

SPECTRAL ANALYSIS METHODS FOR COMPLEX SOURCE MIXTURES

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ORION



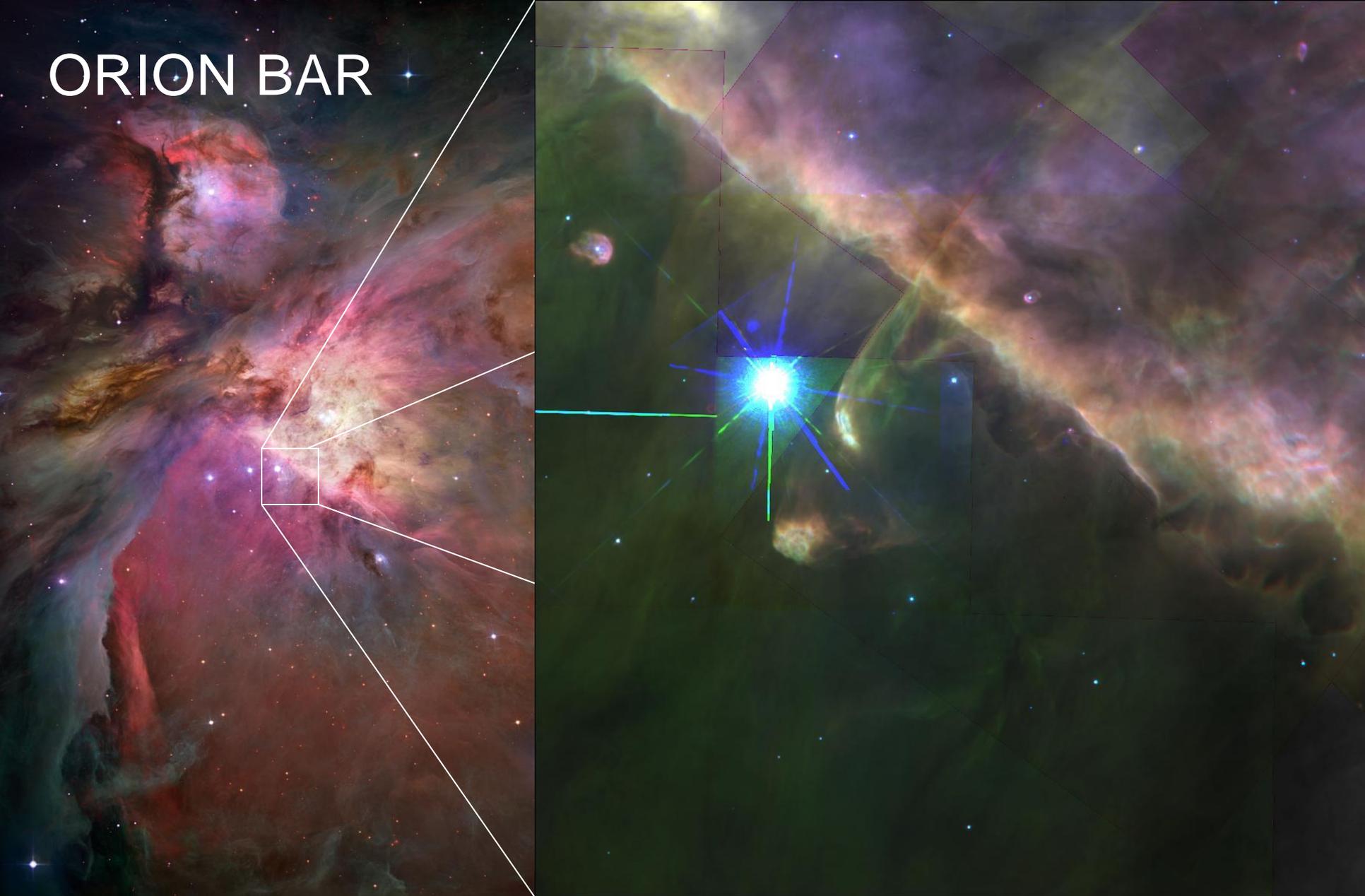
Photo Credit: Matthew Spinelli

ORION NEBULA



HST

ORION BAR



HST

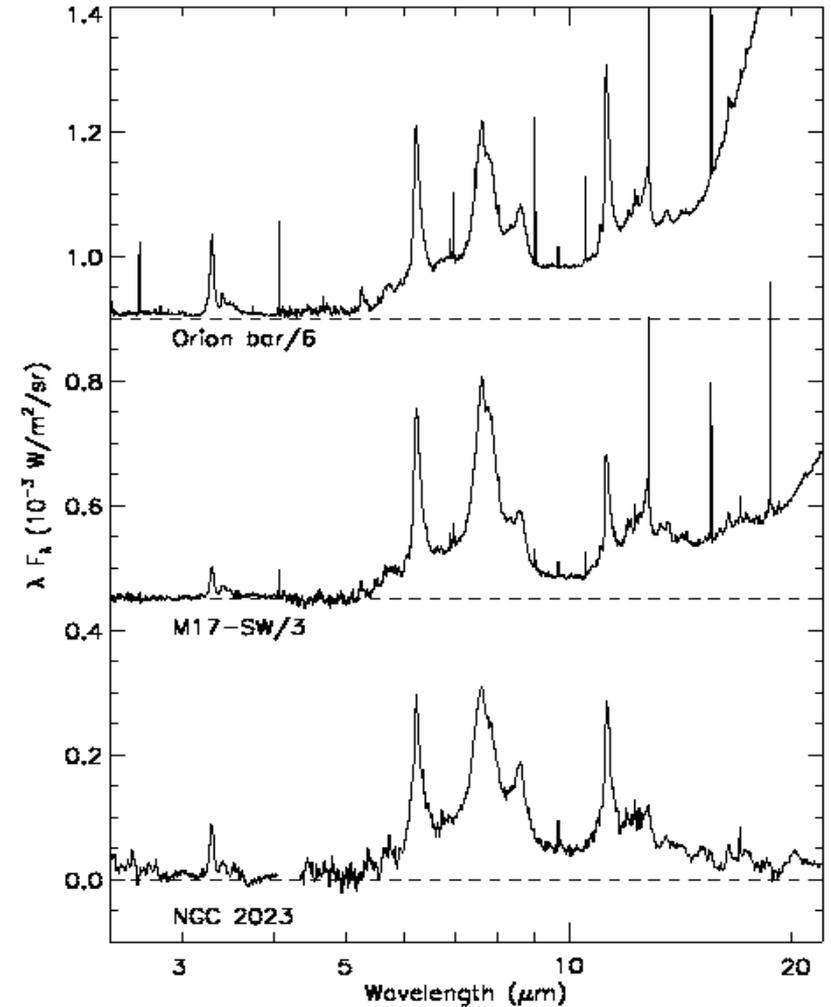
UNIDENTIFIED INFRA-RED EMISSION

UIR emission when there is UV-lit dust

Emission **near** 3.3, 6.2, 7.7, 8.6 and 11.2 μm .

