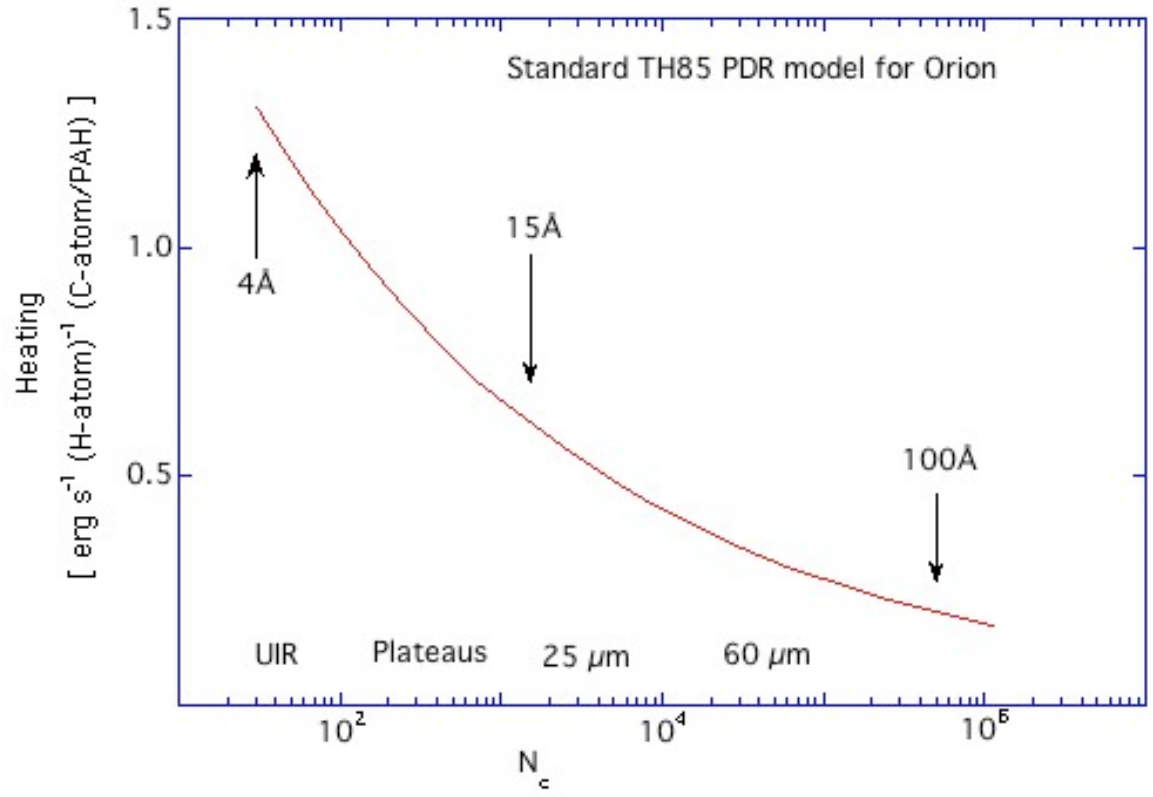
PAHs are the extension of the interstellar grain size distribution into the molecular domain

PAHs and the Heating of the Diffuse ISM



PAHs and Interstellar Clouds

PAHs are important for heating of interstellar gas and hence are a key ingredient for the phase structure of the ISM

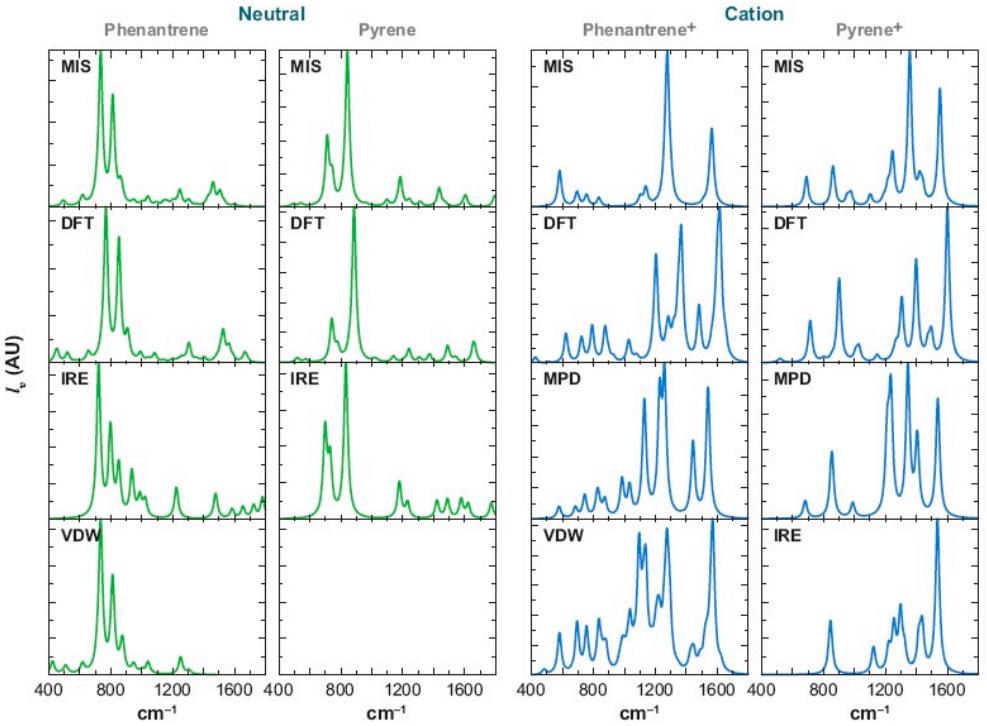


Bakes & Tielens, 1994, ApJ, 427, 822
Wolfire et al, 1995, ApJ, 443, 152

PAH Spectroscopy

Spectroscopy of PAHs

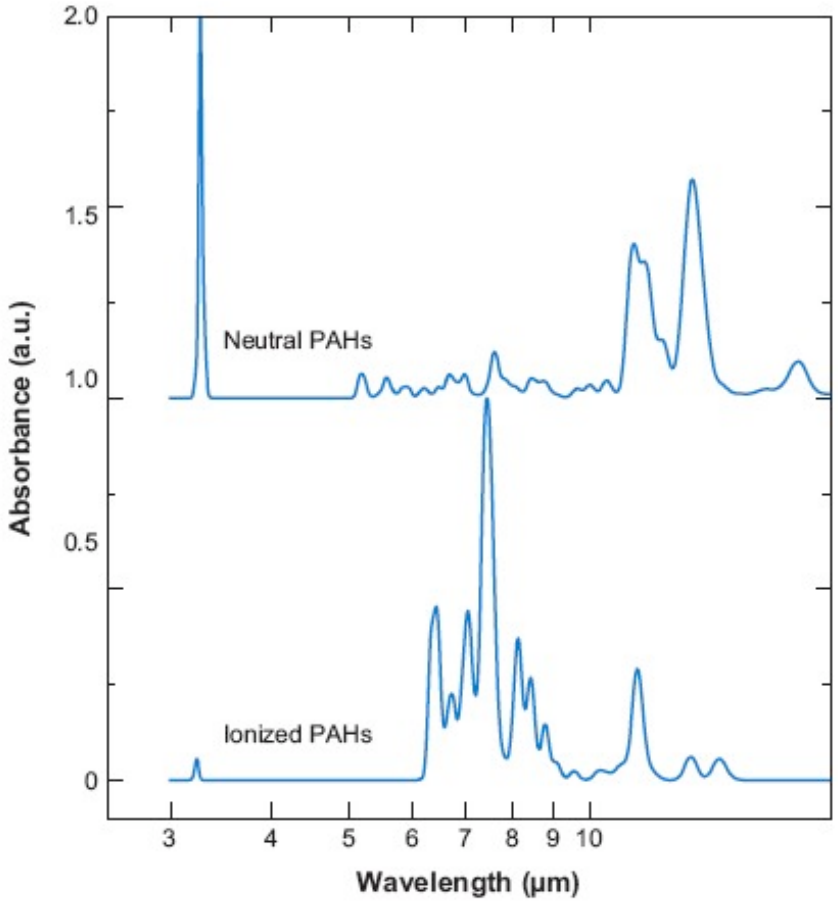
- Wide variety of techniques
- IR fluorescence of vibrationally excited PAHs !
- Neutrals: good agreement in peak position and relative intensity
- Ions: overall agreement but detailed variations
- DFT calculations provide in general reliable results



Oomens et al, 2003, ApJ, 591, 968

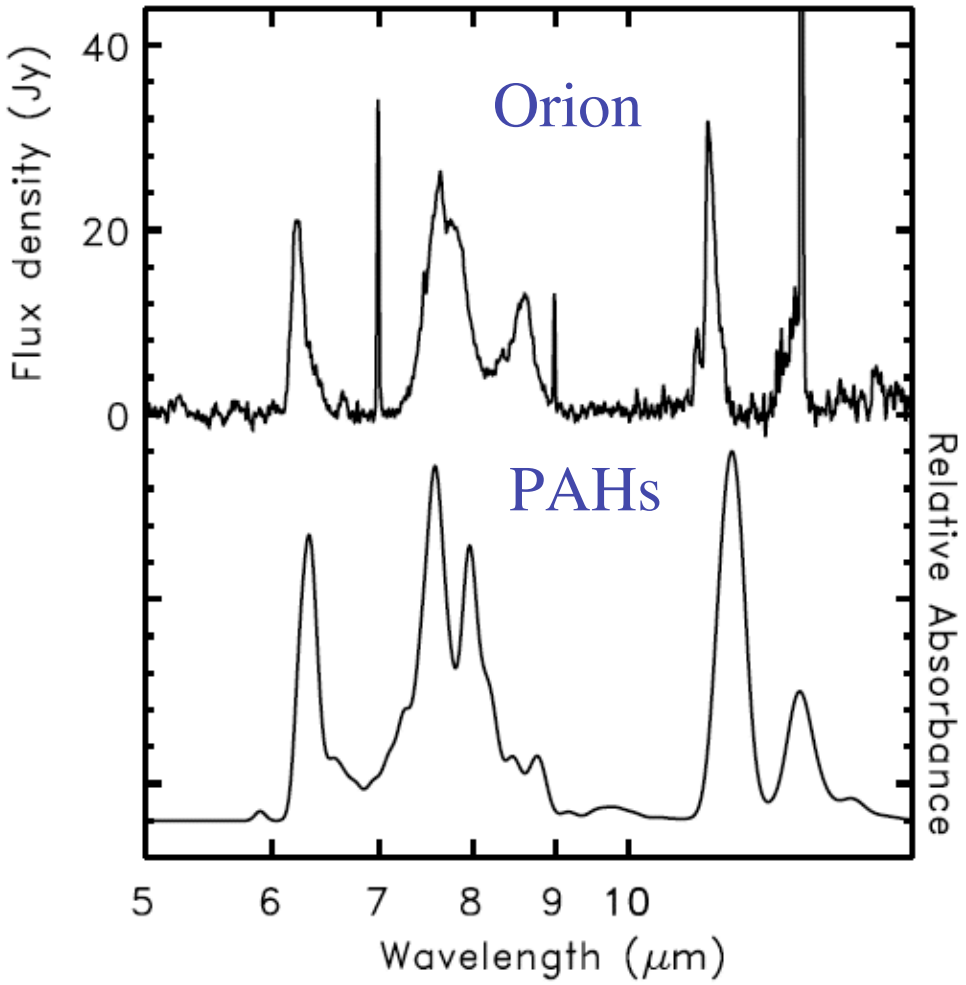
The Spectral Characteristics of PAHs

The PAH spectrum depends on charge state



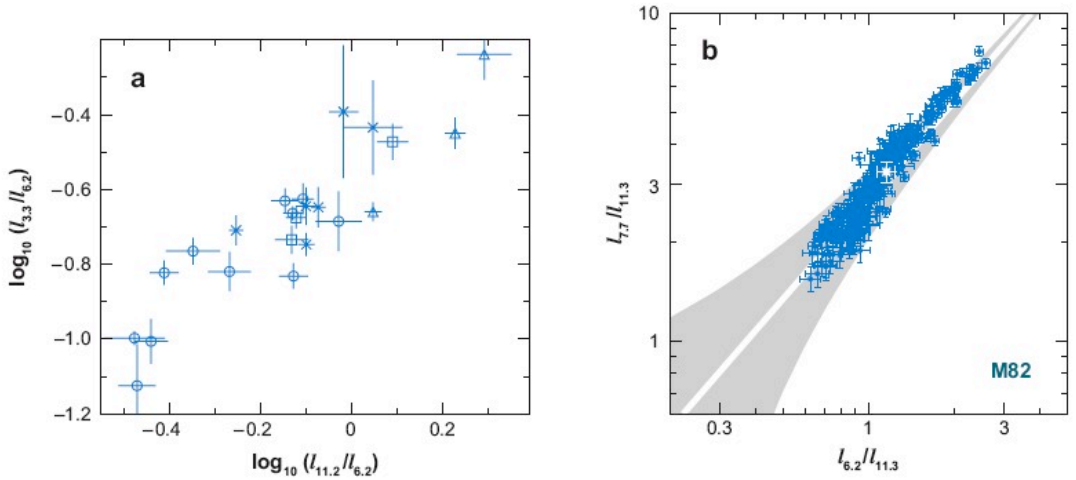
Allamandola et al, 1999, ApJ, 511, L115
Langhoff, 1996, JPC, 100, 2819

