SPECTRAL ANALYSIS METHODS FOR COMPLEX SOURCE MIXTURES

Kevin H. Knuth
Departments of Physics and Informatics
University at Albany
Albany NY

COLLABORATORS

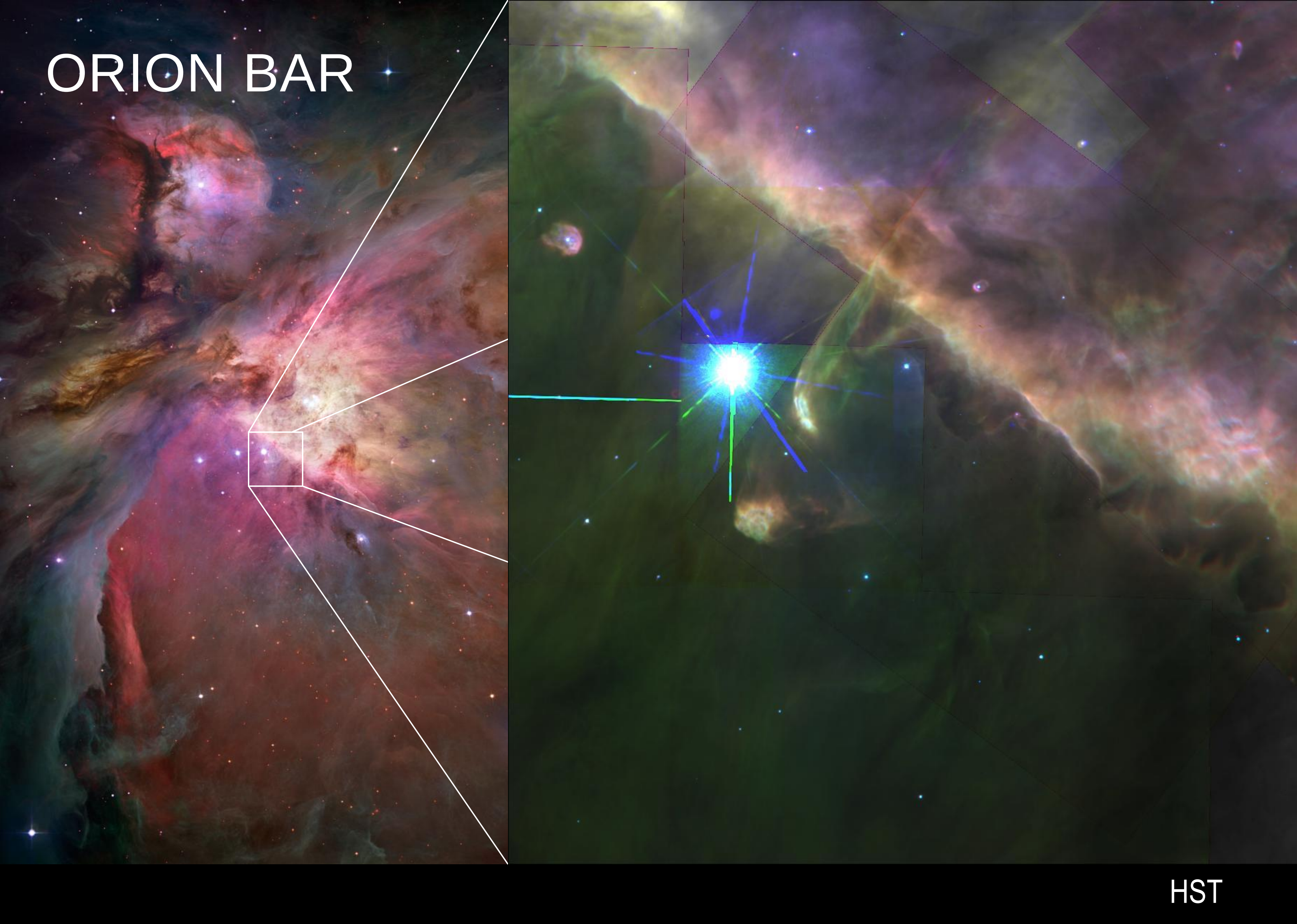
Duane Carbon	NAS NASA Ames Research Center
Joshua Choinsky	UAlbany Physics and Computer Science
Deniz Gencaga	UAlbany Physics (presently CCNY)
Haley Maunu	UAlbany Physics
Brian Nathan	UAlbany Physics (presently University of Texas Dallas)
ManKit Tse	UAlbany Physics