Dying stars, forming stars/planetary systems, ISM

Other galaxies, $z = 2.8$



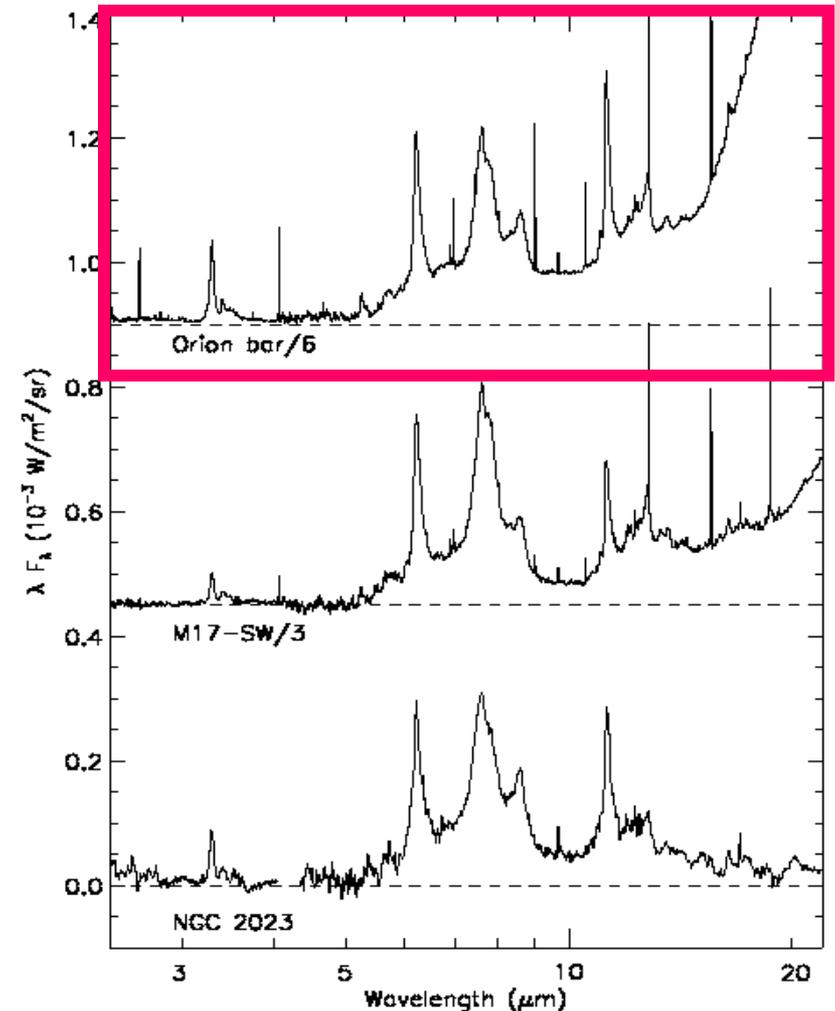
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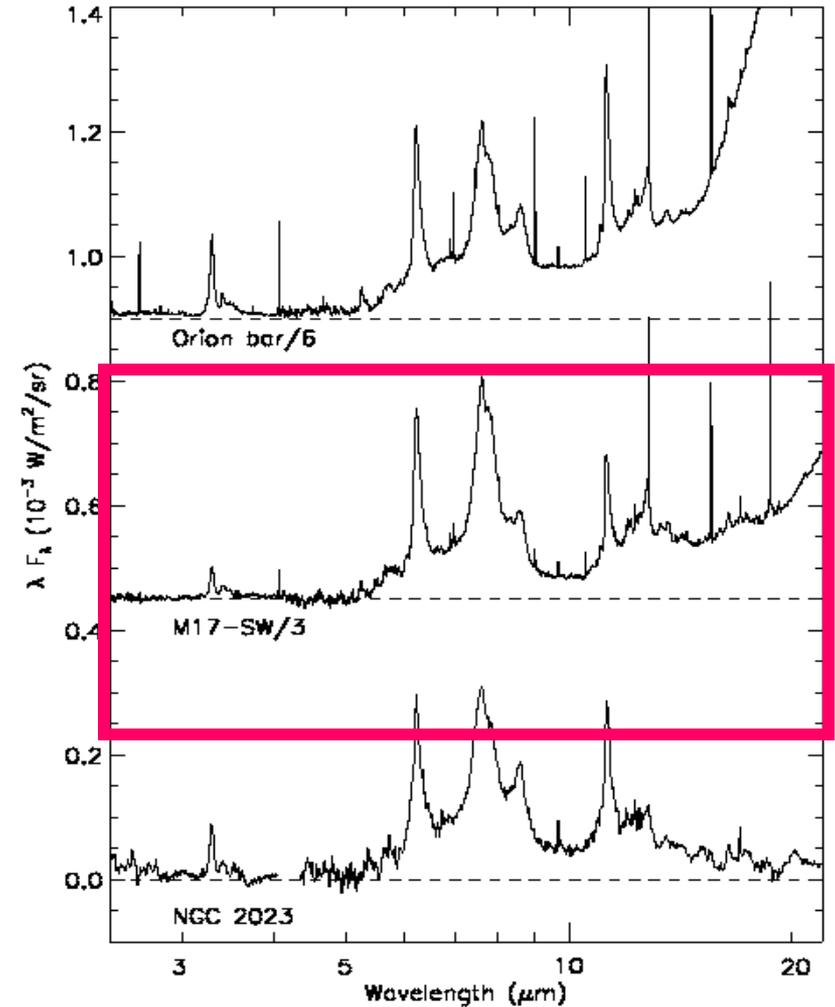
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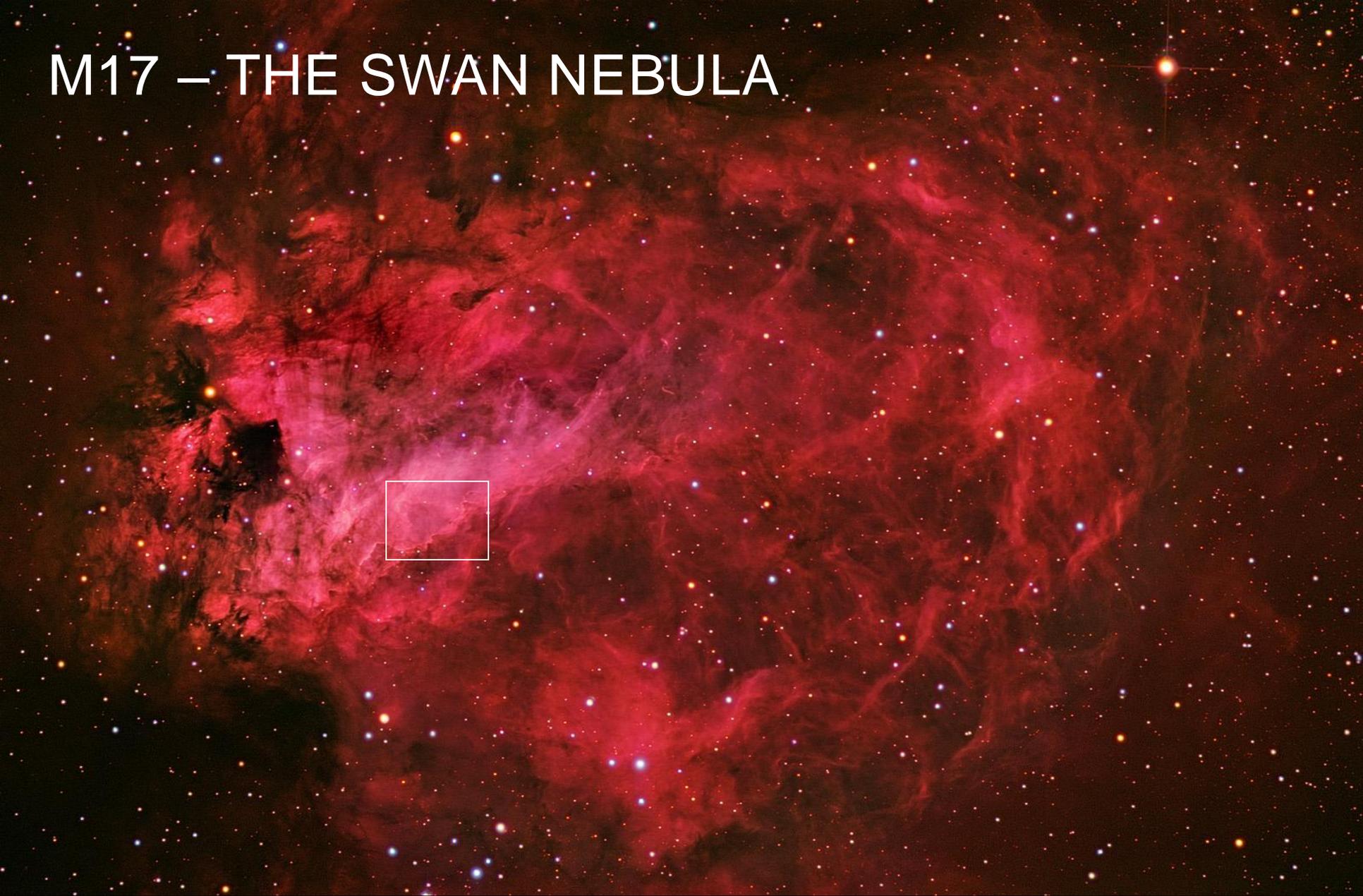


