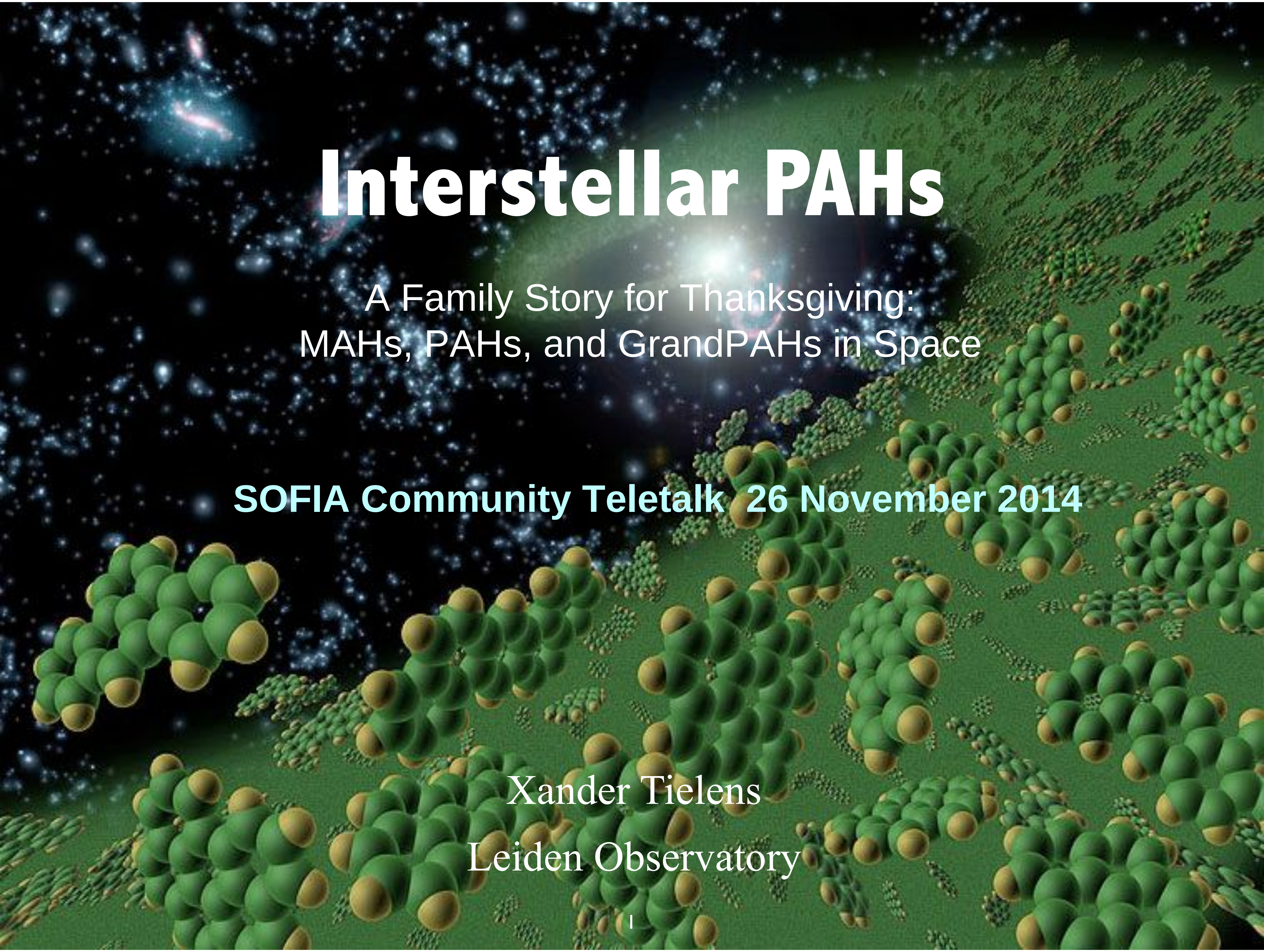


Interstellar PAHs

A Family Story for Thanksgiving:
MAHs, PAHs, and GrandPAHs in Space

SOFIA Community Teletalk 26 November 2014

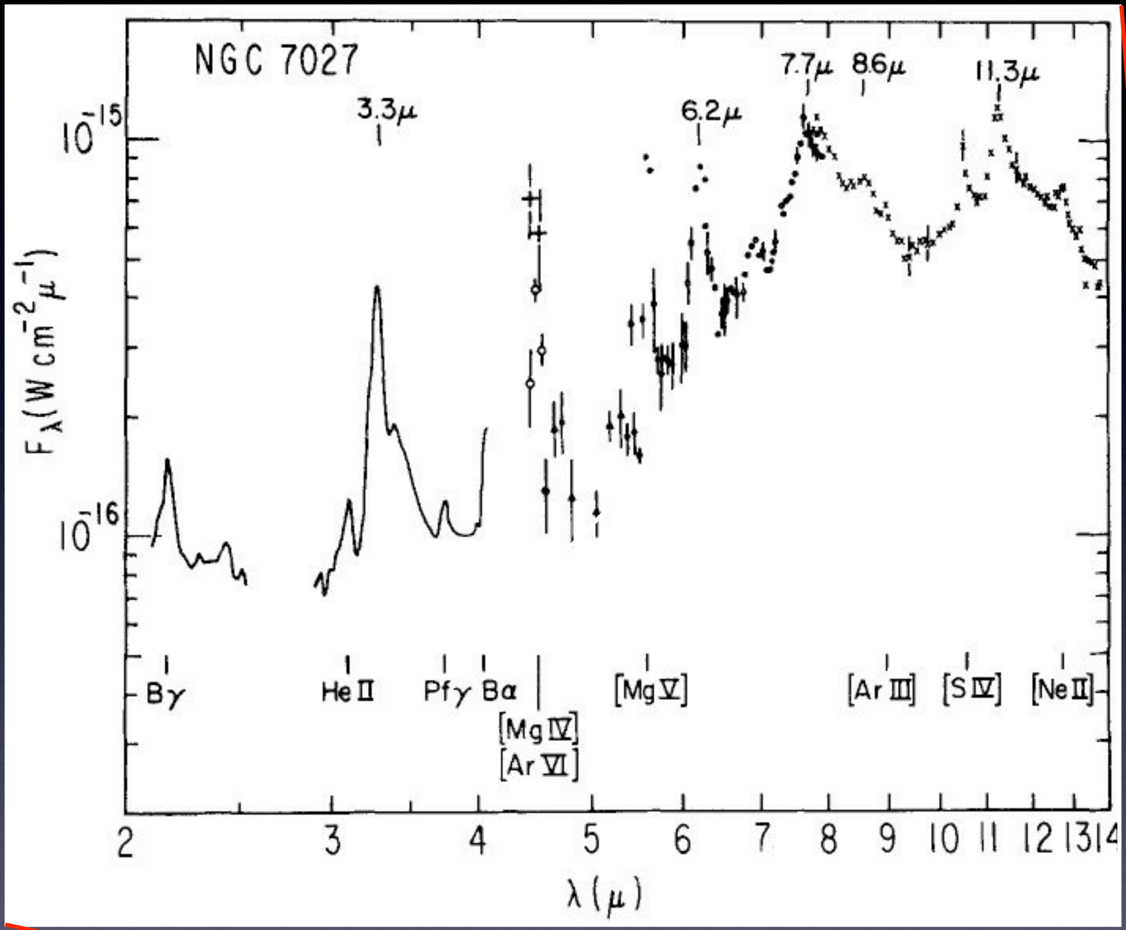
Xander Tielens

Leiden Observatory

The Grand Challenges of Astrochemistry

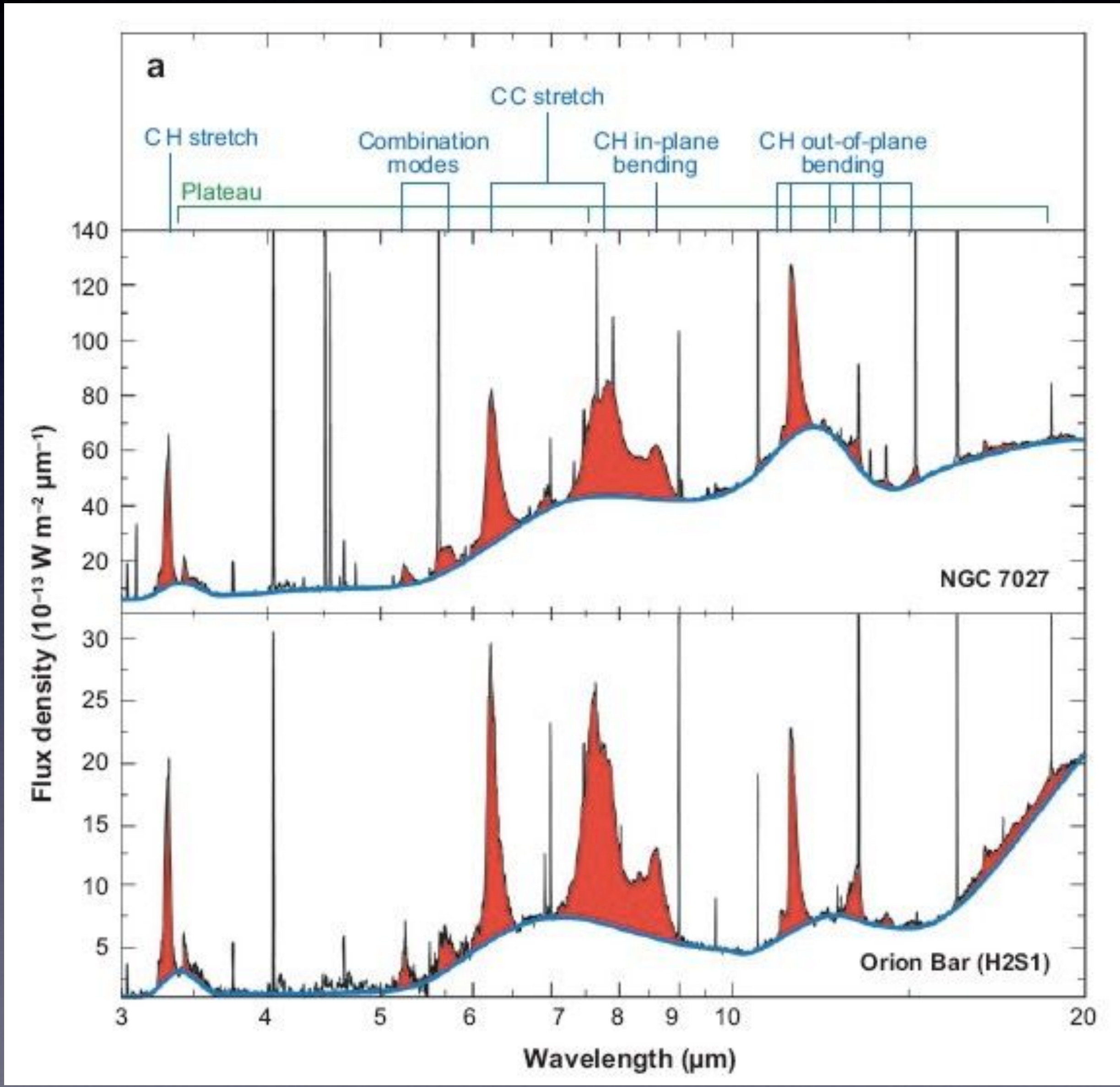
- What is the organic inventory of space, in particular in regions of star and planet formation and how does that relate to the prebiotic origin of life ?
- What is the role of molecules in the evolution of the Universe ?
- How can we use molecules to study the Universe ?