ORION

Photo Credit: Matthew Spinelli

ORION NEBULA

HST


ORION BAR
HST

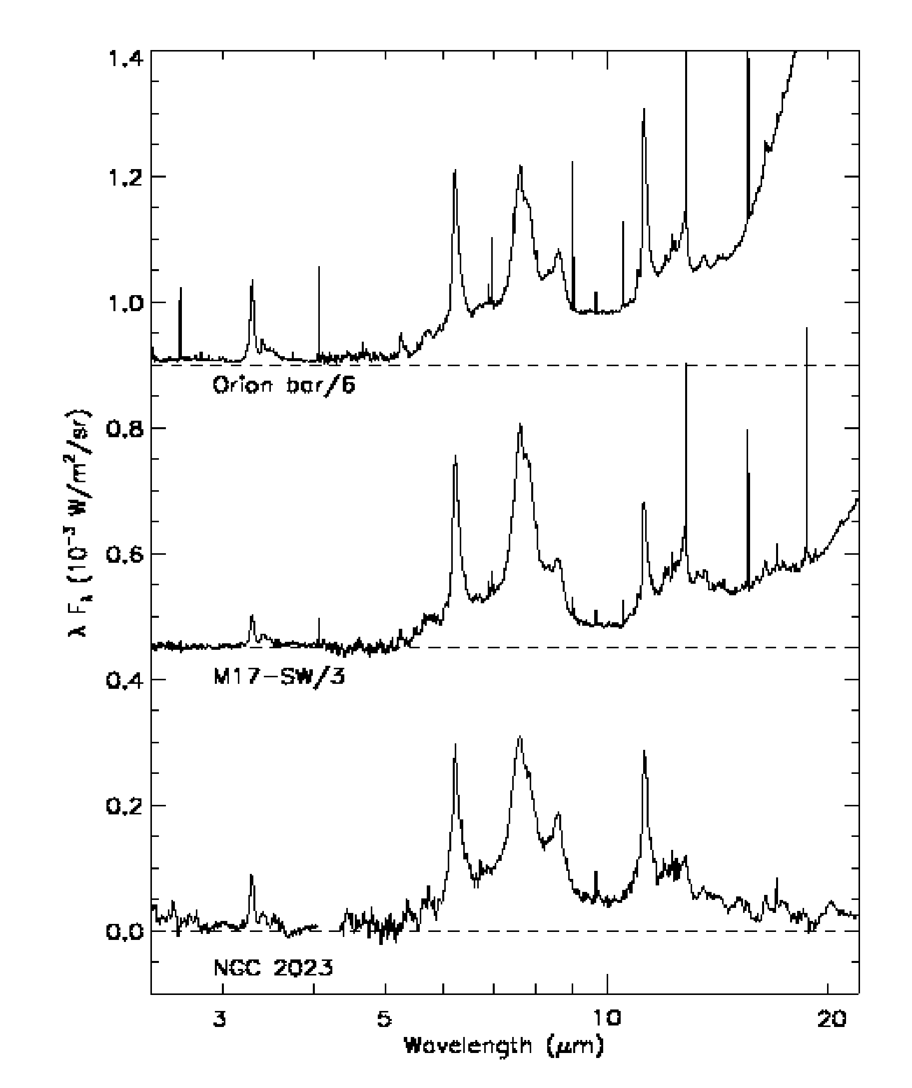
UNIDENTIFIED INFRA-RED EMISSION

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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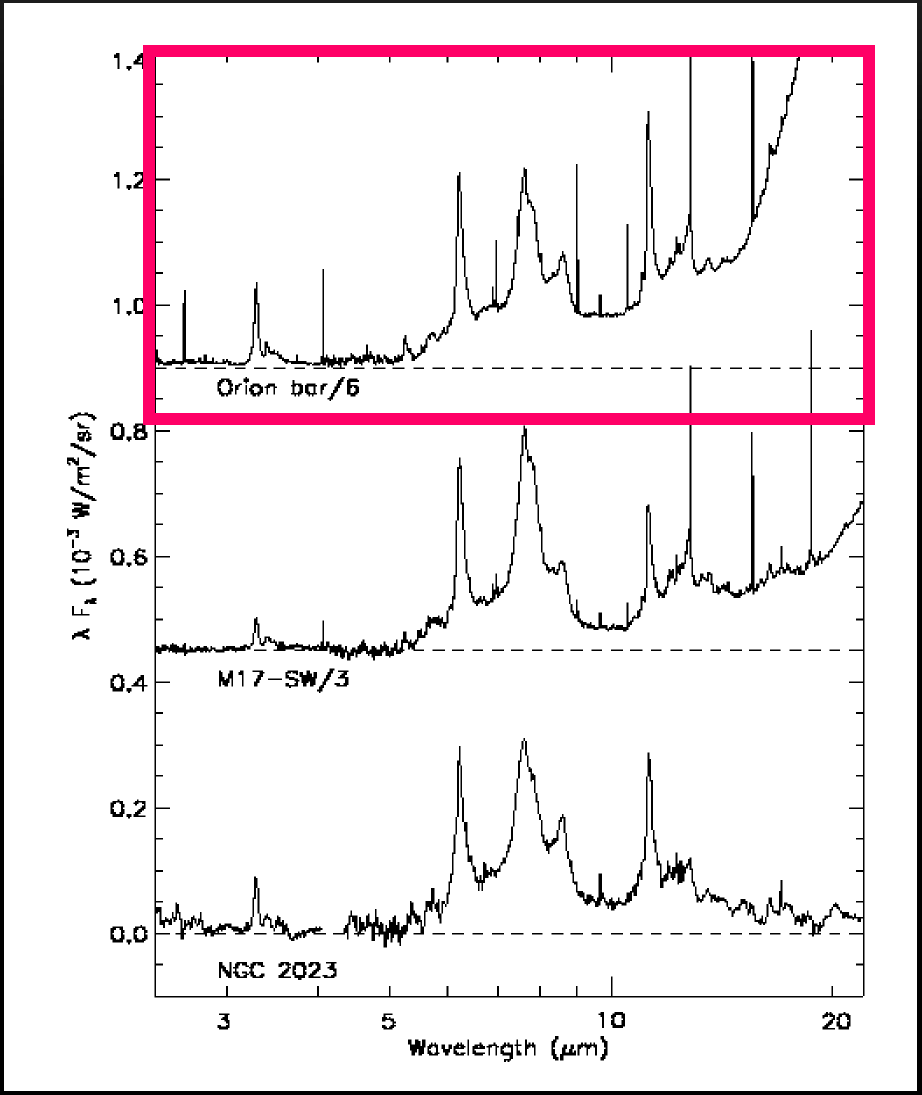

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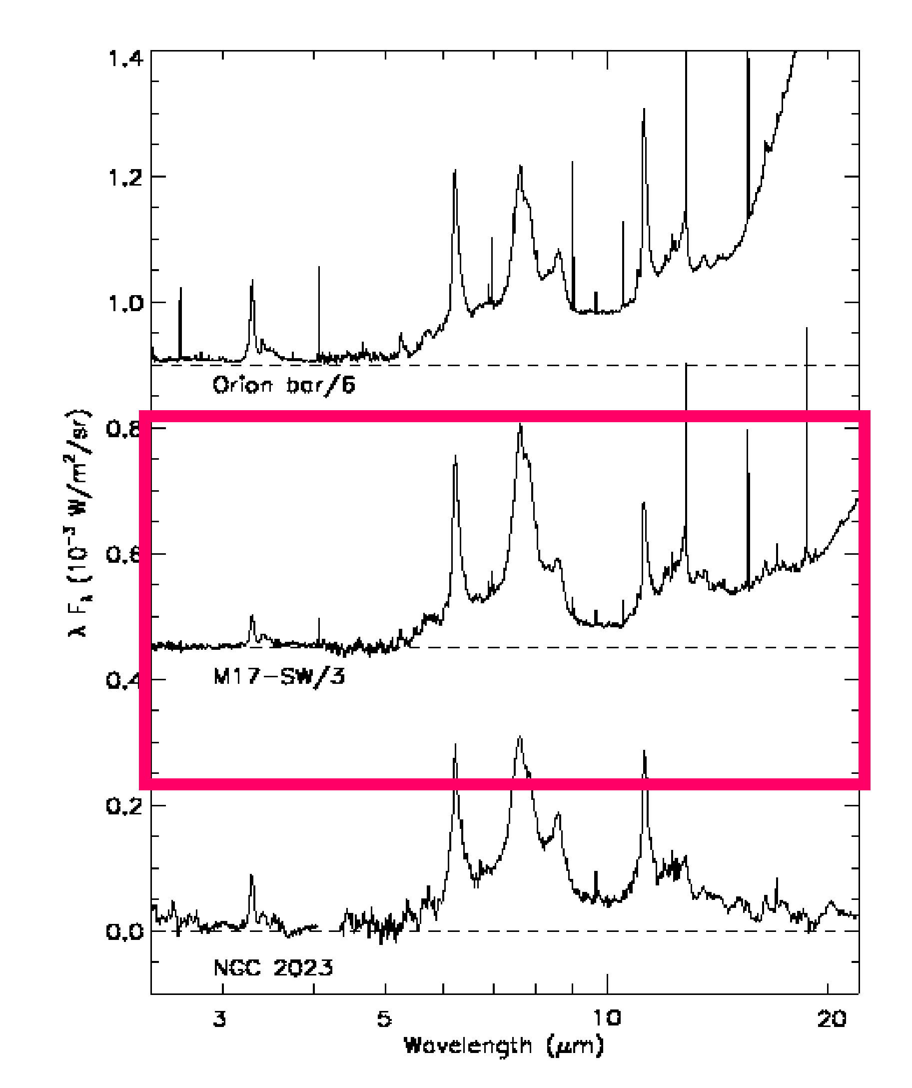
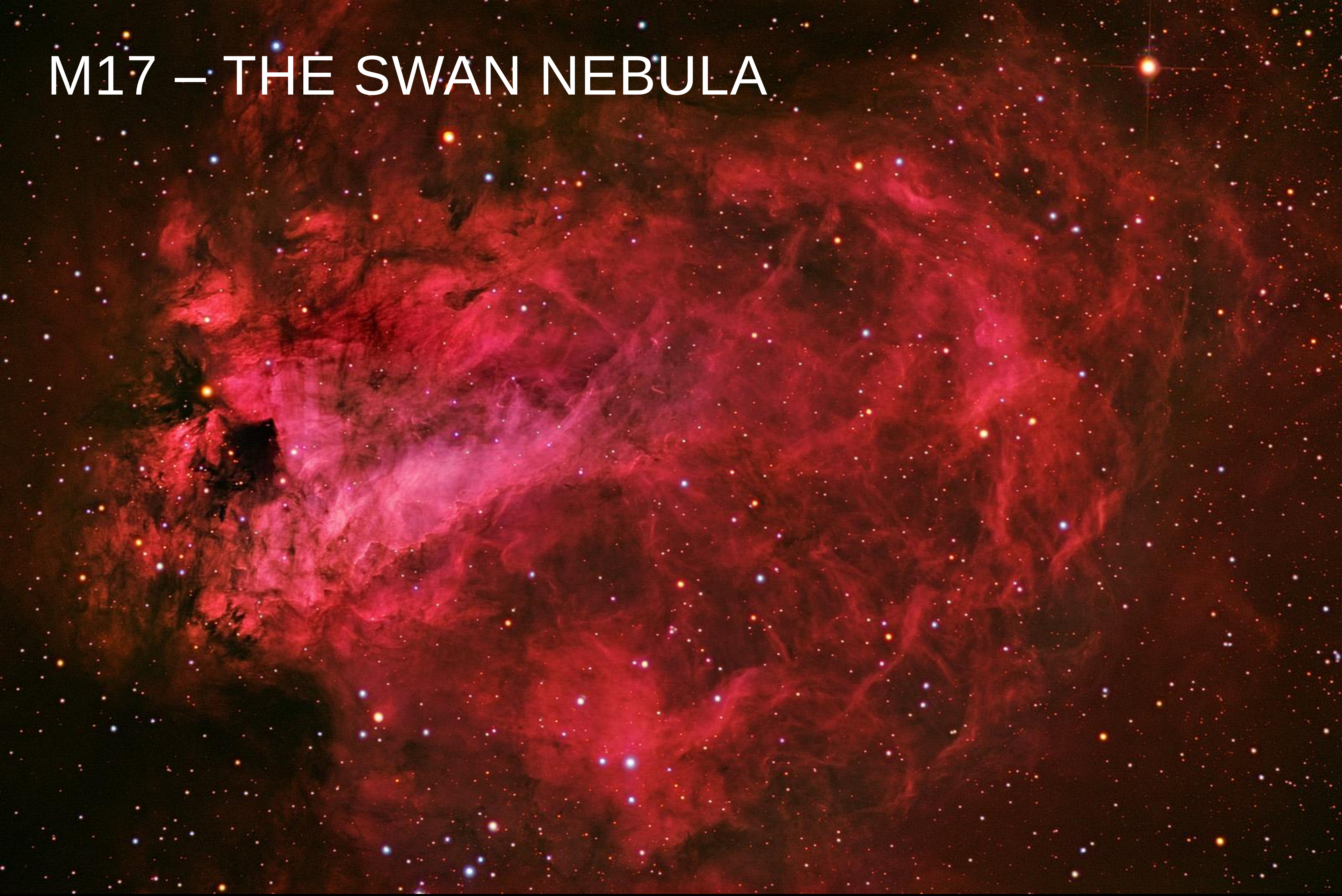