Spectral Characteristics II

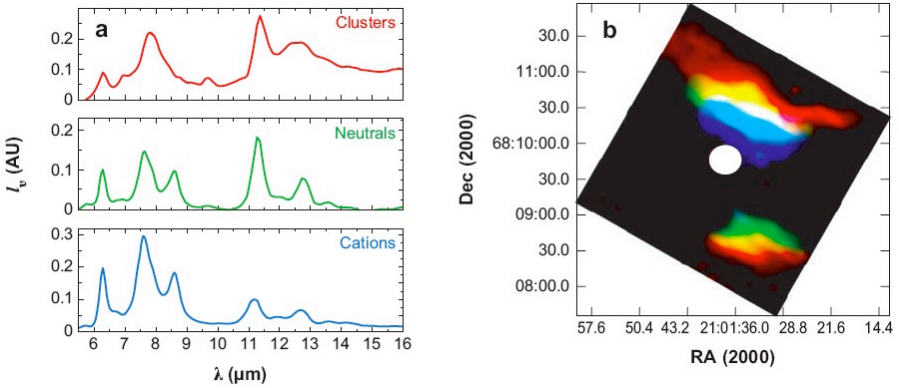


Peeters et al, 2002, A&A,390, 1089

PAH Band Variations



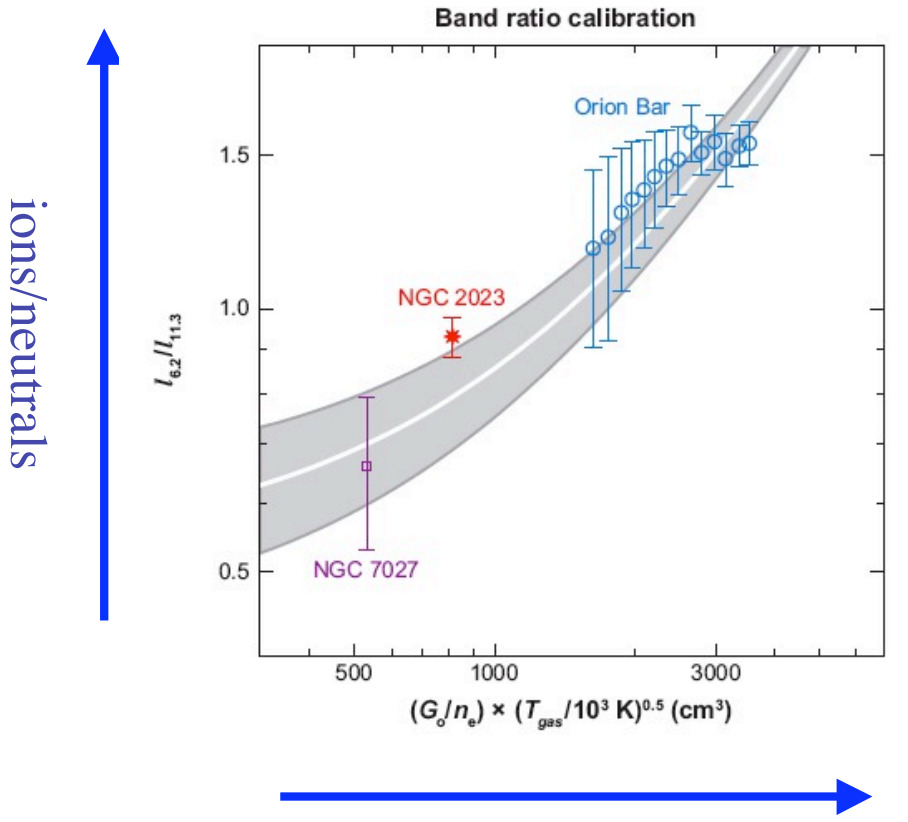
- C-H and C-C modes vary independently



Galliano et al, 2008, ApJ, 679, 310
Hony et al., 2001, A & A, 370, 1030
Bakes et al., 2001, ApJ, 556, 501
Rapacioli et al, 2005, A&A, 429, 193
Berne et al, 2008, A&A, in press

PAH Ionization Balance

- Ratio of C-H/C-C modes measures charge state
- Calibrate PAH band ratios on well-studied PDRs
- Diagnostic atomic and molecular 'PDR' lines
- Implications for photo-electric heating !



Galliano et al, 2008, ApJ, accepted
Hony et al., 2001, A & A, 370, 1030
Bakes et al., 2001, ApJ, 556, 501

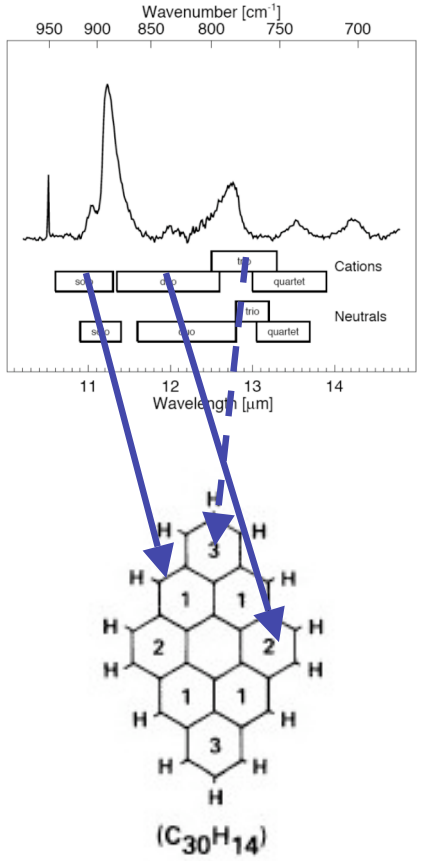
Molecular Structure of PAHs

The role of ionized PAHs

- PAH ionization and photo-electric heating of interstellar gas
  - Phase structure and physical conditions of the diffuse ISM
- PAHs are dominant negative charge carriers in molecular clouds
  - Ambipolar diffusion and onset of star formation
  - Ion-molecule chemistry

Molecular Structure of Interstellar PAHs

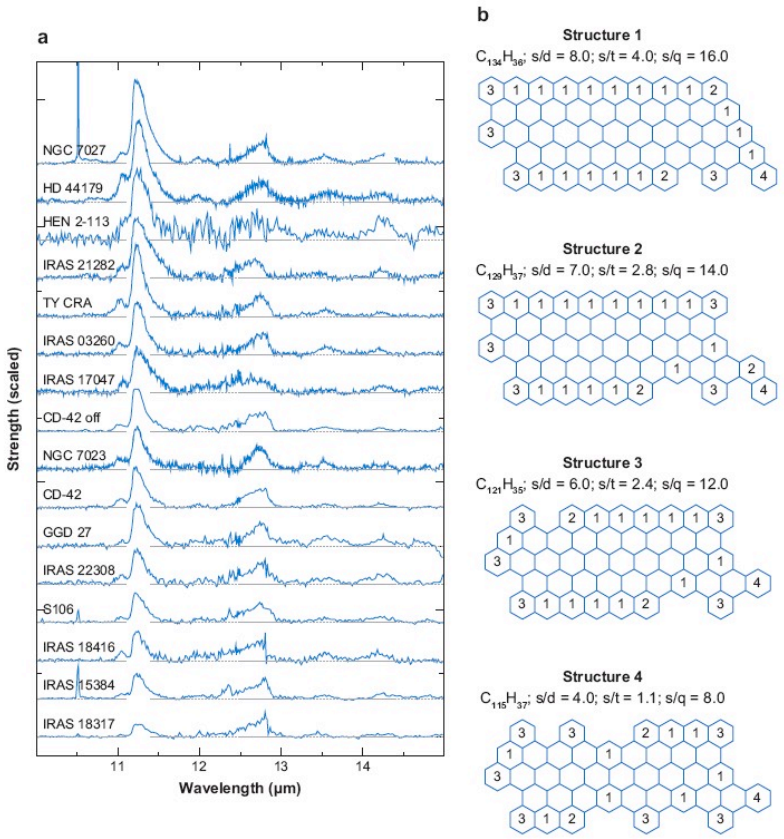
- The out-of-plane bending modes probe the “edge” structure of PAHs
- Spectral pattern is sensitive to “H-adjacency”



- Hony et al, 2001, A&A, 370, 1030
- Hudgins & Allamandola 1999, ApJ, 516, L41

Molecular Structure of Interstellar PAHs

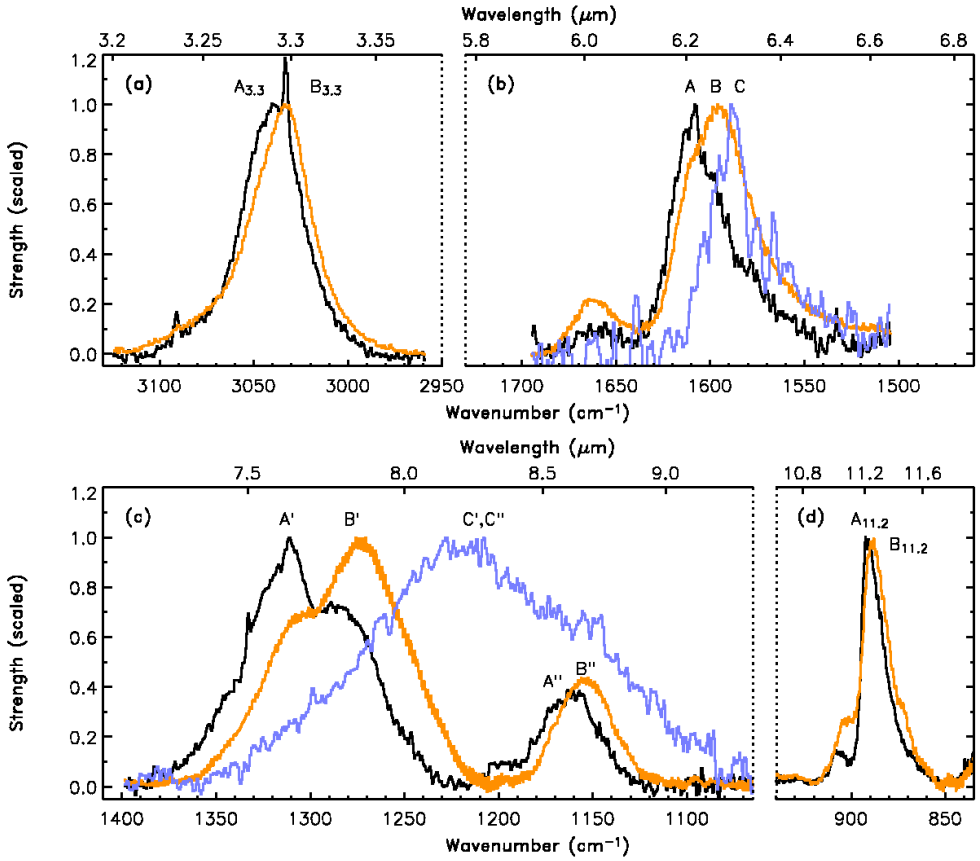
- Interstellar PAH spectrum shows large variations in the oops modes
- Variations in the molecular structure of the emitting PAHs
- Related to physical conditions



Hony et al, 2001, A&A, 370, 1030

PAH Spectral Variations

- Profile variations
- Strongest for CC modes
- Classes A, B, C
- Classes correlate well for CC modes
- Correspond to object type