a trip down memory lane



Russell, Soifer, Willner 1977, ApJ, 217, L149

The incredibly rich spectrum of interstellar PAHs



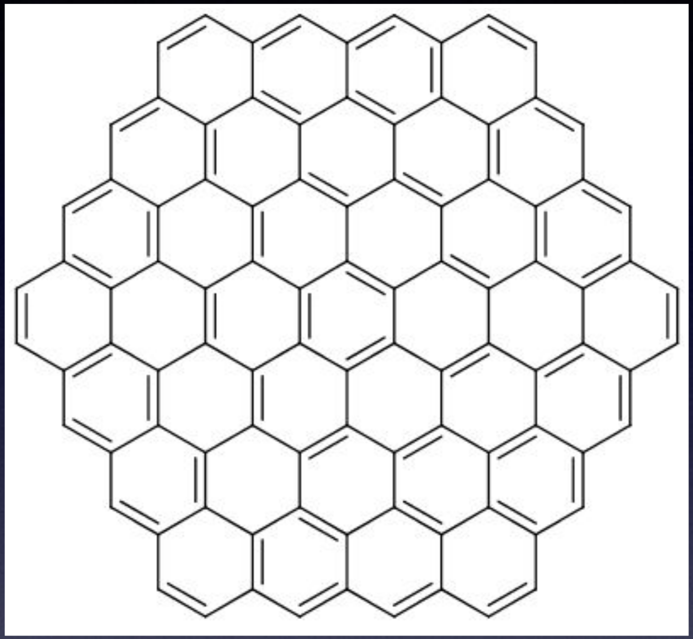
Peeters et al, 2002, A&A,390, 1089

Interstellar PAHs & the IR emission features

- The IR emission features are due to a population of Polycyclic Aromatic Hydrocarbon molecules
- Typical size N_c ~ 50 C-atoms
- some 5-20% of the elemental carbon in space
- Highly aromatic (aliphatic, carbonyl, amine, hydroxyl all less than 2% relative to C or H, respectively)

GrandPAHs

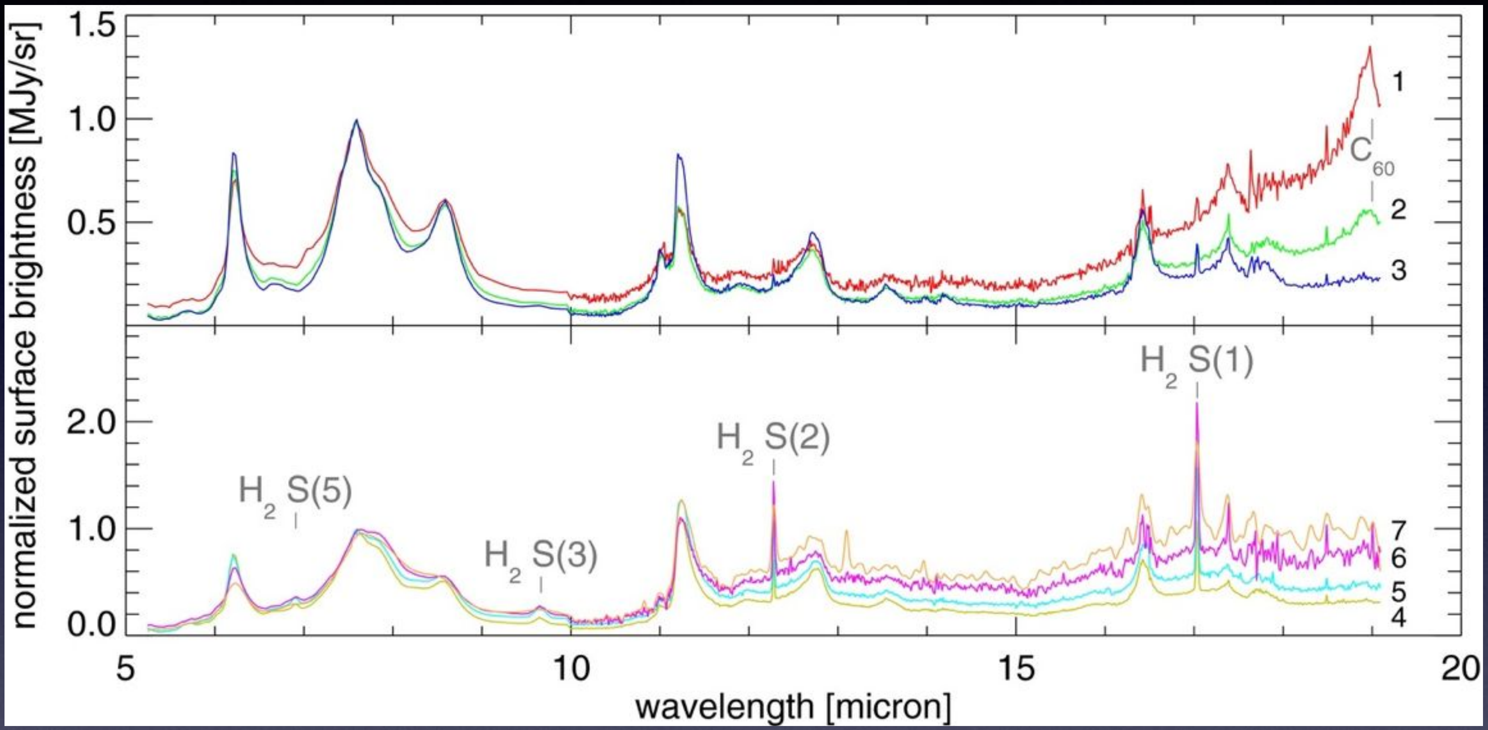
- IR emission spectra are very similar, particular in the "extreme" regions of the ISM
- 15-20 μm region often dominated by a few bands (16.4/17.4/17.8 μm)
- Typical PAH will absorb some 100 Million UV photons over its lifetime ⟶ what can break, will break
- Interstellar PAH family dominated by a few, extremely stable species: the grandPAHs



circumcircumcoronene

Tielens 2008, ARAA, 46, 289

Chemical Variations in NGC 7023

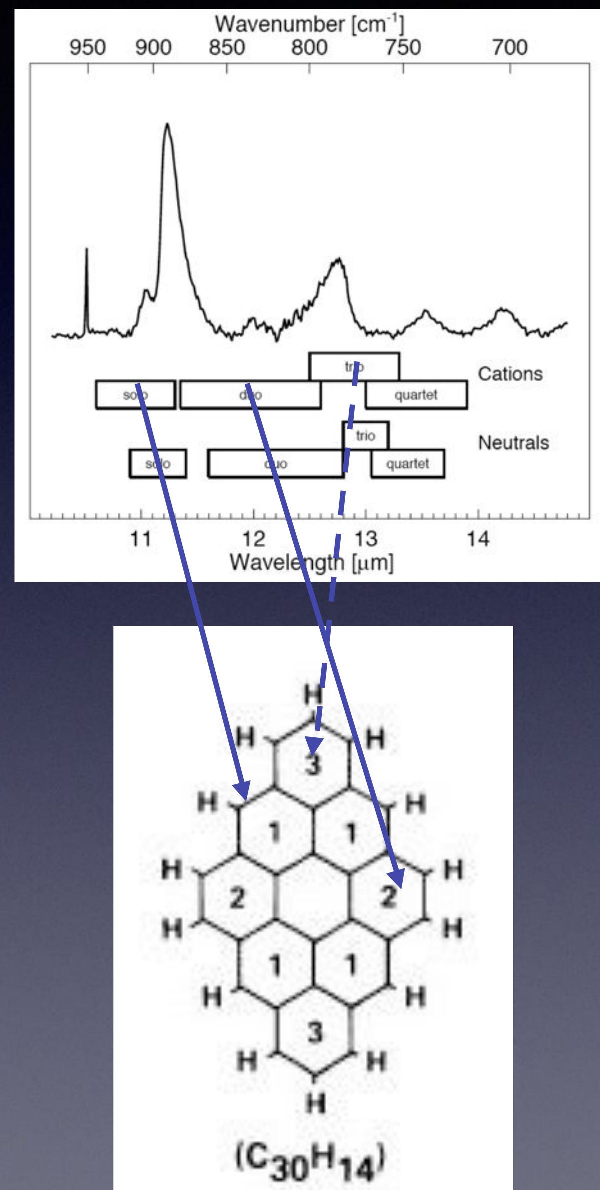


Boersma et al 2014, ApJ, 795, 110

- Spectral variations imply chemical variations:
- 7.6/7.8, 6.2/7.6, & 11.2/12.7 µm bands

Molecular Structure of Interstellar PAHs

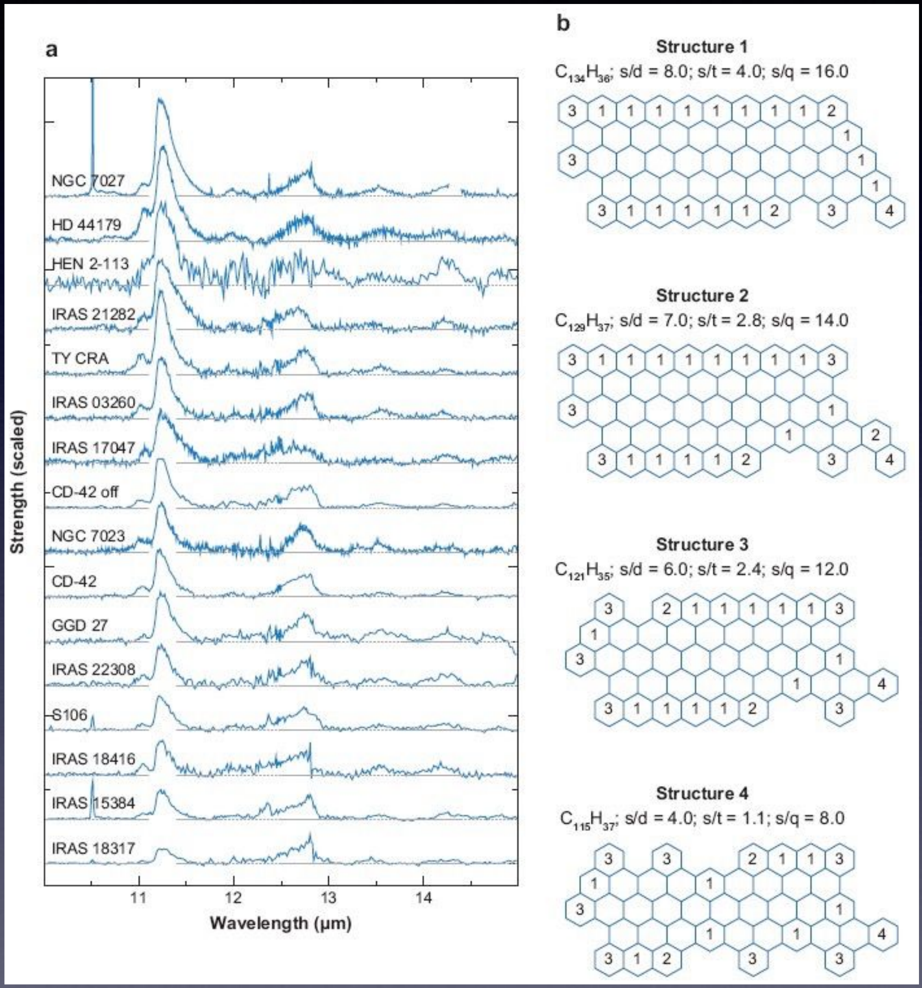
- The out-of-plane bending modes probe the “edge” structure of PAHs
- Spectral pattern is sensitive to “H-adjacency”



