

# Very Large Organic Molecules in Astrophysical Sources: C<sub>60</sub>, PAHs and Nanodiamonds

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# Motivation

## Two ?related problems

### Diffuse Interstellar Bands – unidentified

Absorption (common)  
Emission (rare)

### Infrared Bands: C<sub>60</sub>, PAHs, Nanodiamonds

Emission ('common')  
Absorption (rare or non-existent)

## Are these problems important?

New forms of matter/dust in ISM

Spectroscopic tracer of dust

Organic molecules – implications for origin of life

H<sub>2</sub> formation on grains

Star and planet formation and evolution

External galaxies and early astrochemistry

## Diffuse Band Problem

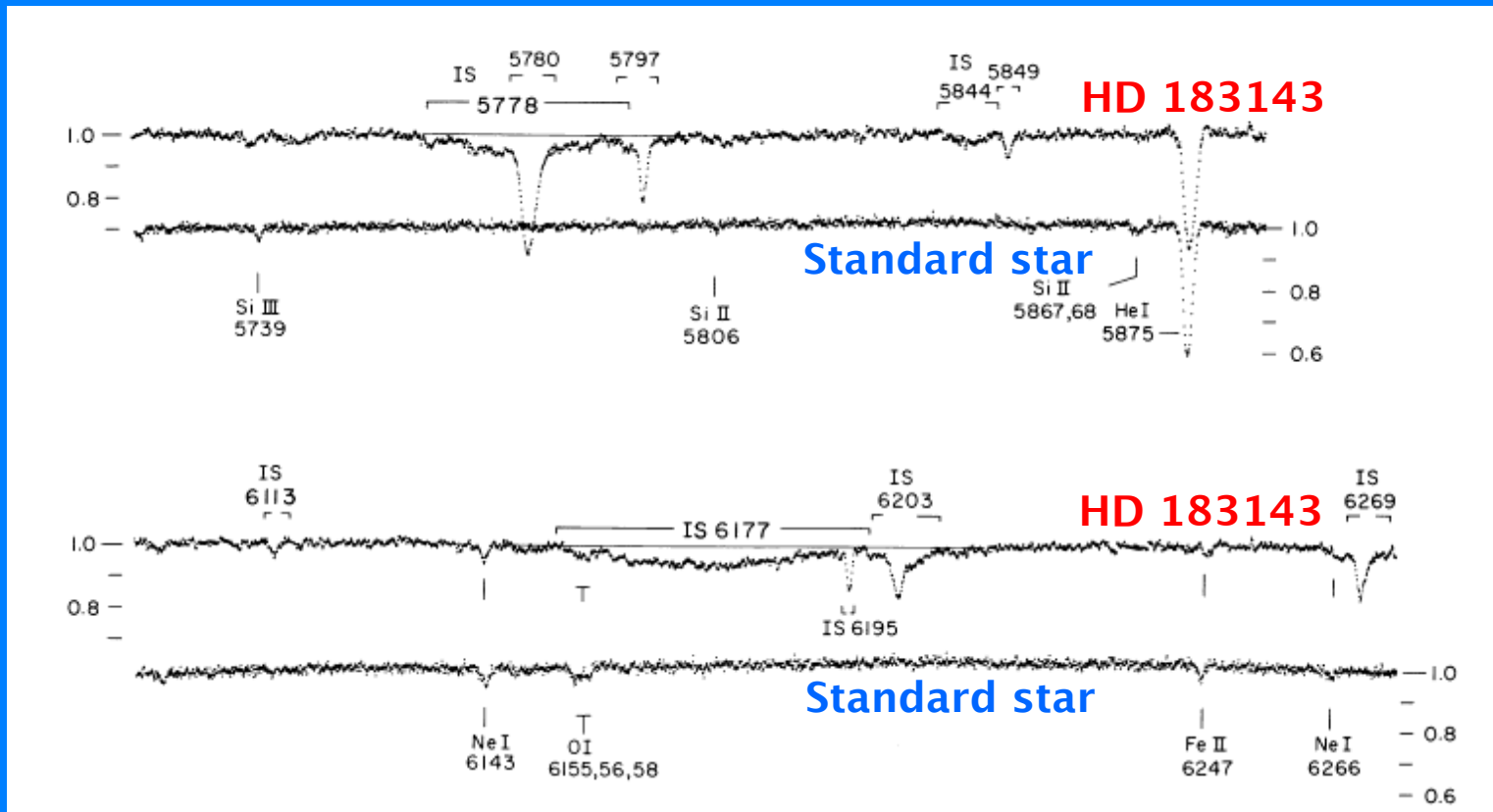
### Mary Lea Heger at Lick Observatory (1919)

### Paul W Merrill (1935)

‘Recent observations at Mount Wilson have disclosed four detached lines whose approximate wave-lengths are 5780.4, 5796.9, 6283.9, and 6613.9 Å; and another one, a vague feature near  $\lambda$ 4427, is suspected.

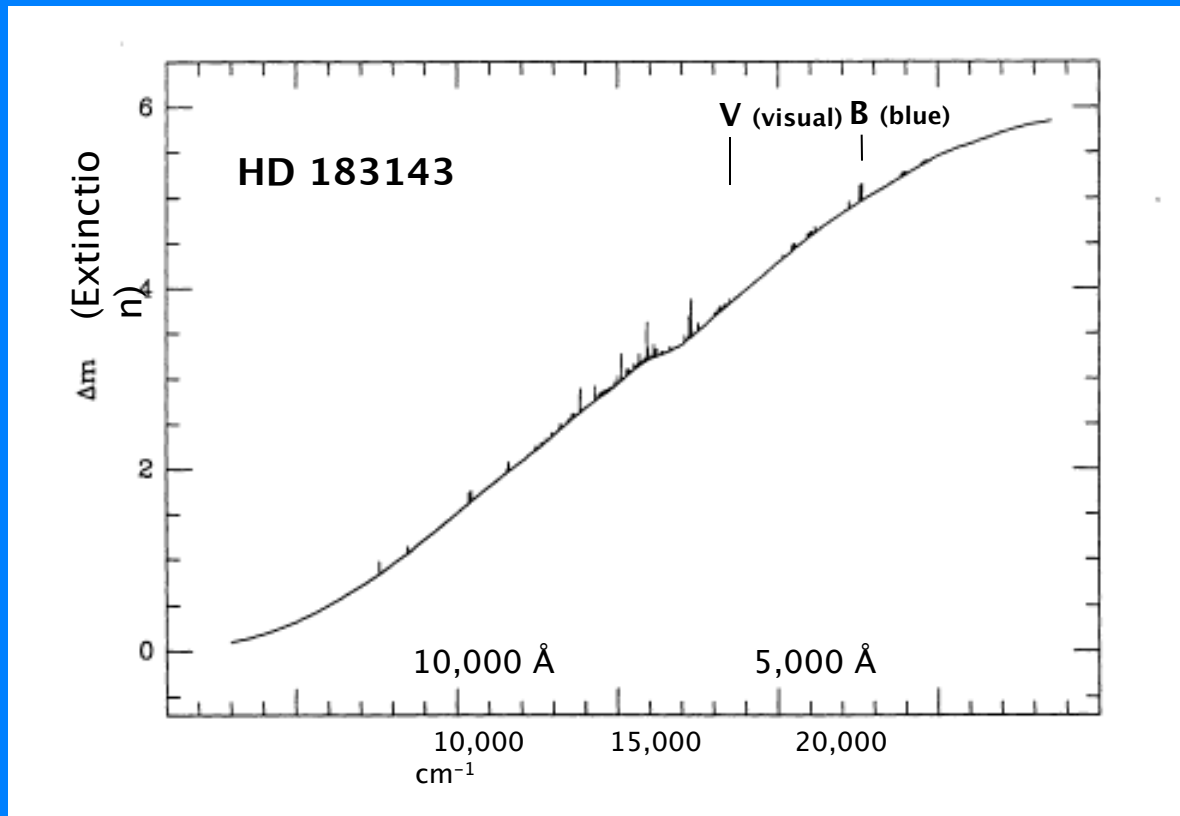
The chemical identification of these lines has not yet been made.’

# George H. Herbig (1975)



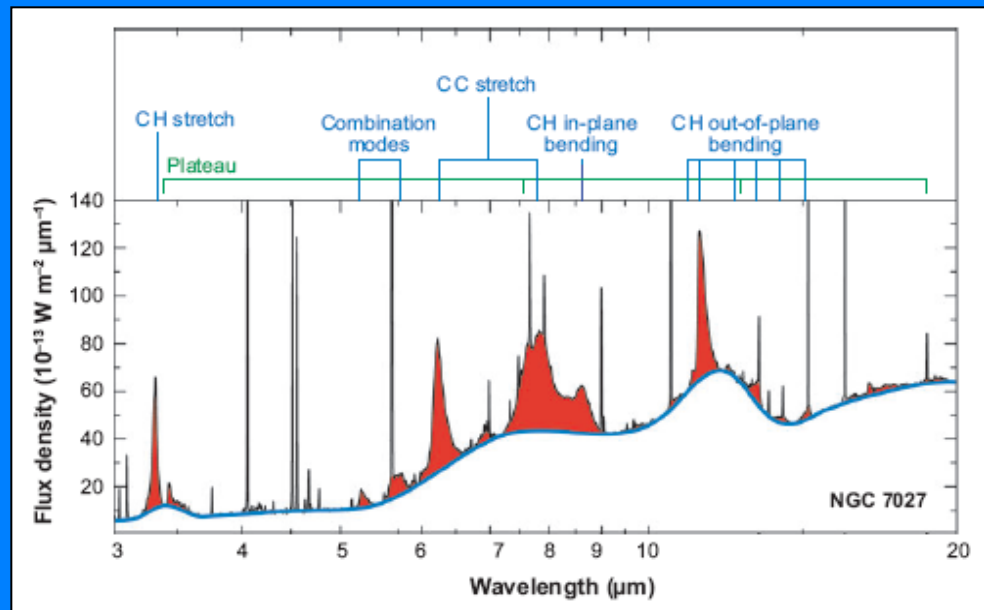
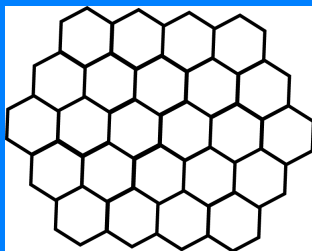
# George H. Herbig (1995)