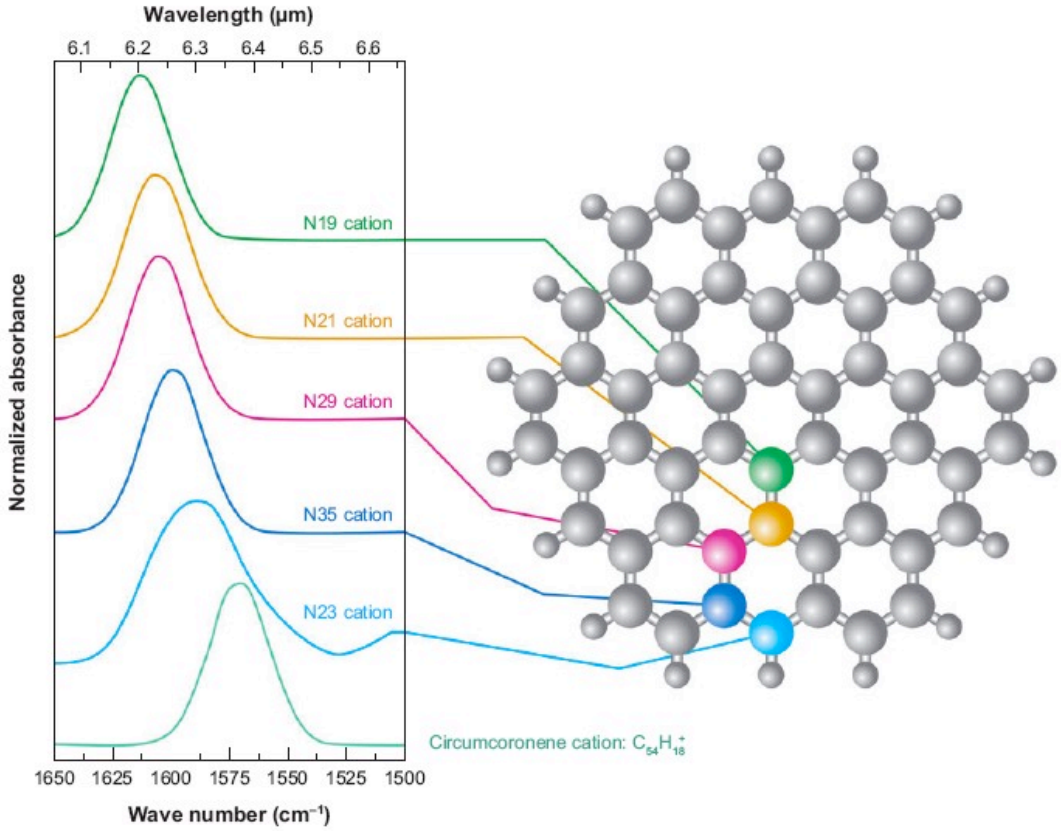


Peeters et al, 2002, A&A, 390, 1089

Chemical Modification of PAHs

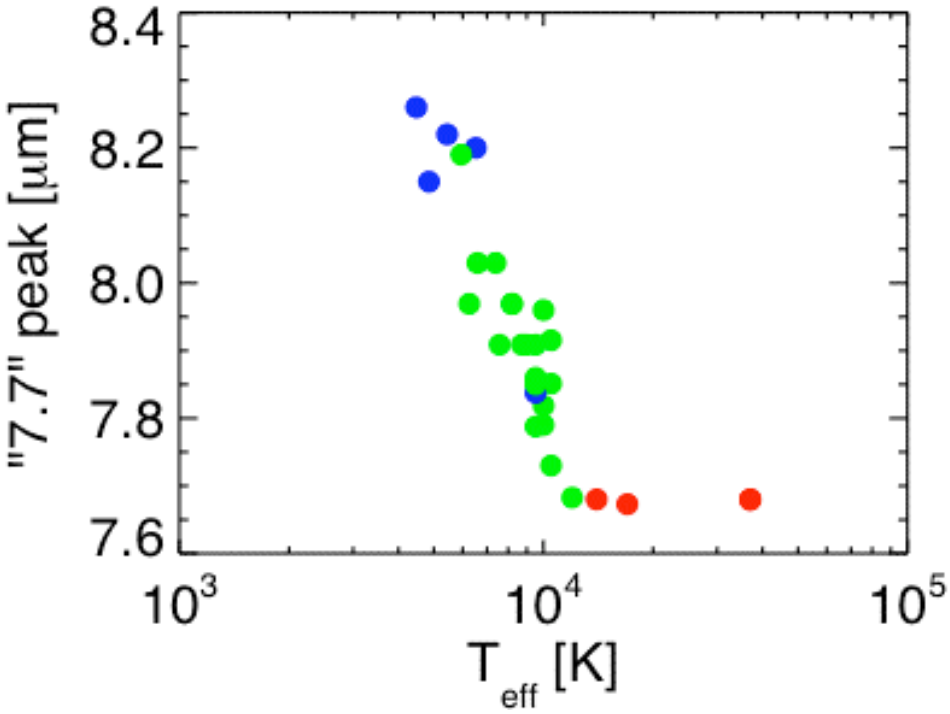
N in the carbon skeleton "shifts" the peak position to higher frequency

Peeters et al., 2002, A&A, 390, 1089



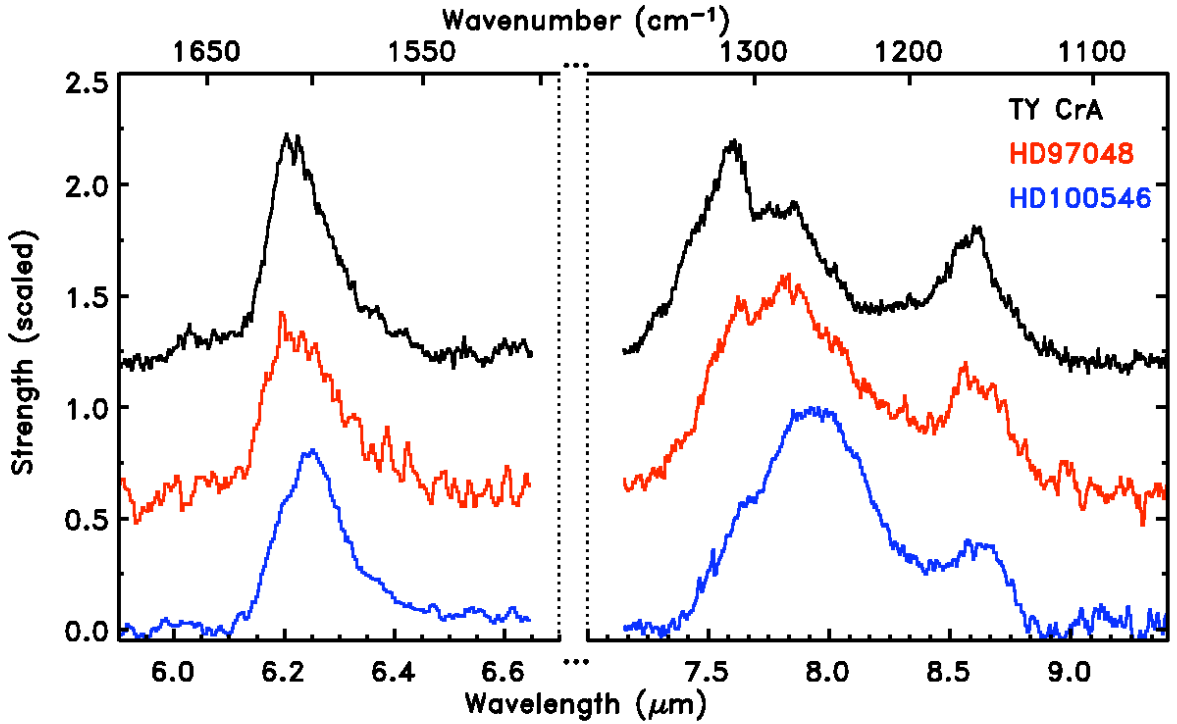
PAHs in Regions of Star Formation

- Peak position of the 7.7 μm band varies depending on source type
- Active chemistry: Aromatic versus aliphatic hydrocarbons or N in the ring
- Balance between reactions with N/C/H and photochemistry



Sloan et al 2007, ApJ, 664, 1144
Boersma et al, 2008, A & A, 484, 241

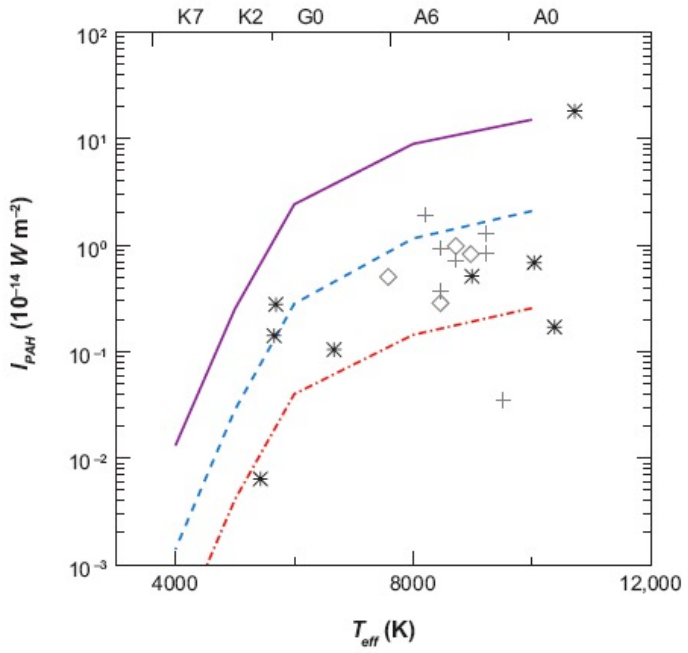
PAHs and Herbig Stars

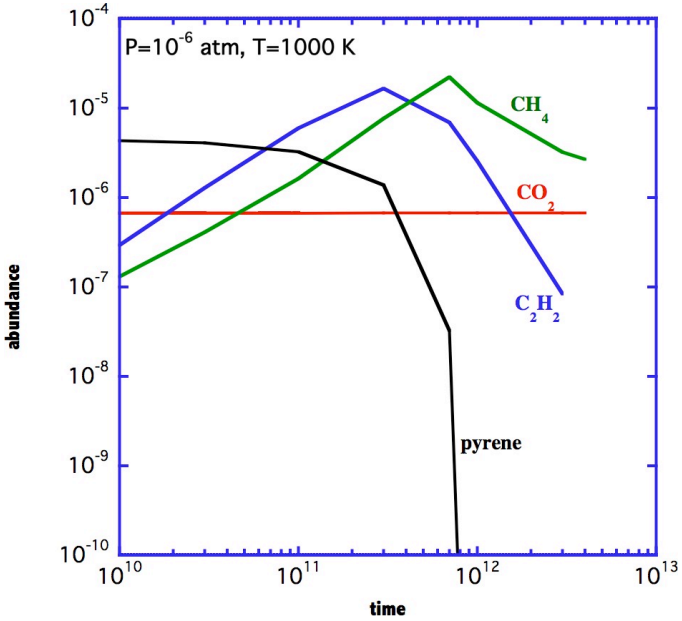


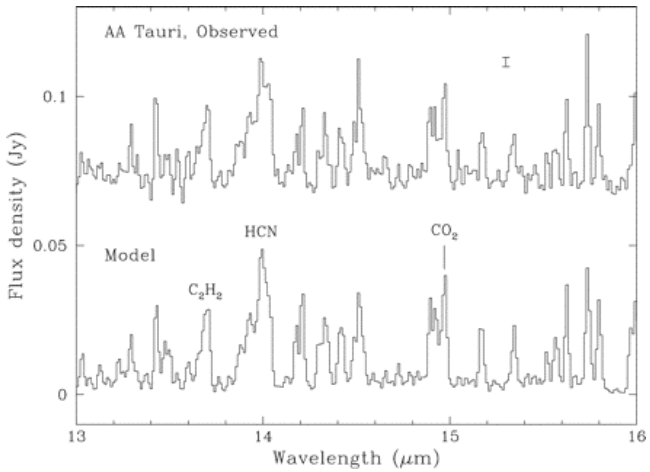
Source	Sp T	Size	Location
TY Cra	B7-B9	~2000 AU	HAeBe in cloud
HD 97048	B9-A0	~100-1000 AU	HAeBe cloud edge
HD 100546	B9	~150 AU	isolated HAeBe star

Boersma et al, 2008, A & A, 484, 241

PAHs & Protoplanetary Disks







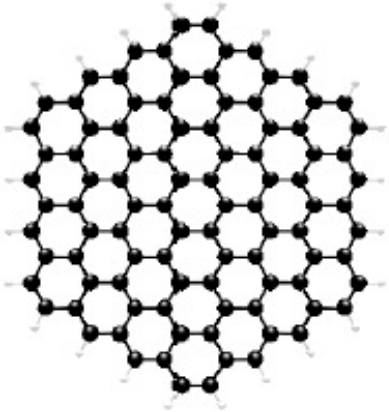
Destruction of PAHs in warm inner nebula creates abundant small hydrocarbons and may be the origin of the “sootline”

Geers et al., 2006, AA, 459, 545
Kress et al, 2010, Adv Sp Res
Carr & Najita, 2008, Science, 319, 1504

GrandPAHs

- IR emission spectra are very similar, particular in the "extreme" regions of the ISM
- 15-20 μm region often dominated by a few bands (16.4/17.4/17.0 μm)
- Typical PAH will absorb some 100 Million UV photons over its lifetime ⟶ what can break, will break
- Interstellar PAH family dominated by a few, extremely stable species