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

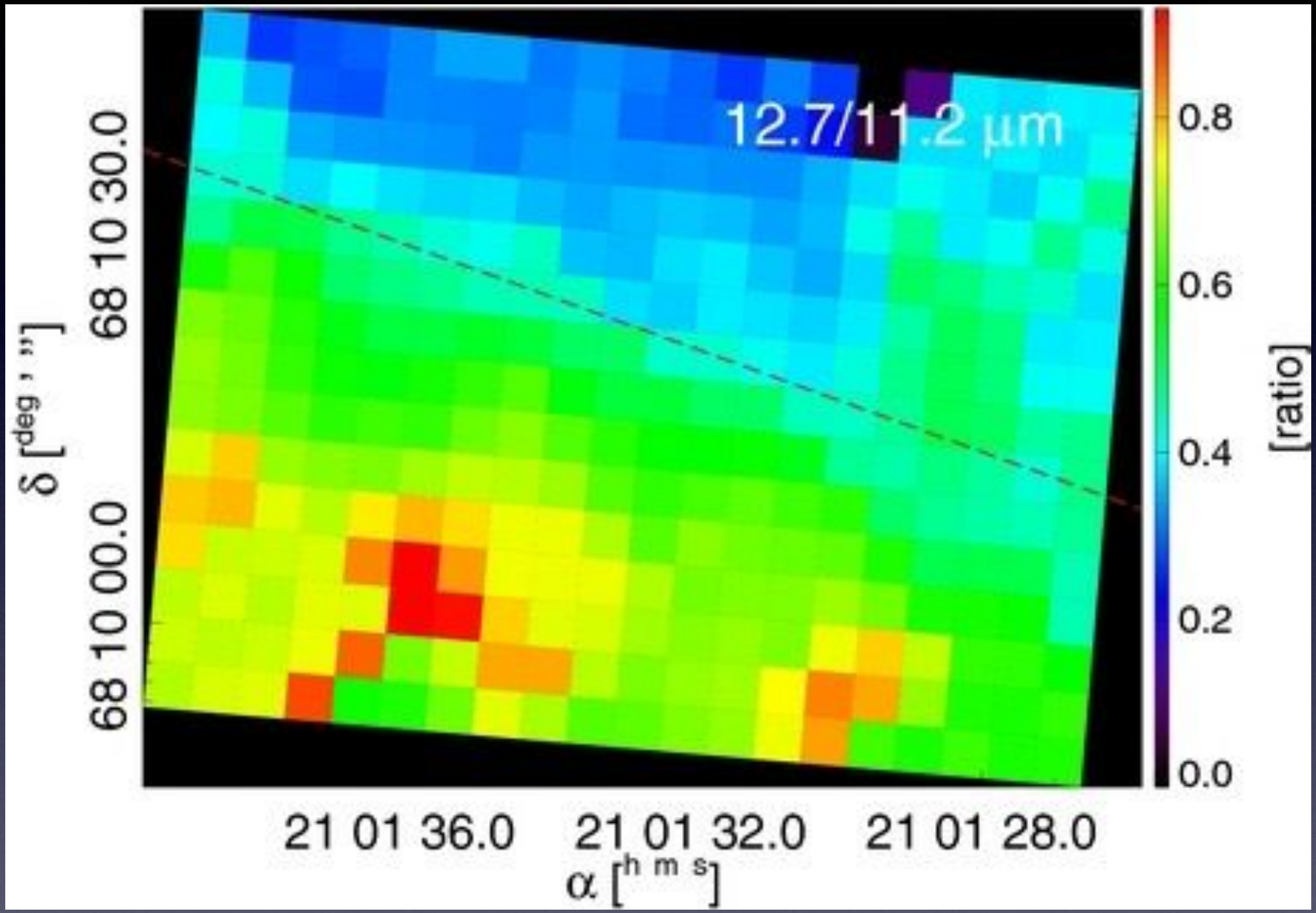
Molecular Structure of Interstellar PAHs

- 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

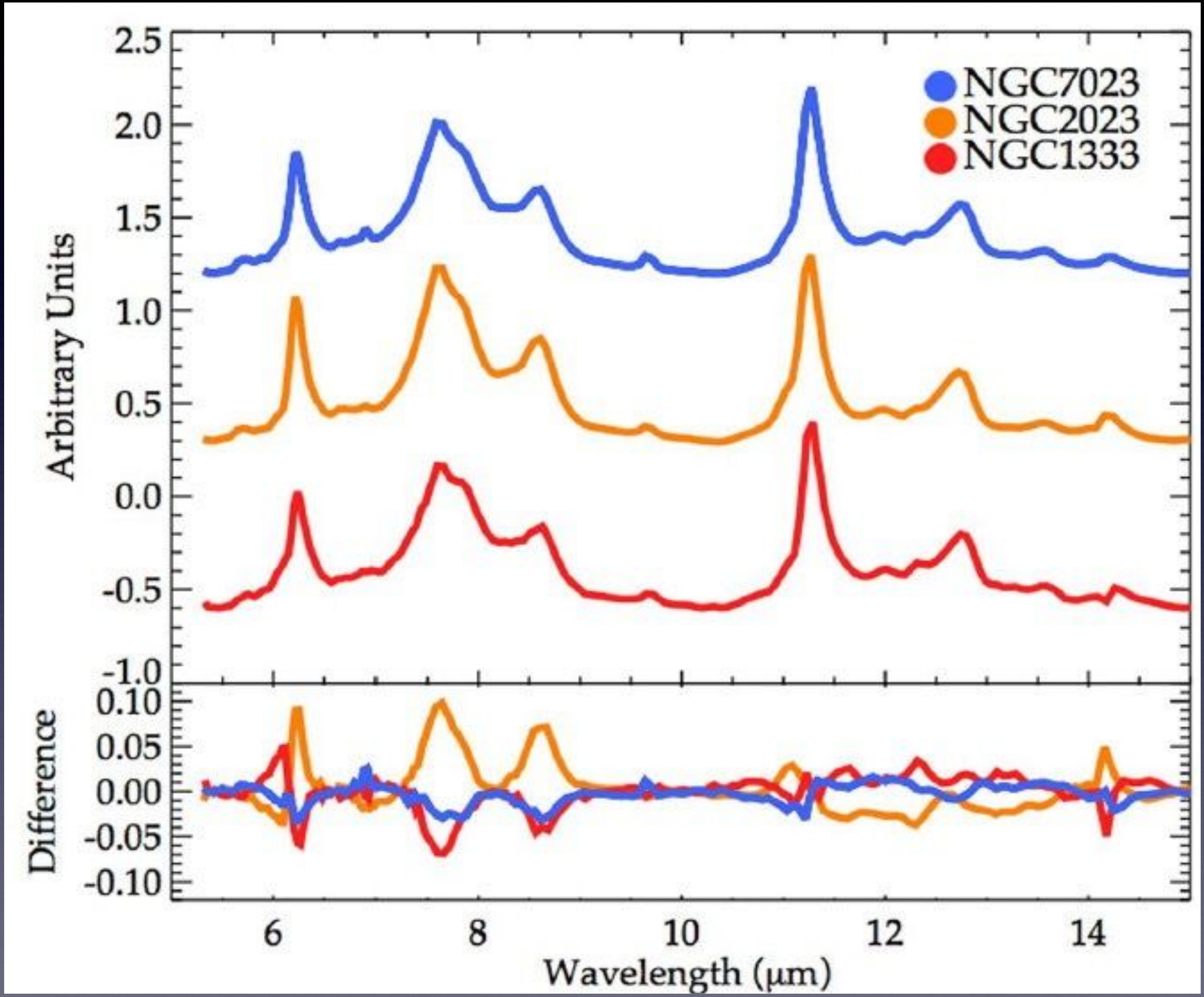
Spectral-spatial variations in NGC 7023



Boersma et al 2014, ApJ, 795, 110

Close to the illuminating star, the emitting PAH population has many more "corners" than straight edges