Extinction curve for HD 183143 with diffuse bands shown

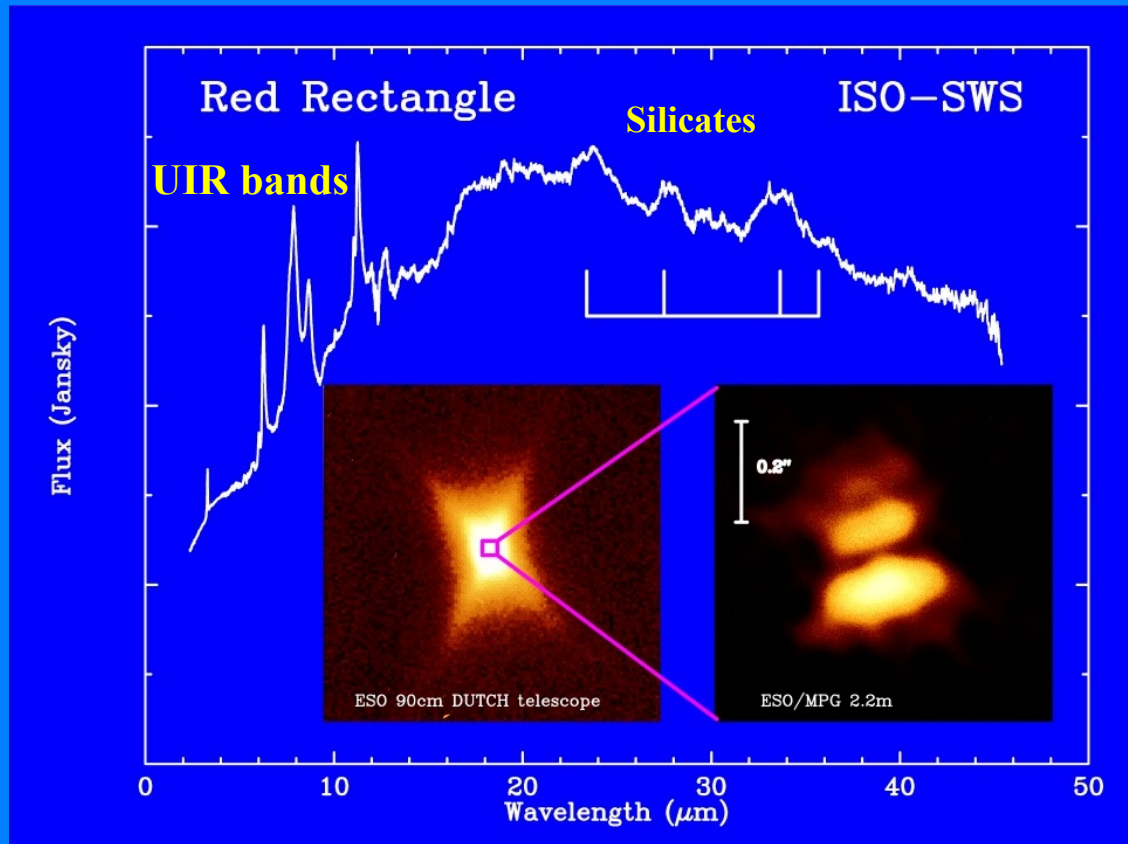


# Infrared Bands due to large carbon molecules

- Emission features
- Common features – UIR bands
- Usually attributed to polycyclic aromatic hydrocarbons (PAHs)

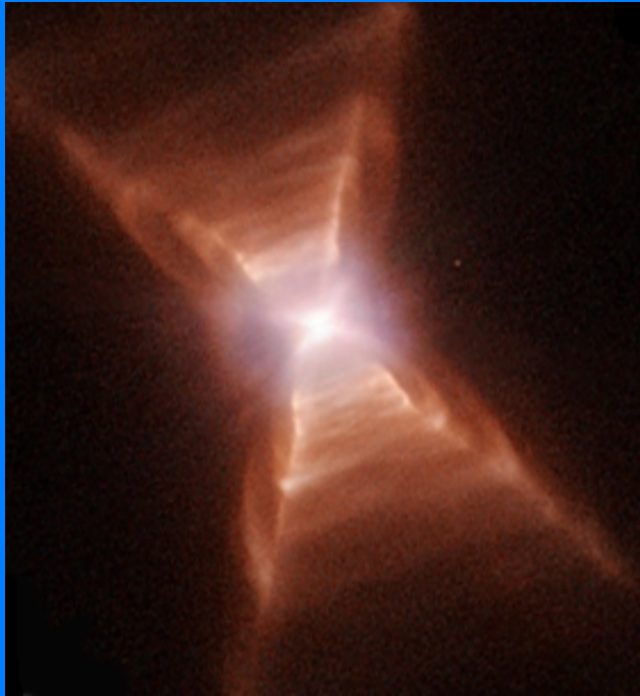


# Infrared Space Observatory (ISO) spectrum + ESO images

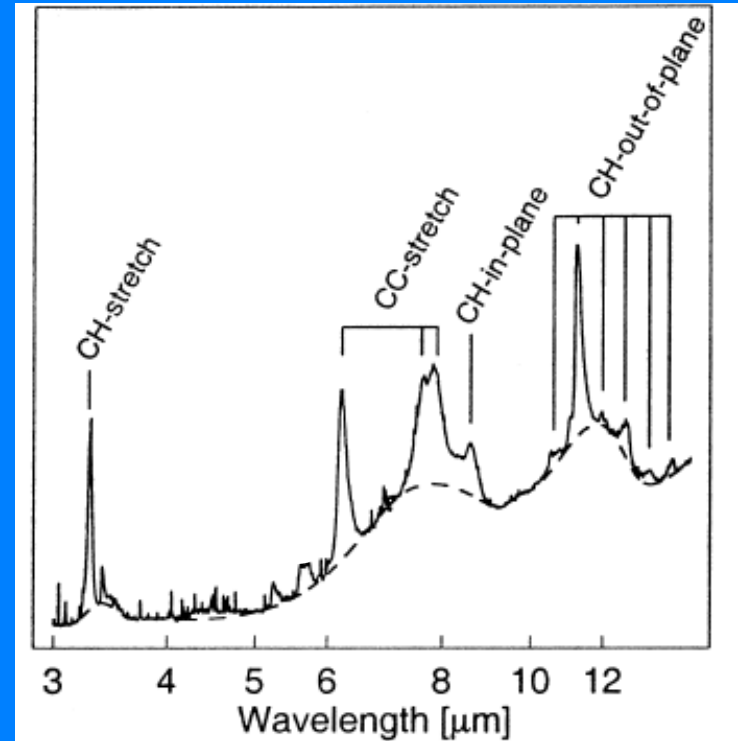




# UIR bands



HST image 2004, NASA, ESA & H. Van Winckel and M. Cohen



Typical spectrum

# Red Rectangle

## Star

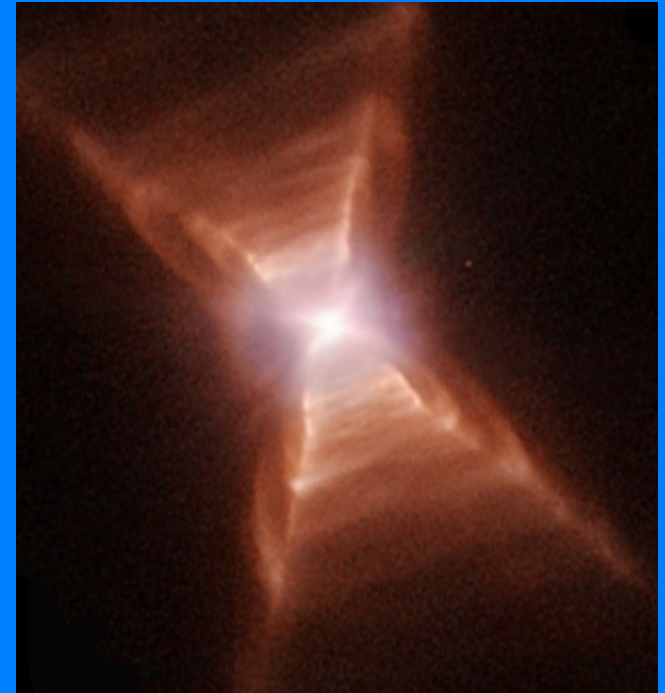
- Central star A0, Fe poor
- Binary – period  $318 \pm 3$  days
- Bipolar outflow from binary system

## Nebula and disk

- Nebula (C-rich)
- Circumbinary disk (O-rich)

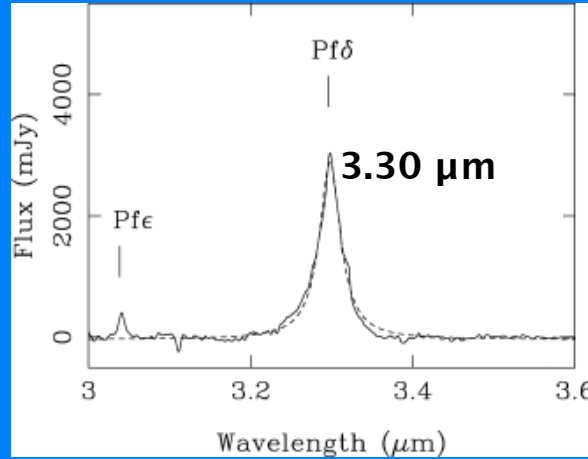
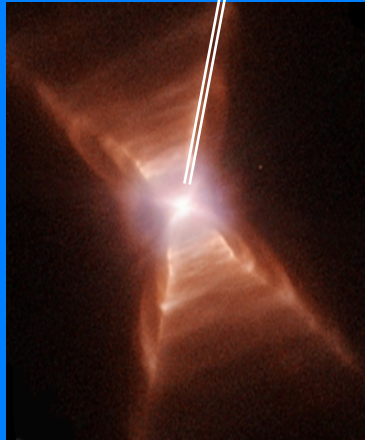
## IR spectral Features