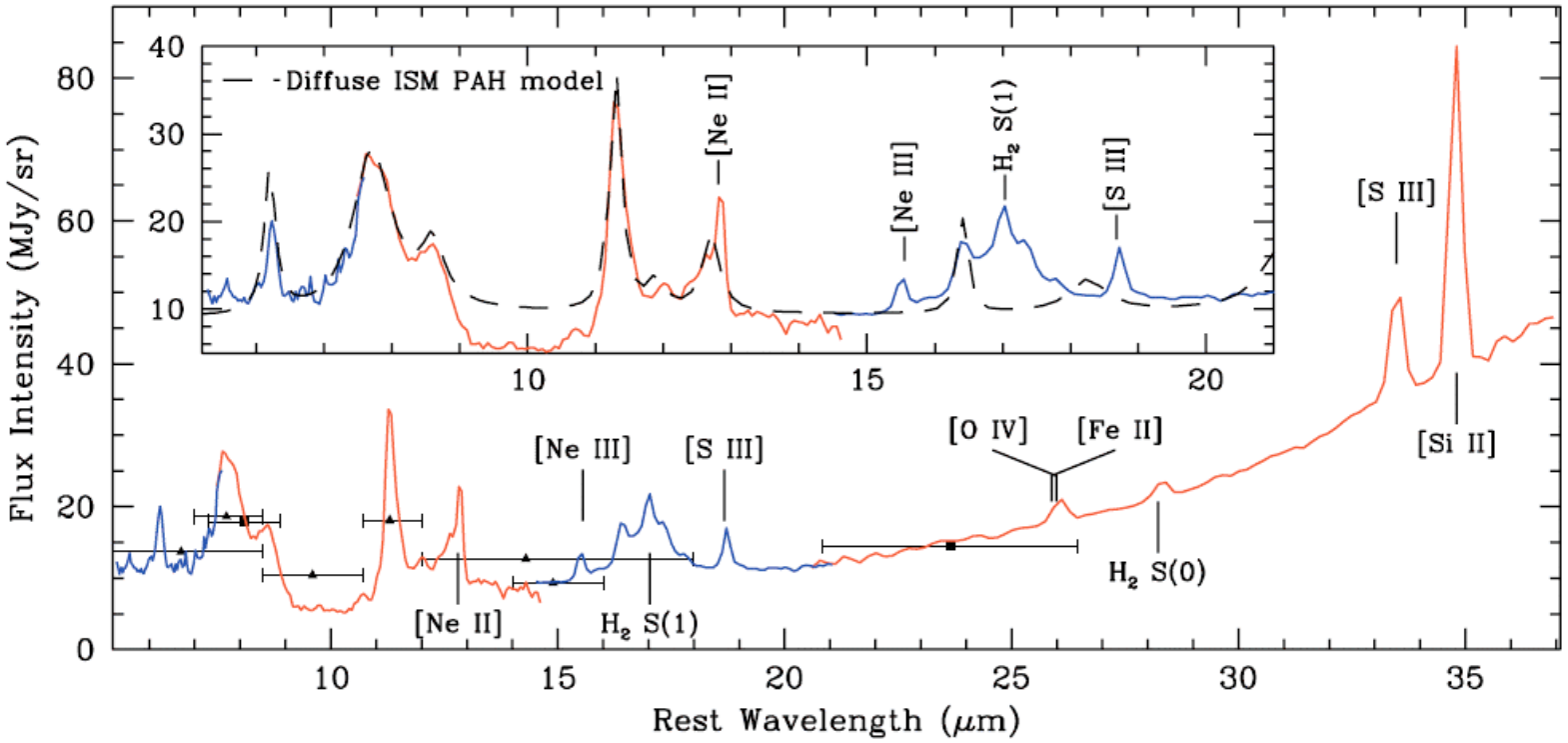
$C_{96}H_{24}$



PAHs & Star Formation Activity

PAHs in Galaxies

NGC 7331

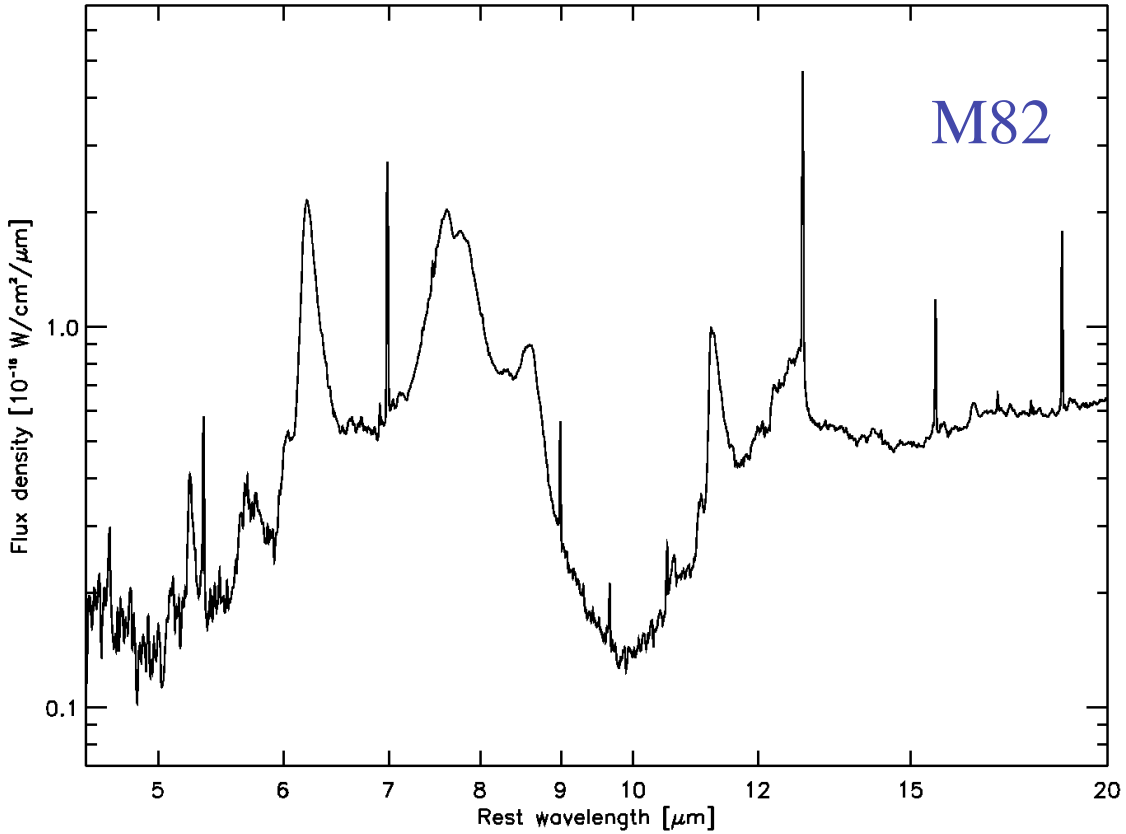


Moderate star formation activity: $L_{IR}/L_{opt} \sim 1$

Galaxy-wide SFR ~ 1 M_o/yr

Smith et al., 2004, ApJS, 154, 199

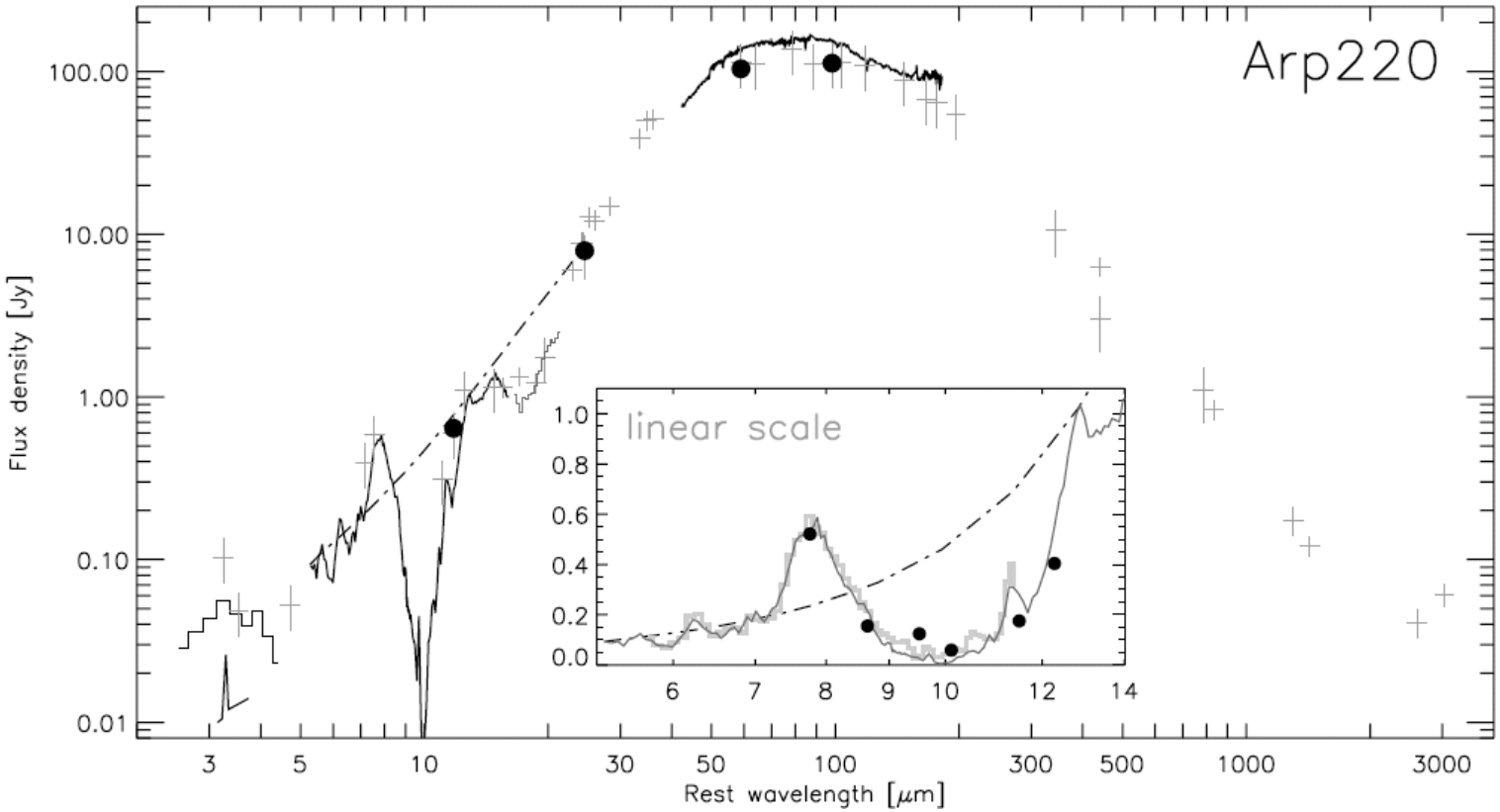
PAHs in Starburst



Starburst galaxy: $L_{IR}/L_{opt} \sim 40$
Nuclear SFR ~ 1 M_o/yr

Spoon, 2003, PhD thesis

PAHs in ULIRGs

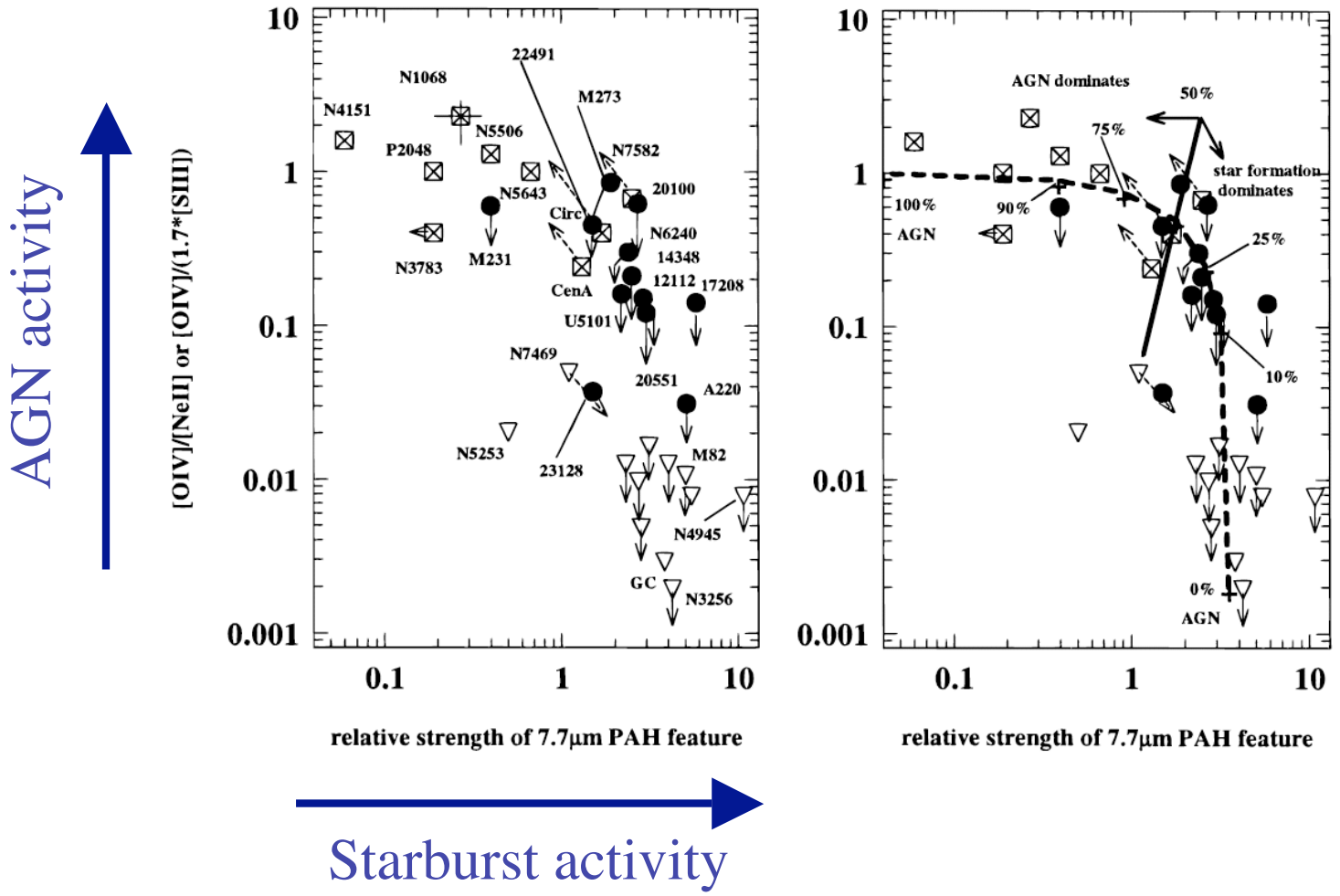


ULIRGs have $L_{IR}/L_{OPT} \sim 400$

SFR ~ 10^3 M_o/yr

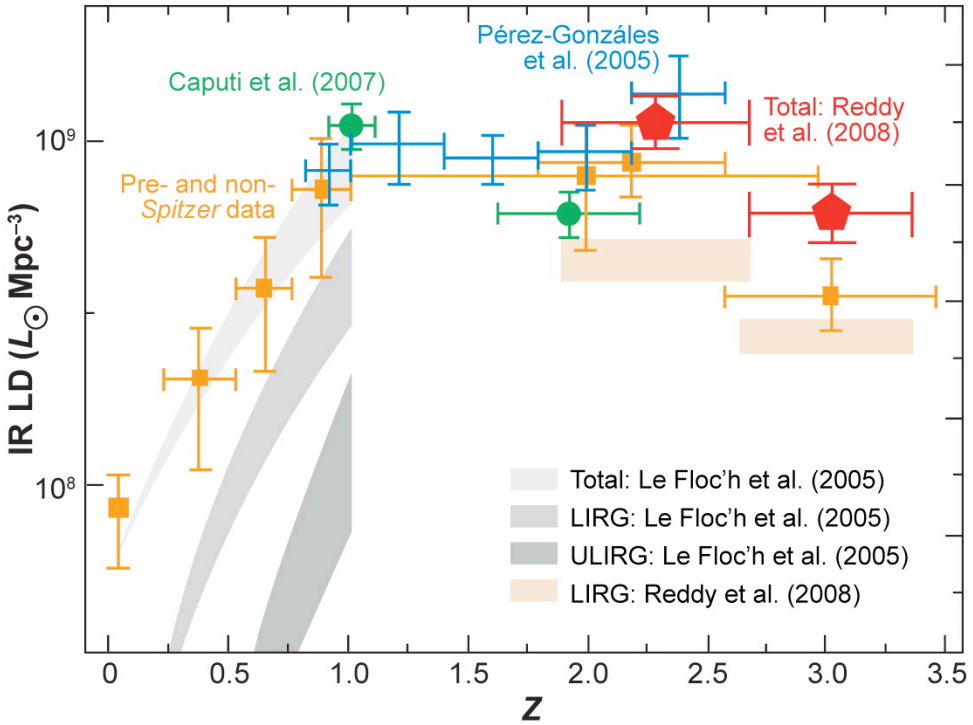
Spoon et al., A&A, 2004, 414, 873

PAHs as a Measure of Starburst Activity



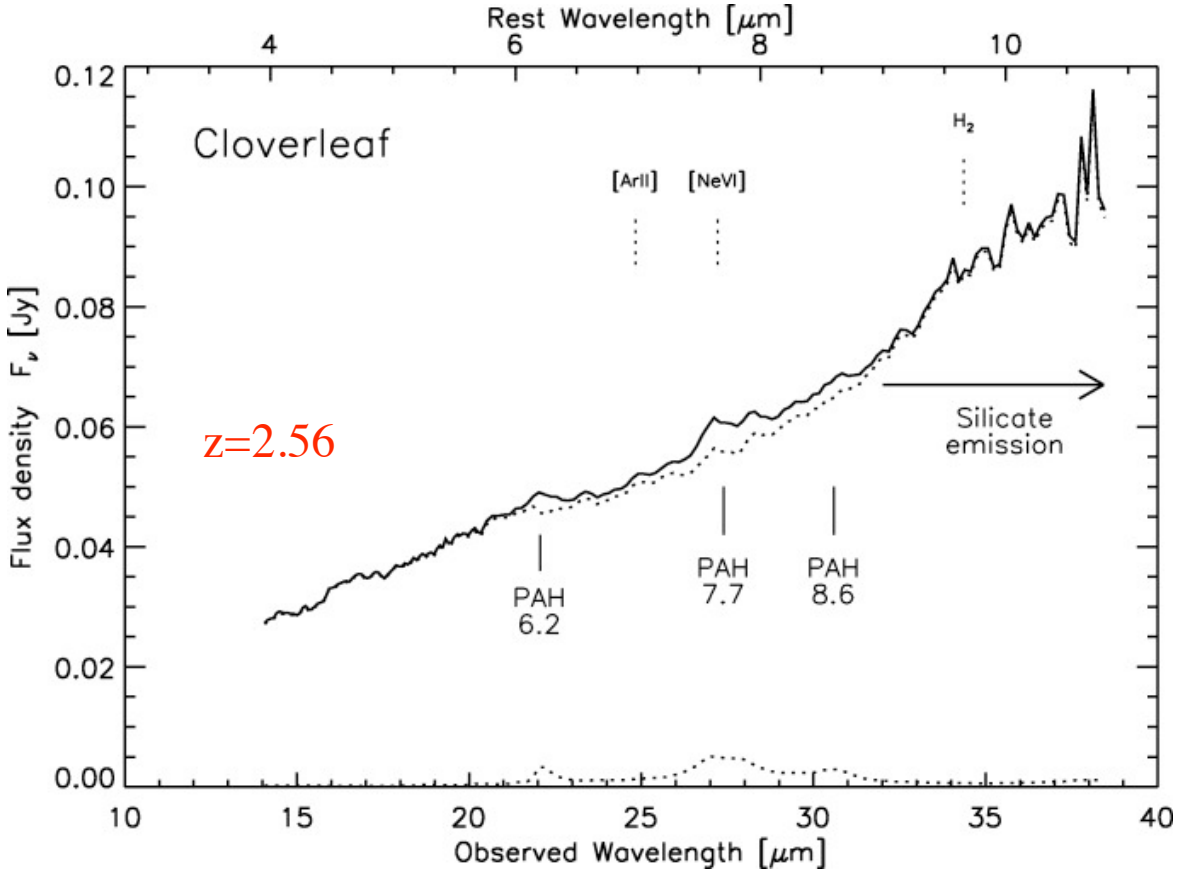
Genzel et al., 1999, ApJ, 498, 579

The Star Formation History of the Universe