PAH Spectra at the Brightest Spots of Reflection Nebulae

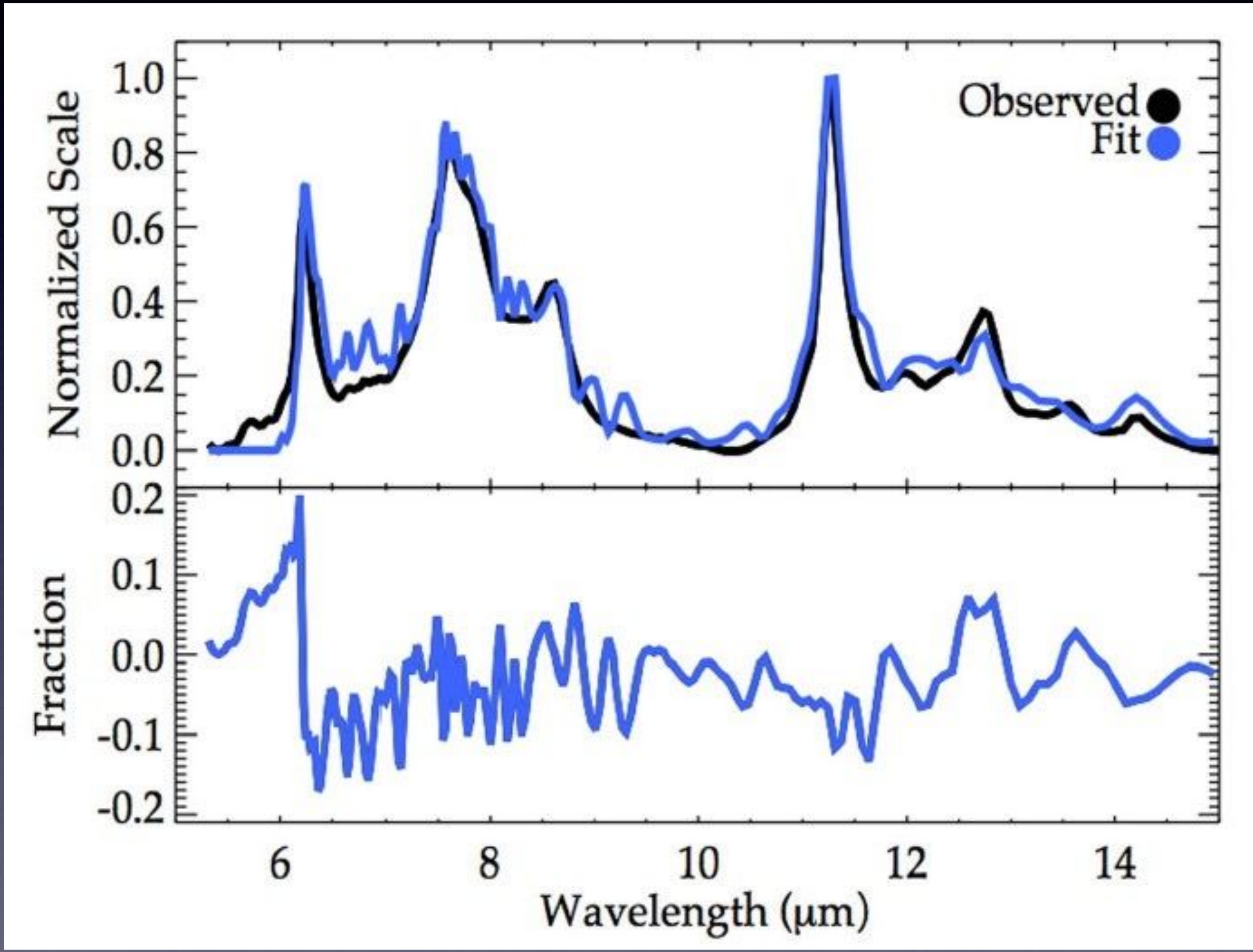


incredibly similar spectra

Werner et al, 2009, AAS, 412.15
Andrews et al, 2014, submitted

PAH Database Fit: Baserun

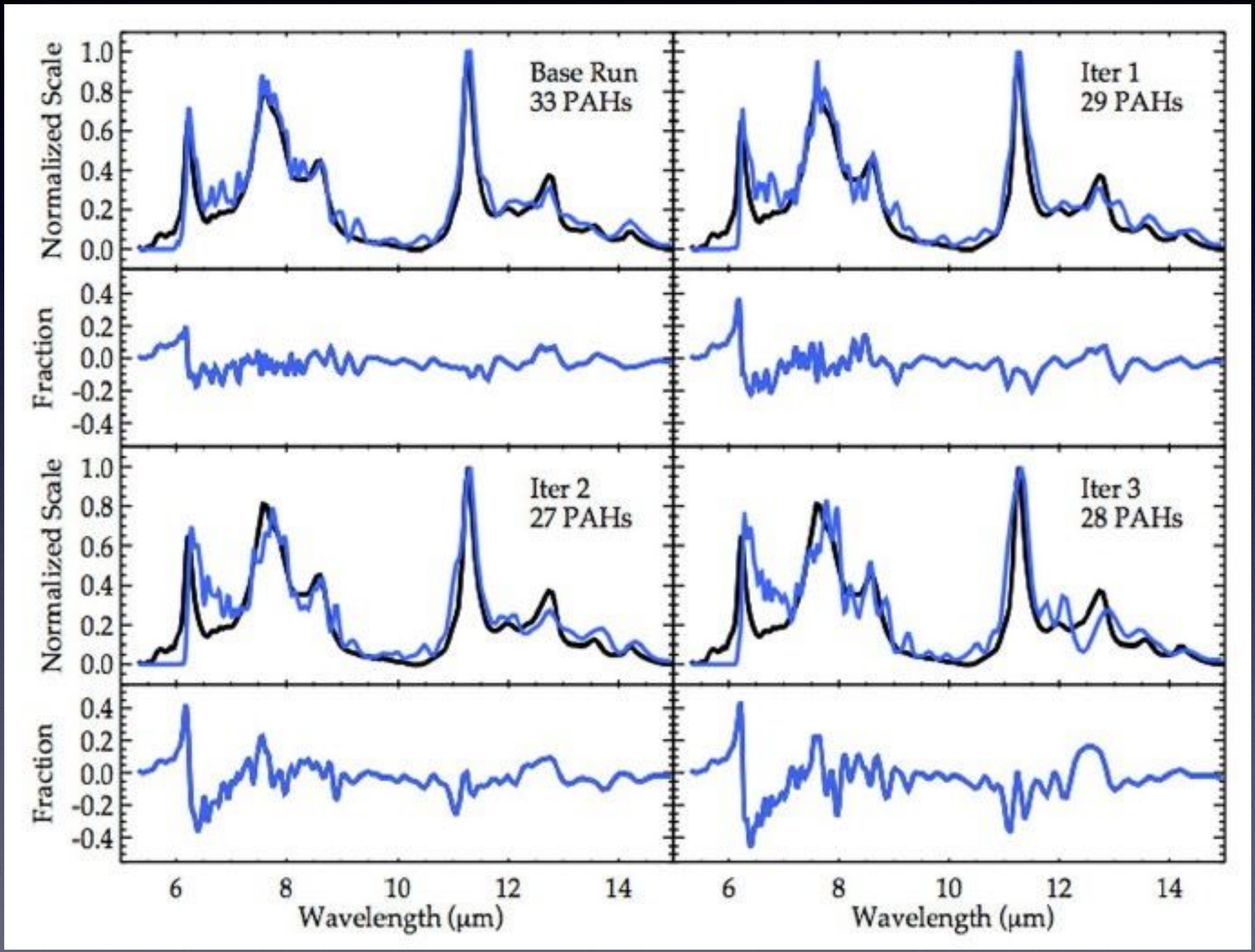
Andrews et al, 2014, submitted



http:www.astrochem.org/pahdb

The NASA Ames PAH database provides a convenient tool to probe the characteristics of the emitting PAH population

PAH Database Fit: Sequential Baseruns

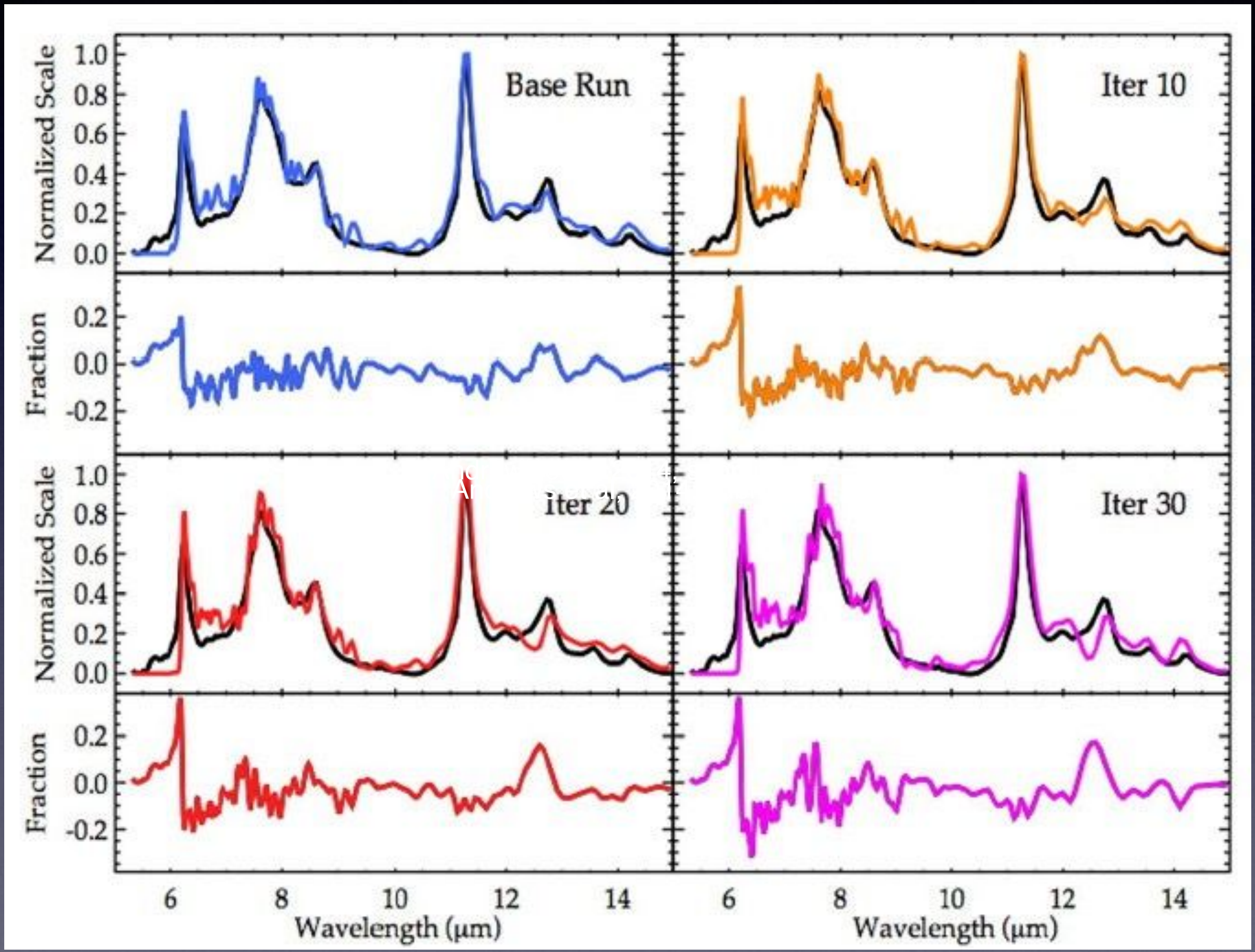


Andrews et al, 2014, submitted

Sequential fits: Removing the selected PAHs from the previous fits produces lower quality fit: Limited number of PAHs can produce good fit

PAH Database Fit: Sequential fits by removing most abundant PAH

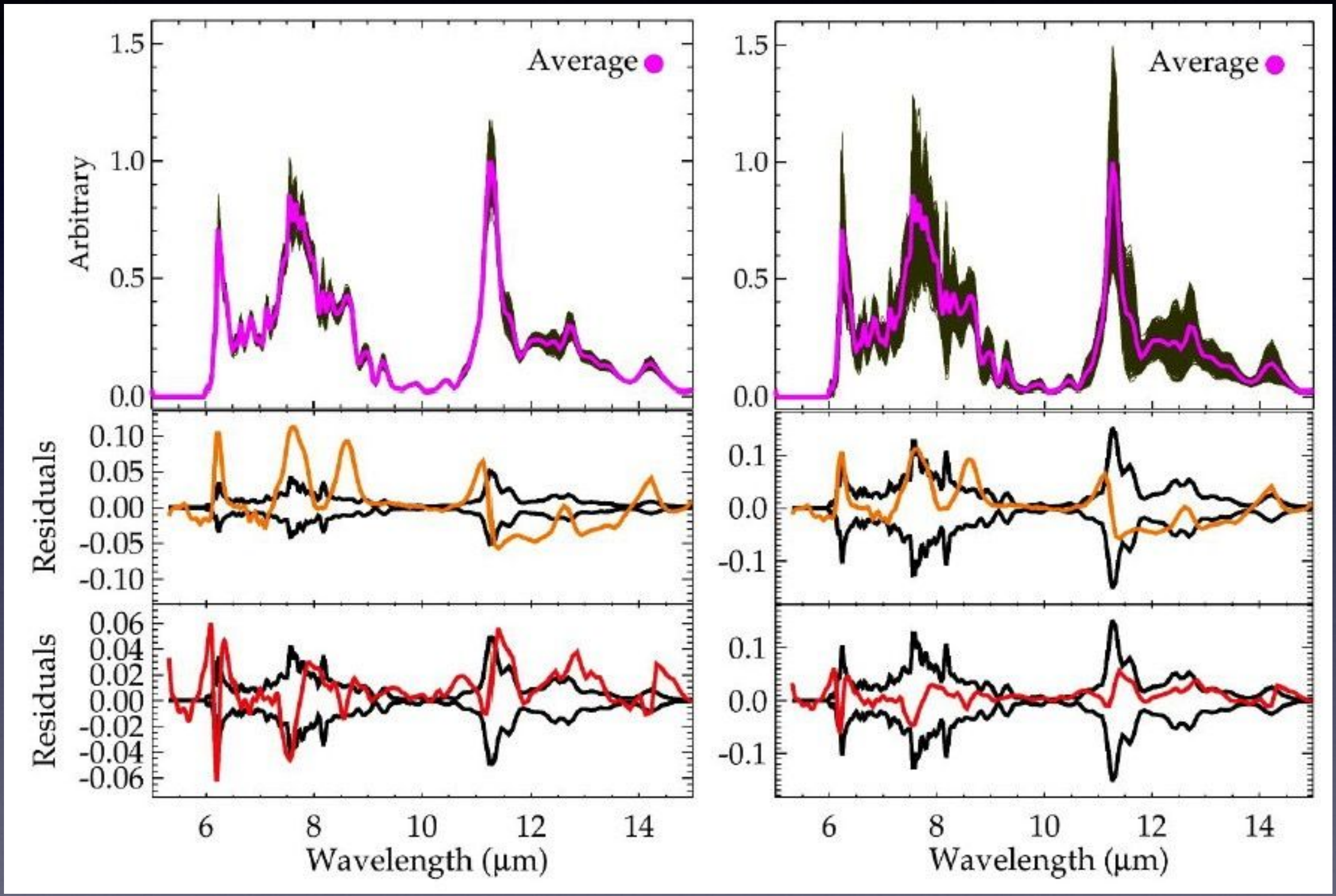
Andrews et al, 2014, submitted



Subtle variations in the emission characteristics of individual PAHs

PAH Database Fit: observed variations in the 3 RNe

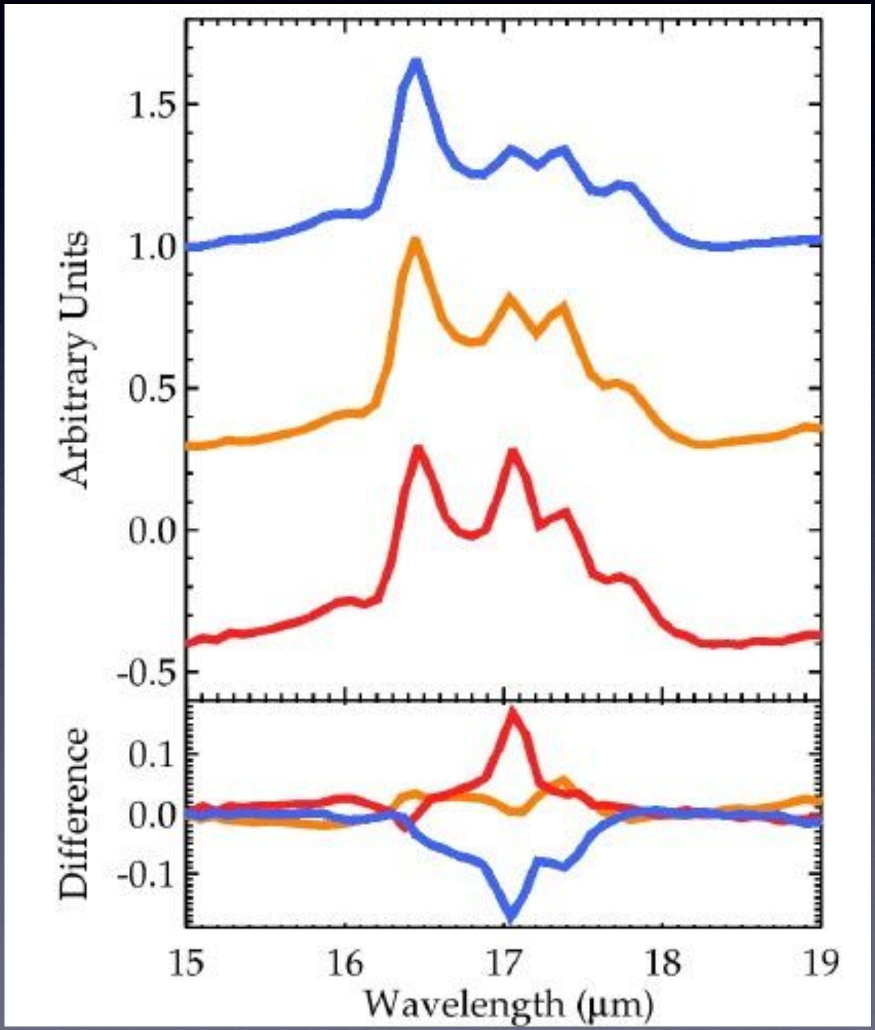
Andrews et al, 2014, submitted



The observed small variations in the spectra of the 3 reflection nebulae imply less than 30% variations in the abundances of the PAHs in the baserun fit.