- Unidentified infrared emission (UIR) – PAHs
- Silicate emission (disk)

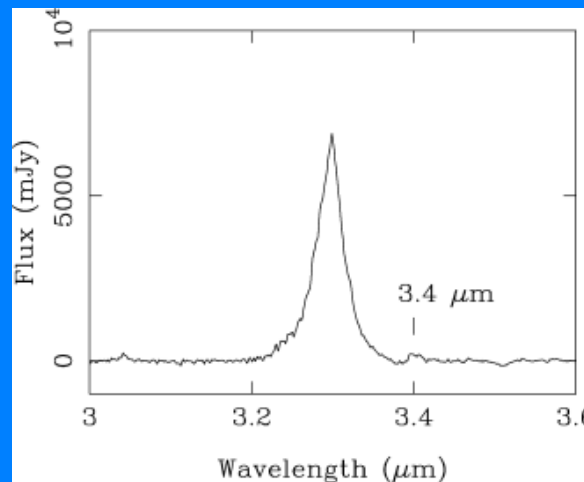


HST optical image 2004, NASA, ESA & H. Van Winckel and M. Cohen

# Spectroscopy: 3.3 $\mu\text{m}$ feature (C—H stretch)

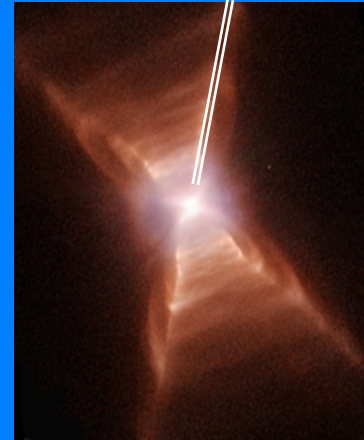
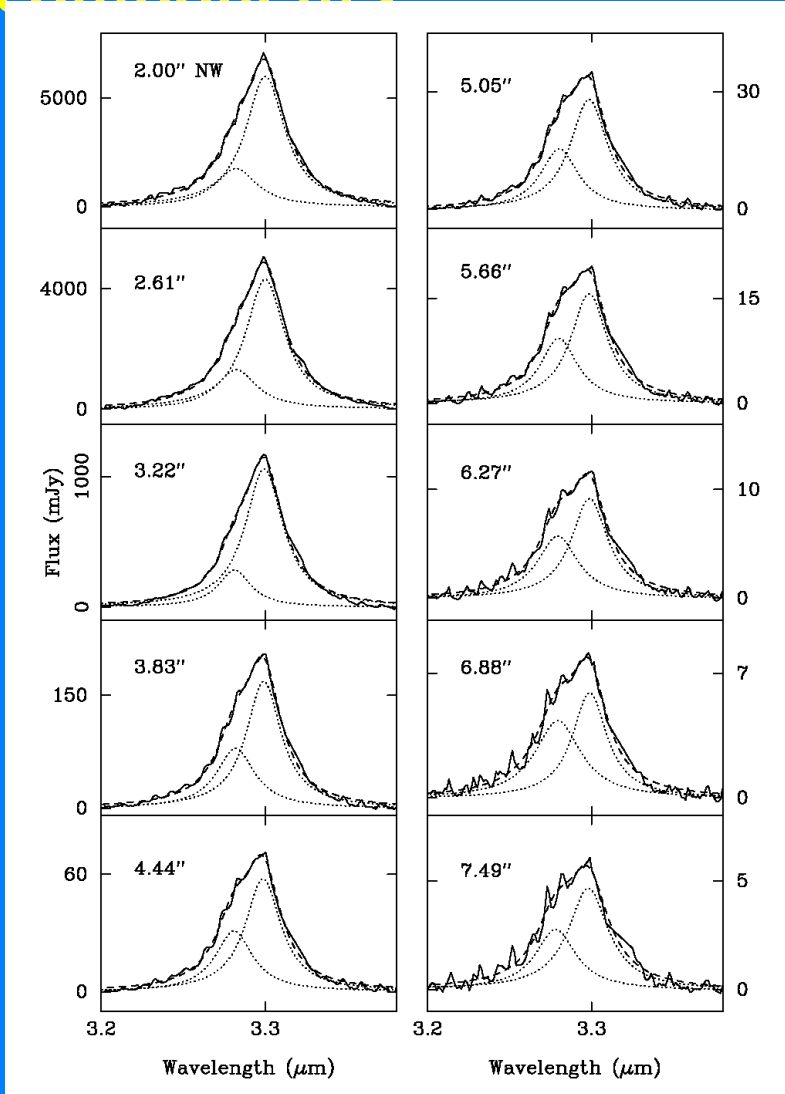


On-star  
Good Lorentzian fit



2" offset

# 3.3 $\mu\text{m}$ band C-H stretch – two-components

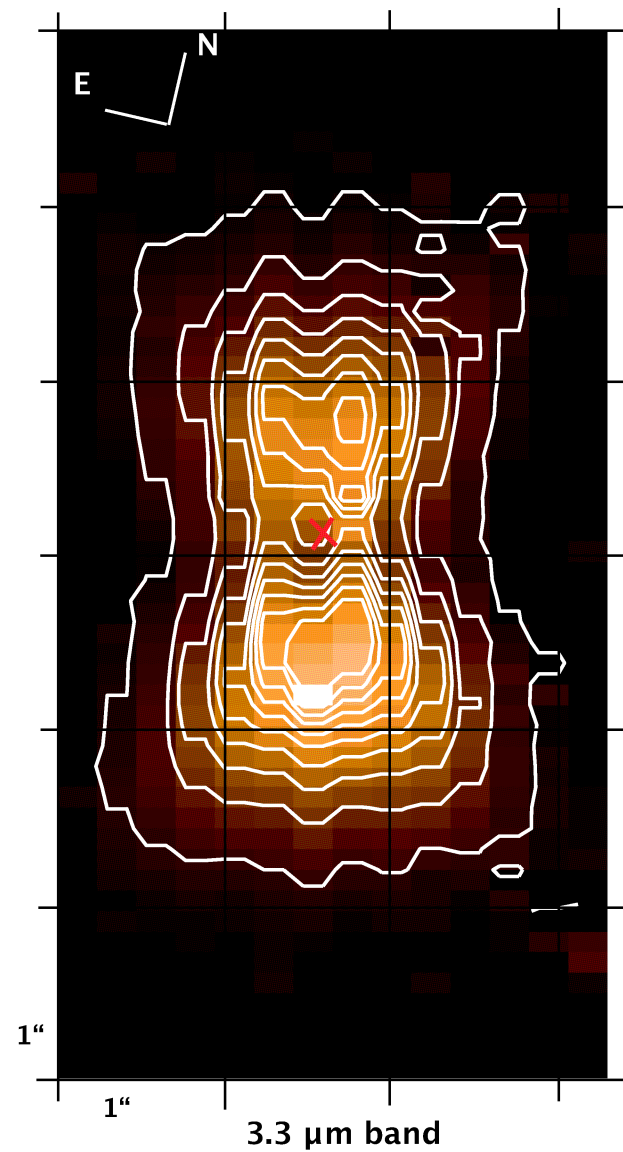
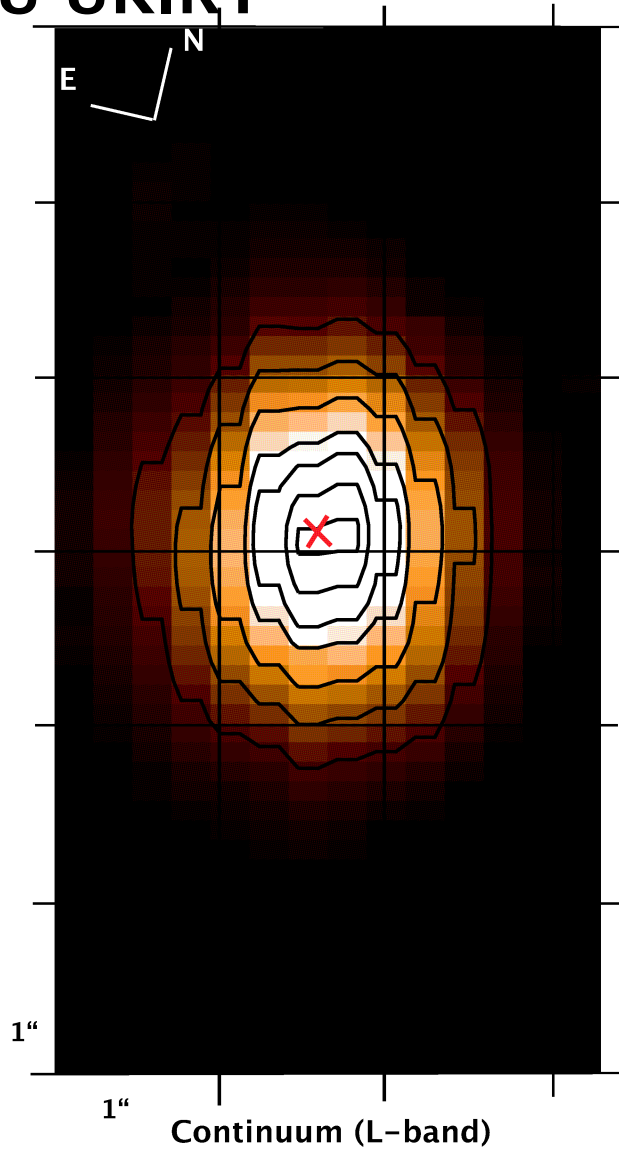