Soifer BT, et al. 2008.
Annu. Rev. Astron. Astrophys. 46:201–40

PAHs in the Early Universe

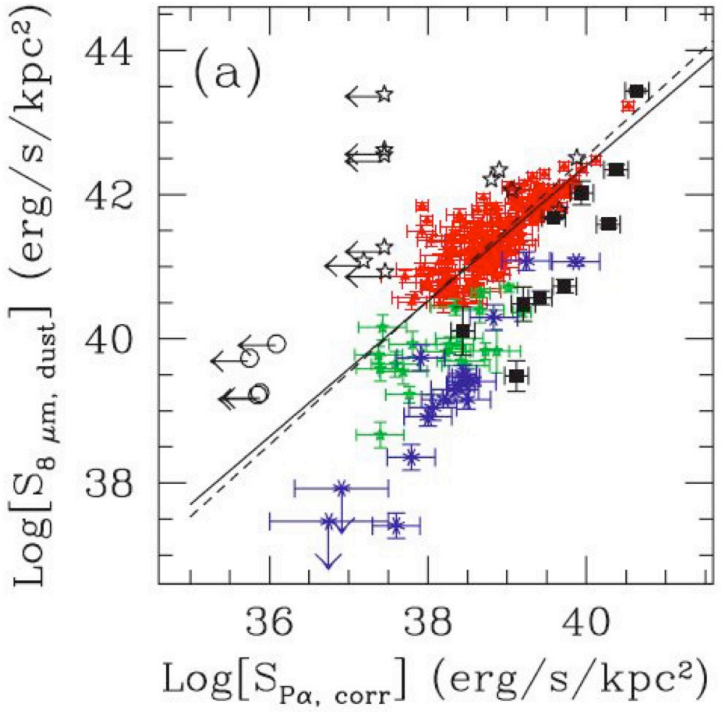


SFR ~ 10^3 M_o/yr

Lutz et al, 2007, ApJ, 661, L25

PAHs & Star Formation Rate

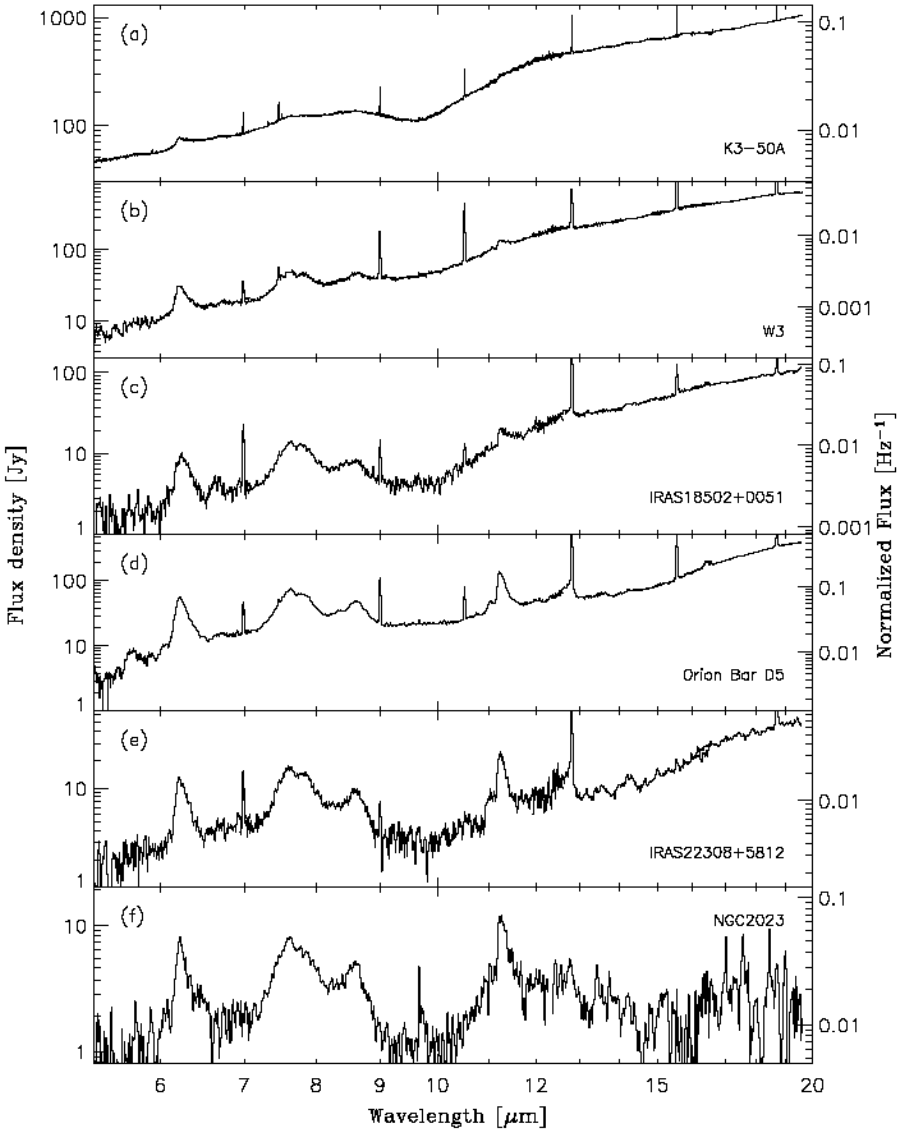
- PAH intensity in galaxies calibrated against HI recombination line
- PAHs are OK, but be wary
- Dependence on:
  - Metallicity
  - AGN
  - Starburst activity



- Calzetti et al, 2007, ApJ, 666, 870

Metallicity: high, intermediate, low

PAHs in PDRs

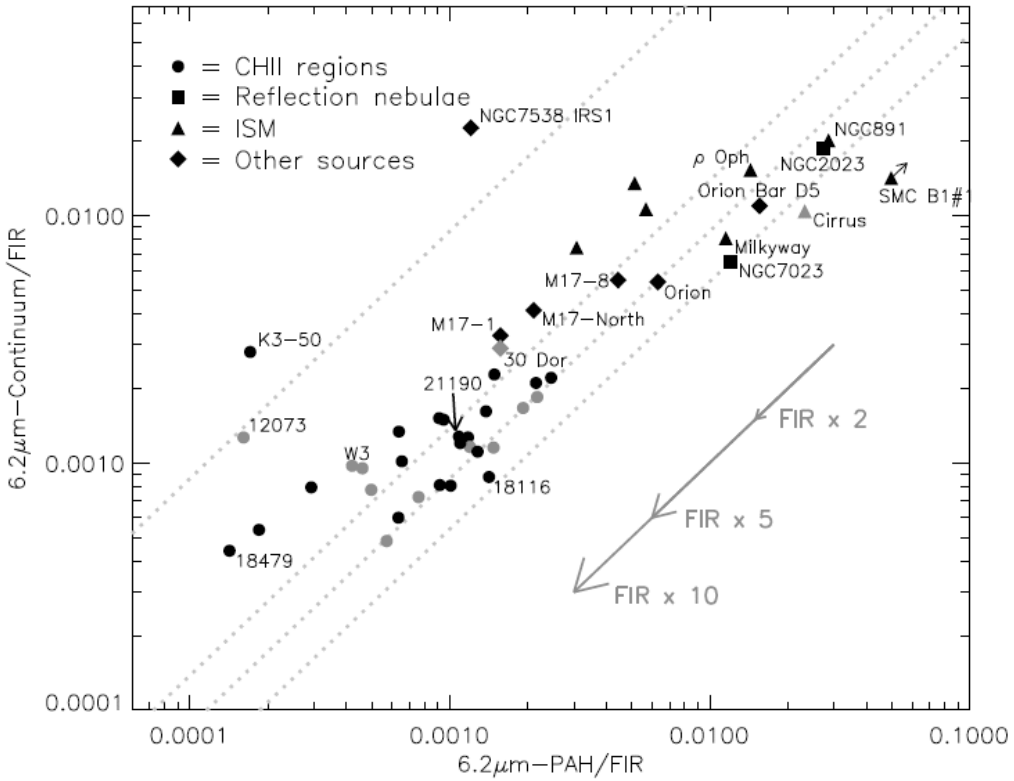


Peeters et al, 2002, A&A,390, 1089

Diagnostic Diagrams

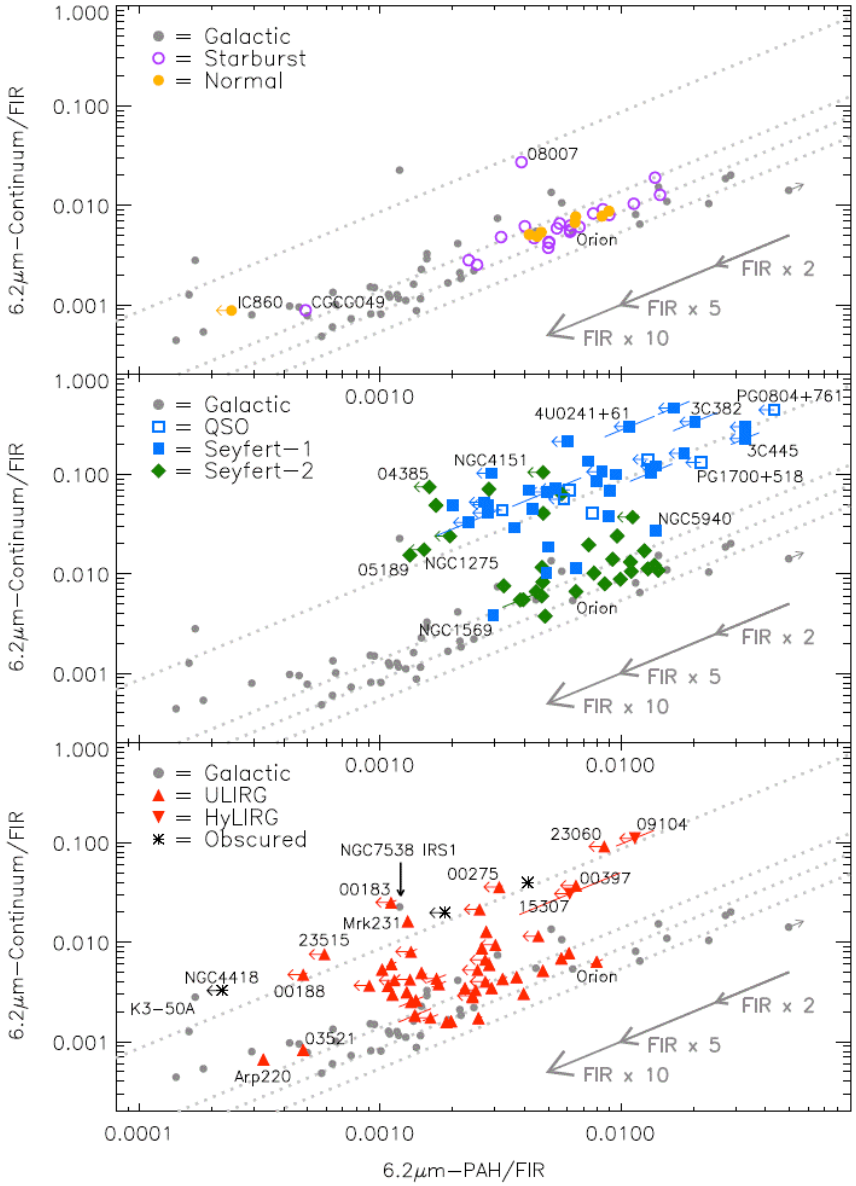
Sample of galactic HII regions

- feature/continuum = ~constant
- feature/FIR varies by two orders of magnitude
- Correlates with star formation characteristics