The 16-18 µm Bands

- Observations reveal very similar spectra for these 3 RNe (except for H_2 line at 17 µm)
- Carbon skeletal modes
- Most molecules show complex spectra with several bands
- Bands are molecule specific
- Evidence for (compact) grandPAHs



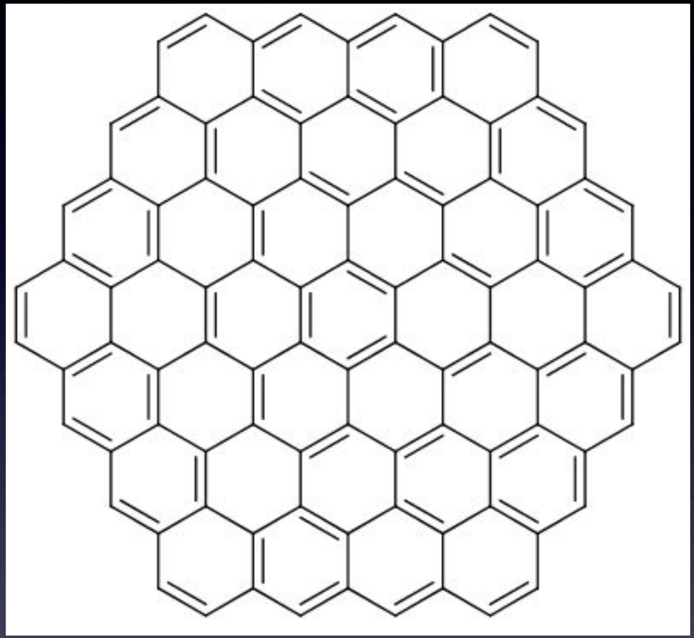
Ricca et al, 202012, ApJ, 754, 75
Andrews et al, 2014, submitted

Evidence for GrandPAHs

IR emission spectra are very similar in these 3 RNe

Database analysis:

- Limited number of species can contribute
- Subtle spectral variations among intrinsic PAH spectra imply very limited differences between PAH populations
- Abundance variations are less than 30%



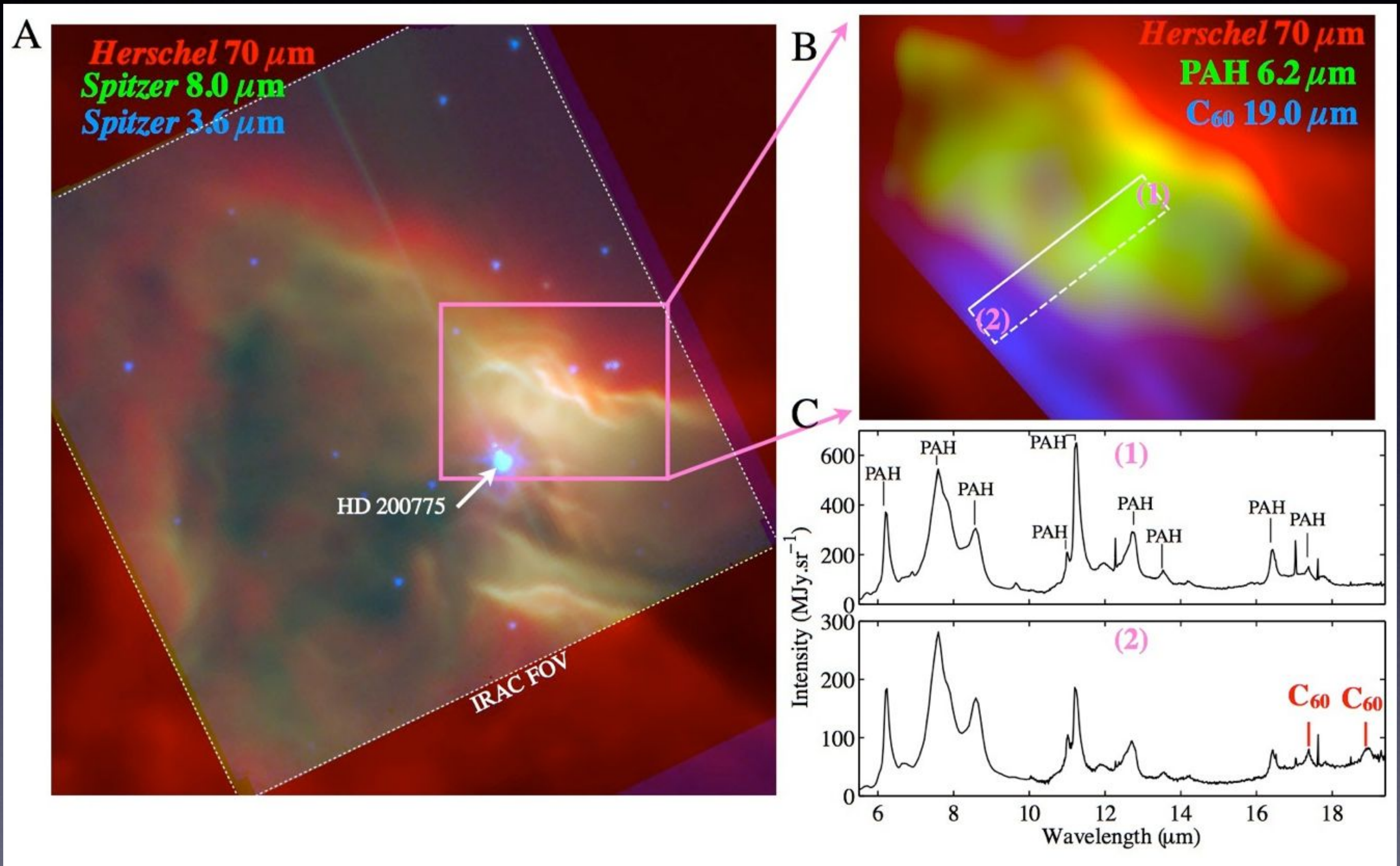
circumcircumcoronene

15-20 μm region dominated by a few bands (16.4/17.4/17.8 μm)