M17 – THE SWAN NEBULA



Bernd Flach-Wilken and Volker Wendel

M17 – THE SWAN NEBULA



Bernd Flach-Wilken and Volker Wendel

M17



HST

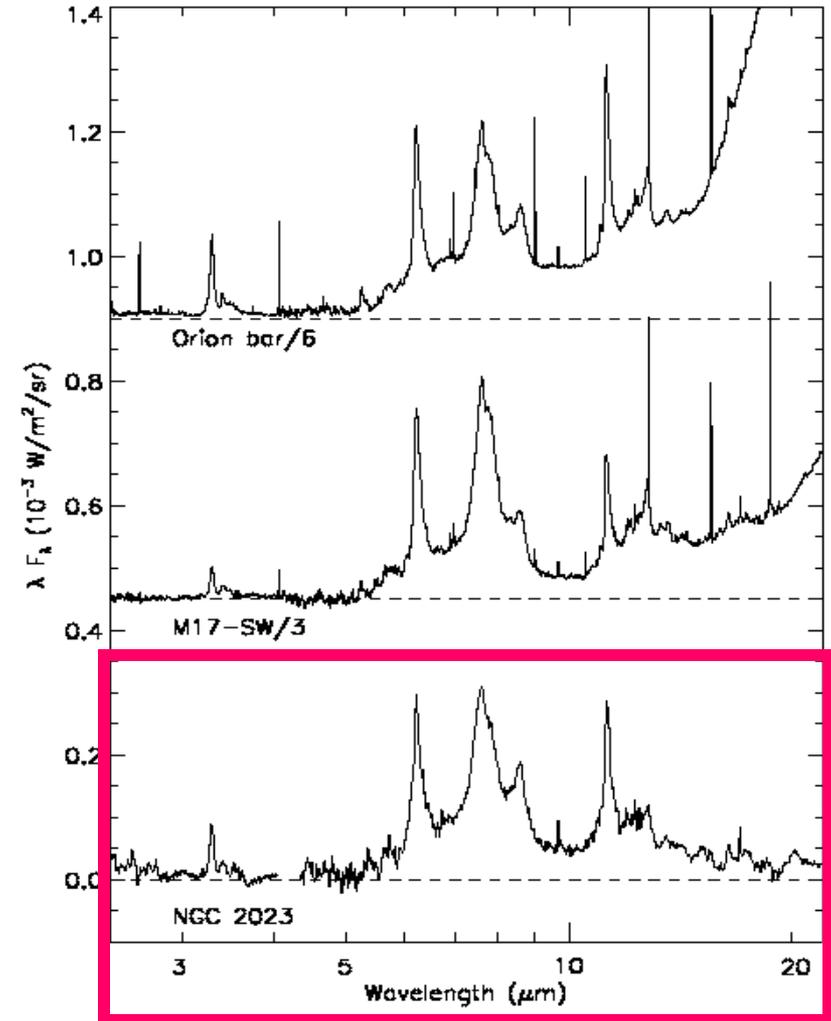
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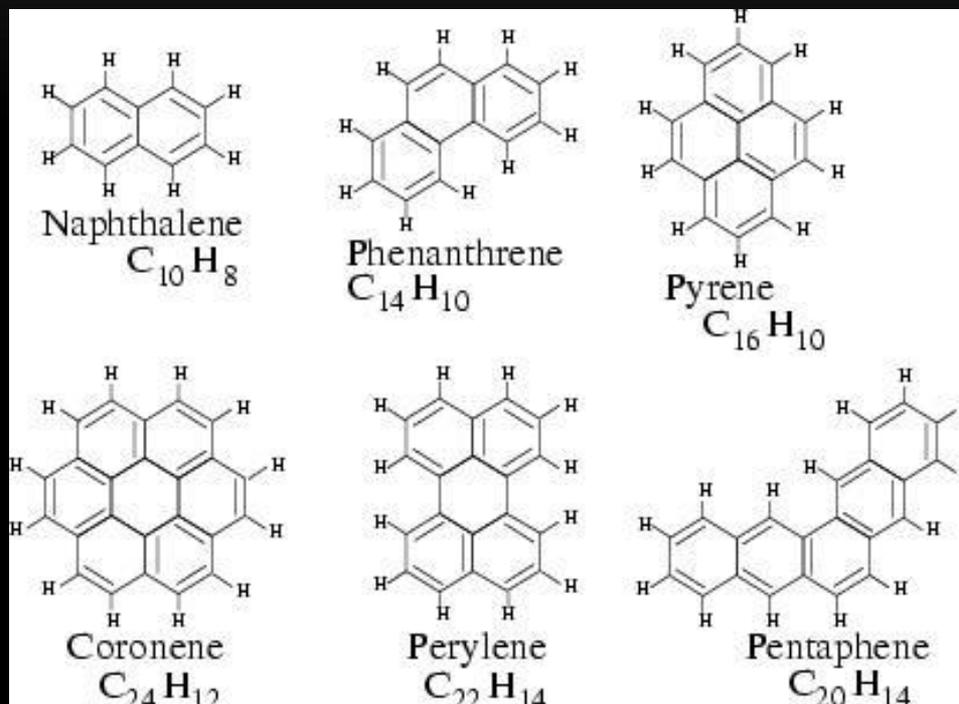
NGC 2023



Russell Croman

PAHS: SOURCES OF UIR EMISSIONS

Polycyclic Aromatic Hydrocarbons



Molecular bands near correct wavelengths

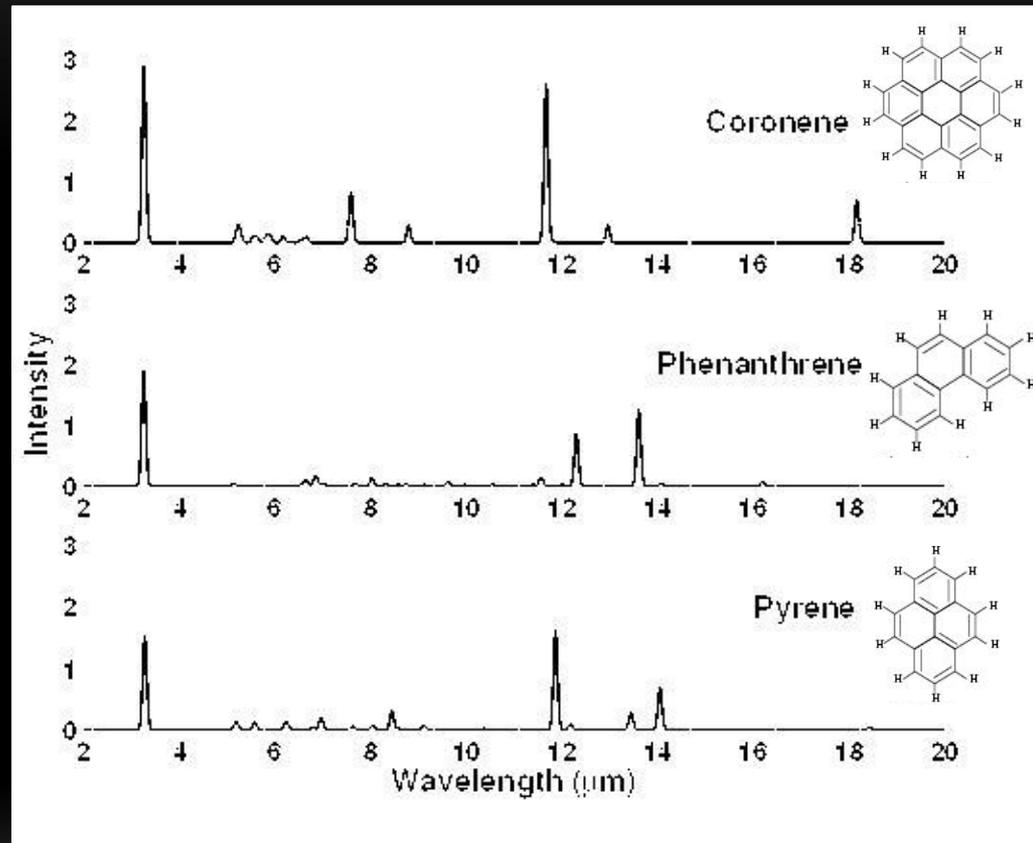
Reasonable physical model for UV-driven IR emission

EVERY PAH IS AN INDIVIDUAL

Spectra for ~1000 PAH species known
from lab or theoretical work

neutral, ions, and D, N, Fe,
Mg-substituted

Each PAH has unique spectral features



WHY ARE PAHS INTERESTING?

10-20% of all carbon atoms in the Interstellar Medium (ISM) are in PAH molecules

For this reason, PAH emissions are found in almost every cosmic environment in which there are concentrations of dust illuminated by ultraviolet radiation

They could be used to characterize the conditions of the ISM, and could be used as a tracer of star formation in the Milky Way

PAHs now appear to be important molecules on the pathway to life

PAH IDENTIFICATION PROBLEM

No astrophysical source shows the unique signature of any identifiable **known** PAH

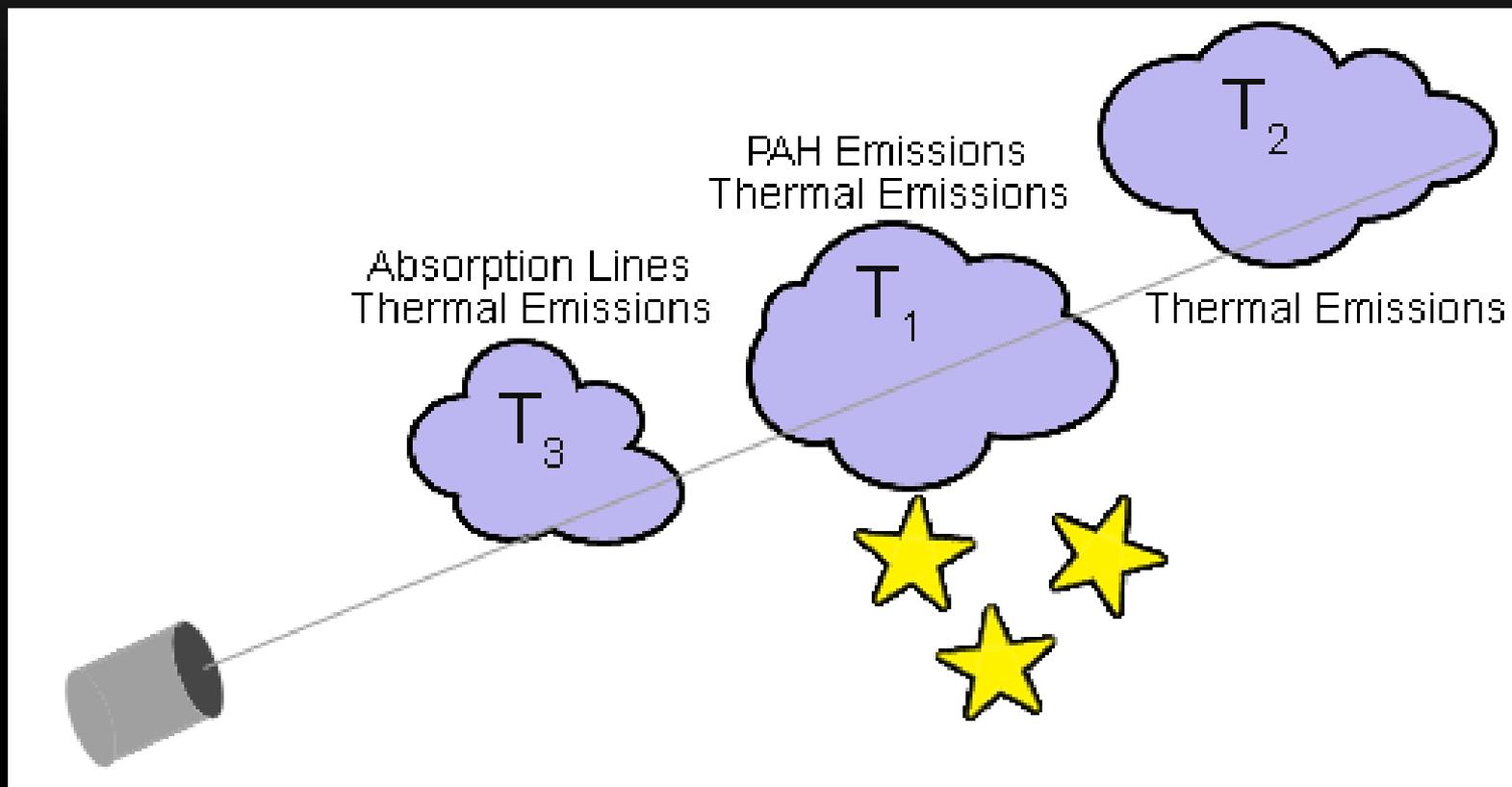
Astrophysical sources appear to have:

