The spectral characteristics of the PAH emission features

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Outline

• Introduction
• PAH Intensities: 6.2, 7.7, 8.6
• Decomposition of the 7-9 $\mu$ m region
• Spatial Sequence
• Comparison of observations with PAH database
• Summary
• SOFIA & PAHs
Discovery: IR emission bands

Evolved star

Red Rectangle
HD44179

NASA-HST

Gillett et al. 1973; Russel et al. 1978
Incredibly rich IR emission bands

Peeters et al. 2004

NGC 7027 evolved star

NASA-HST

Star forming region Orion

NASA, JPL-Caltech, University of Toledo
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
PAH excitation & relaxation

- Excited by photon absorption, relax through IR vibrational modes
- Not molecule specific 
  \[ \rightarrow \text{no single molecule identified} \]

\[ a = 25\text{Å} \quad \tau_{abs} = 5 \times 10^4 \text{ s} \approx 13.9 \text{ h} \]

Draine & Li 2001

NASA Ames Astrochemistry Laboratory
Life cycle

The Lifecycle of Organic Carbon in the Interstellar Medium

Stellar Birth

Dense Cloud

Stellar Death

Diffuse Interstellar Medium

IRAS22272+5435

BD+30°3639

Diffuse ISM

NGC 7023

Orion Bar

Planetary Formation

5 6 7 8 9 10 15

Wavelength (µm)

5 6 7 8 9 10 15

Wavelength (µm)

5 6 7 8 9 10 15

Wavelength (µm)
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 \(\rightarrow\) gas-phase abundances
  - Surface chemistry
- PAHs are used as a tracer for star formation
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

IR Spectral Database

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

Experimental data from carbonaceous species

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

Duley et al., Pino et al. Jager et al.
Observational characteristics

PAH emission:
- is variable:
  - (relative) intensity
  - peak position & profile
- depends on environment, physical conditions
Well-known PAH intensity correlations

- from source to source
  
  $11.2 \text{ vs. } 3.3$

- $6.2 \text{ vs. } 7.7$

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

Hony (Peeters) et al. 2001
Well-known PAH intensity correlations

- within extended sources

\[ \begin{align*}
6.2 & \text{ vs. } 7.7 \\
6.2 & \text{ vs. } 7.7 \\
8.6 & \text{ vs. } 7.7
\end{align*} \]

Peeters et al., 2015

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”

Evolved star

Star forming region

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

compact PAHs with smooth edge structure

more irregular

Large neutral PAHs
NGC 2023

- Reflection Nebula
- illuminating star: B1.5V star HD 37903
- distance of 350 pc
- a FUV radiation field of $\sim 500 \times 10^4$ $G_0$ 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 $\mu$m
  - $R=\sim60-128$
- **SH:**
  - 10-20 $\mu$m
  - $R=\sim600$

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

Contours
Black: 11.2
Pink: 7.7
7-9 $\mu$m decomposition

North

South

G7.6 & G8.6
G7.8 & G8.2
7-9 $\mu$m decomposition

best correlation:

G7.6 & G8.6

weaker correlation:

G7.8 & G8.2

North

South
7-9 $\mu$m 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

  $\uparrow$

  7.8 is related to 8.2

- They arise from at least two PAH subpopulations with spatially distinct morphologies
7-9 \( \mu m \) extremes

Spatial distribution varies:
- with \( \lambda \) across bands
- between 2 extremes at 7.35 and 8.1 \( \mu m \)
- 8.1 \( \mu m \) \sim 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

Whelan (Peeters) et al. 2013
Break-down between 6.2 & 7.7?

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Stock, Peeters et al. 2013
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

Stock, Peeters et al. 2013
Morphology of PAH emission changes

Increasing distance from the star

7.35 extreme,
8.6, G7.6, G8.6
6.2, 7.7
G7.8, G8.2
8.1 extreme

BUT 6.2 – 7.7 breakdown inside some star-forming regions

2 extremes in 7-9 \( \mu m \) 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:
  - 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

Increasing distance from the star

2 extremes in 7-9 μm PAH emission
4 Gaussian decomposition
- Reveals variation beyond charge state (neutrals - ions):

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

BUT 6.2 – 7.7 breakdown inside some star-forming regions
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

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 \( \mu \) m 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 \( \mu \) m 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  \( \text{(Bauschlicher; Peeters et al. 2008, 2009)} \)
  - 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 $\lambda$ across PAH bands

• 7-9 $\mu$m 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.
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)