M17 – THE SWAN NEBULA



Bernd Flach-Wilken and Volker Wendel

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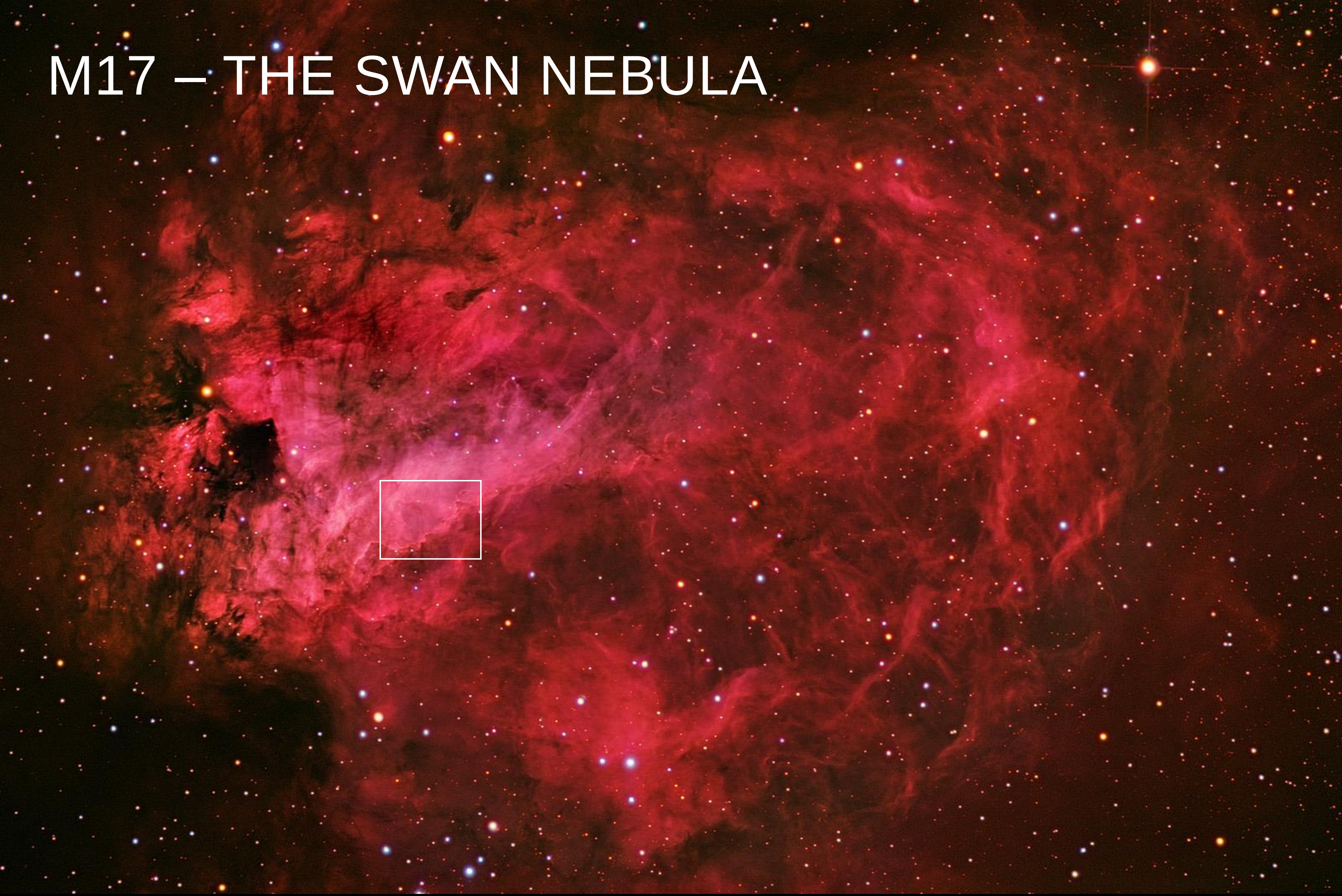

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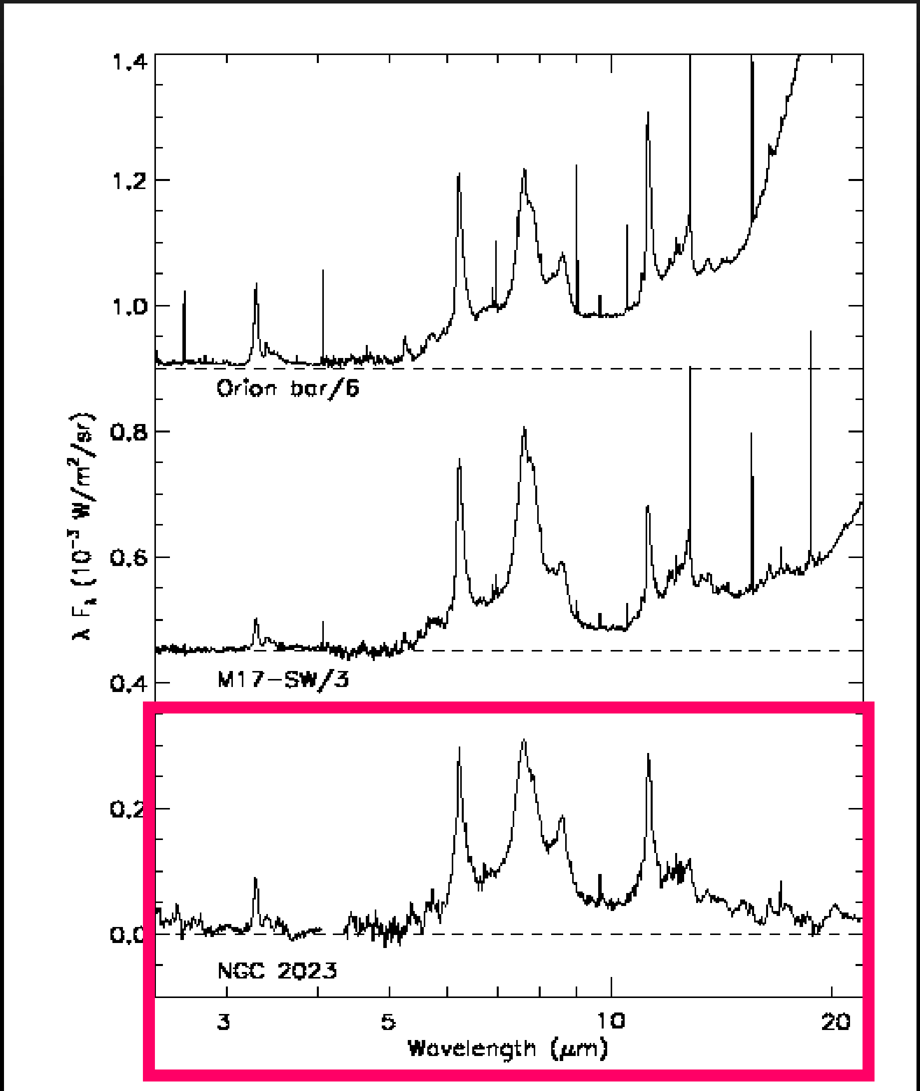
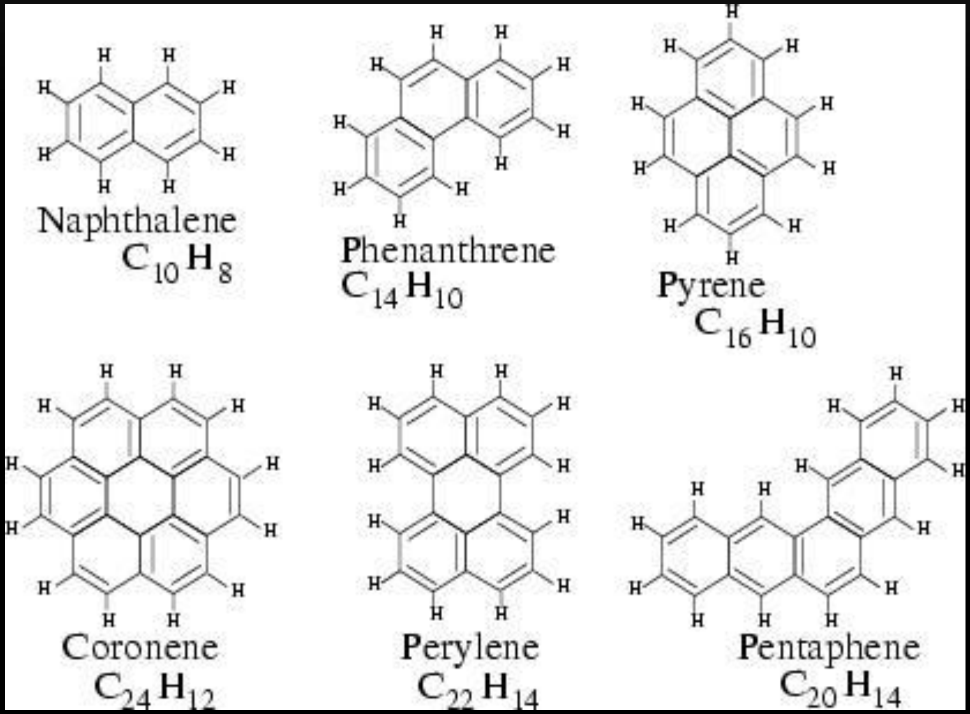