- multiple PAH species present

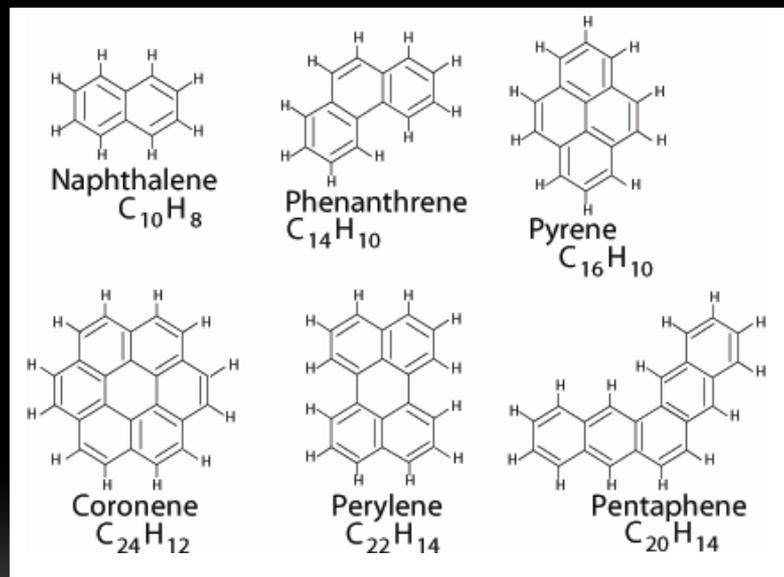
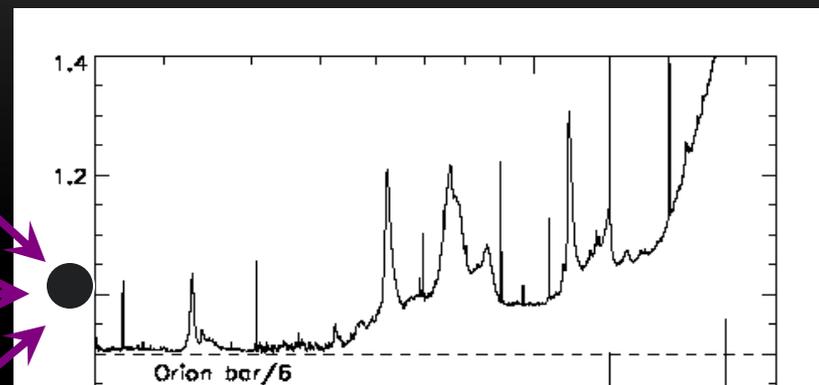
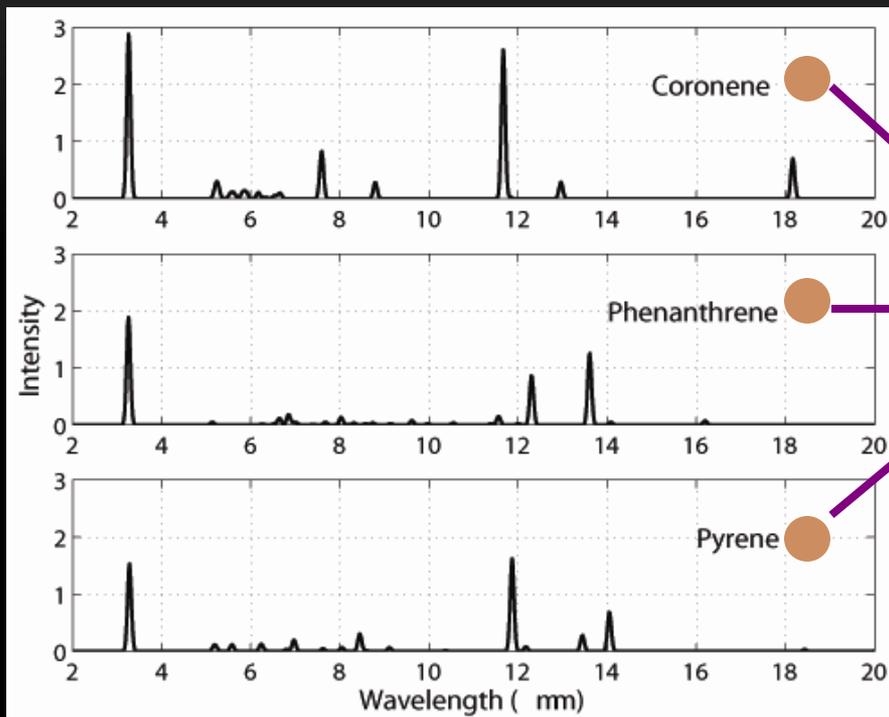
- different PAH-species concentrations depending on:

 - UV-intensity, temperature, and composition

COMPLEX SPECTRA



NUMEROUS PAH SPECIES



Any number of thousands of PAH species can contribute to an observed spectrum.

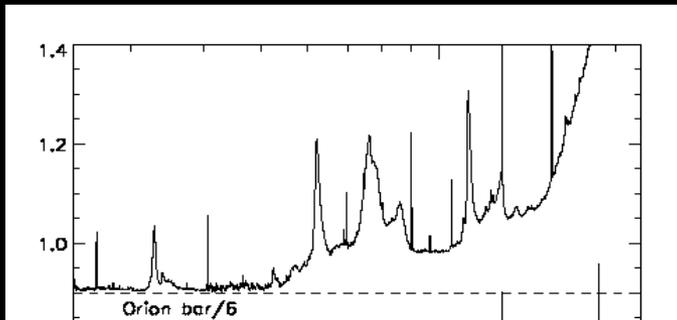
MODELING IMPORTANT FEATURES

$$F(\lambda) = \sum_{p=1}^P c_p \delta_p PAH_p(\lambda) + \sum_{k=1}^K A_k Planck(\lambda; T_k) + \sum_{g=1}^G A_g N(\lambda; \bar{\lambda}_g, \sigma_g)$$

PAH contributions

c_p – PAH concentration

δ_p – PAH presence (YES or NO)



MODELING IMPORTANT FEATURES

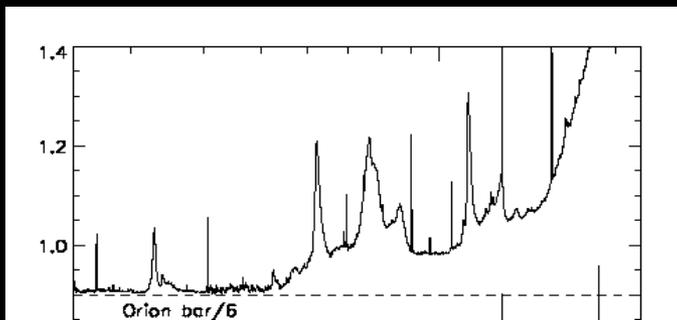
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Planck Blackbody Radiators

A_k – Planck Amplitude

T_p – Planck Temperature



$$Planck(\lambda; T_k) = \sqrt{\frac{\lambda_{\max}}{\lambda}} \frac{\exp(hc / \lambda_{\max} kT) - 1}{\exp(hc / \lambda kT) - 1}$$

MODELING IMPORTANT FEATURES

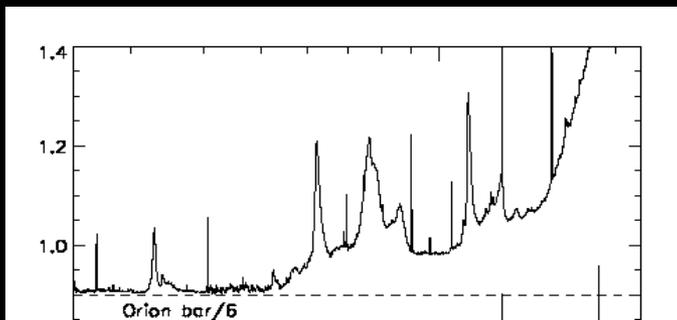
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Mixture of Gaussians

A_g – Gaussian Amplitude

– Gaussian Mean

– Gaussian Mean



MODELING IMPORTANT FEATURES

$$F(\lambda) = \sum_{p=1}^P c_p \delta_p PAH_p(\lambda) + \sum_{k=1}^K A_k Planck(\lambda; T_k) + \sum_{g=1}^G A_g N(\lambda; \bar{\lambda}_g, \sigma_g)$$

1. PAH contributions (and atomic and ionic transitions)
2. Planck Radiators
3. Mixture of Gaussians

These three models describe the spectrum to first order.