3.30  $\mu\text{m}$  and 3.28  $\mu\text{m}$

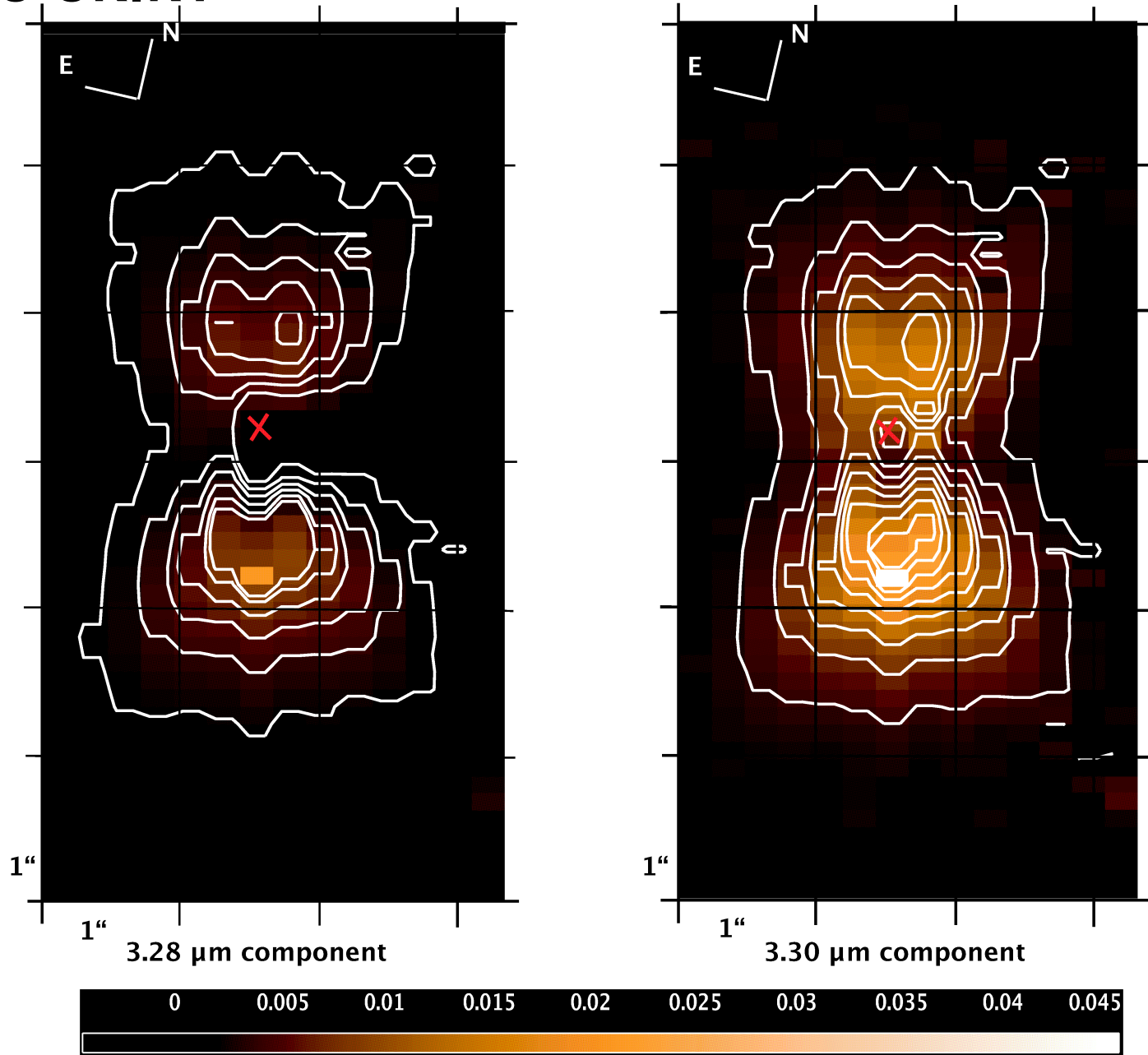
$\Delta \sim 0.02 \mu\text{m}$

Small PAHs – a few rings

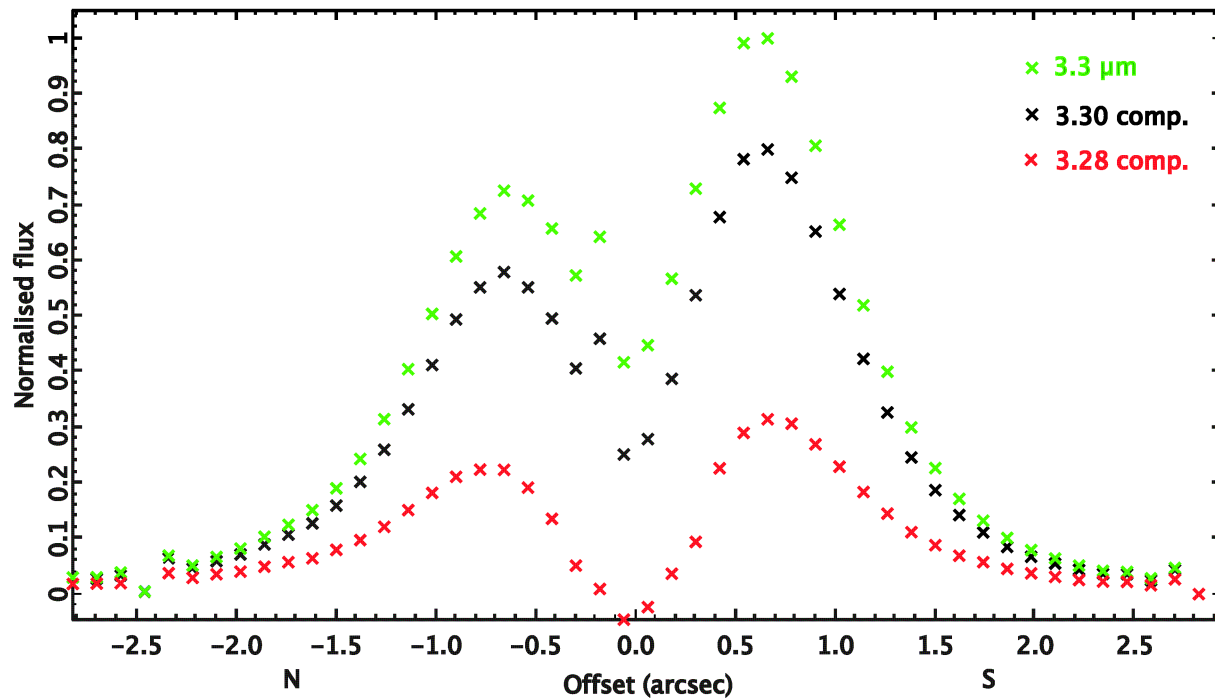
# IFU UKIRT



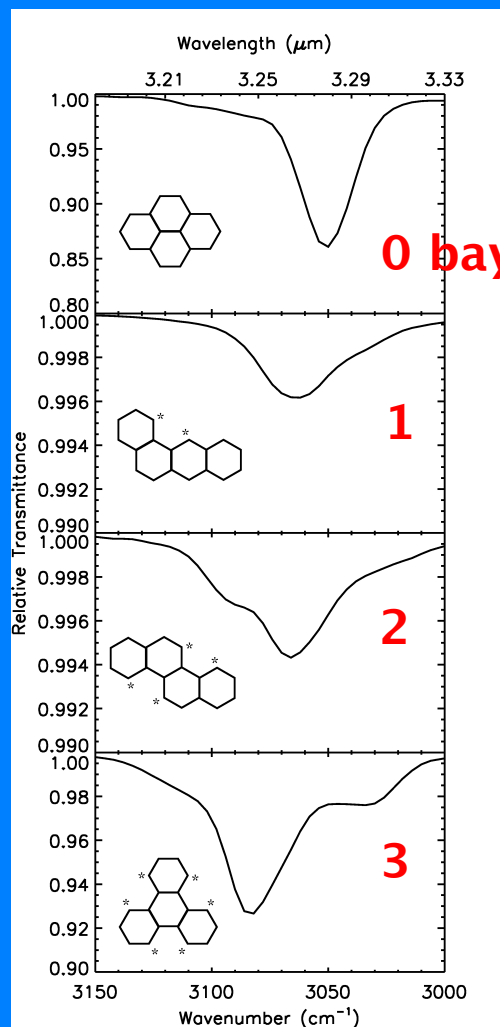
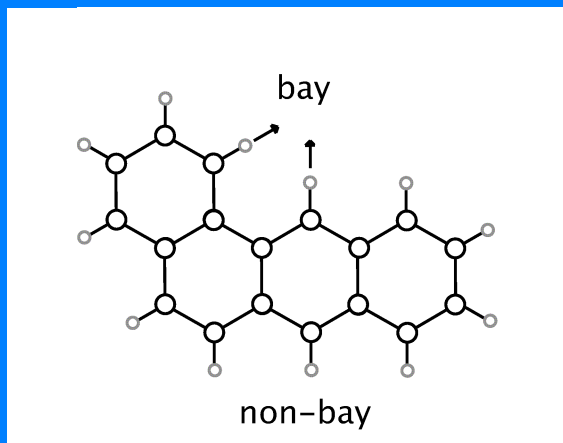
# IFU UKIRT