Russell Croman

PAHS: SOURCES OF UIR EMISSIONS

Polycyclic Aromatic Hydrocarbons



Molecular bands near correct wavelengths

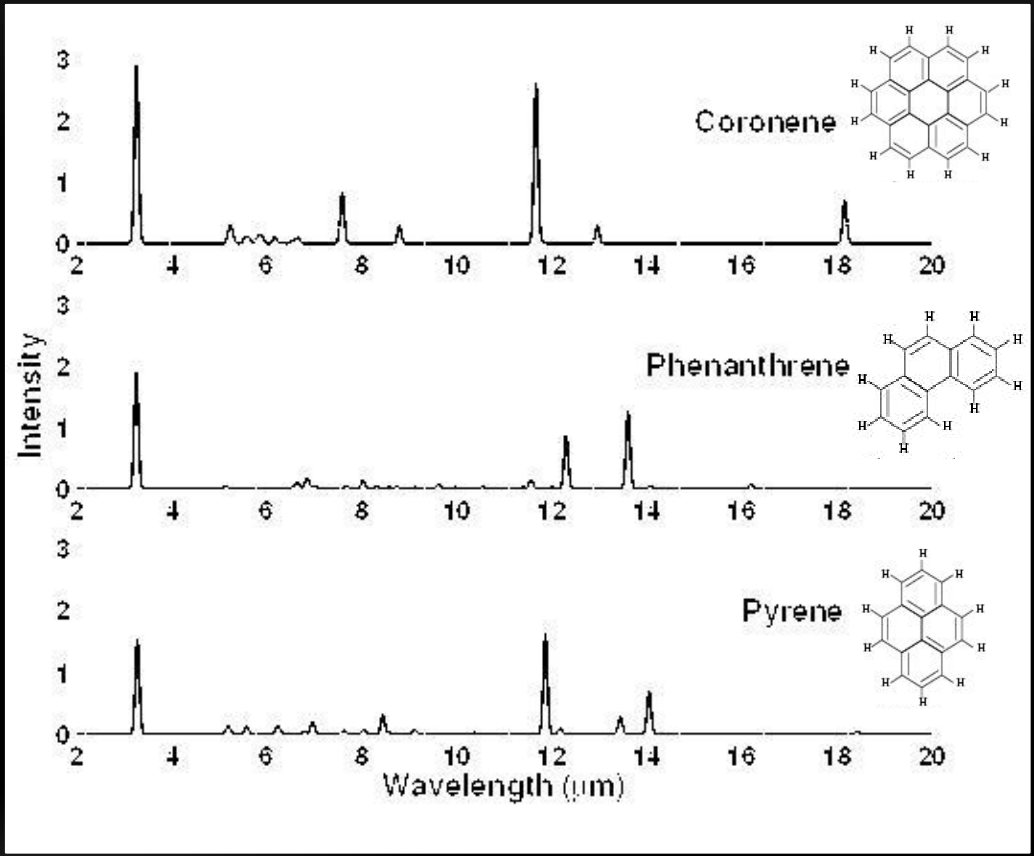
Reasonable physical model for UV-driven IR emission