PAHS POSE UNIQUE DIFFICULTIES

Most source separation problems consist of multiple mixtures and a handful of unknown sources with unknown contributions.

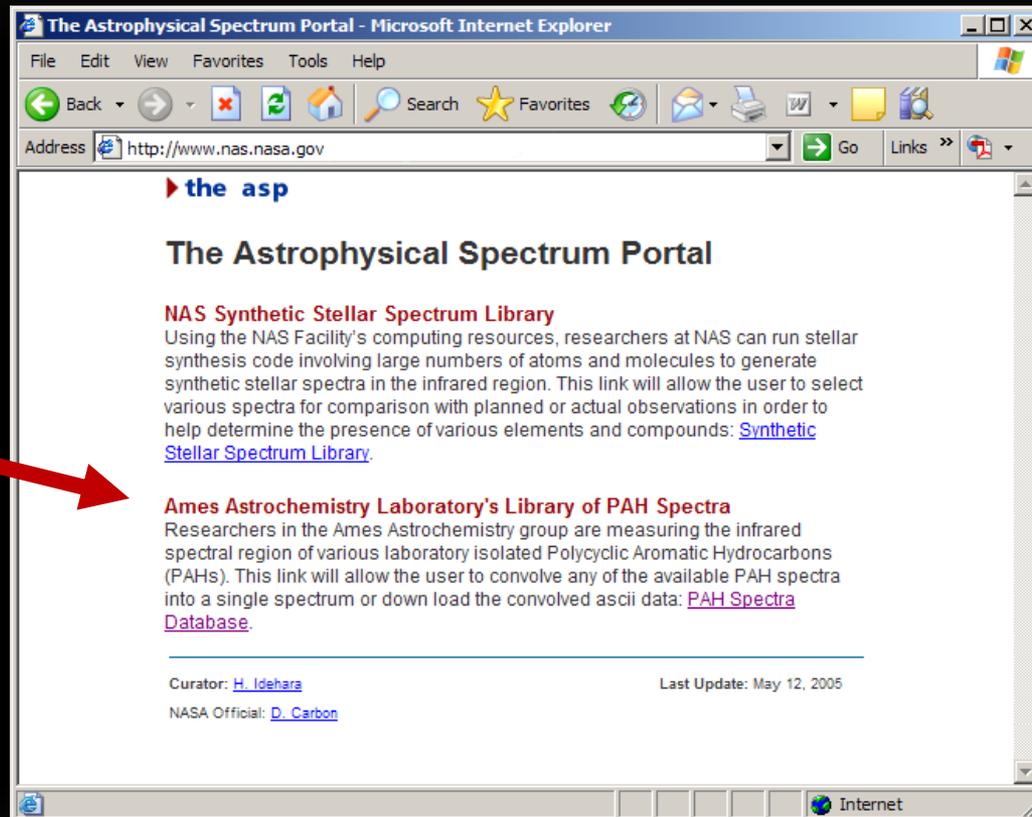
PAH spectral source separation consists of one mixture and numerous known sources with unknown contributions (and even some unknown sources).

There are potentially 100s to 1000s of species present.

- How do we tell which ones?
- How do we deal with the large number of spectra?

ASTROPHYSICAL SPECTRUM PORTAL

The PAH spectra database at NASA Ames Research Center contains
~1000 PAH spectra



The screenshot shows a Microsoft Internet Explorer browser window titled "The Astrophysical Spectrum Portal - Microsoft Internet Explorer". The address bar shows "http://www.nas.nasa.gov". The page content includes:

- the asp**
- The Astrophysical Spectrum Portal**
- NAS Synthetic Stellar Spectrum Library**
Using the NAS Facility's computing resources, researchers at NAS can run stellar synthesis code involving large numbers of atoms and molecules to generate synthetic stellar spectra in the infrared region. This link will allow the user to select various spectra for comparison with planned or actual observations in order to help determine the presence of various elements and compounds: [Synthetic Stellar Spectrum Library](#).
- Ames Astrochemistry Laboratory's Library of PAH Spectra**
Researchers in the Ames Astrochemistry group are measuring the infrared spectral region of various laboratory isolated Polycyclic Aromatic Hydrocarbons (PAHs). This link will allow the user to convolve any of the available PAH spectra into a single spectrum or down load the convolved ascii data: [PAH Spectra Database](#).
- Curator: [H. Idehara](#)
- NASA Official: [D. Carbon](#)
- Last Update: May 12, 2005

A red arrow points from the left side of the image to the "Ames Astrochemistry Laboratory's Library of PAH Spectra" section.

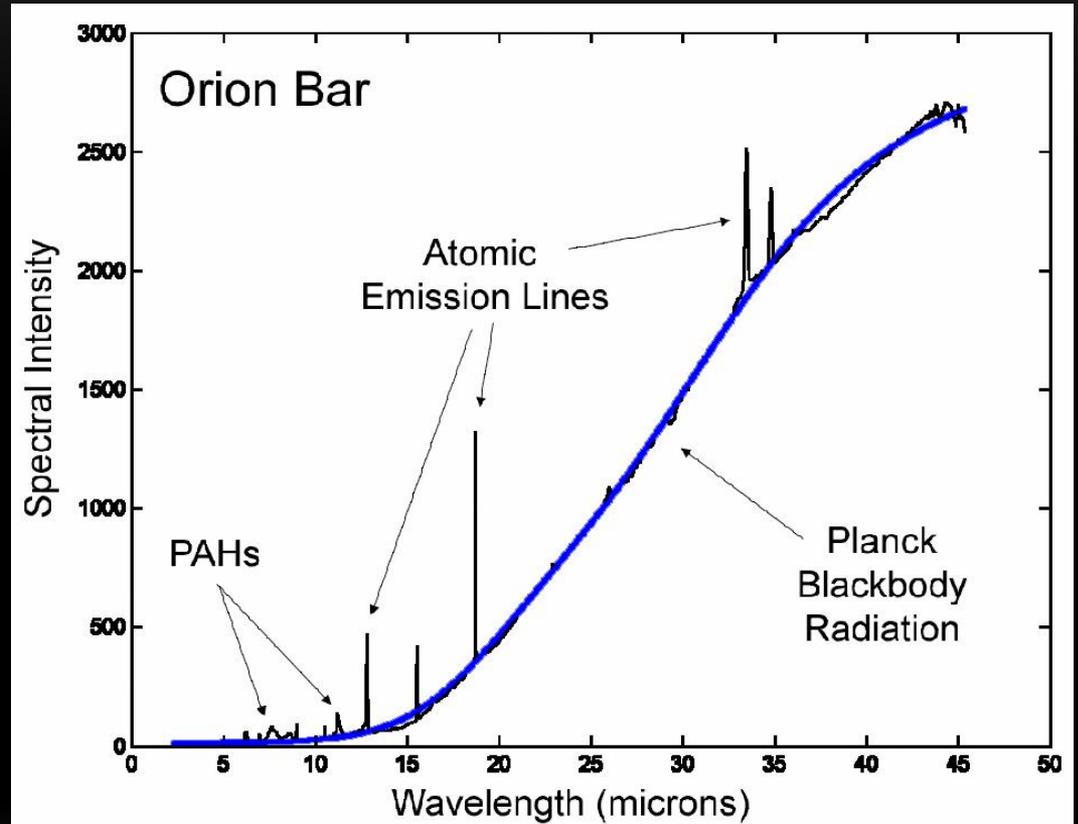
ESTIMATING PLANCK BLACKBODIES

ESTIMATING PLANCK BLACKBODIES

This figure shows a spectrum taken from the Orion Bar

The black curve is the original data, the blue curve is the background estimation.

One blackbody radiator is at a temperature of 61.043 ± 0.004 K, and there is possibly a second (36.3% chance), at a temperature around 18.8 K.