# N-S cut: 3.3 $\mu\text{m}$ band (total) and its two components



# Bay and non-bay hydrogens

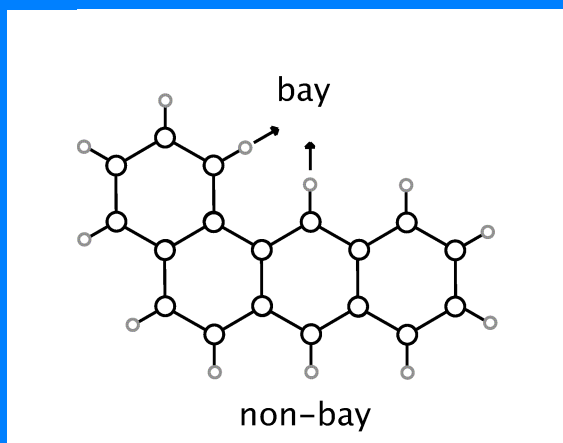


500 K

NIST Chemistry database

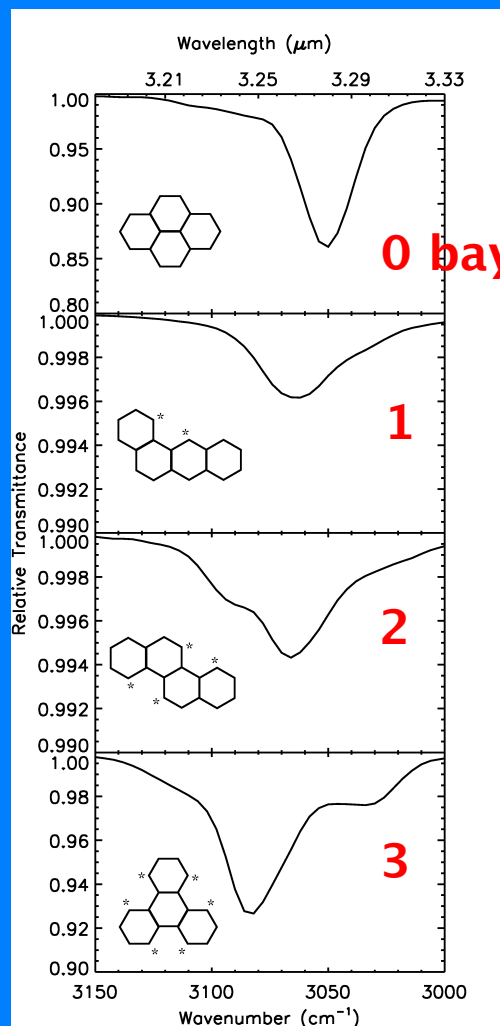


# Bay and non-bay hydrogens



3.30  $\mu\text{m}$  ..non-bay (on star) *e.g.* pyrene

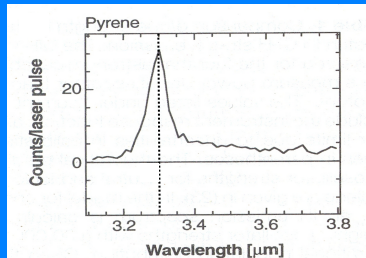
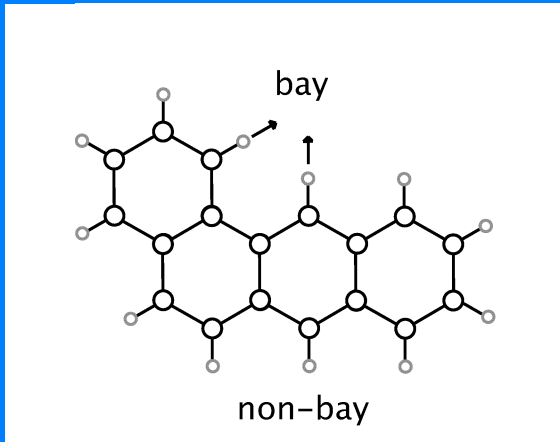
3.28  $\mu\text{m}$  ..bay (grows off-star)



500 K

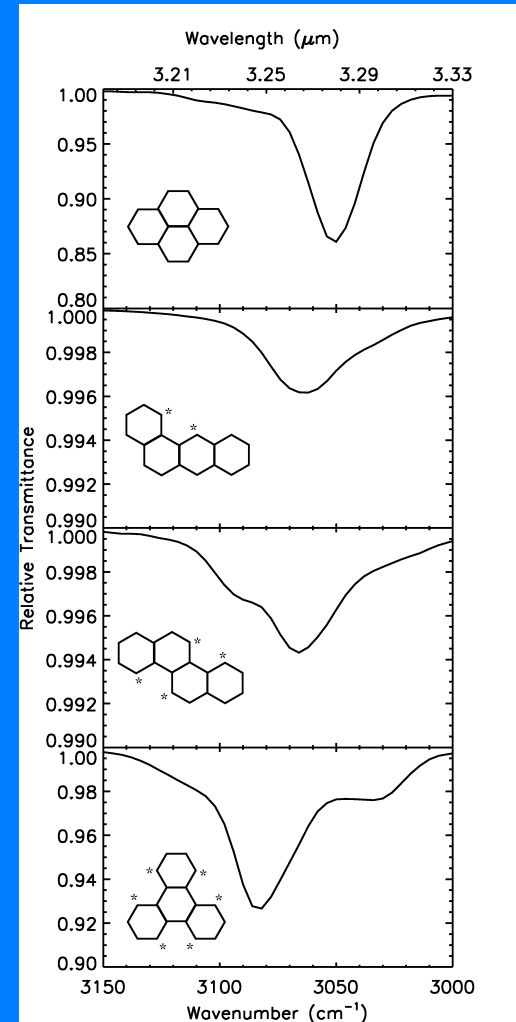
NIST Chemistry database

# Bay and non-bay hydrogens



Schlemmer et al. (1994)

UV pumped IR emission -  
higher T - falls at 3.30  
 $\mu\text{m}$



500  
K

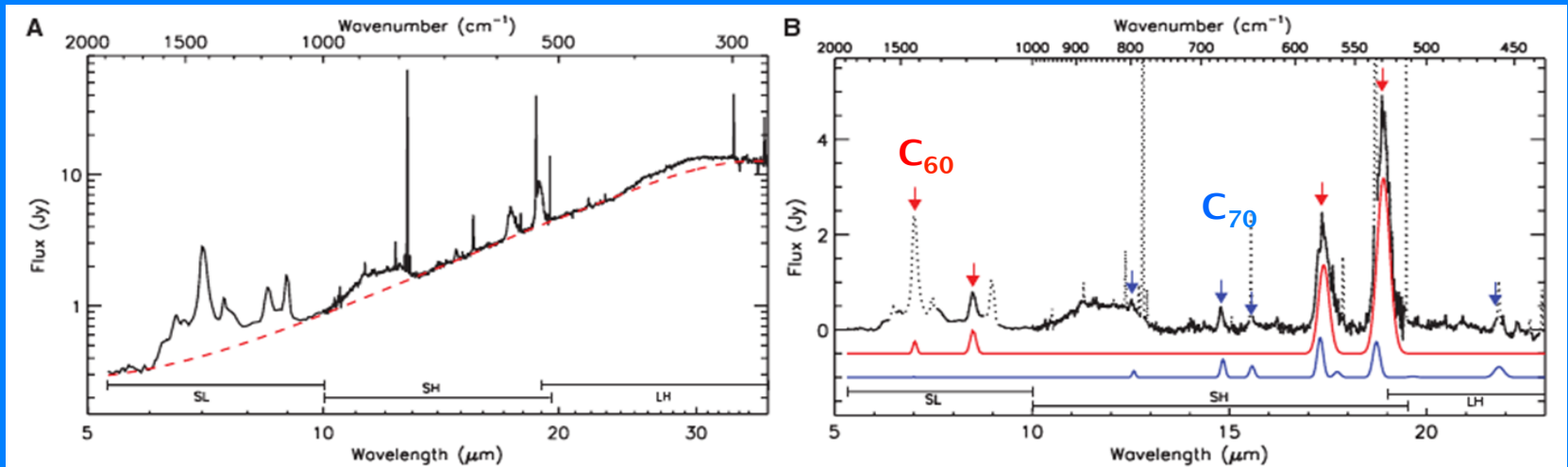
NIST Chemistry database

# C<sub>60</sub>

- C<sub>60</sub> – molecule discovered in 1985 (Kroto et al.)
- Macroscopic quantities – 1990 (Krätschmer et al.)
- Infrared spectrum – 4 bands ~ 7.0, 8.5, 17.4, 18.9 μm
- Two bands in NGC 7023 noted in Werner et al. (2004); discussed in detail in 2007 (Sellgren et al.)
  
- 2010
  - Sellgren et al. report 3<sup>rd</sup> band – confirmation (also in NGC 2023)
  - Cami et al. report C<sub>60</sub> and C<sub>70</sub> in young planetary nebula Tc 1

$C_{60}$

- Tc 1 *Spitzer* data



# C<sub>60</sub>

- C<sub>60</sub> – also discovered in.....
- PNe in Milky Way and Magellanic Clouds (Garcia–Hernandez et al. 2010, 2011)
- One (possibly two) RCB stars (Garcia–Hernandez et al. 2011)
- PPN (Zhang & Kwok 2011)
- ‘Veil’ region of Orion Nebula (Rubin et al. 2011)
- Several post–AGB objects (Gielen et al. 2011)
- Binary XX Oph (Evans et al. 2011)
- Our work.. YSOs, Herbig Ae/Be star and an unusual post–AGB star

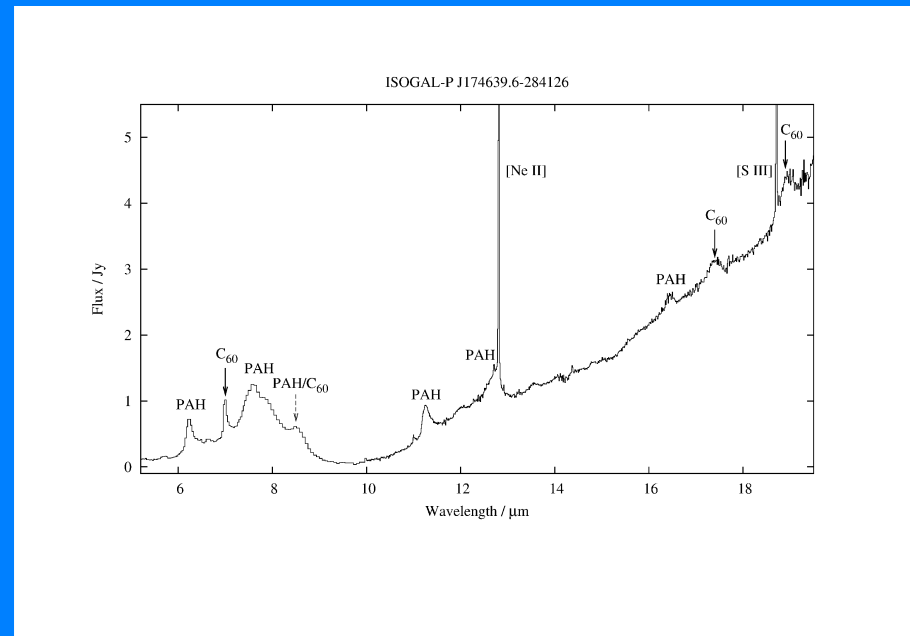
# C<sub>60</sub> objects with *Spitzer* programmes