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

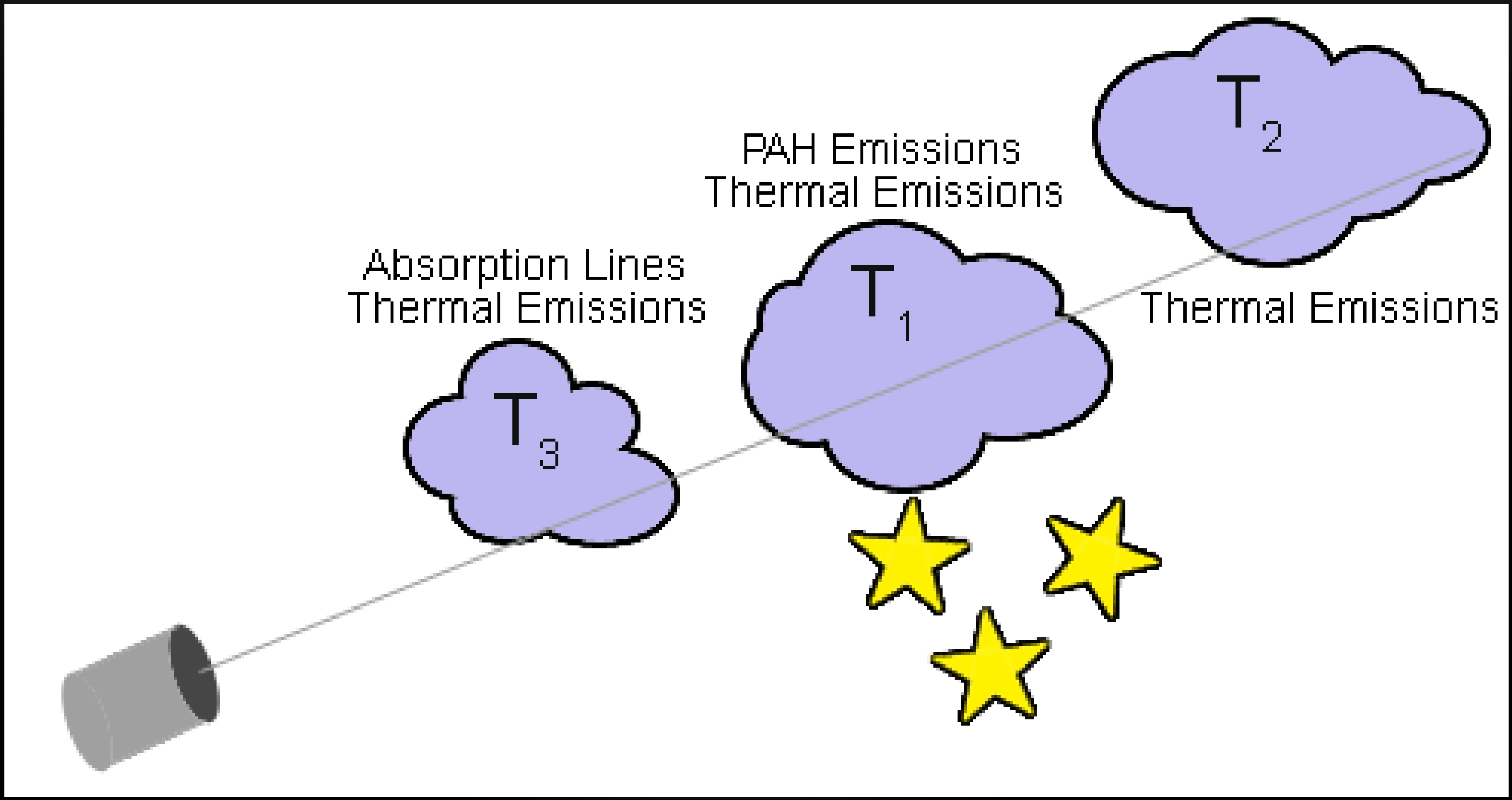
PAH IDENTIFICATION PROBLEM

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

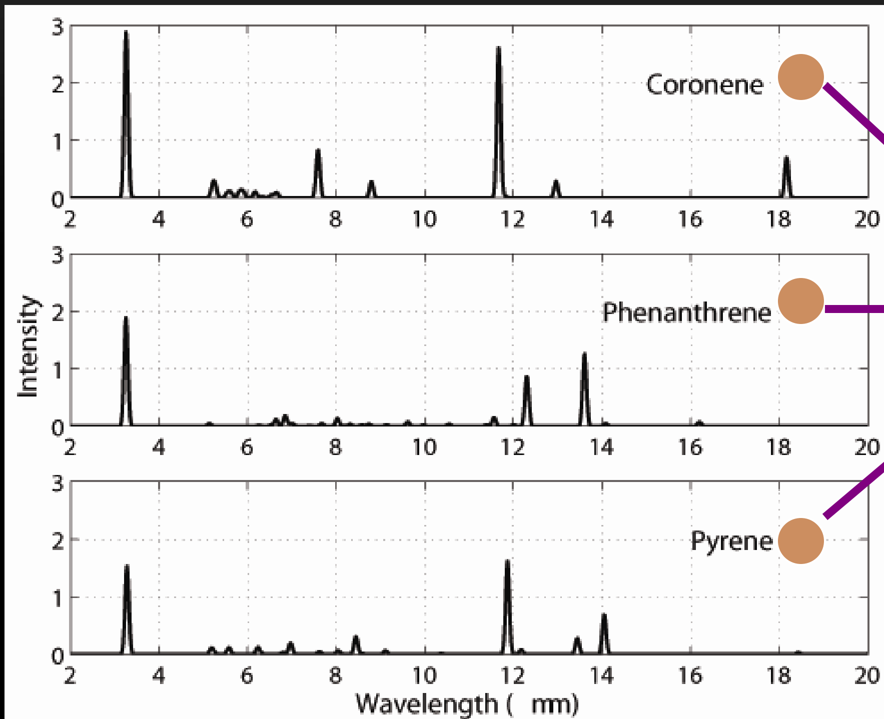
Astrophysical sources appear to have:

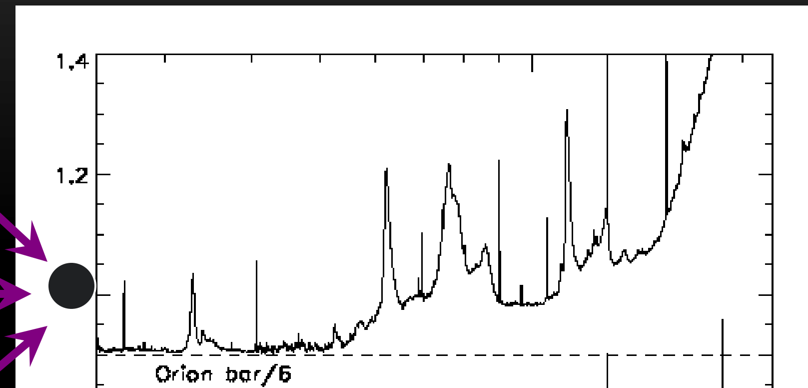
- multiple PAH species present
- different PAH-species concentrations depending on:
  - UV-intensity, temperature, and composition

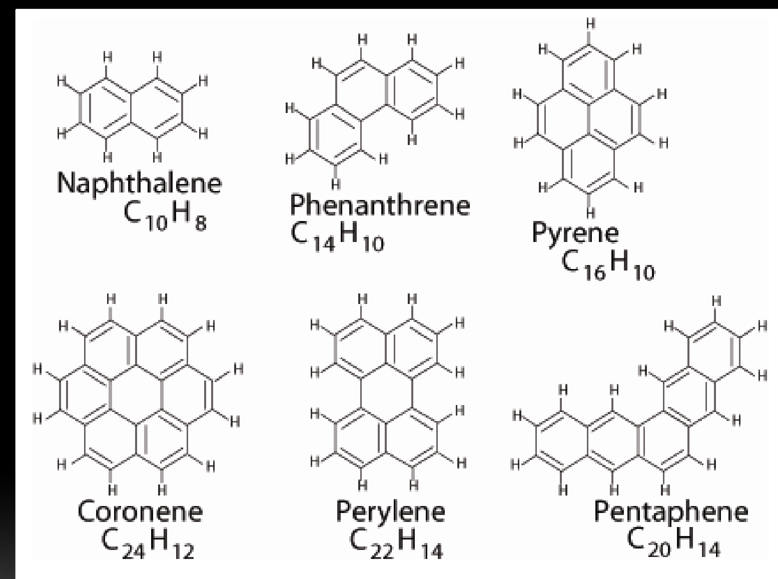
COMPLEX SPECTRA



NUMEROUS PAH SPECIES







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

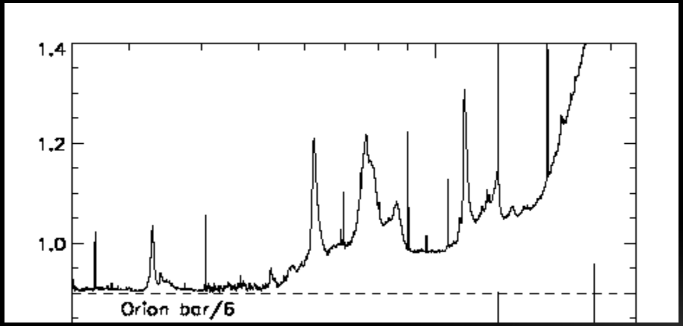
MODELING IMPORTANT FEATURES

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

PAH contributions

c_p – *PAH concentration*

δ_p – *PAH presence (YES or NO)*



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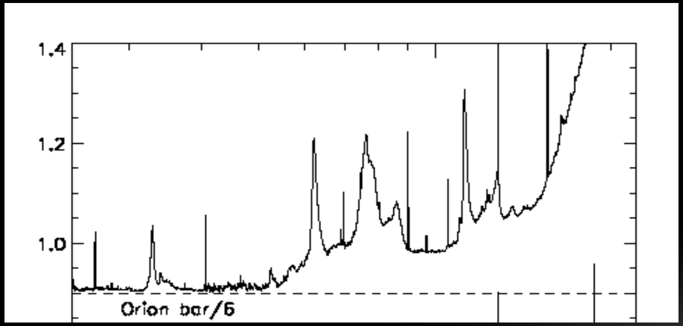
Planck Blackbody Radiators

A_k – *Planck Amplitude*

T_p – *Planck Temperature*



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

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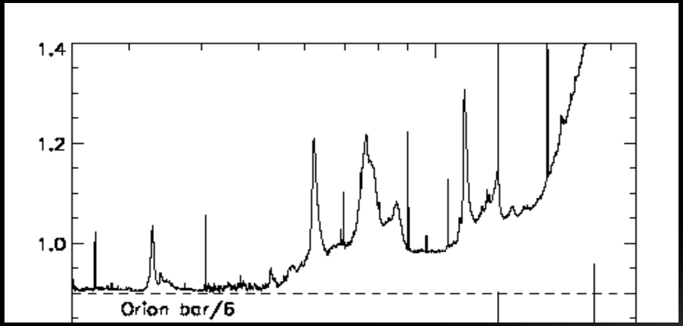
Mixture of Gaussians

A_g – *Gaussian Amplitude*

– *Gaussian Mean*

– *Gaussian Mean*



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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.

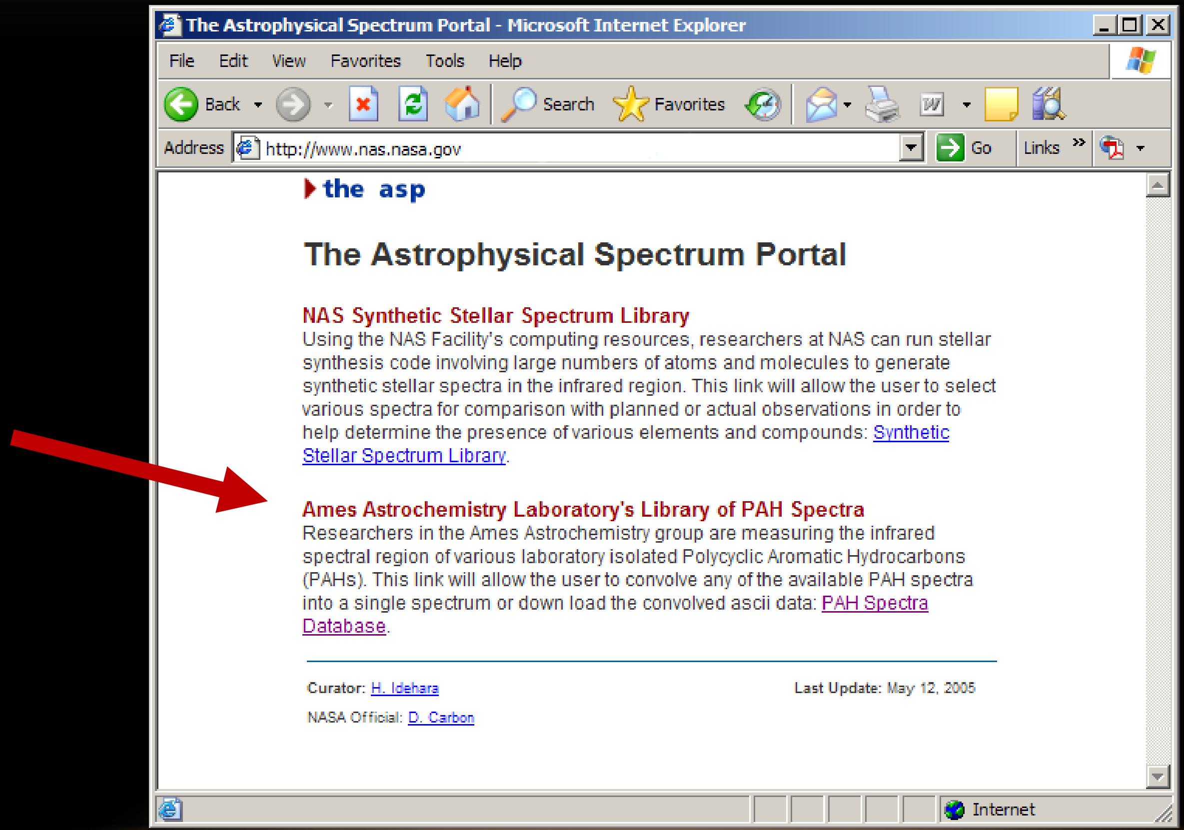
PAH spectral source separation consists of one mixture and numerous known sources with unknown contributions (and even some unknown sources).