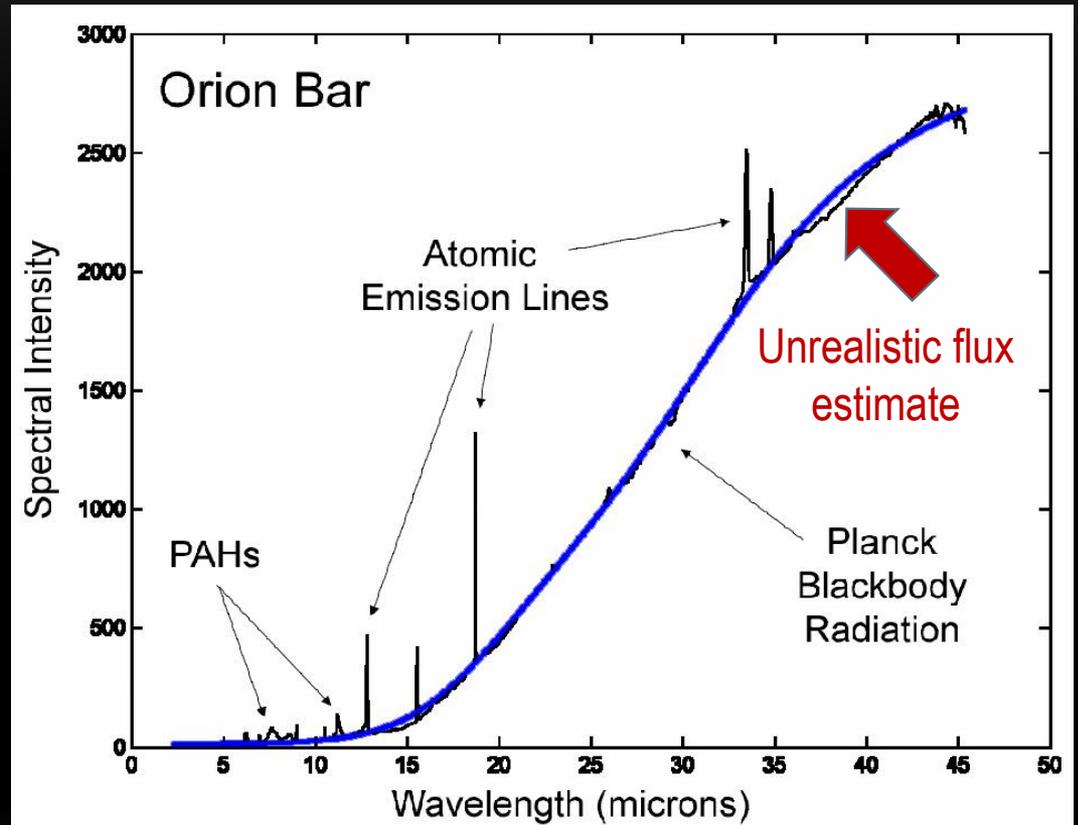


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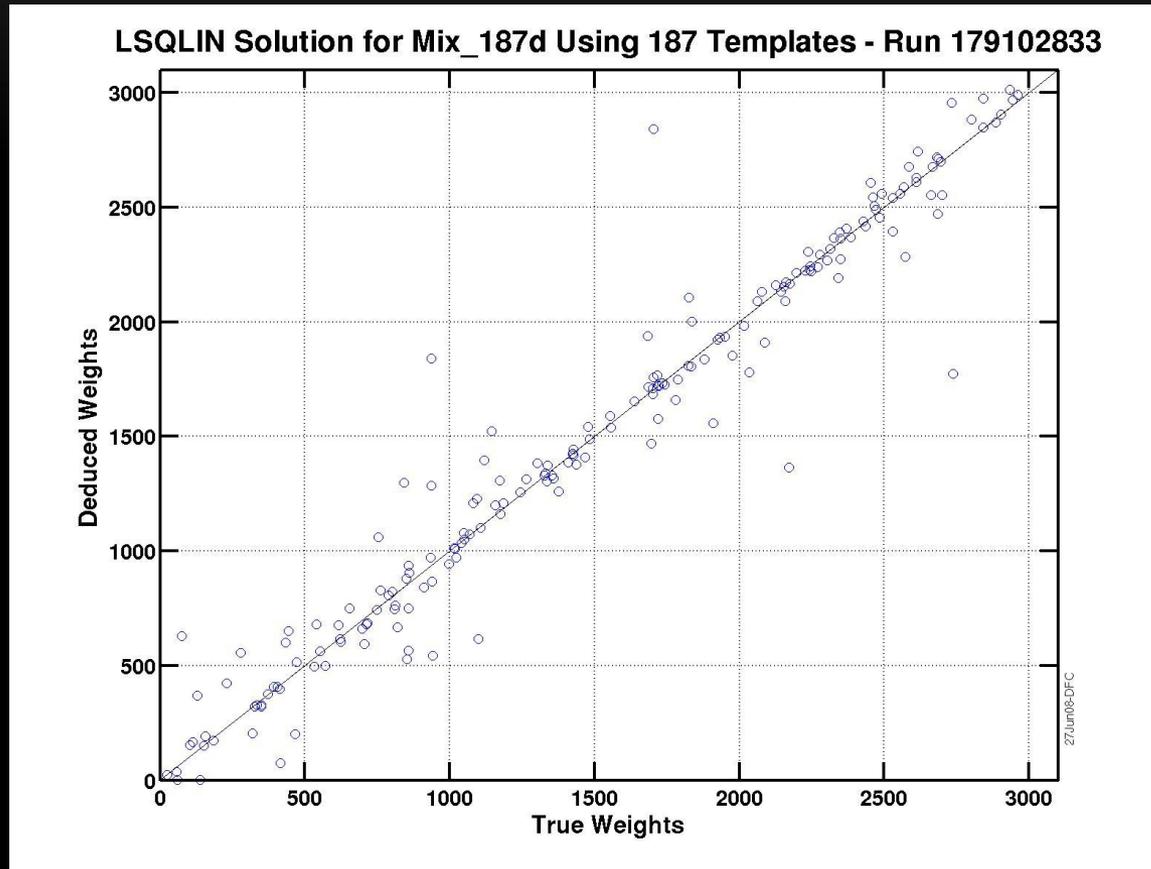
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ESTIMATING PAHS