**Table 1.** Coordinates and photometry for the targets with C<sub>60</sub> emission bands. Right ascension, declination, and near-infrared magnitudes are taken from the 2MASS catalogue (Skrutskie et al. 2006); mid-infrared magnitudes (where available) are from the *Spitzer* IRAC survey of the Galactic centre (Ramírez et al. 2008). *Spitzer* programme numbers and Principal Investigator (PI) names are given for the IRS observations used in this study.

| Name                         | RA          | Dec         | <i>J</i> | <i>K</i> | [3.6] | [4.5] | [5.8] | [8.0] | Programme (PI)     |
|------------------------------|-------------|-------------|----------|----------|-------|-------|-------|-------|--------------------|
| Embedded YSOs:               |             |             |          |          |       |       |       |       |                    |
| ISOGAL-P J174639.6-284126    | 17:46:39.60 | -28:41:27.0 | > 13.8   | 12.95    | 10.28 | 8.83  | 7.38  | 5.58  | 40230 (Ramírez)    |
| SSTGC 372630                 | 17:44:42.76 | -29:23:16.2 | > 16.0   | 12.87    | 10.31 | 8.82  | 7.67  | 6.48  | 40230 (Ramírez)    |
| 2MASS J06314796+0419381      | 06:31:47.96 | +04:19:38.2 | 14.01    | 10.67    | -     | -     | -     | -     | 50146 (Keane)      |
| Other targets:               |             |             |          |          |       |       |       |       |                    |
| HD 97300 (Herbig Ae/Be star) | 11:09:50.03 | -76:36:47.7 | 7.64     | 7.15     | -     | -     | -     | -     | 2 (Houck)          |
| HD 52961 (post-AGB object)   | 10:18:07.52 | -28:29:30.7 | 16.06    | 15.42    | -     | -     | -     | -     | 3274 (Van Winckel) |
| HR 4049 (post-AGB object)    | 07:03:39.63 | +10:46:13.1 | 6.32     | 5.53     | -     | -     | -     | -     | 93 (Cruikshank)    |

$C_{60}$

- YSO in Central Molecular Zone in Galactic Centre
- PAHs
- Ne II, S III
- $C_{60}$  at 18.9 and 17.4  $\mu\text{m}$
- $C_{60}$  at 7.0  $\mu\text{m}$  (Ar II)

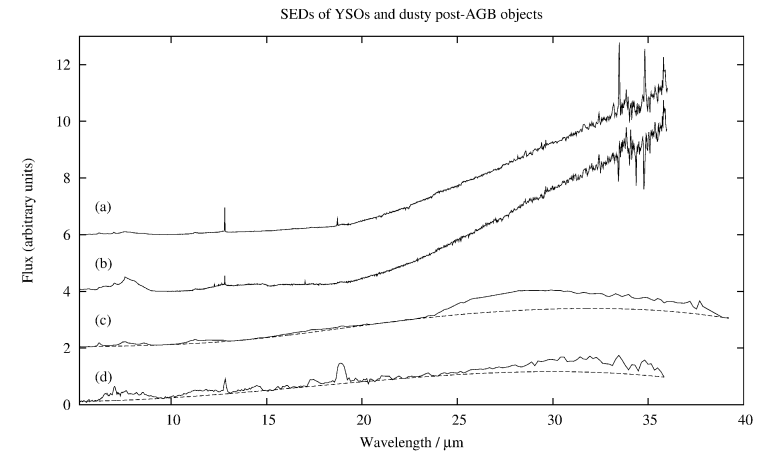
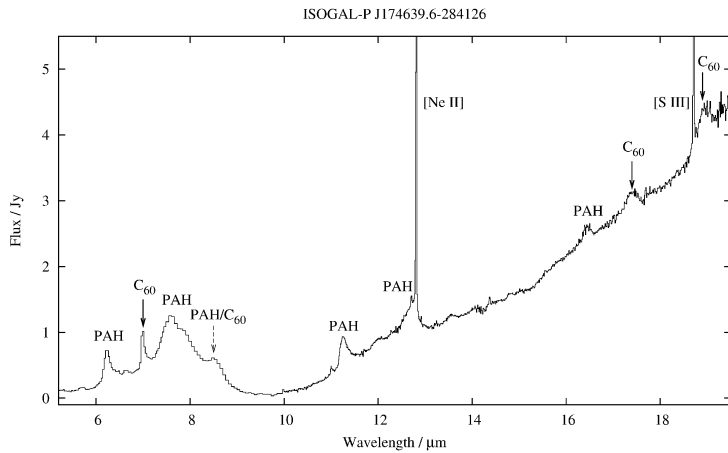


C<sub>60</sub>

- YSO in Central Molecular Zone

## SEDs of YSOs and post-AGB objects (a) ISOGAL

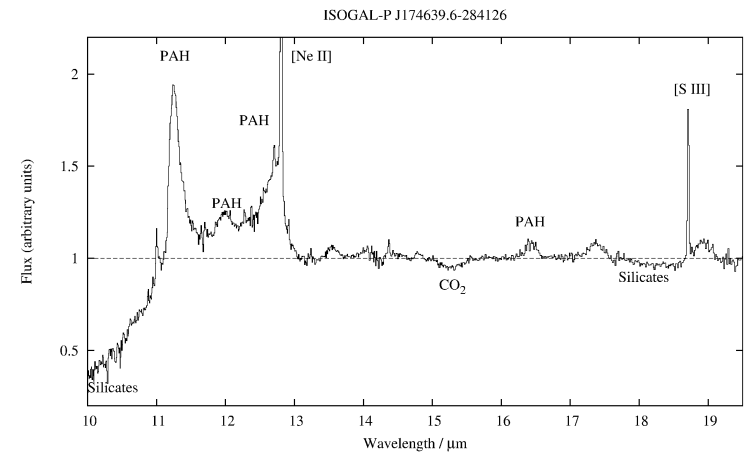
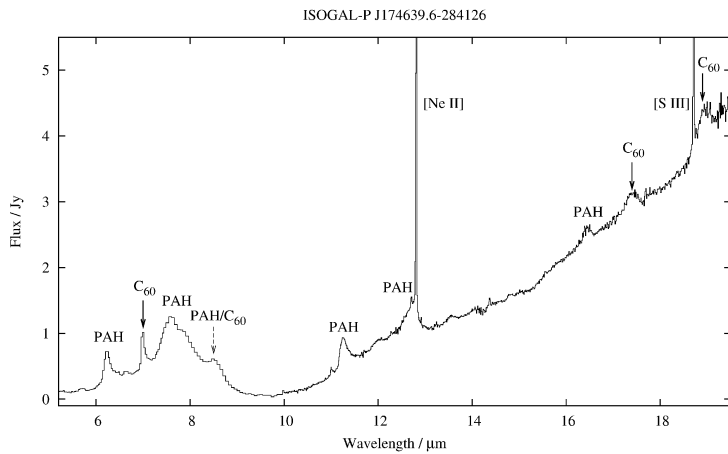
object





C<sub>60</sub>

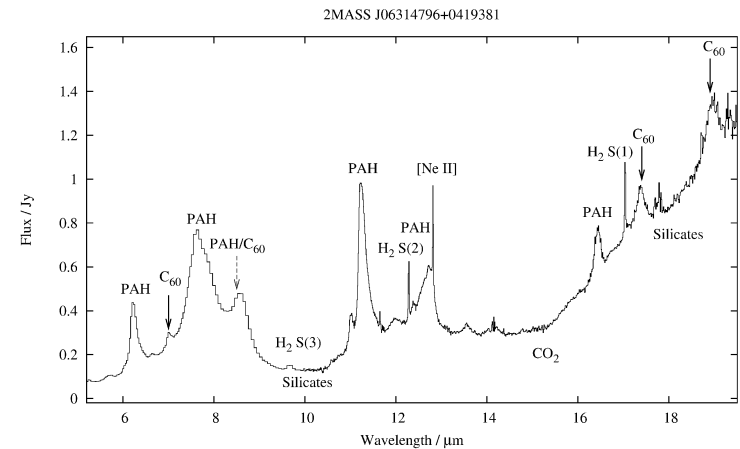
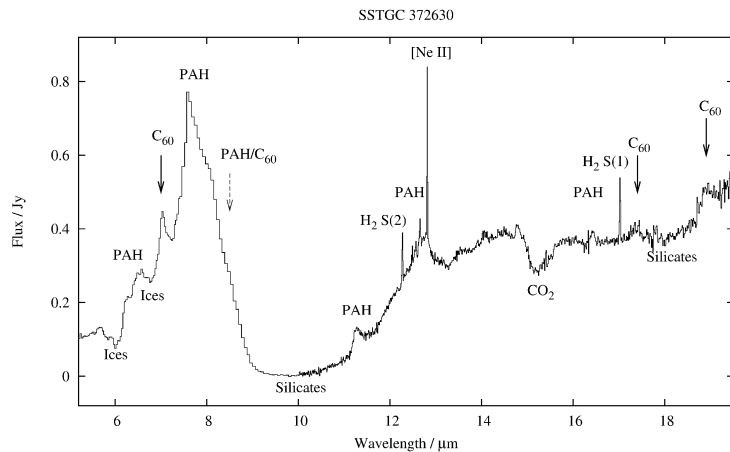
- YSO in Central Molecular Zone
- Silicate and CO<sub>2</sub> ice absorption bands