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



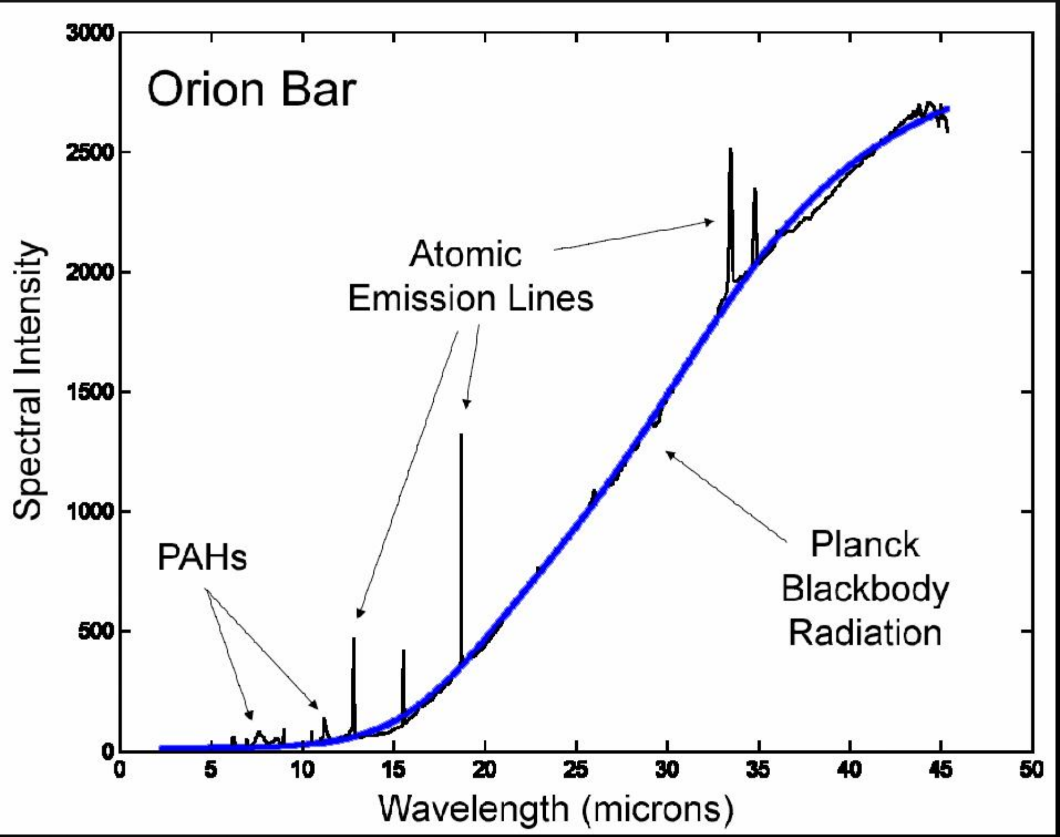
ESTIMATING PLANCK BLACKBODIES

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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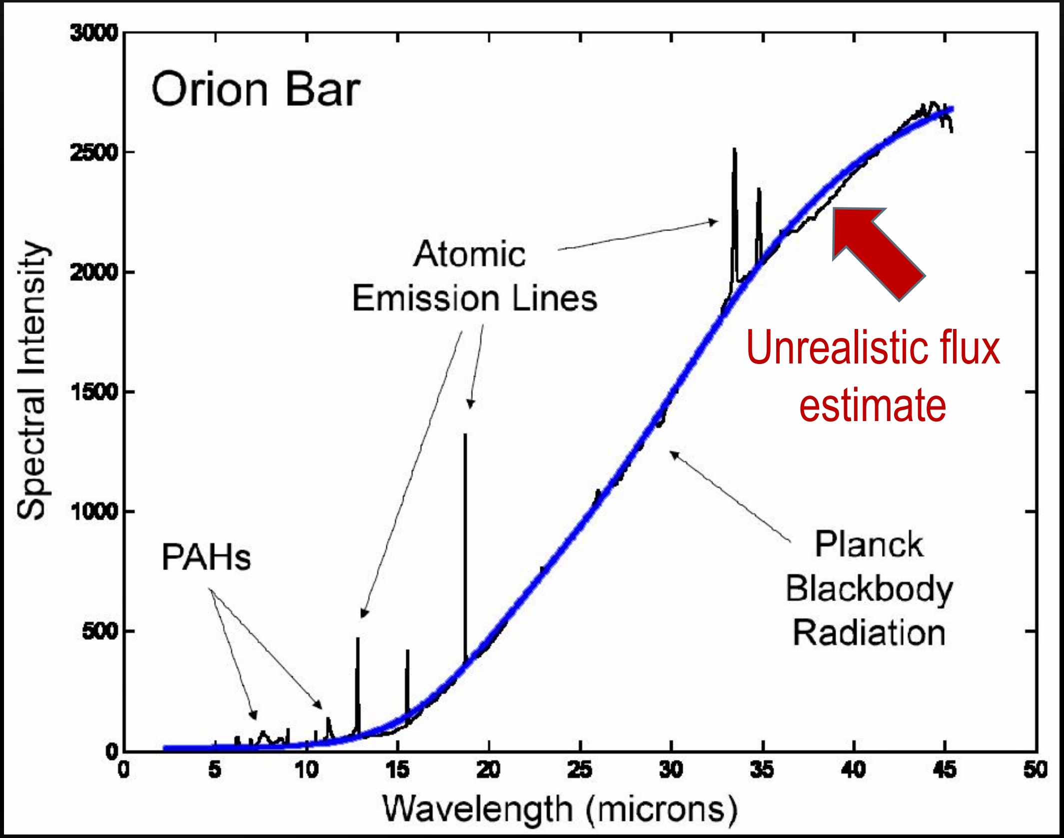
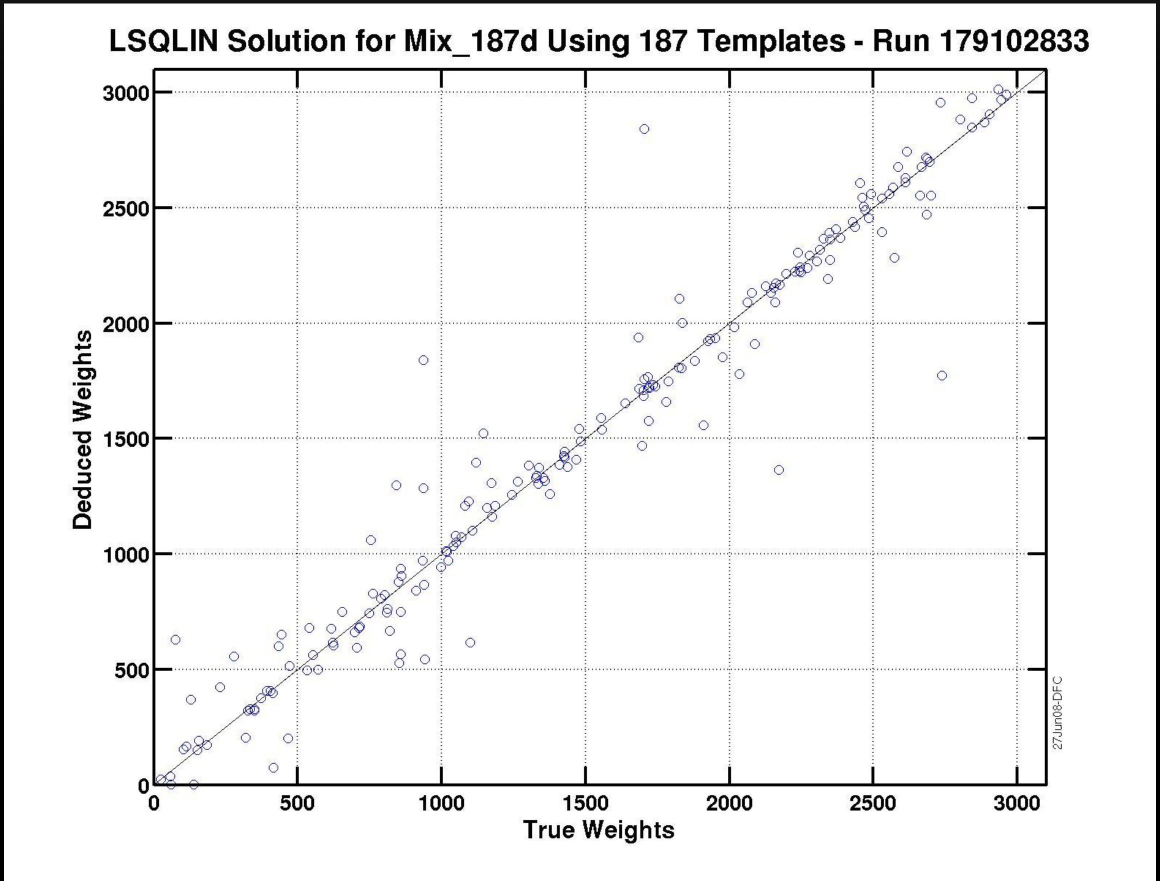