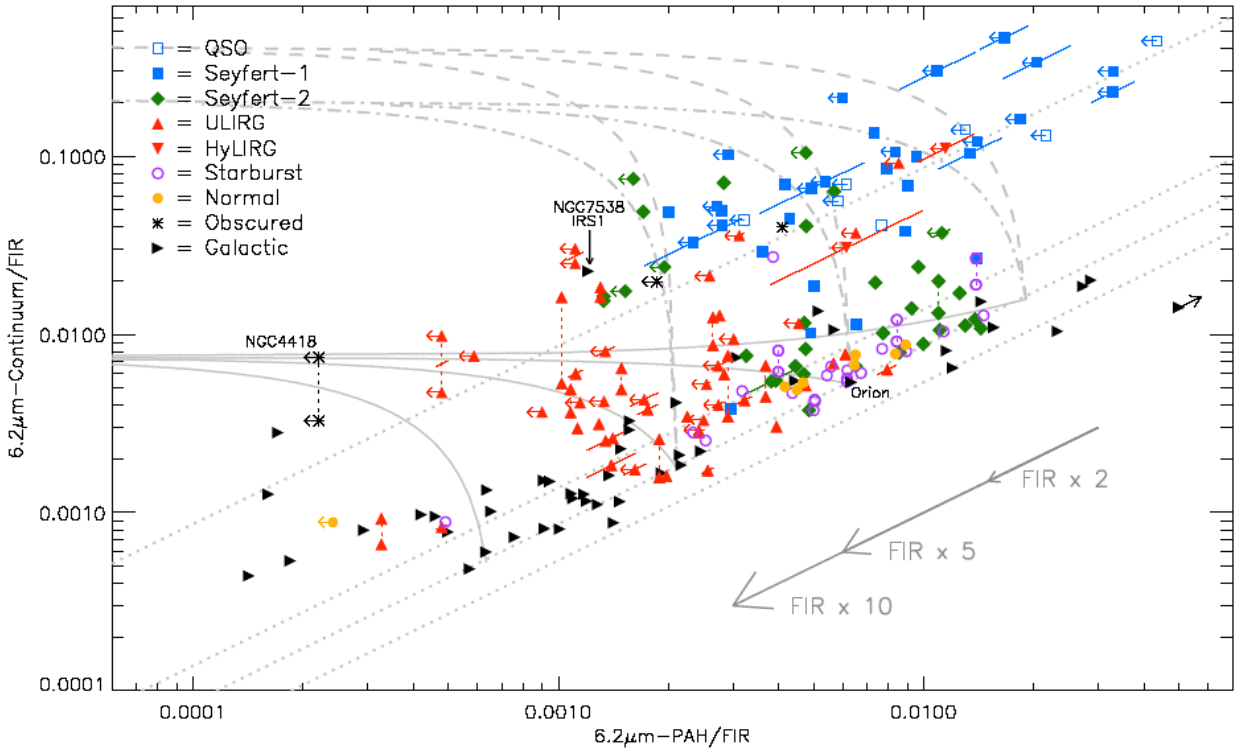
Peeters et al, 2004, ApJ, 613, 986

PAHs in Galaxies



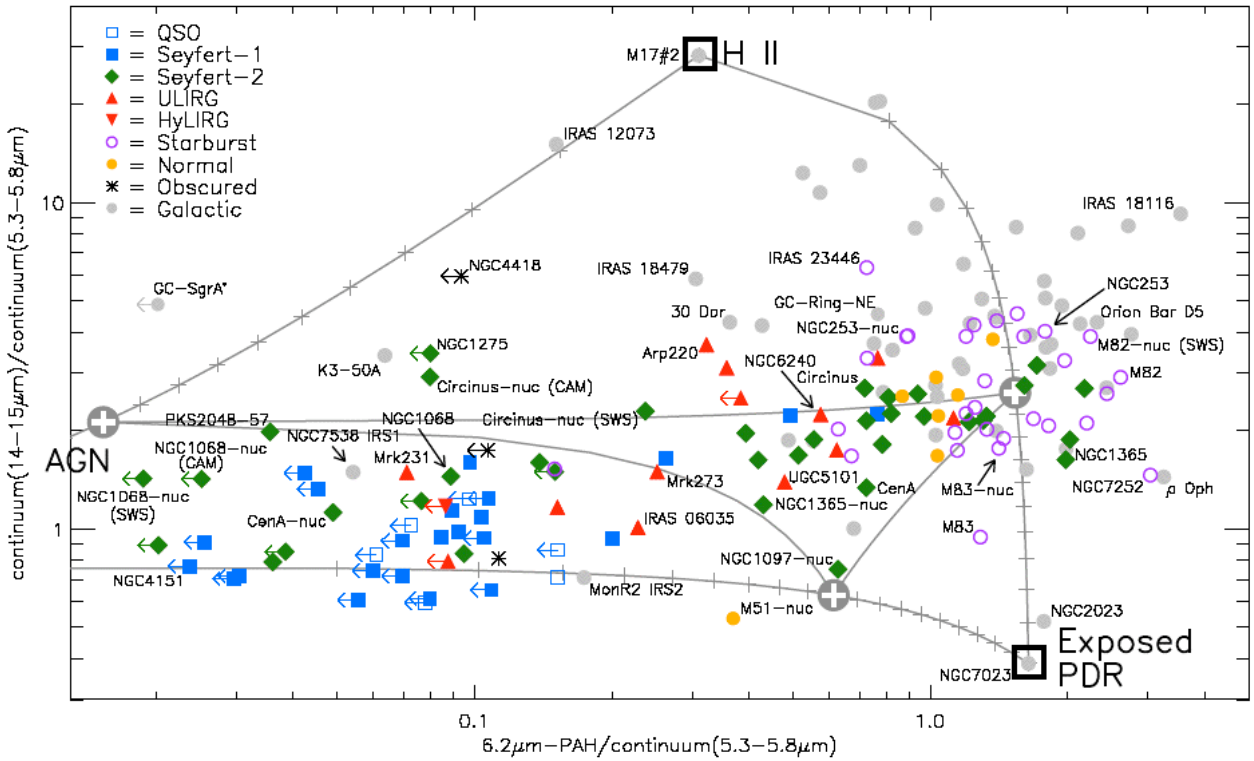
Peeters et al, 2004, ApJ, 613, 986

Mix and Match



Peeters et al, 2004, ApJ, 613, 986

Templates



Laurent et al., 2000, A&A, 359, 887

SUMMARY

- PAHs are ubiquitous in the ISM of galaxies
  - HII regions, reflection nebulae, planetary nebulae, galactic nuclei, …
  - Diffuse ISM, molecular cloud surfaces, general ISM
  - Star burst galaxies, ULIRGs, lensed & submm galaxies
- PAHs are active “players” in the ISM of galaxies
  - Photoelectric effect on PAHs (regulates phases of the ISM)
  - PAHs regulate ionization structure of molecular clouds
  - PAHs regulate molecular abundances, ambipolar diffusion, cooling…
- PAHs trace the conditions in the ISM of galaxies
  - Spectral characteristics of PAHs reflect local physical conditions through charge state (!) and molecular structure (gas phase reactions and photolysis ?)
- PAHs provide “dyes” for star formation
  - PAHs are a partially calibrated tracer of star formation rate
  - Have to account for deeply embedded star formation

Future

- What are the spectroscopic signatures of large PAH molecules and how do they depend on the molecular structure ?
- What is the relation between the chemical and physical characteristics of large molecules (size, charge state, excitation) and the physical conditions of a region ?
- How can we translate these observational characteristics into astronomers tools to reveal the physical conditions in regions near and far ?
- What does that tell us about the processes taking place in the universe ?
- What does that tell us about the organic inventory of the Universe and in particular the habitable zone of regions of planet formation ?

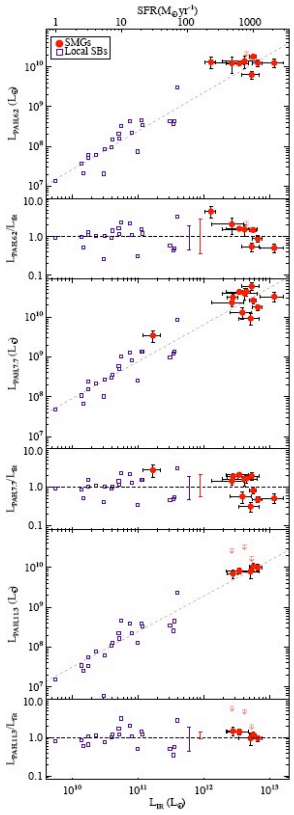
Key Questions on PAHs

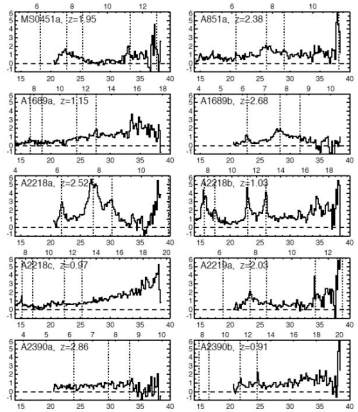
- Are interstellar PAHs an important source of organic molecules in meteorites, comets, interplanetary dust particles, and other Solar system bodies ? Are PAHs an important reservoir of carbonaceous species in other planet forming environments or are PAHs rapidly destroyed in the habitable zone ?
- Do the PAHs represent a separate chemical route towards complex molecules or are they formed by the same reactions that make small interstellar molecules ? Are PAHs the building blocks of very small and big grains ? Is the photolysis of PAHs an important source of small molecules in the ISM ?
- Is the photo-electric effect on PAHs an important heating agent for interstellar gas ? Does the presence or absence of PAHs change the character of the cloud and intercloud phases and structure as well as the star formation characteristics of the ISM of galaxies ?
- Are PAHs the dominant charge carriers in molecular clouds ? Do they therefore control the ambipolar diffusion process that enables the collapse of molecular cloud cores ? As the most abundant anions, do PAHs influence the formation of other species through ion-molecule reactions ?
- Are PAHs destroyed in AGN toroids by X-ray photons and what is the timescale for this process? Is the presence of PAHs evidence for the absence of AGN activity ?
- What causes the spectral variations of PAHs in regions of massive star formation and how does that depend on the local conditions ? Can we use the observed PAH features as an astronomical tool that measures the physical and chemical conditions in regions of massive star formation, including ULIRGs and galaxies at high red-shift ? Is the absence of PAHs evidence for the absence of starformation activity ?