- A few, large, compact PAHs dominate the population

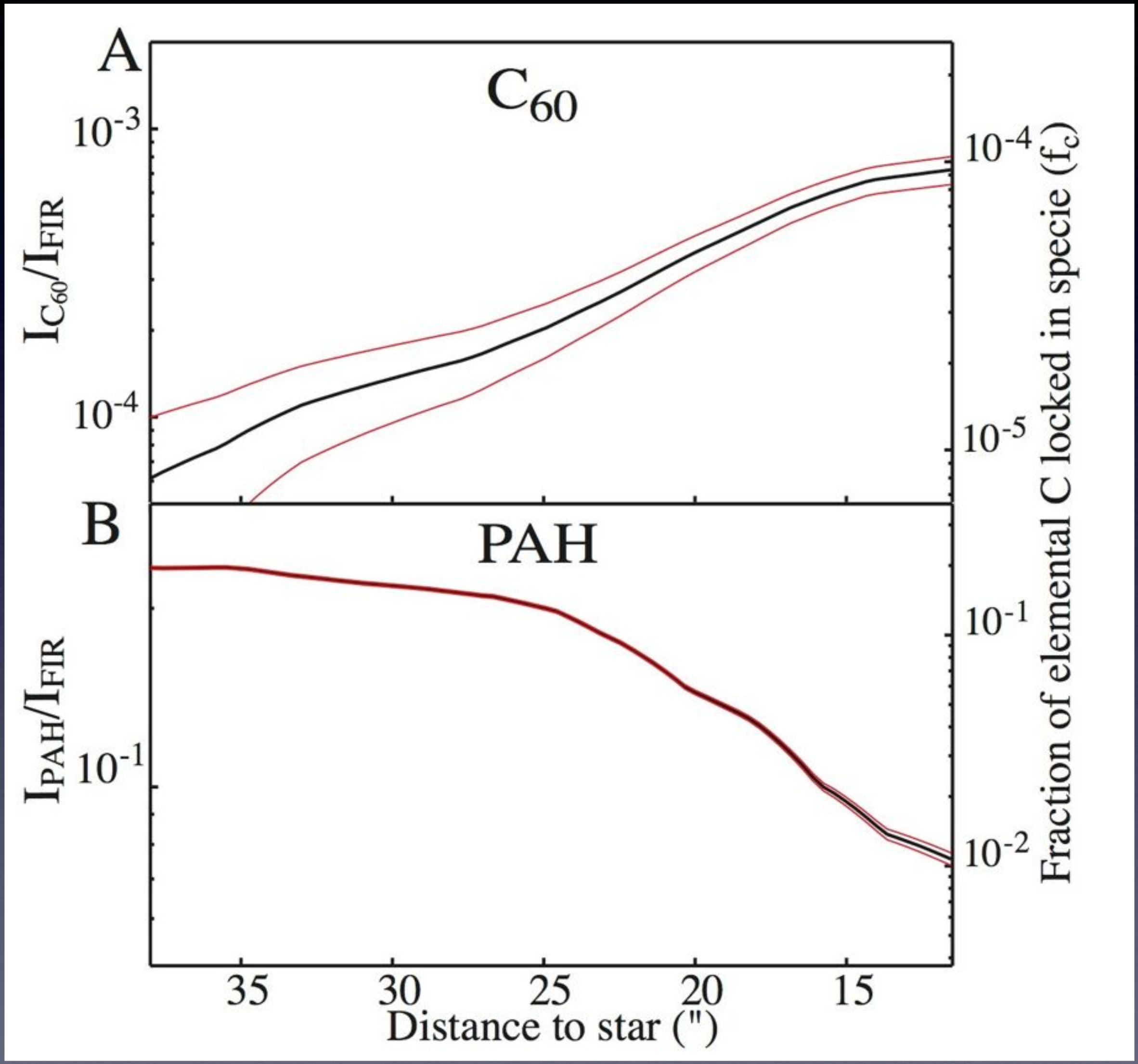
Andrews et al, 2014, submitted

PAHs & C_{60} in NGC 7023



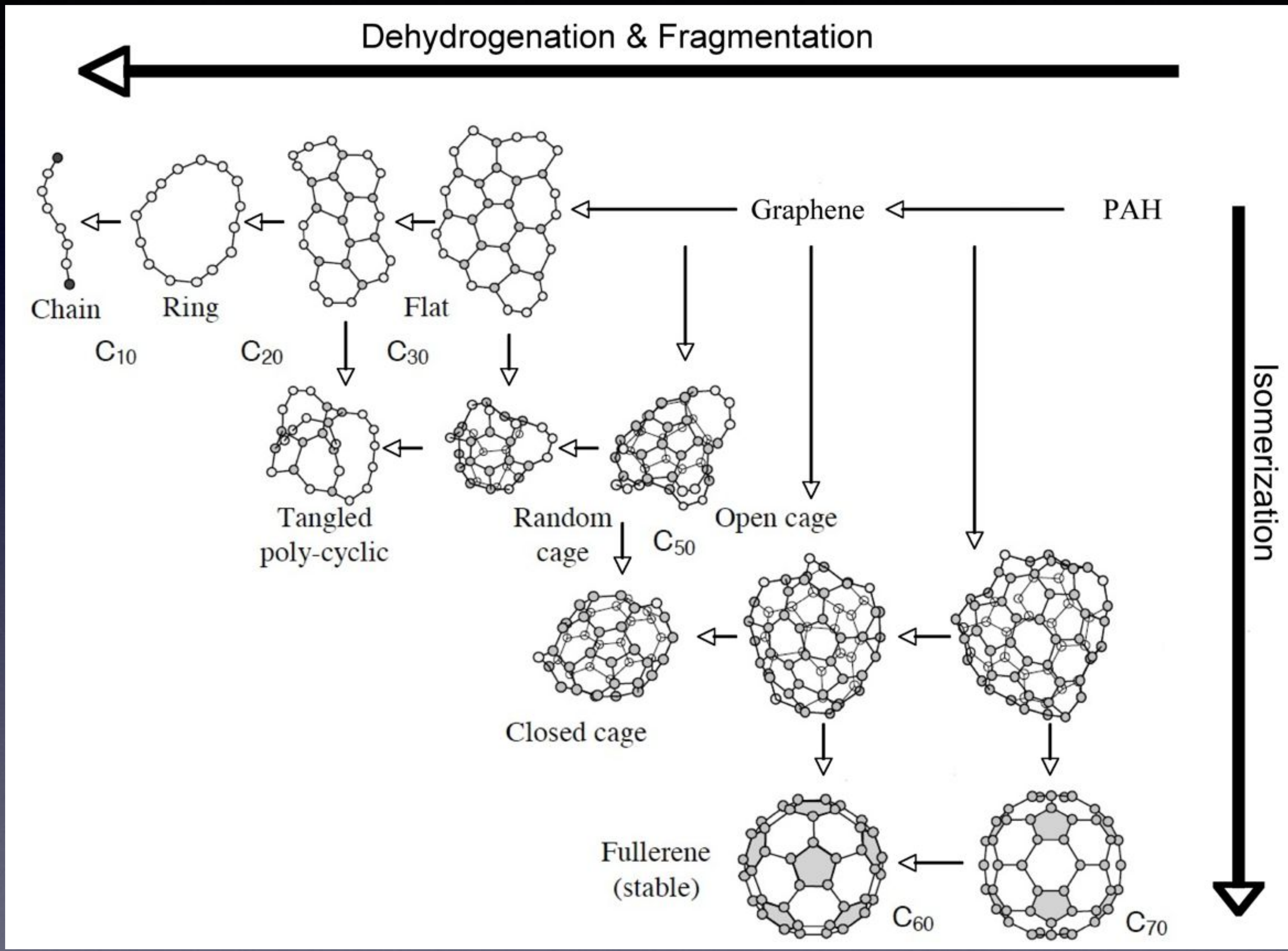
Berne & Tielens, 2012, PNAS, 109, 401

PAHs & C_{60} Abundance



Berne & Tielens, 2012, PNAS, 109, 401

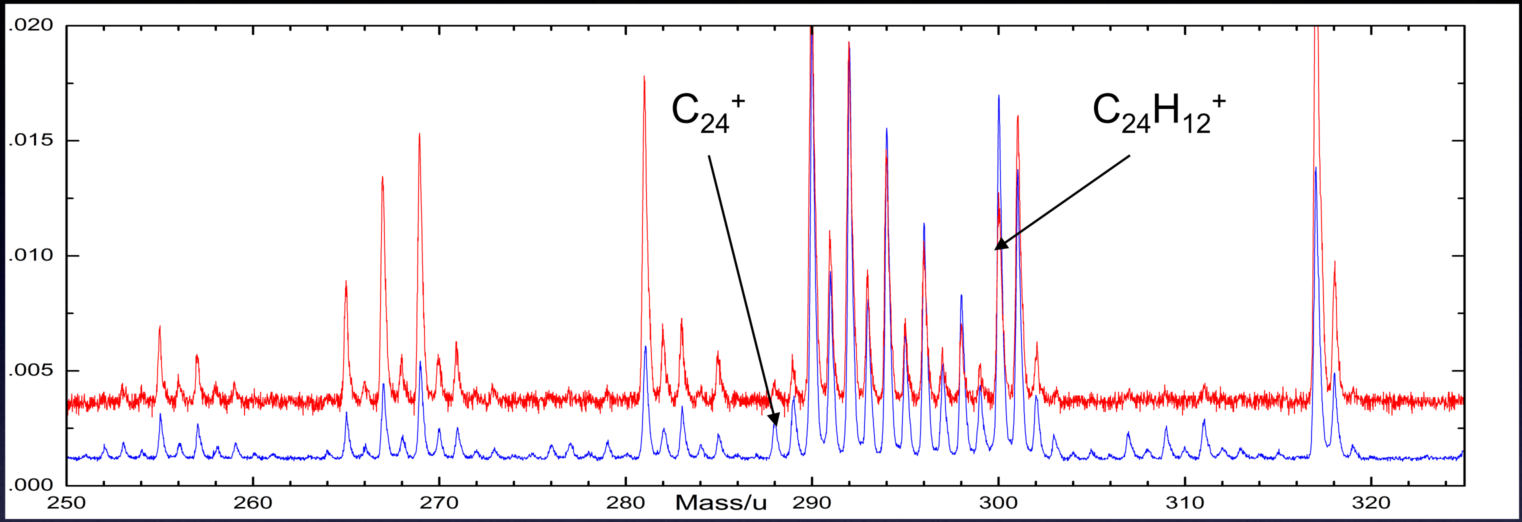
PAHs as a source of "small" Molecules



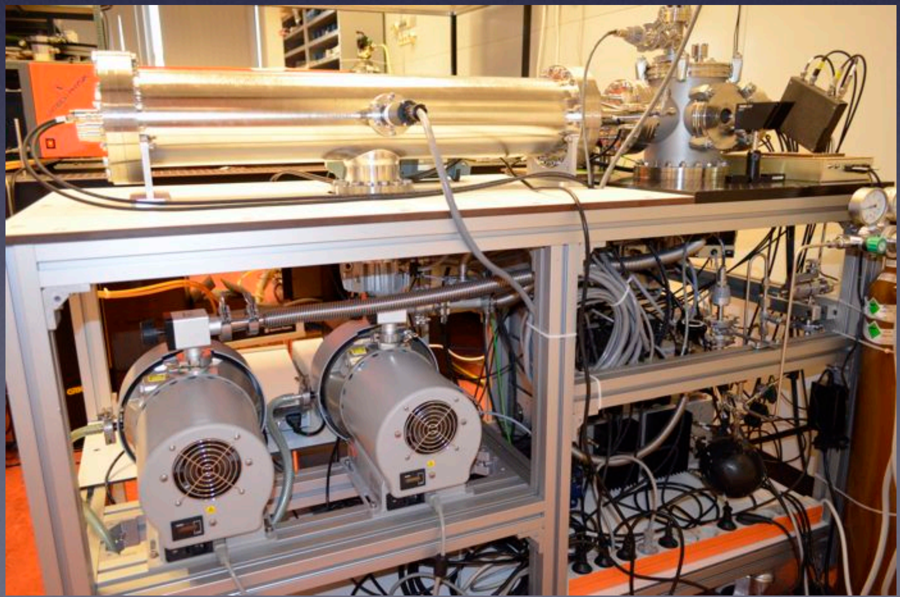
Pety et al 2005, A&A, 435, 885
Berne & Tielens, 2012, PNAS, 109, 401

PAKs & UV fotonen leidt tot fragmentatie & isomerizatie

PAH photolysis

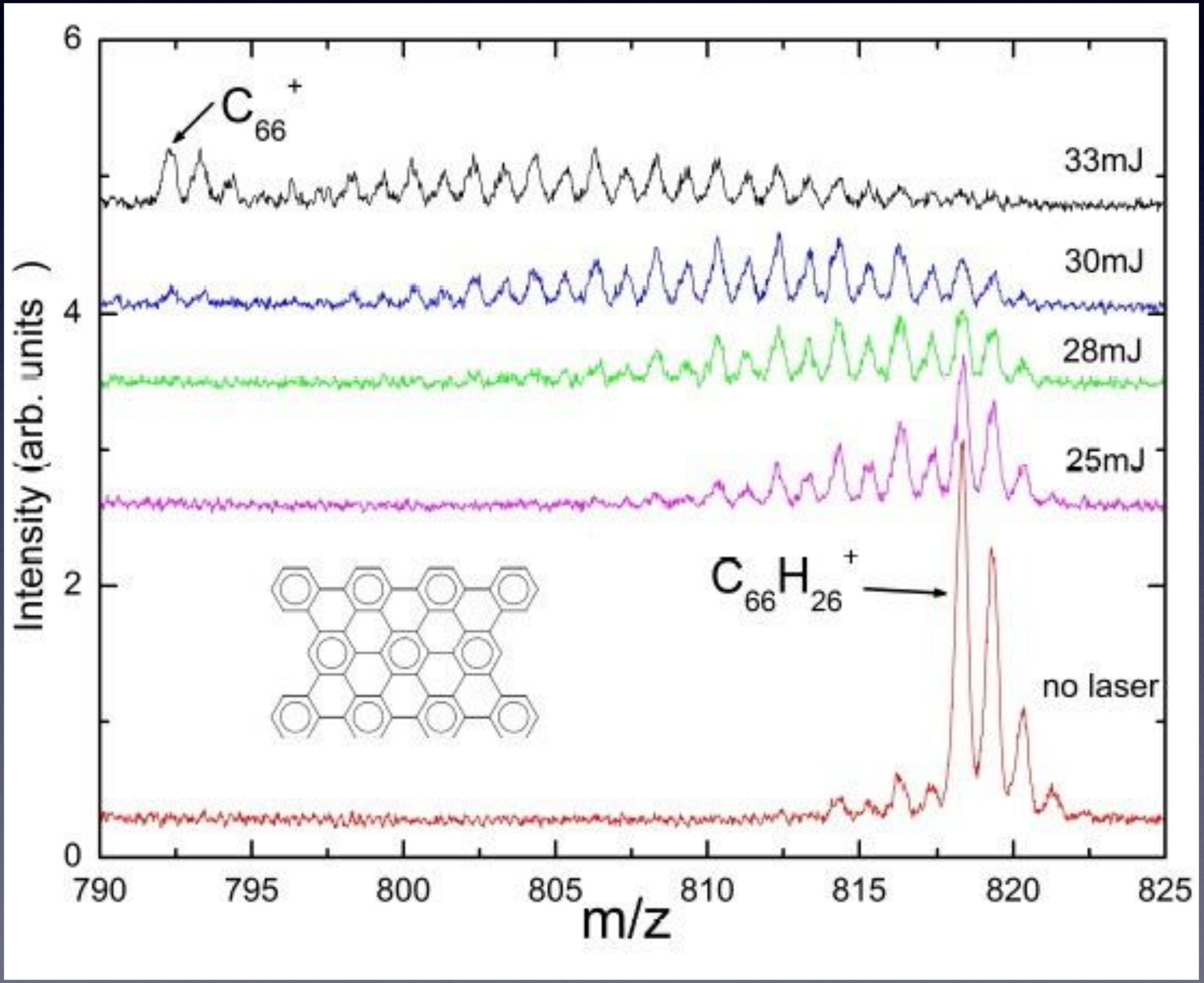


- Highly excited PAHs fragment
- Weakest link goes first
- Products will be investigated through laser action spectroscopy at Felix/ Nijmegen and in the Laser Center in A'dam
- From PAHs to graphene to C_{60}