ESTIMATING PAHS

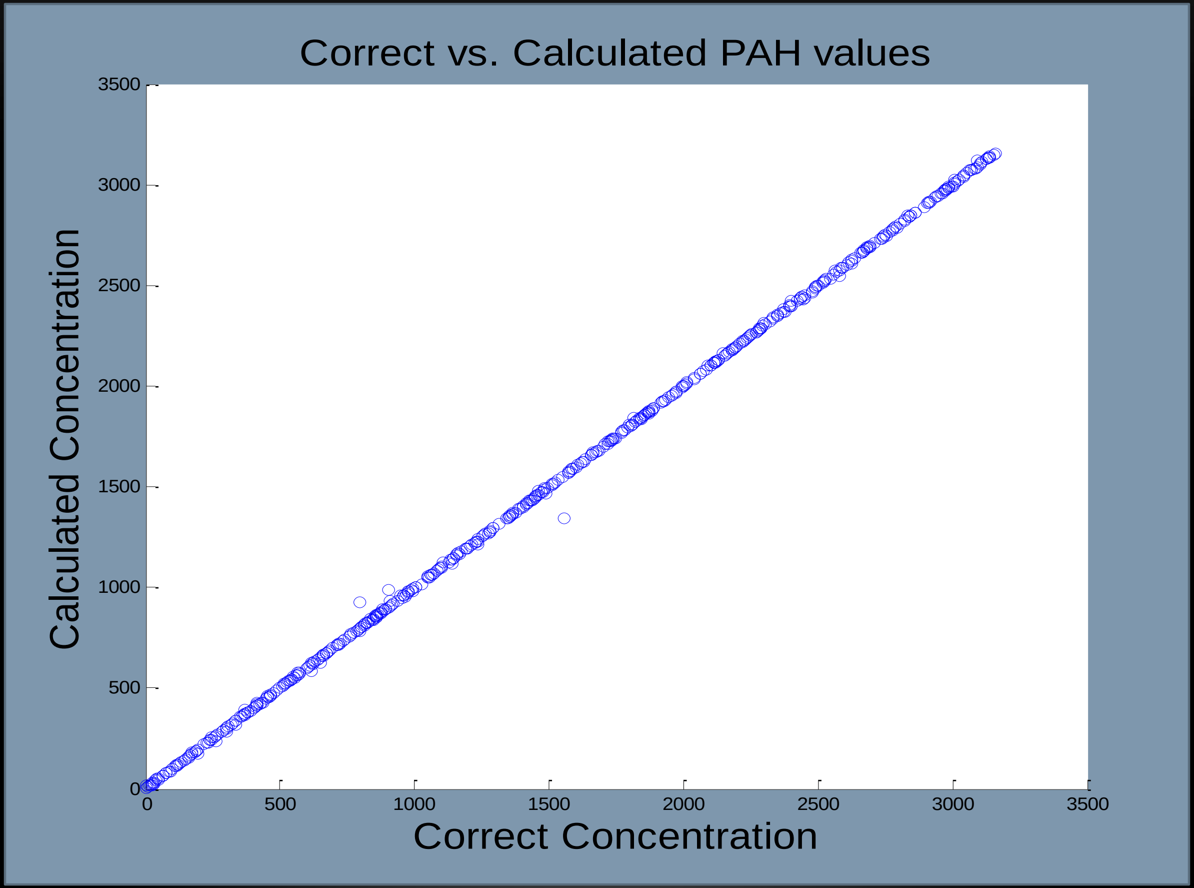
LINEAR LEAST SQUARES

187 PAHs in a synthetic mixture



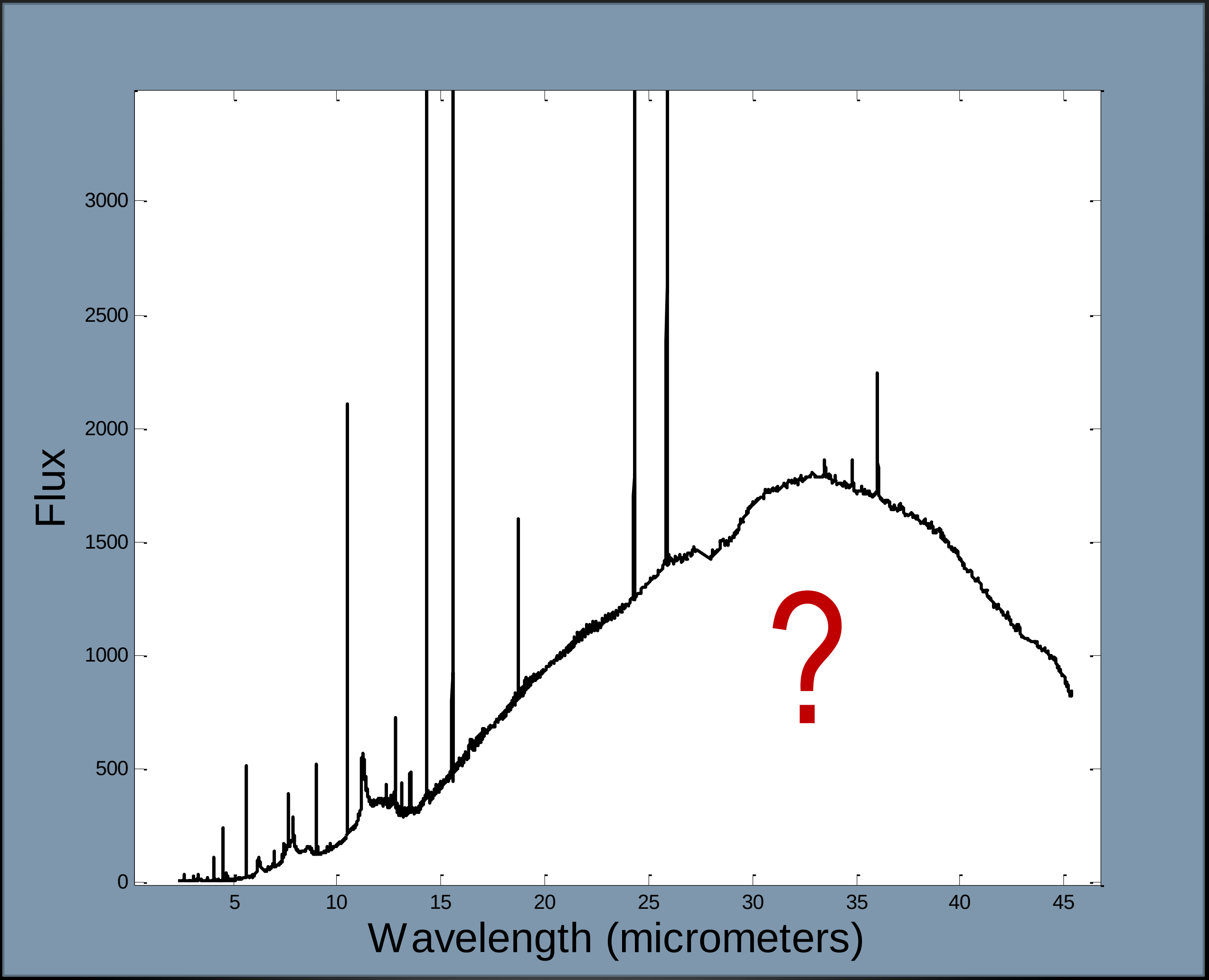
METROPOLIS HASTINGS MCMC

187 PAHs in a synthetic mixture

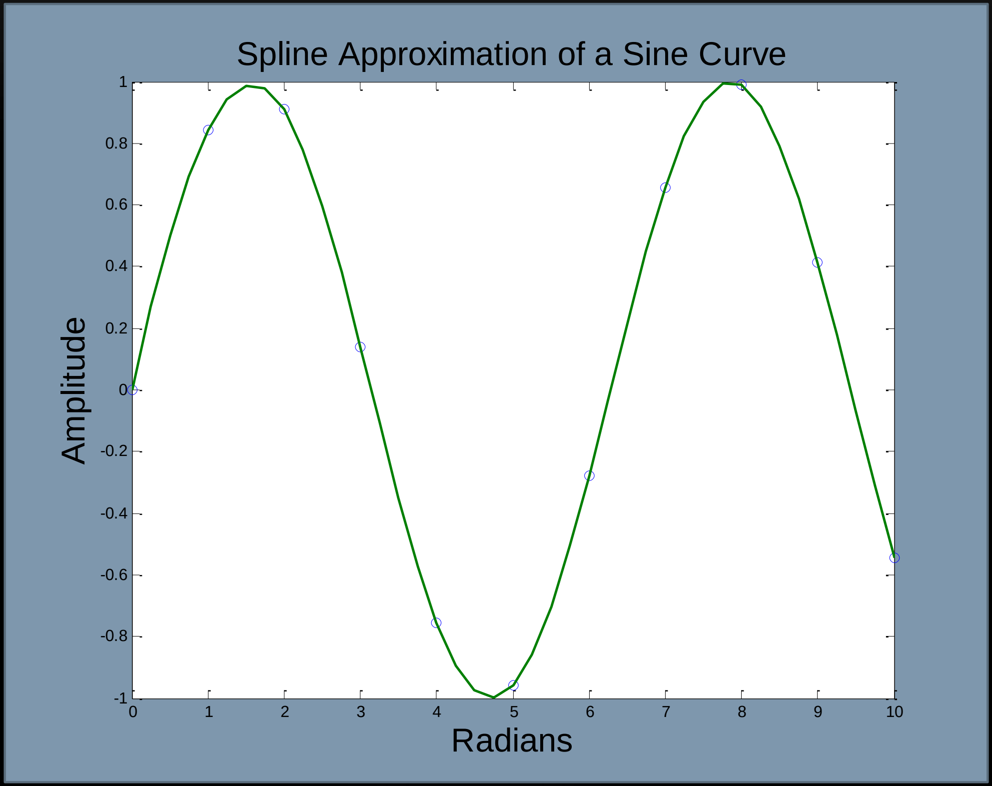


ESTIMATING BACKGROUND

WHAT TO DO WITH BACKGROUND?



SPLINE MODEL



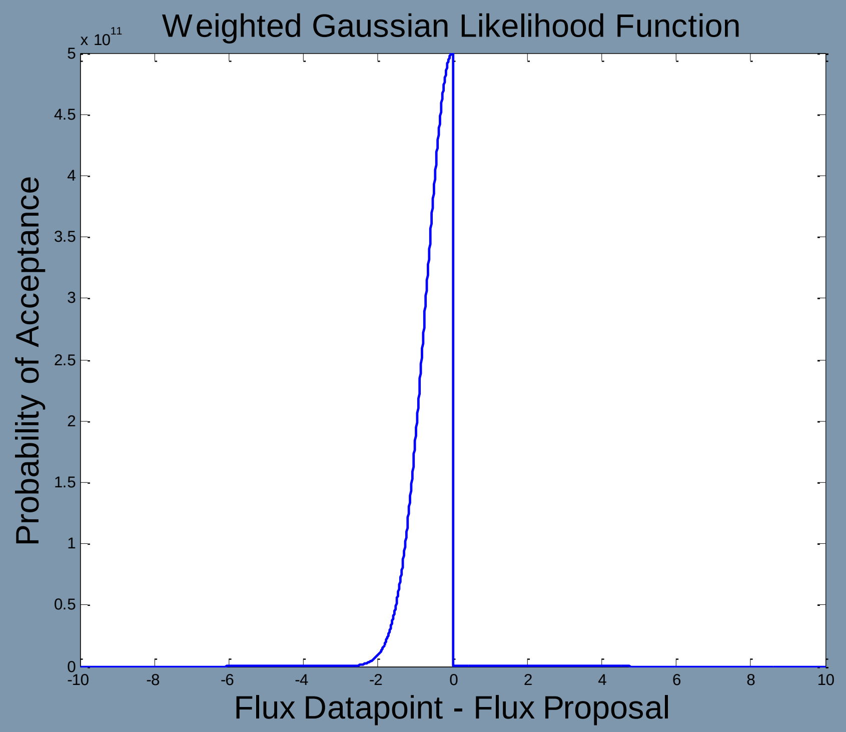