C<sub>60</sub>

## YSO in Central Molecular Zone Nebula

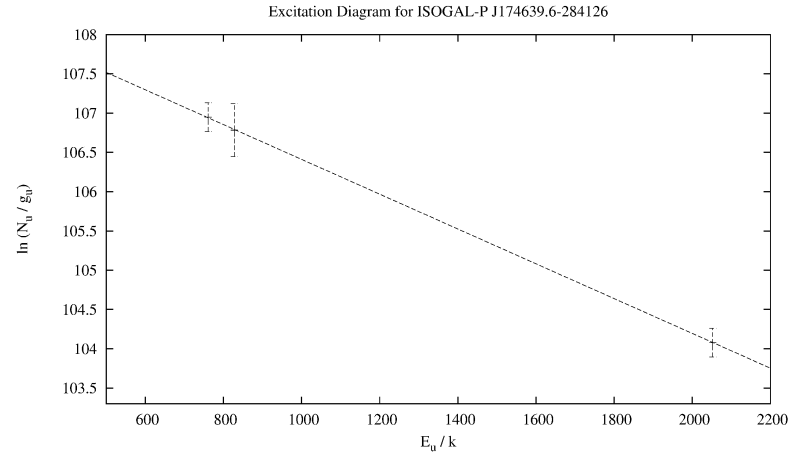
## Candidate YSO in Rosette Nebula



# C<sub>60</sub> – excitation mechanism

- Thermal

$$N_u \propto g_u \exp(-E_u/kT)$$



**Table 3.** Observed vibrational band intensity ratios, inferred vibrational temperatures for YSOs and comparison with predicted photo-excited band ratios of Sellgren et al. (2010).  $T_{\text{vib}}^{\text{C}}/K$  and  $T_{\text{vib}}^{\text{I-G}}/K$  are the vibrational temperatures derived from the C<sub>60</sub> band strengths used by Cami et al. (2010) and obtained by Iglesias-Groth, Cataldo & Manchado (2011), respectively.

| Object†                         | $I_{7.04}/I_{18.9}$ | $I_{17.4}/I_{18.9}$ | $T_{\text{vib}}^{\text{C}}/K$ | $T_{\text{vib}}^{\text{I-G}}/K$ |
|---------------------------------|---------------------|---------------------|-------------------------------|---------------------------------|
| ISOGAL-P J174639.6-284126 (CMZ) | $\sim 0.42^a$       | 0.53                | $\leq 450^a$                  | $\leq 500^a$                    |
| SSTGC 372630 (CMZ)              | $\leq 0.70^b$       | $\sim 0.59^b$       | $\leq 540^b$                  | $\leq 620^b$                    |
| 2MASS J06314796+0419381         | 0.29                | 0.48 <sup>c</sup>   | 410                           | 450                             |

# C<sub>60</sub> – excitation mechanism

- Photo (UV) excitation
- As invoked for PAH IR emission

**Table 3.** Observed vibrational band intensity ratios, inferred vibrational temperatures for YSOs and comparison with predicted photo-excited band ratios of Sellgren et al. (2010).  $T_{\text{vib}}^{\text{C}}/K$  and  $T_{\text{vib}}^{\text{I-G}}/K$  are the vibrational temperatures derived from the C<sub>60</sub> band strengths used by Cami et al. (2010) and obtained by Iglesias-Groth, Cataldo & Manchado (2011), respectively.

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| 2MASS J06314796+0419381         | 0.29                | 0.48 <sup>c</sup>   | 410                           | 450                             |
| Photon energy/eV                |                     |                     |                               |                                 |
| 5                               | 0.46-0.58           | 0.28-0.38           |                               |                                 |
| 10                              | 0.76-0.94           | 0.28-0.38           |                               |                                 |
| 15                              | 0.97-1.20           | 0.29-0.38           |                               |                                 |

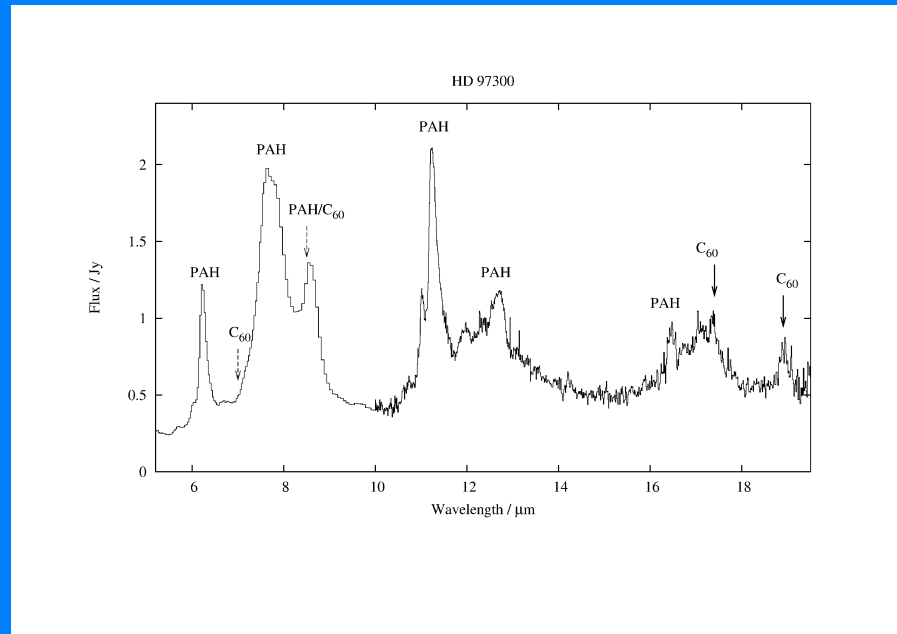
<sup>a</sup> Value when 60% contribution to 7.0  $\mu\text{m}$  feature from [Ar II] is removed (see text).

<sup>b</sup> Silicate and ice absorptions affect continuum level definition.

<sup>c</sup> Ratio when contribution of 20% from PAH feature at 17.4  $\mu\text{m}$  is removed.

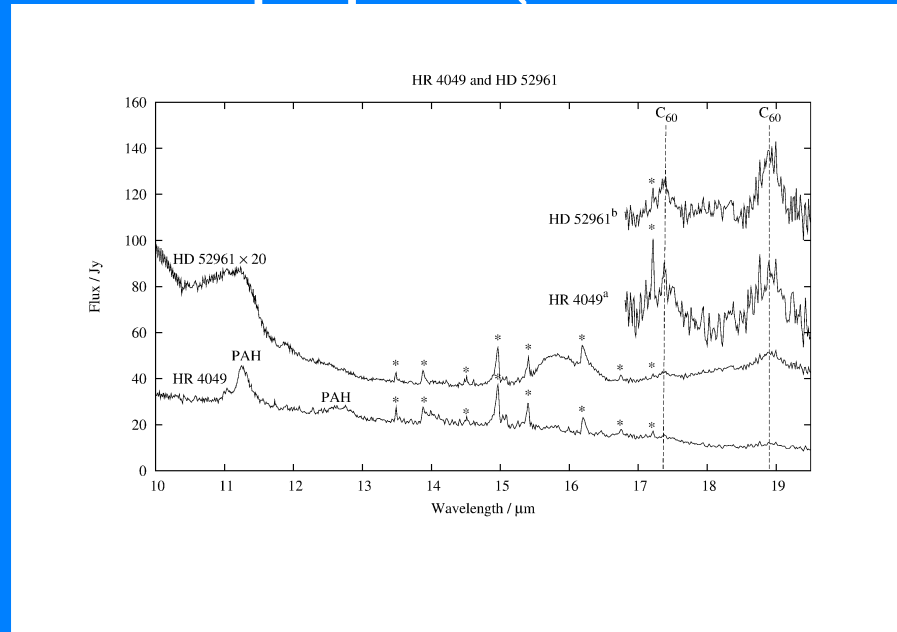
# C<sub>60</sub> – pre-main-sequence star

- Herbig Ae/Be star HD 97300
- PAHs + C<sub>60</sub>
- Very cool C<sub>60</sub> (from weakness of 7.0 μm band)



# C<sub>60</sub> in unusual post-AGB stars

- Mixed chemistry post-AGB stars
- These two stars show IR emission from nanodiamonds – very rare
- ? C<sub>60</sub> and nanodiamond formation linked
- Carbon onion pressure cell proposal (Goto et al. 2009)

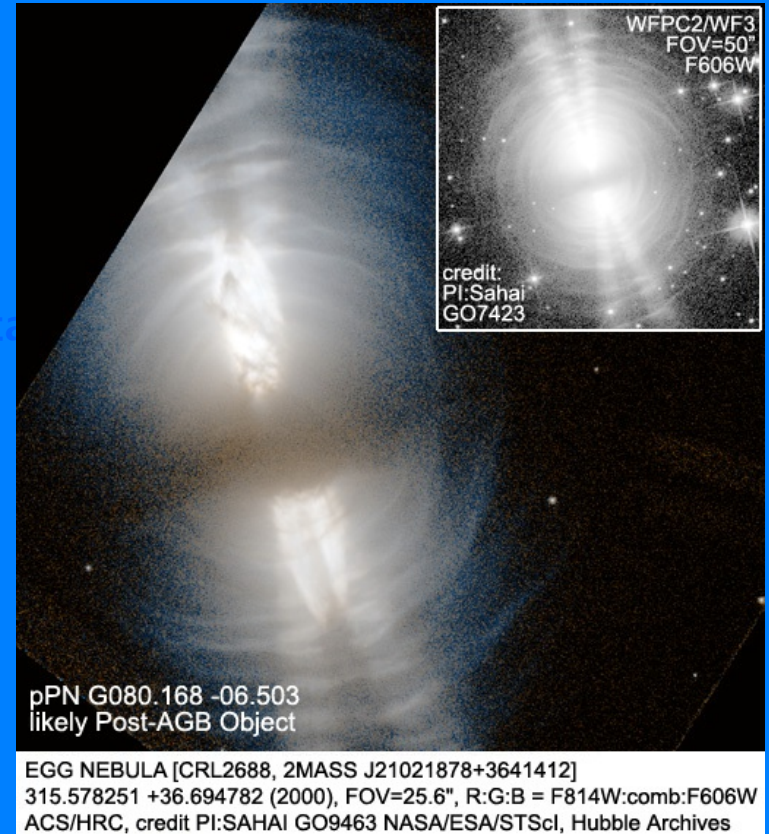


# $C_{60}$ formation

- Uncertain
- Micelotta et al. (2010) – shock-induced formation from PAHs
- Chuvilin et al. (2010) TEM experiments
  - Dehydrogenation of a PAH/graphene
  - Formation of a 5-membered ring
  - Curvature to form  $C_{60}$