From PAHs to C_{60}

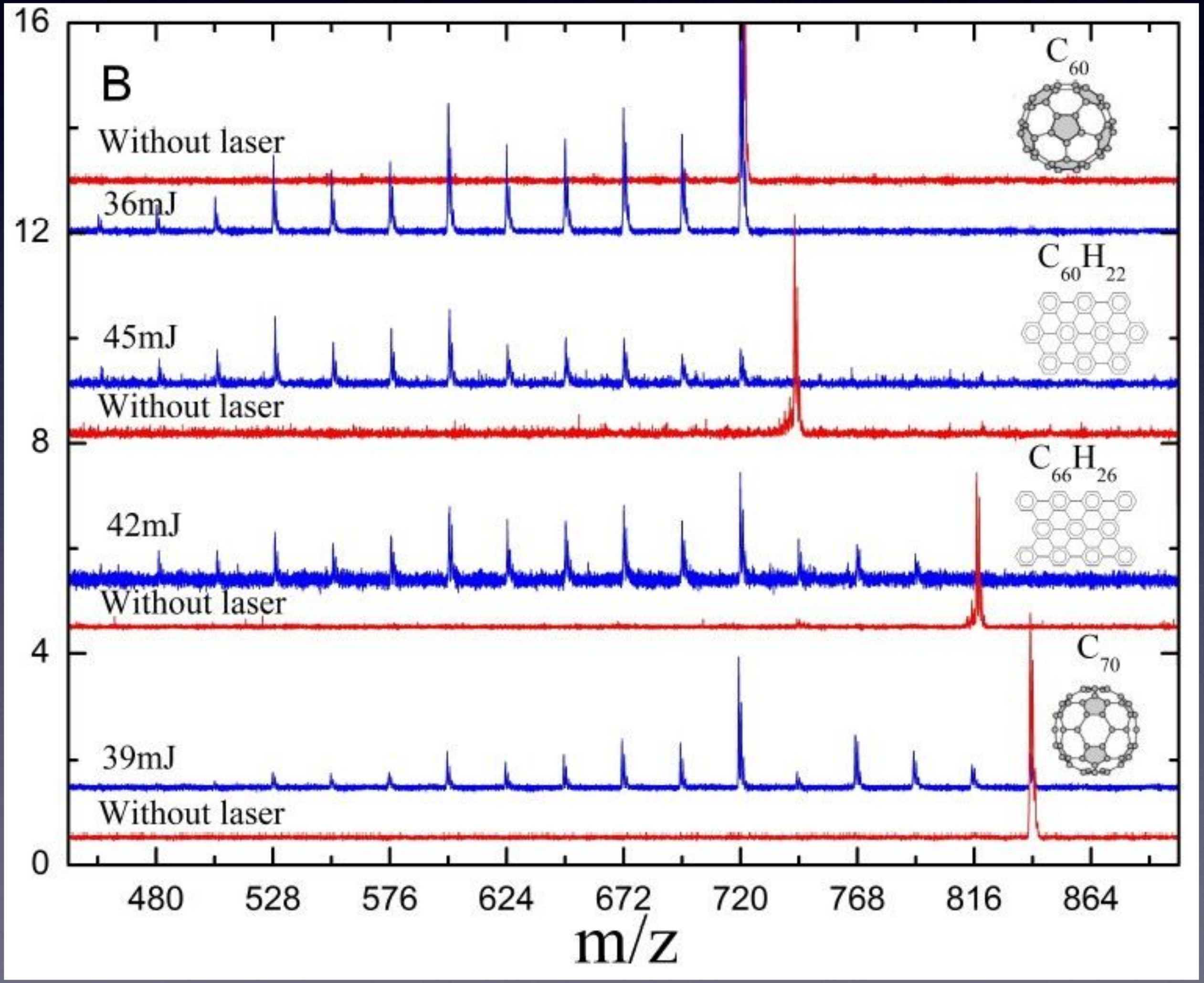
UV photolysis at 355 nm



Zhen et al, 2014, ApJL, in press

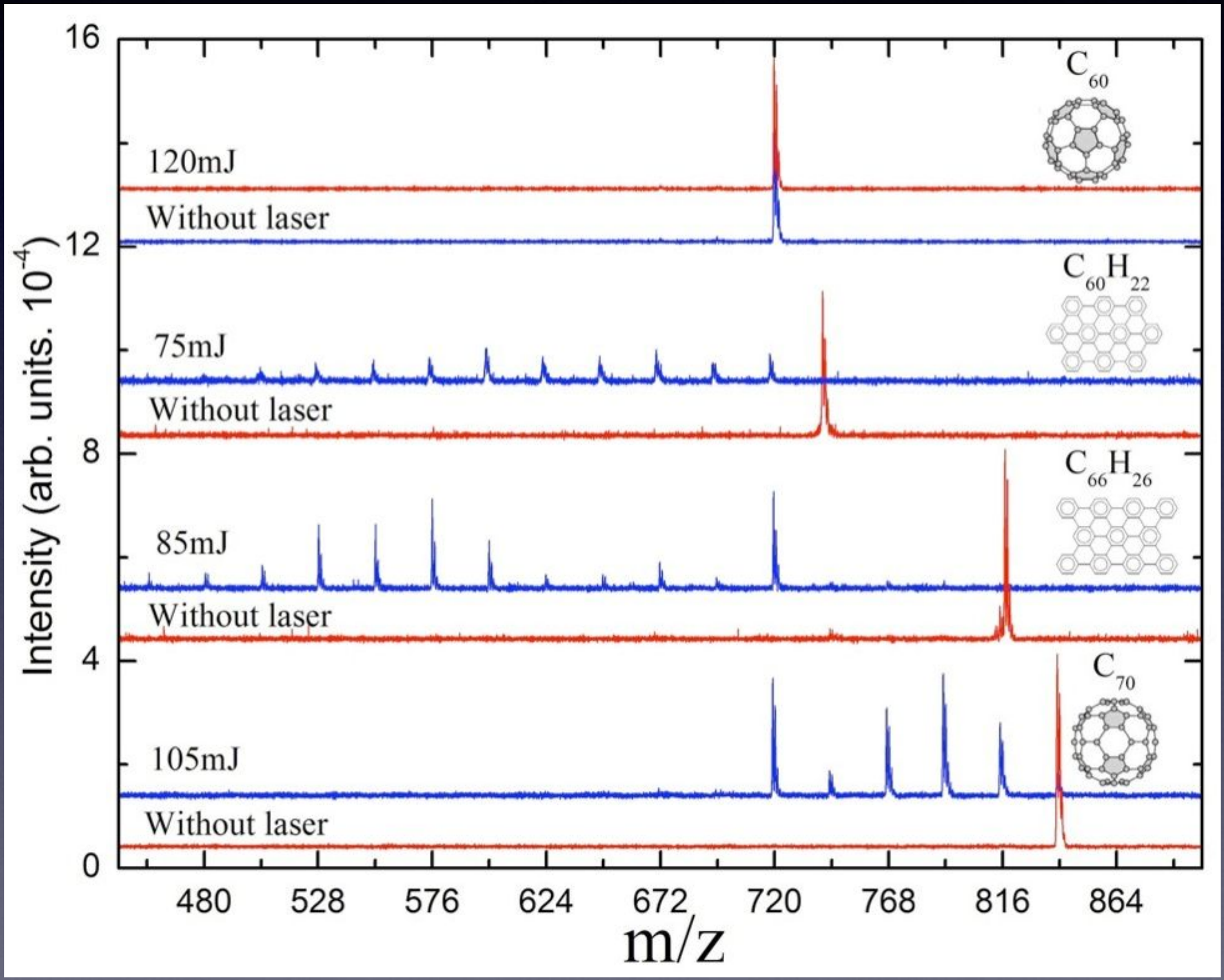
From PAHs to C_{60}

UV photolysis at 355 nm



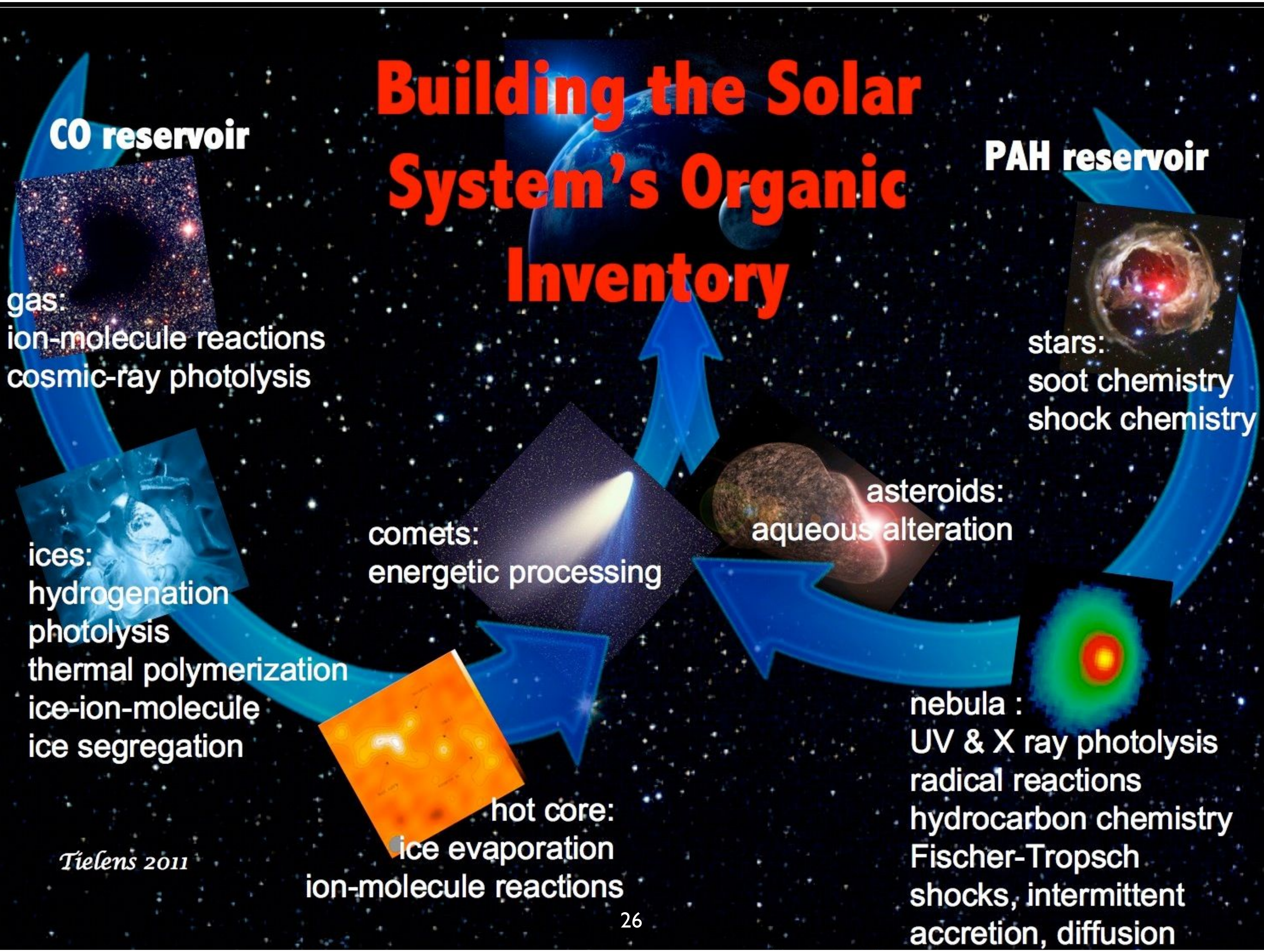
Zhen et al, 2014, ApJL, in press

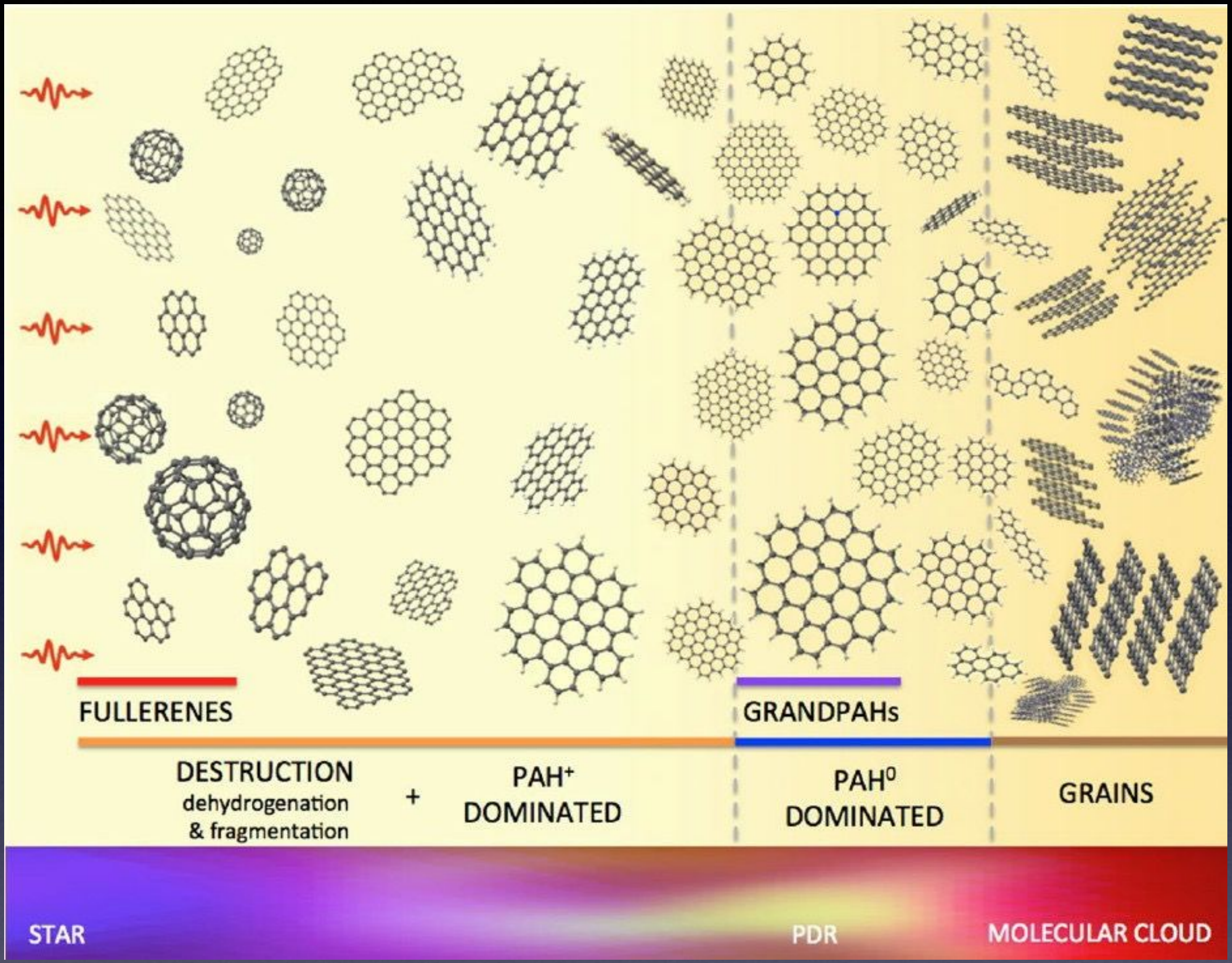
From PAHs to C_{60}



UV photolysis of PAHs

- Weakest link goes first: strip of H's and form graphene flakes
- Followed by sequential steps of C_2 loss
- After loss of first C_2, isomerization to cages becomes important
- PAHs with $N_c>62$ will form C_{60} very efficiently (~20%)
- In NGC 7023, PAH destruction far outweighs C_{60} formation: initial PAH population skewed towards $N_c<62$


Building the Solar System's Organic Inventory
CO reservoir
PAH reservoir
gas:
ion-molecule reactions
cosmic-ray photolysis
stars:
soot chemistry
shock chemistry
asteroids:
aqueous alteration
comets:
energetic processing
ices:
hydrogenation
photolysis
thermal polymerization
ice-ion-molecule
ice segregation
nebula :
UV & X ray photolysis
radical reactions
hydrocarbon chemistry
Fischer-Tropsch
shocks, intermittent
accretion, diffusion
hot core:
ice evaporation
ion-molecule reactions
Tielens 2011



Schematic of PAH evolution in NGC 7023