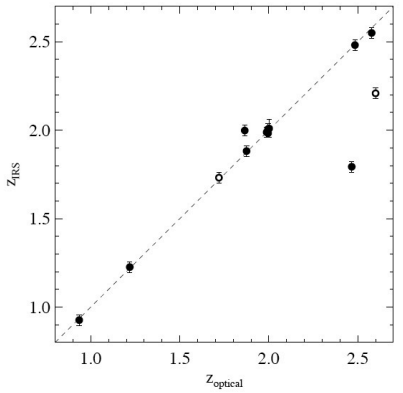
MIRI: PAHs Measuring the Star Formation History of the Universe

- PAHs as tracers of redshift
- PAHs as quantitative measures of the star formation rate

$$\mathrm{SFR}\,[\mathrm{M_\odot yr^{-1}}] \simeq 10^{-7}\, L_{\mathrm{PAH,6.2}}\,[\mathrm{L_\odot}].$$



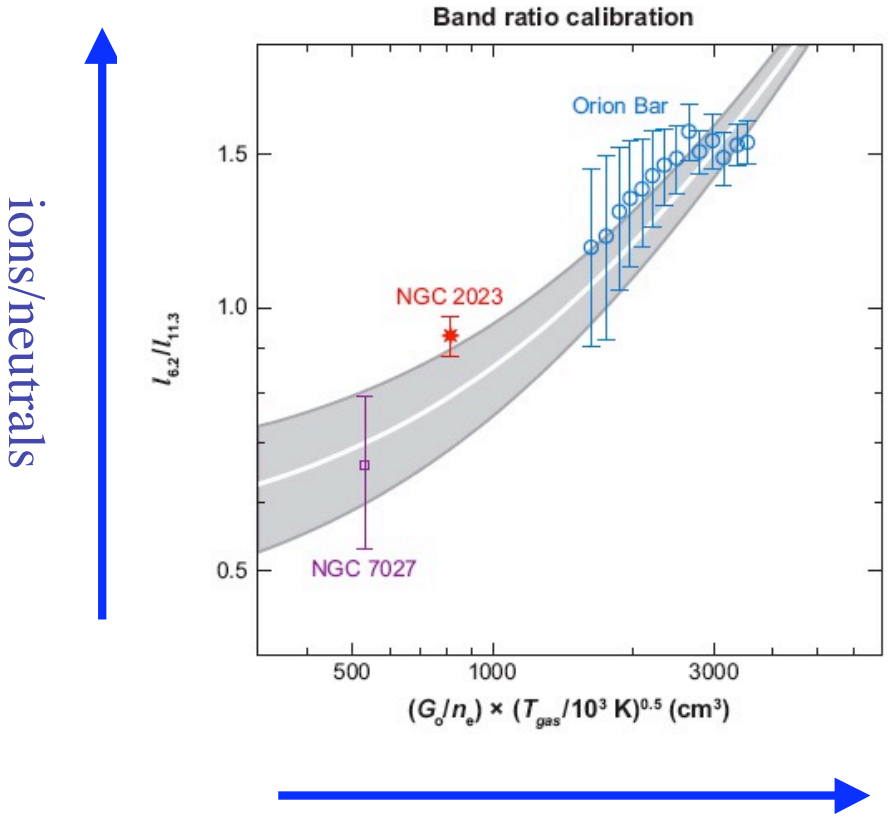




Pope et al, 2008, ApJ, 675, 1171
Rigby et al, 2008, ApJ, 675, 262

MIRI: PAHs Measuring the Conditions of Star Formation in the Universe

Calibrated PAH "tools" will probe the physical conditions in regions of star formation

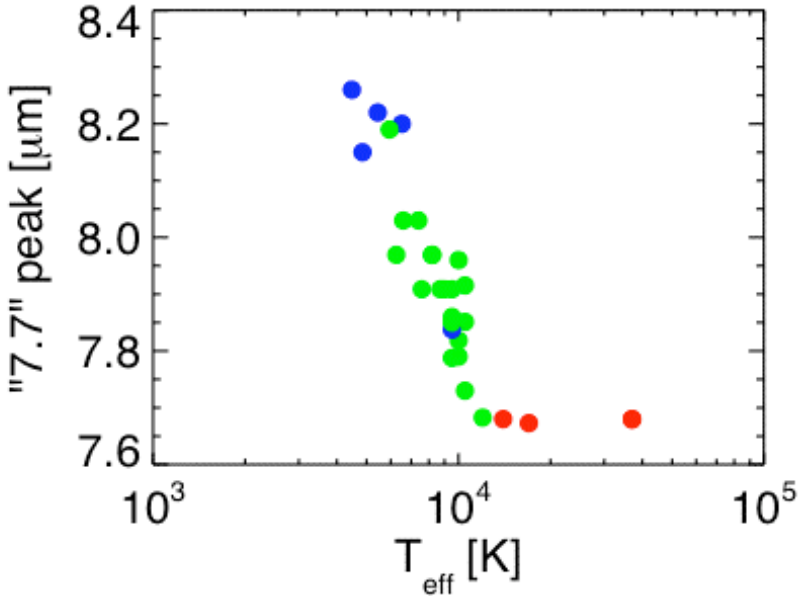


Galliano et al, 2008, ApJ, 679, 310
Hony et al., 2001, A & A, 370, 1030
Bakes et al., 2001, ApJ, 556, 501

JWST & PAHs in Planet Forming Disks

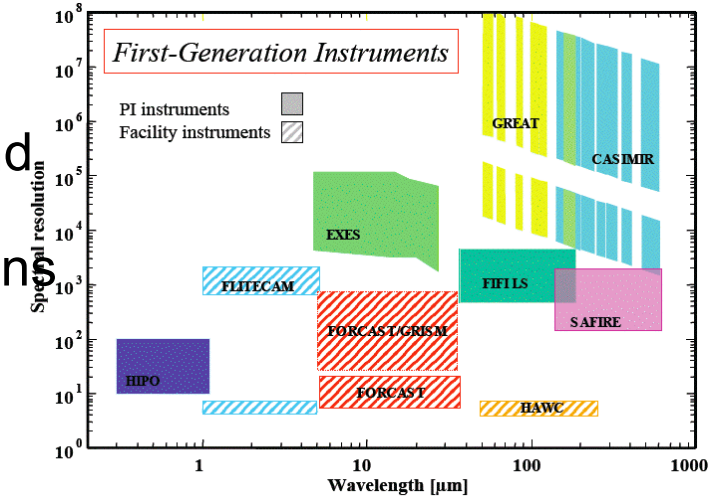
MIRI/JWST will be able to probe the spectral & chemical evolution of PAHs in regions of star and planet formation

- Chemical inventory
- Chemical processes:
  - UV/ X-ray/thermal
- Physical processes:
  - mixing/lightning/shocks



Developing PAHs as Astronomical Tools

- Mid-IR spectral imaging in CH and CC PAH bands to measure ionization parameter coupled with diagnostic (PDR) gas lines, and far-IR dust continuum mapping and CII and OI cooling line to measure physical conditions and heating efficiency



SOFIA's discovery space

- Spitzer has spectrally mapped the PAH features in a wide range of galactic and extragalactic regions
- Herschel can probe the physical conditions in the PAH emission zones
- JWST will find PAHs all the way back to when the Universe was young
- SOFIA: wide wavelength coverage, wide range of spectral resolution, wide array of instruments is the ultimate "PAH-tool machine"

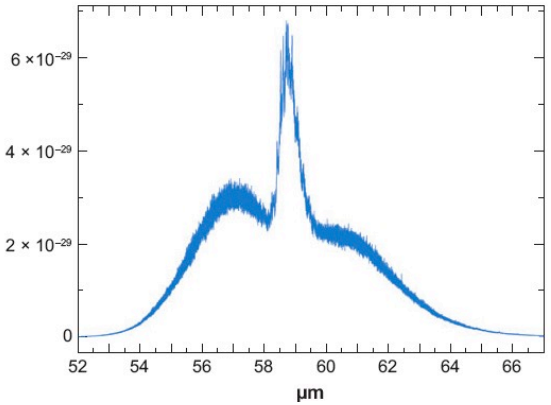
Looking for the 'GrandPAH'

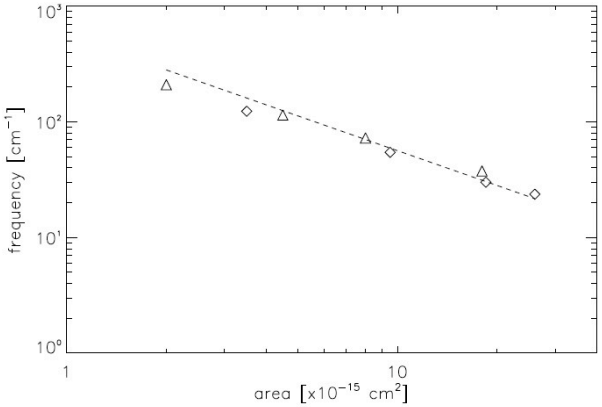
The interstellar PAH family seems to be dominated by a few, large, very stable, compact PAHs

Identification of specific PAHs

- Electronic spectra & DIBs
- Pure rotational spectra
- Drumhead modes: Lowest-lying vibrational state will emit when the modes have decoupled

SOFIA/Herschel

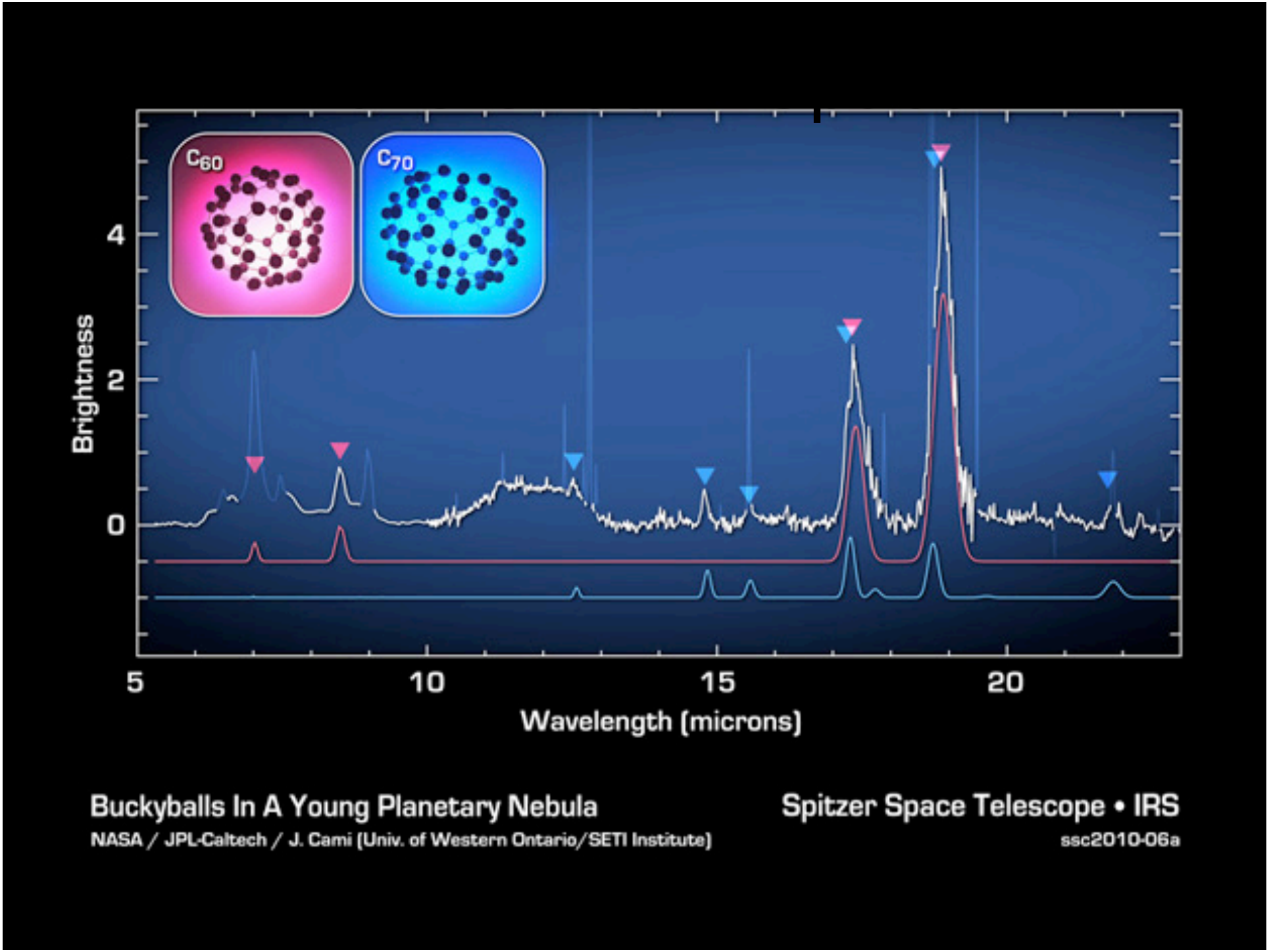




Mulas et al, 2006, A & A, 456, 161
Boersma et al, 2010, in prep

GrandPAH II

- If GrandPAHs truly exist, identification is key:
  - Molecular specific properties control the role of interstellar PAHs
  - Interstellar PAHs as prebiotic species
  - Interstellar PAHs and the organic inventory of planetary systems
  - Markers of abiotic complexity

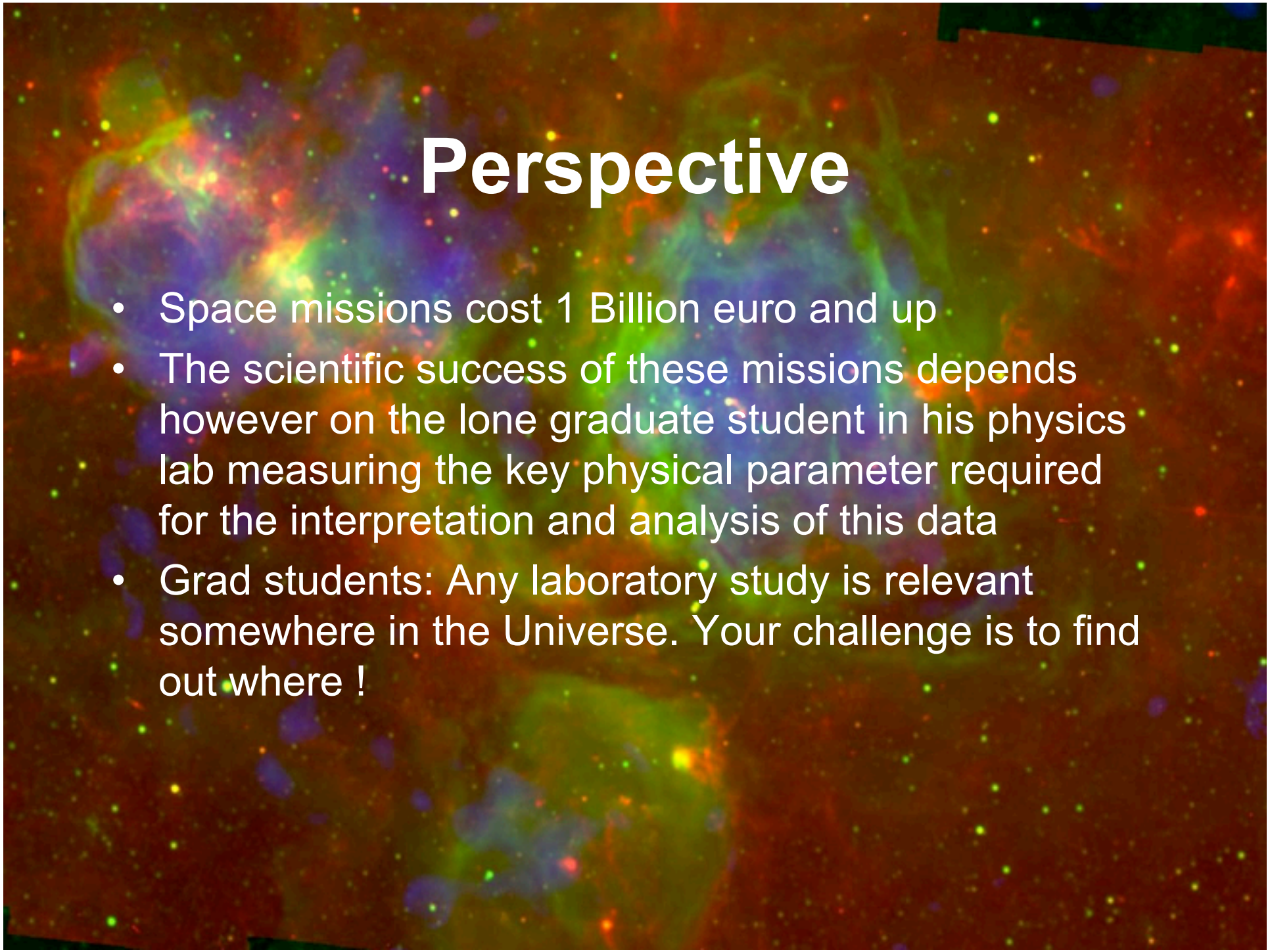


Buckyballs In A Young Planetary Nebula

NASA / JPL-Caltech / J. Cami (Univ. of Western Ontario/SETI Institute)