# SOFIA

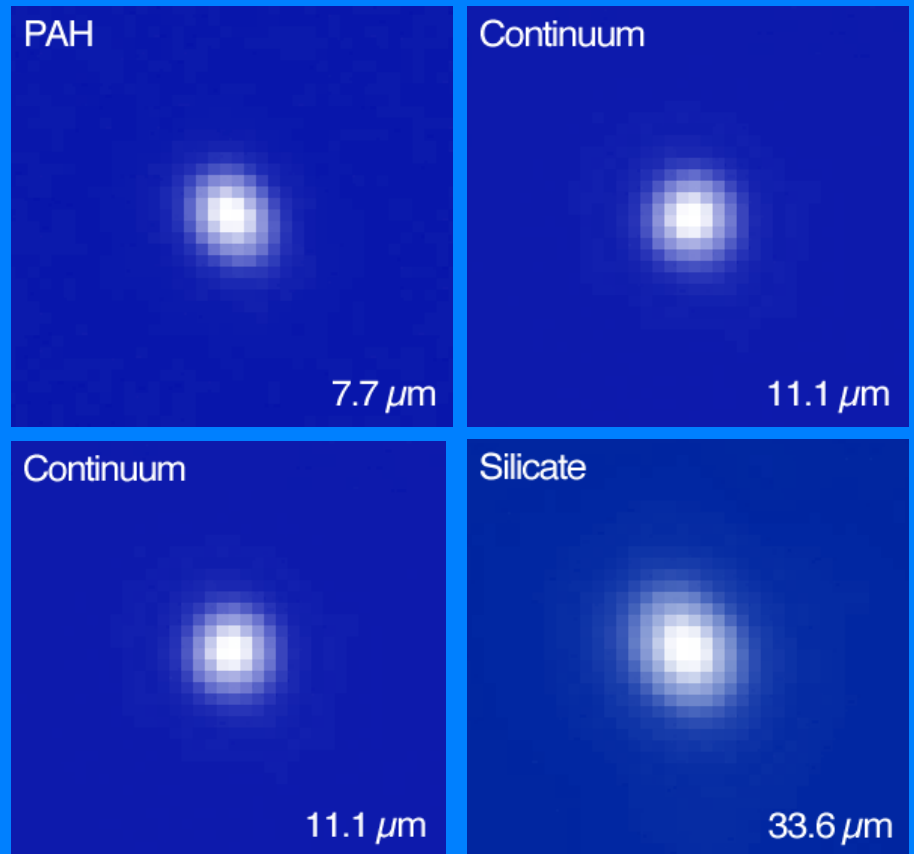
- Multi-filter imaging of post-AGB objects
- AFGL 2688 – the Egg Nebula
- Edge-on circumstellar disk
- Complex bipolar outflow
- Crystalline silicates, PAH features, and acetylene



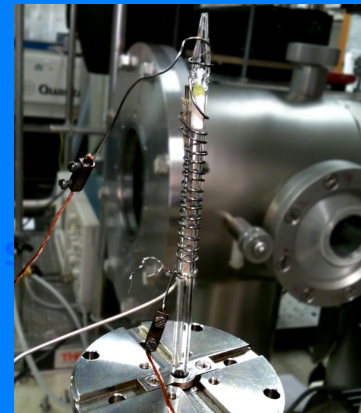
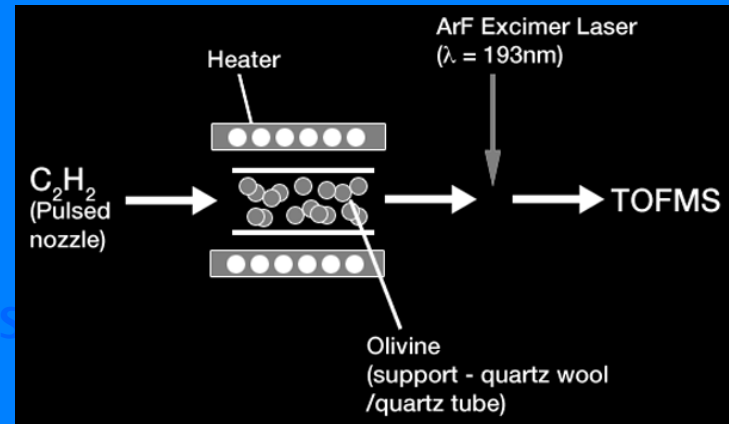
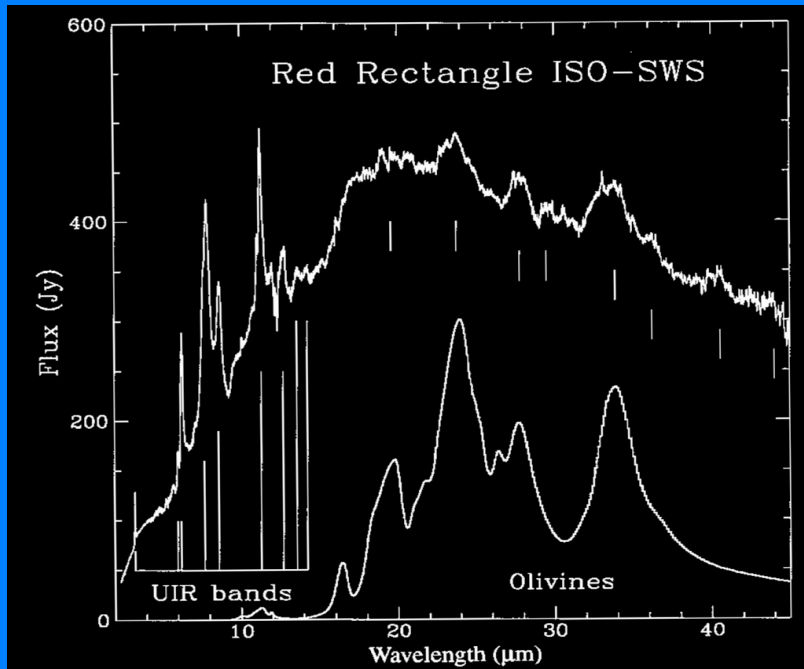


# SOFIA Observations

- PAH and silicates elongated
- PAHs and silicates – chemistry linked?



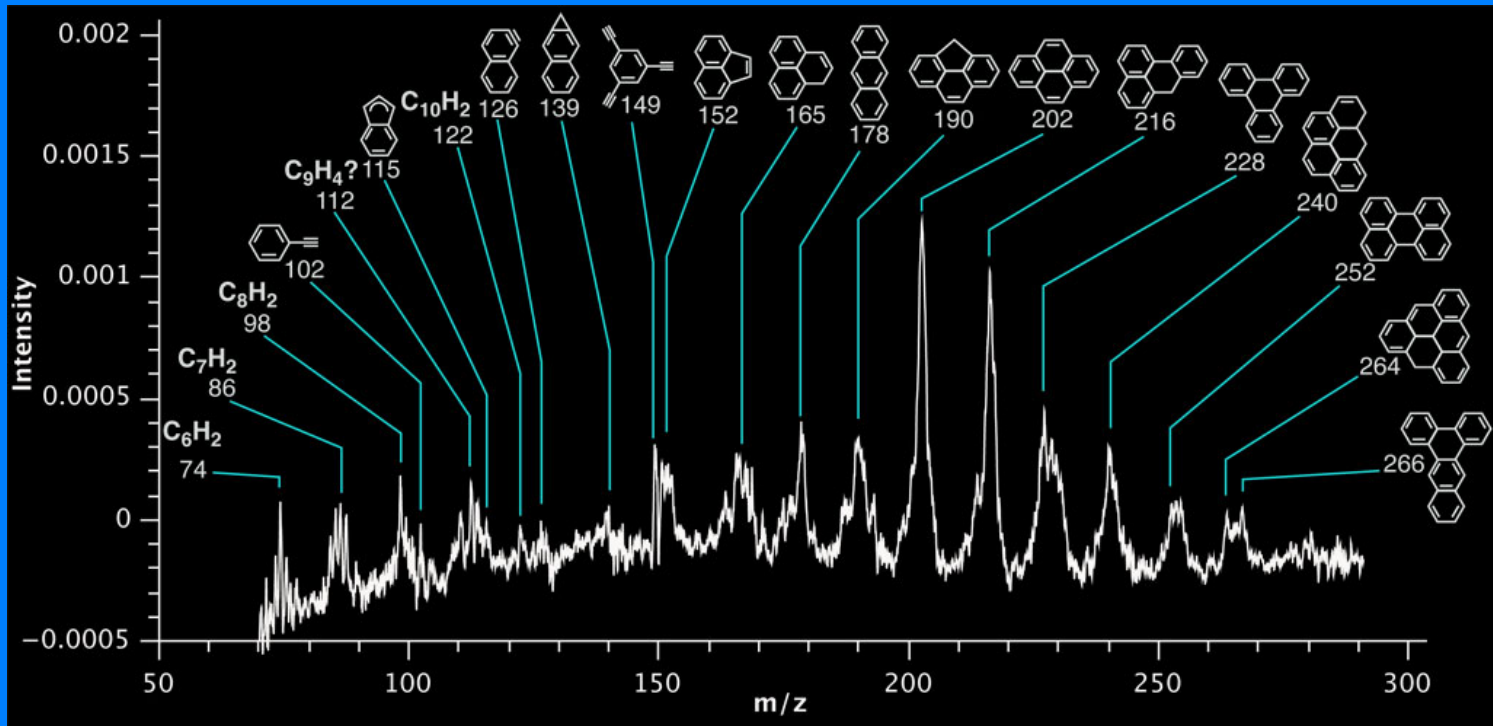
# PAH formation



Standard s

Collaboration with Cheung et al. at Hong Kong University

# Mass spectrometry results



## Future – SOFIA

- Spectroscopy!
- Thanks

Standard star