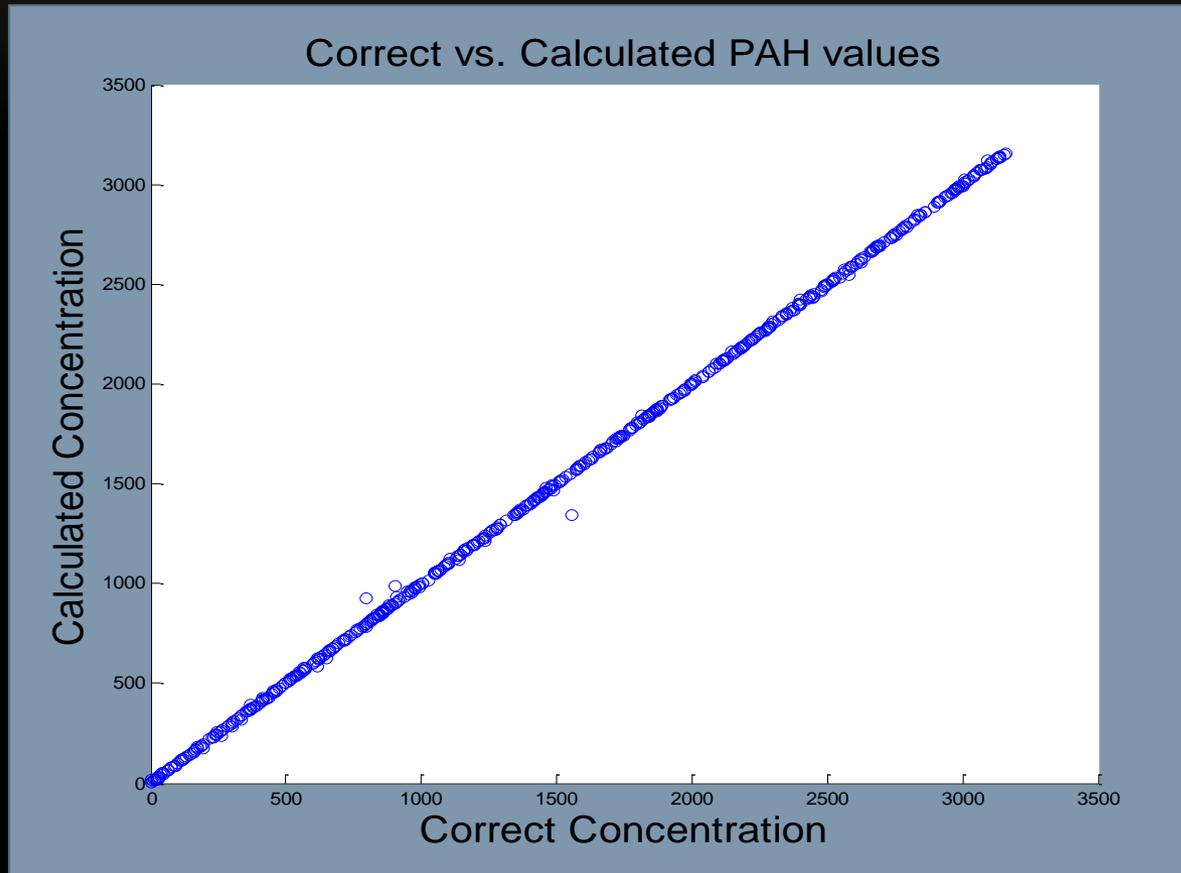
LINEAR LEAST SQUARES

187 PAHs in a synthetic mixture



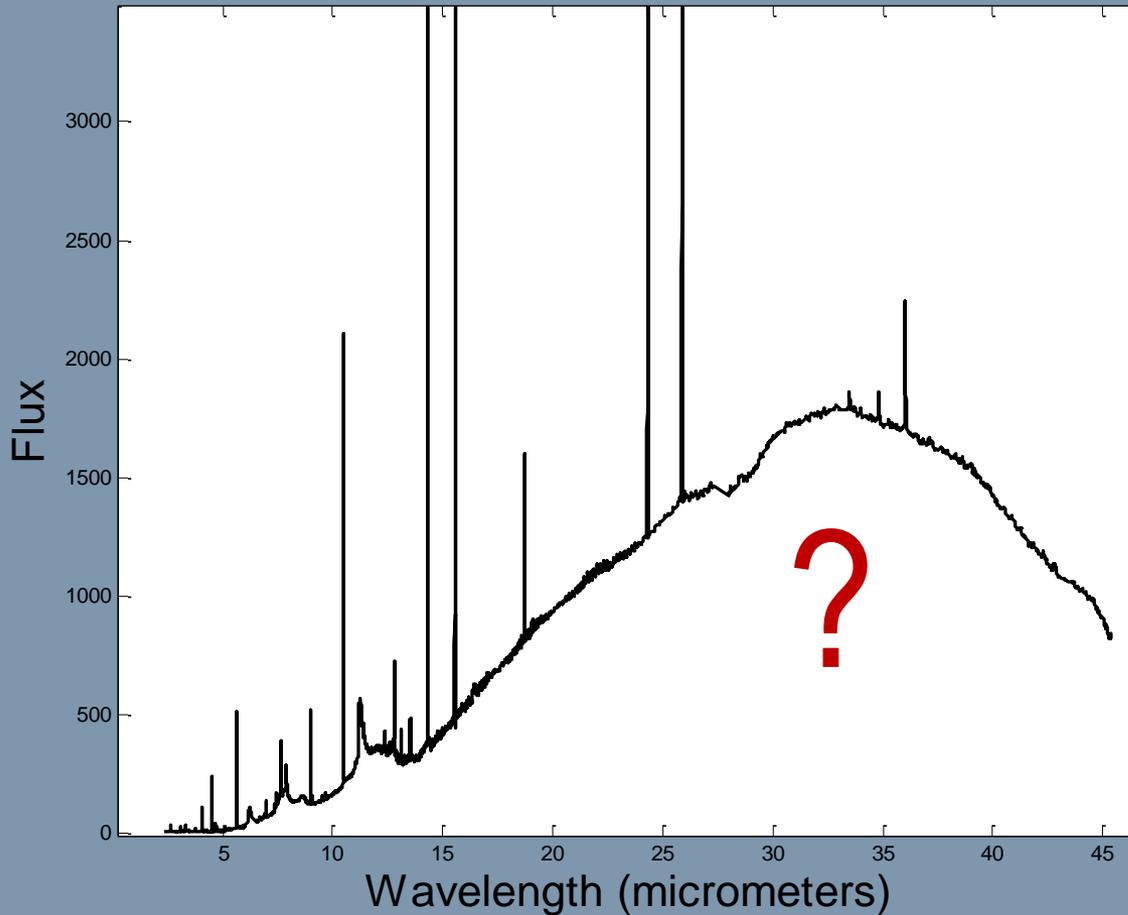
METROPOLIS HASTINGS MCMC

187 PAHs in a synthetic mixture

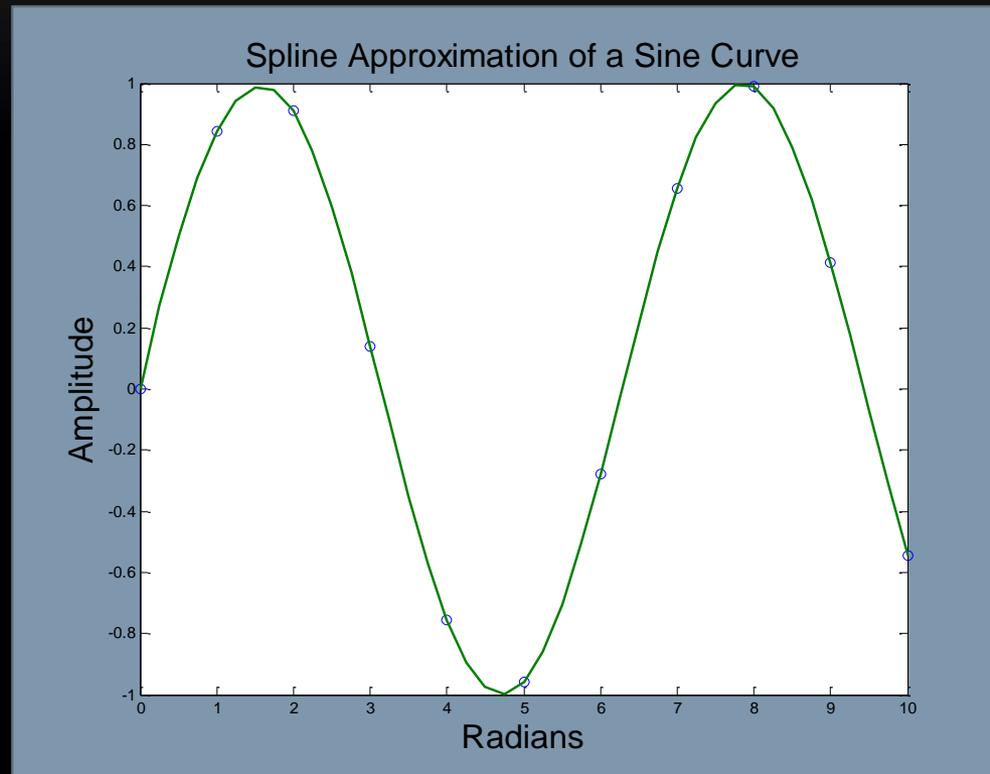


ESTIMATING BACKGROUND

WHAT TO DO WITH BACKGROUND?



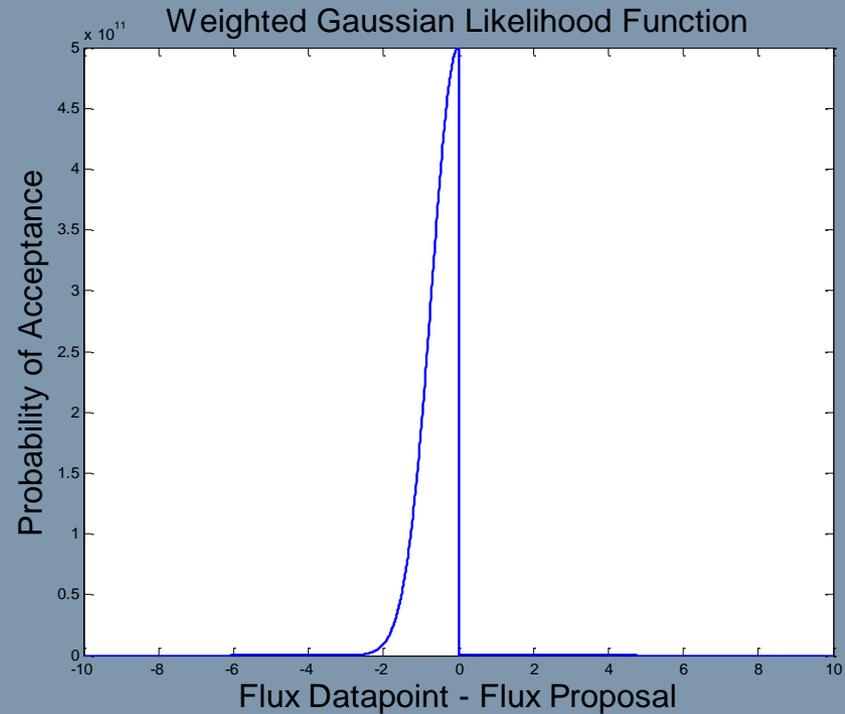
SPLINE MODEL



PIECEWISE GAUSSIAN LIKELIHOOD

$$\text{if } y_{pred} - y_{data} \leq 0$$
$$\exp\left(-\frac{(y_{pred} - y_{data})^2}{2\sigma^2}\right)$$

$$\text{if } y_{pred} - y_{data} > 0$$
$$\exp\left(-\frac{(y_{pred} - y_{data})^2}{10^6 \cdot 2\sigma^2}\right)$$