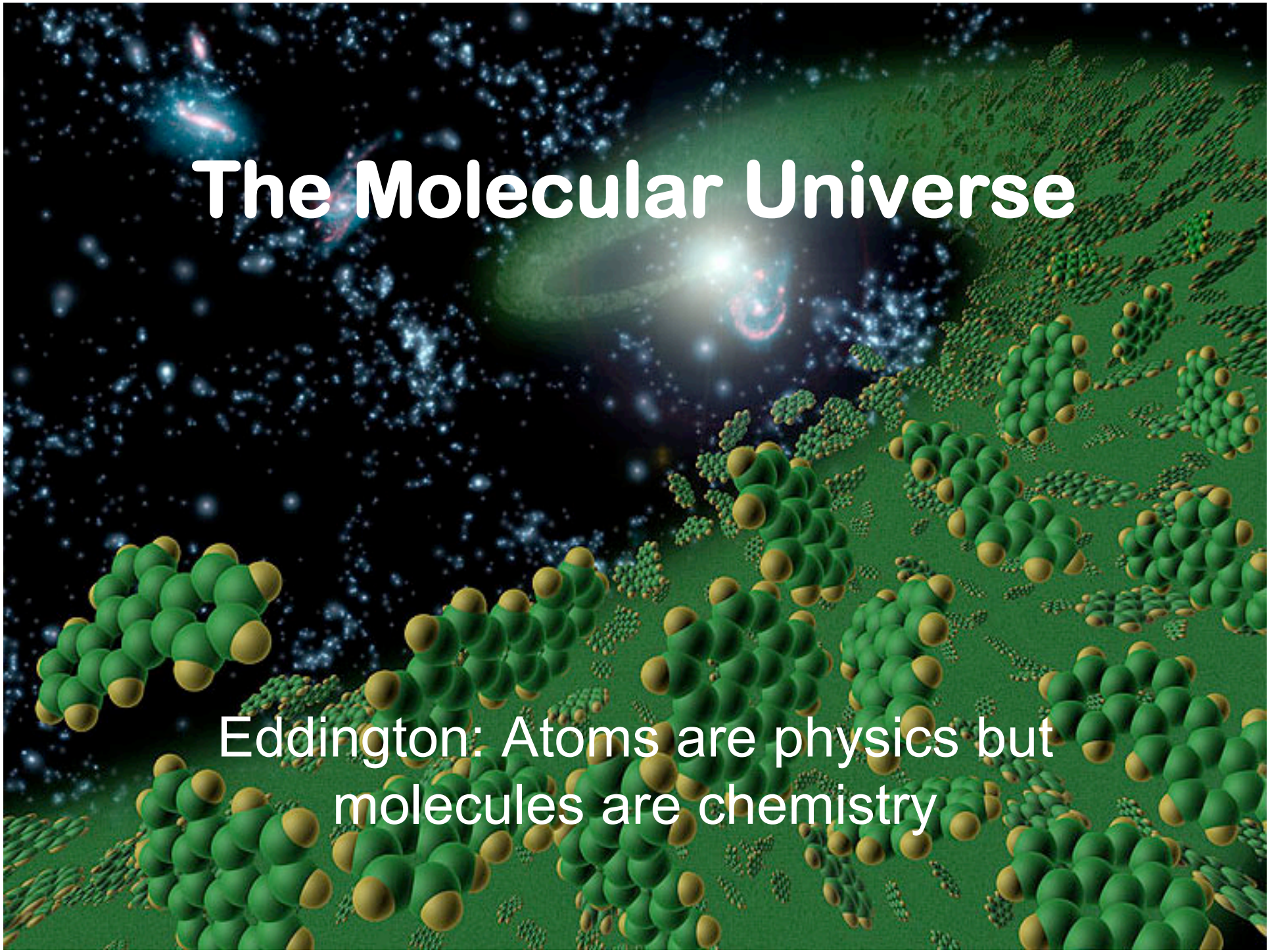
Spitzer Space Telescope • IRS

ssc2010-06a



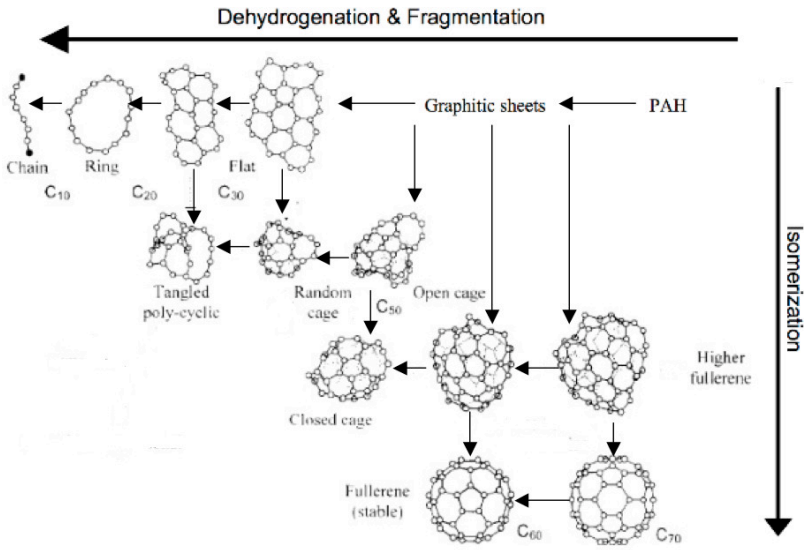
Perspective

- Space missions cost 1 Billion euro and up
- The scientific success of these missions depends however on the lone graduate student in his physics lab measuring the key physical parameter required for the interpretation and analysis of this data
- Grad students: Any laboratory study is relevant somewhere in the Universe. Your challenge is to find out where !

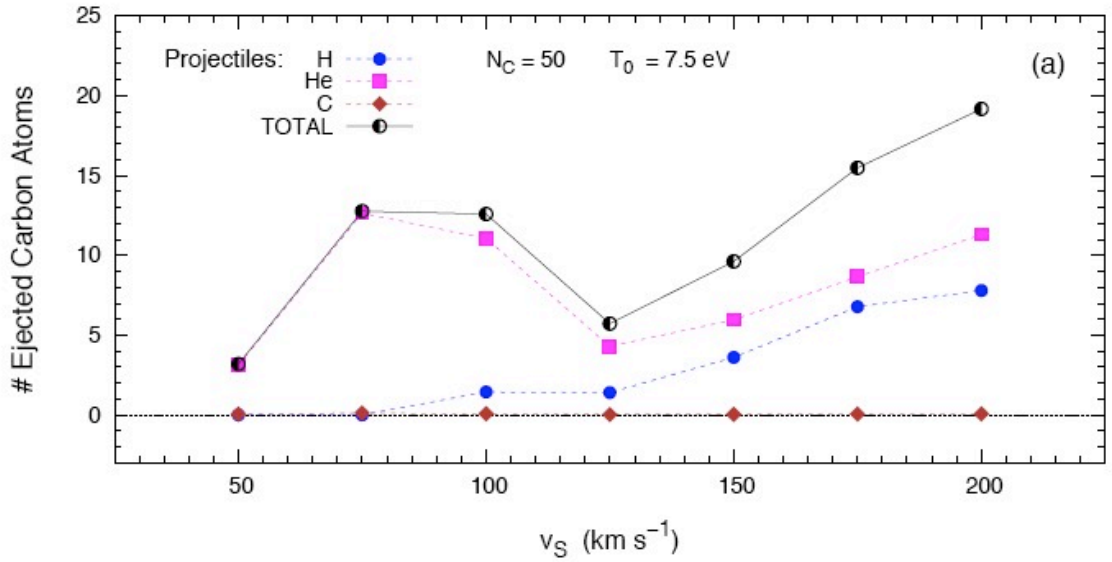

The Molecular Universe
Eddington: Atoms are physics but molecules are chemistry

PAHs as source of interstellar moelcules

- PAHs are injected by C-rich AGB stars as part of the soot formation process
- In the ISM, over ~100 Myr, PAHs are processed by UV photons “concentrating” the PAH family into its strongest members, the GrandPAHs
- This process will be a source of related compounds including small hydrocarbons, sheets, cages, rings, and chains
- The DIB carriers are likely “hidden” in chemical scheme



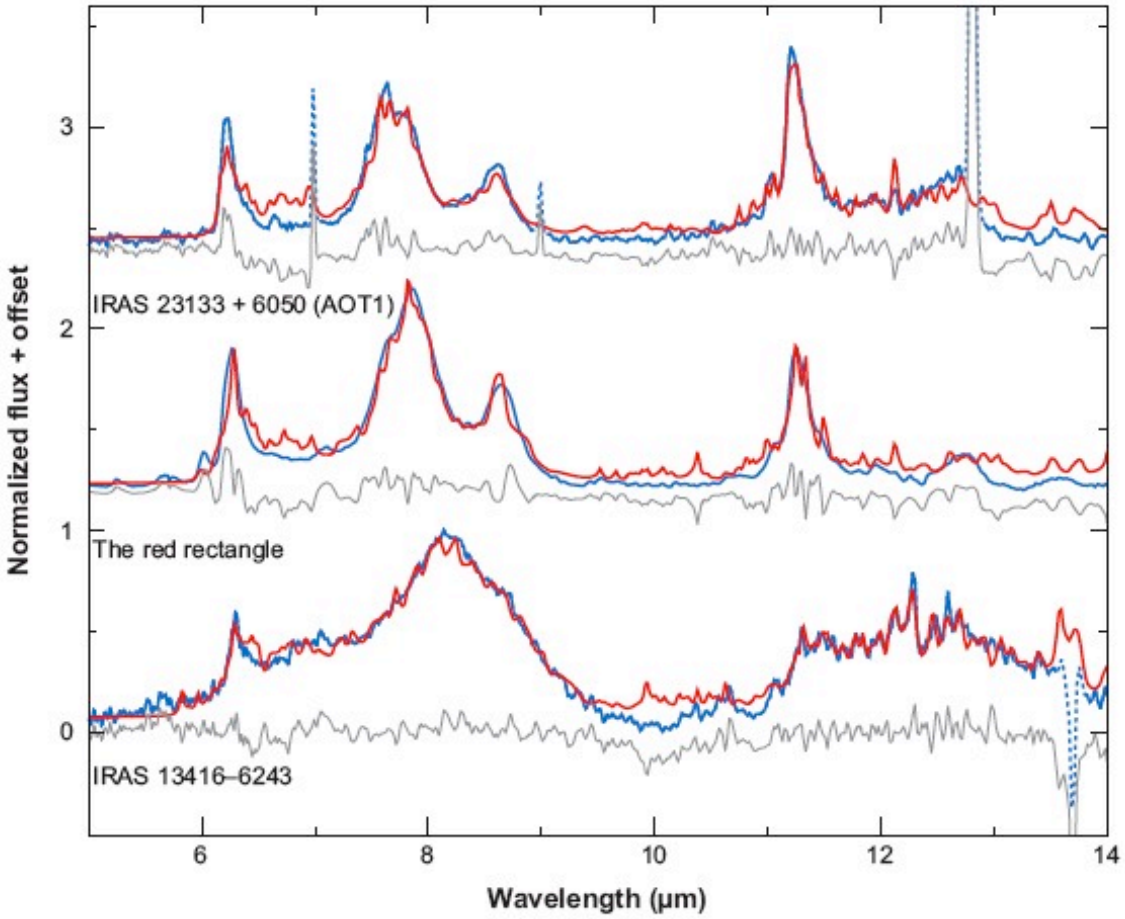
PAHs and Shocks



- Nuclear knock on collisions by helium results in loss of ~10 C-atoms
- Gas phase reactions and UV photolysis will lead to further “gardening” of the PAH population

Micelotta et al, 2008, in prep

Spectral Fits



- Cami et al, 2008, in prep

- http://www.astrochem.org/pahdata
- http://astrochemistry.ca.astro.it/database