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 ?

SOFIA & Looking for mr 'grandPAH'

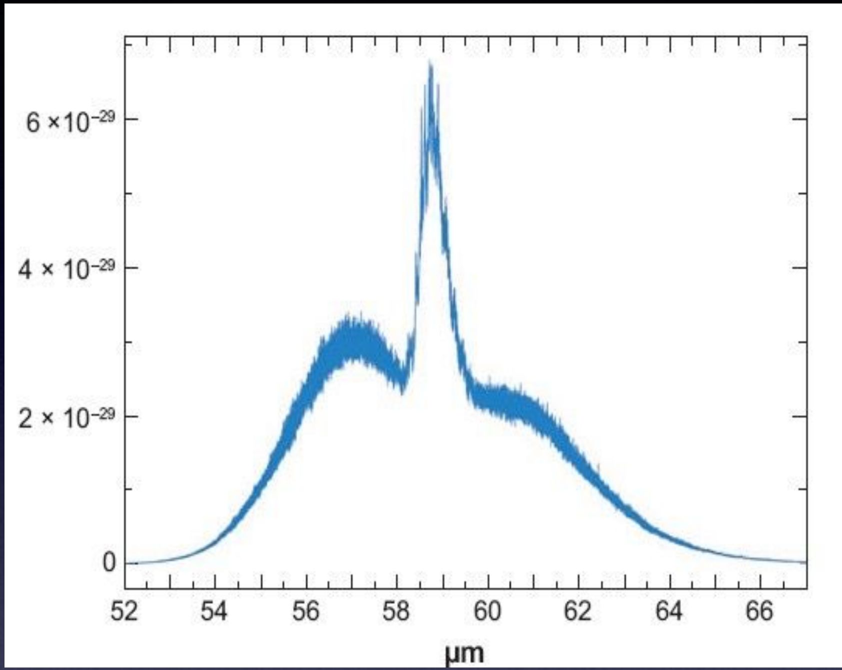
The interstellar PAH family seems to be dominated by a few, large, very stable, compact PAHs

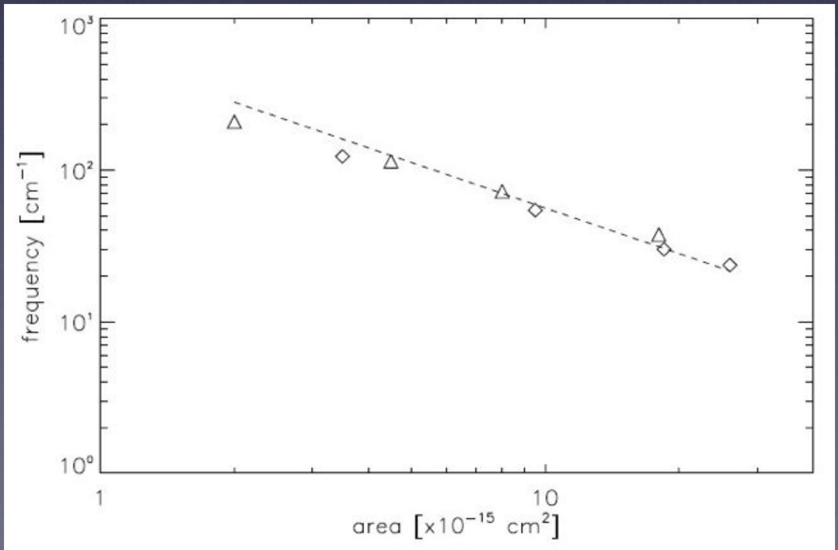
Identification of specific PAHs

- Pure rotational spectra: Anomalous microwave emission
- Drumhead or jumping jack modes: Lowest-lying vibrational state will emit when the modes have decoupled and will show rotational substructure

Observing strategy with future instruments on SOFIA

- Wide wavelength coverage at moderate resolution
- High spectral resolution within limited spectral range
- Target brightest spots in RNe

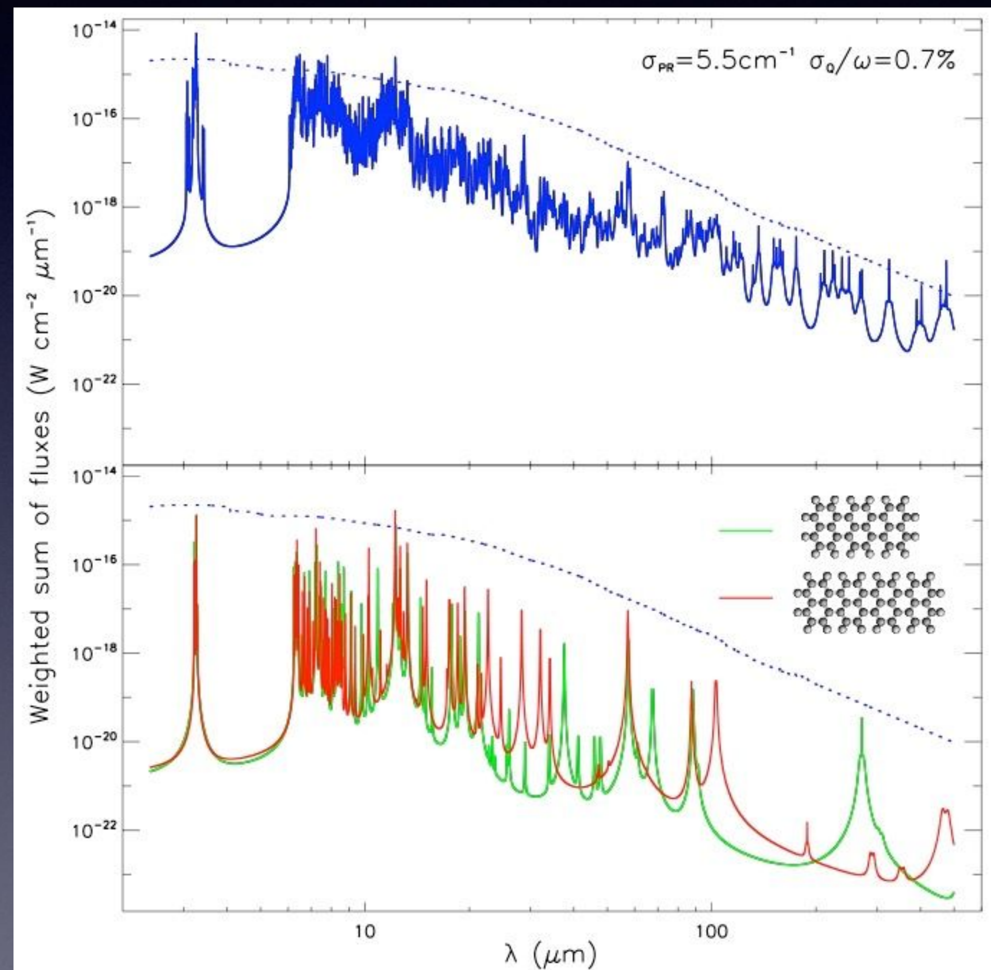




Mulas et al, 2006, A & A, 456, 161, Boersma et al, 2010, A&A, 511, A32, Ricca et al, 2012, ApJ, 754, 75

SOFIA & Looking for mr 'grandPAH'

- The far-IR 'drum head' or Jumping Jack modes are highly molecule specific
- Only SOFIA has the potential to measure all vibrational modes of interstellar PAHs
- Requirements: Moderate resolution (R=200-1000) spectroscopy from 5-200 µm
- High resolution follow up using GREAT to resolve P-Q-R branch structure of lowest vibrational transitions



Calculated spectrum for the Red Rectangle

Mulas et al, 2006, A & A, 456, 161