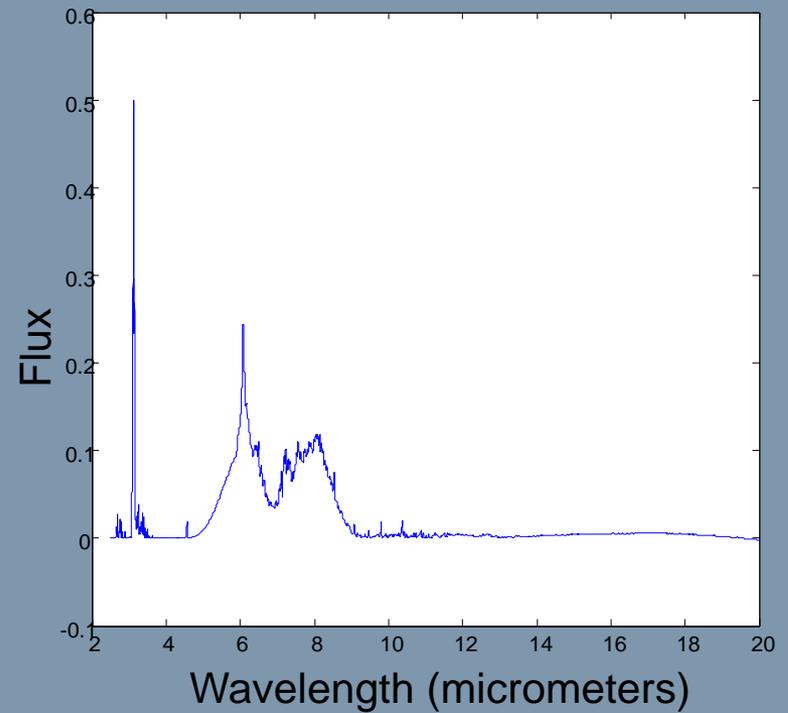
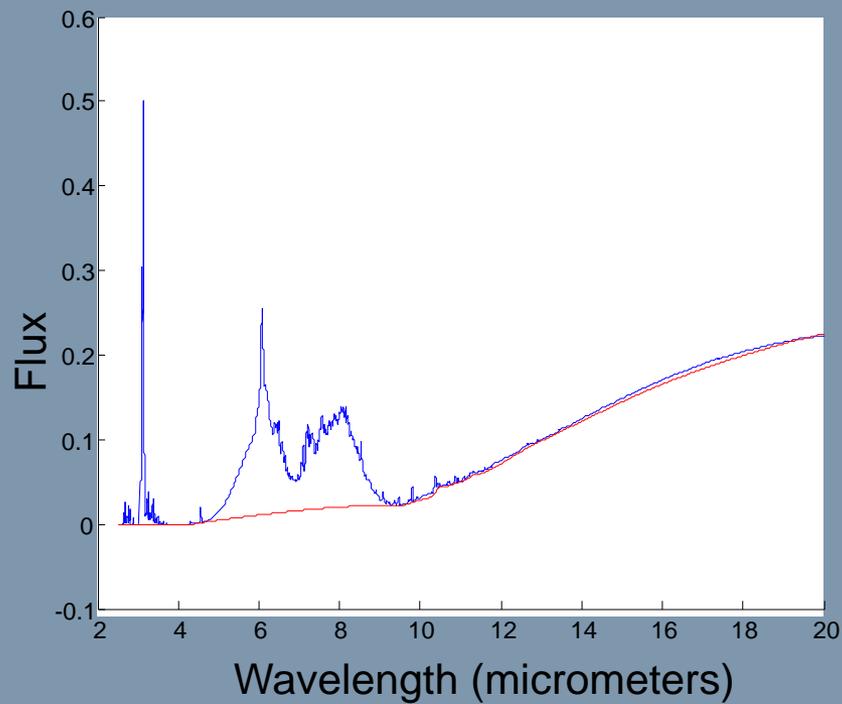
SMOOTHNESS PRIOR (OPTIONAL)

Gaussian Prior on the Integral of the Second Derivative

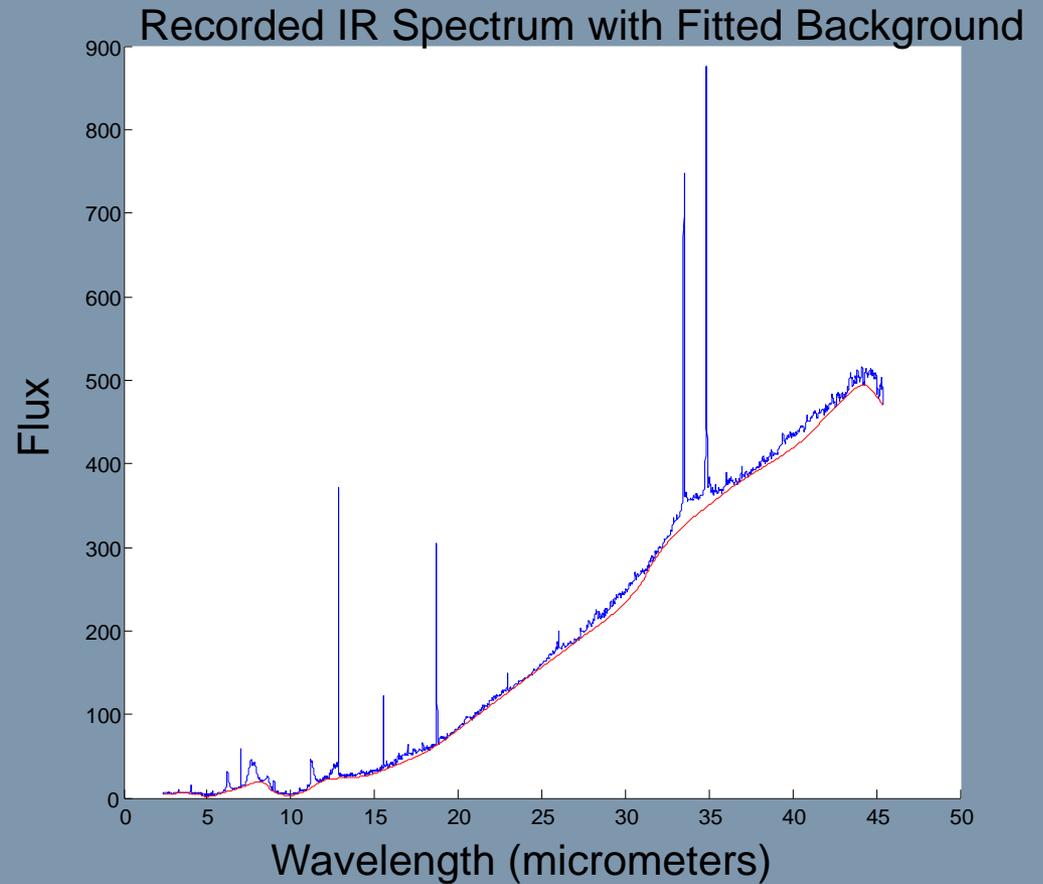
$$\text{Prior} \propto \exp\left(\frac{-\left(\int y''(\lambda)d\lambda\right)^2}{2\nu^2}\right)$$

$$\int y''(\lambda)d\lambda \approx \left(\frac{1}{N-2}\right) \sum_{i=1}^{N-2} \frac{y(i) - 2y(i+1) + y(i+2)}{(x(i+2) - x(i+1))(x(i+1) - x(i))}$$

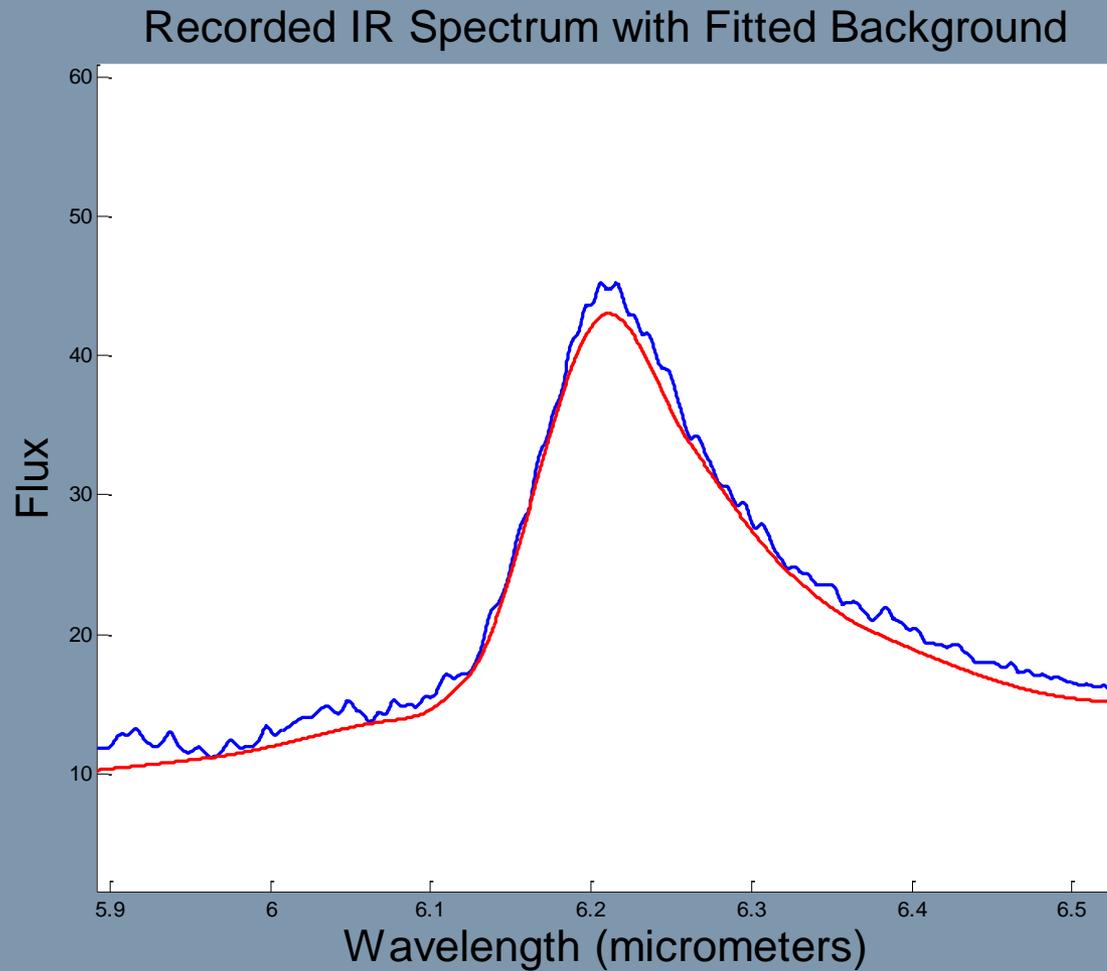
SYNTHETIC BACKGROUND REMOVAL



M82 STARBURST



PORTION OF THE ORION BAR



LIVE DEMO

FUNDED BY:

NASA SCIENCE MISSION DIRECTORATE
APPLIED INFORMATION RESEARCH PROGRAM (AISR)
05-AISR05-0143 (KNUTH PI, CARBON CO-I)