PIECEWISE GAUSSIAN LIKELIHOOD

$$\text{if } \; y_{pred} - y_{data} \leq 0$$

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

$$\text{if } \; y_{pred} - y_{data} > 0$$

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



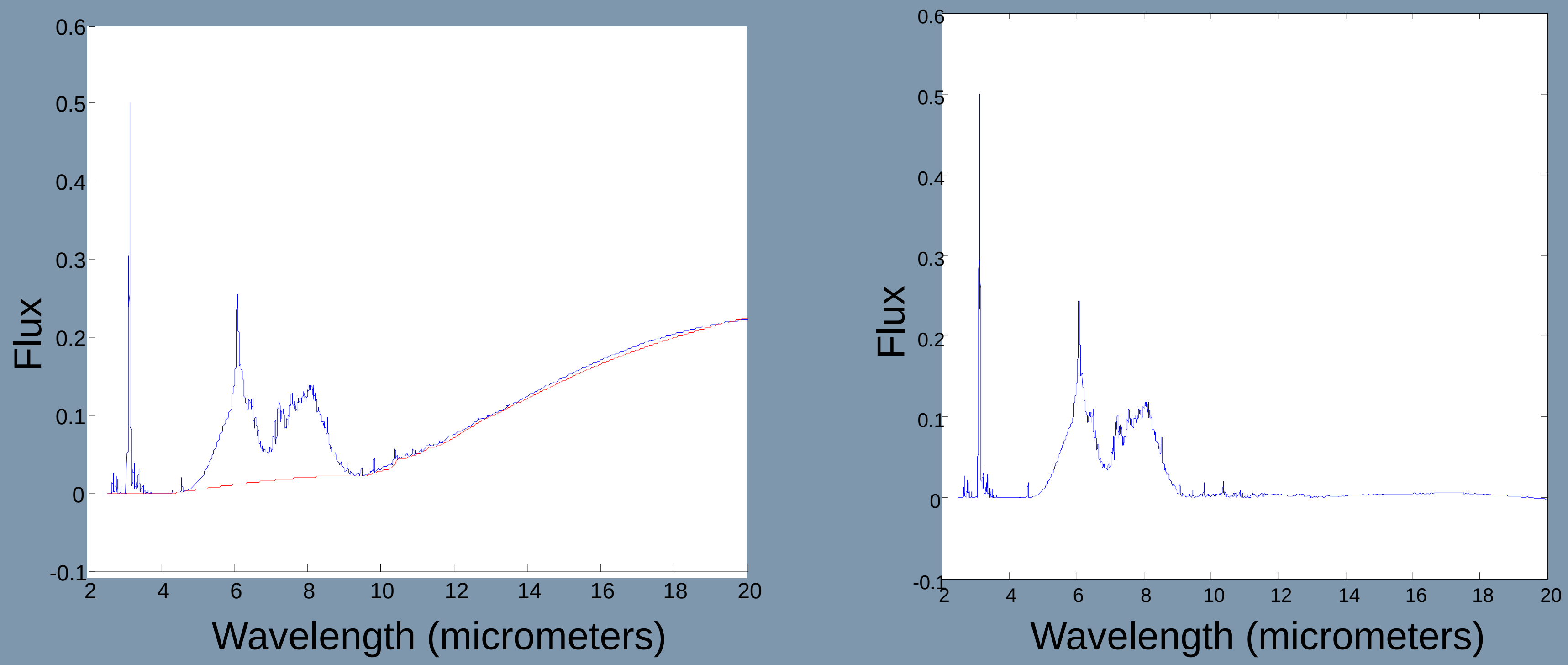
SMOOTHNESS PRIOR (OPTIONAL)

Gaussian Prior on the Integral of the Second Derivative

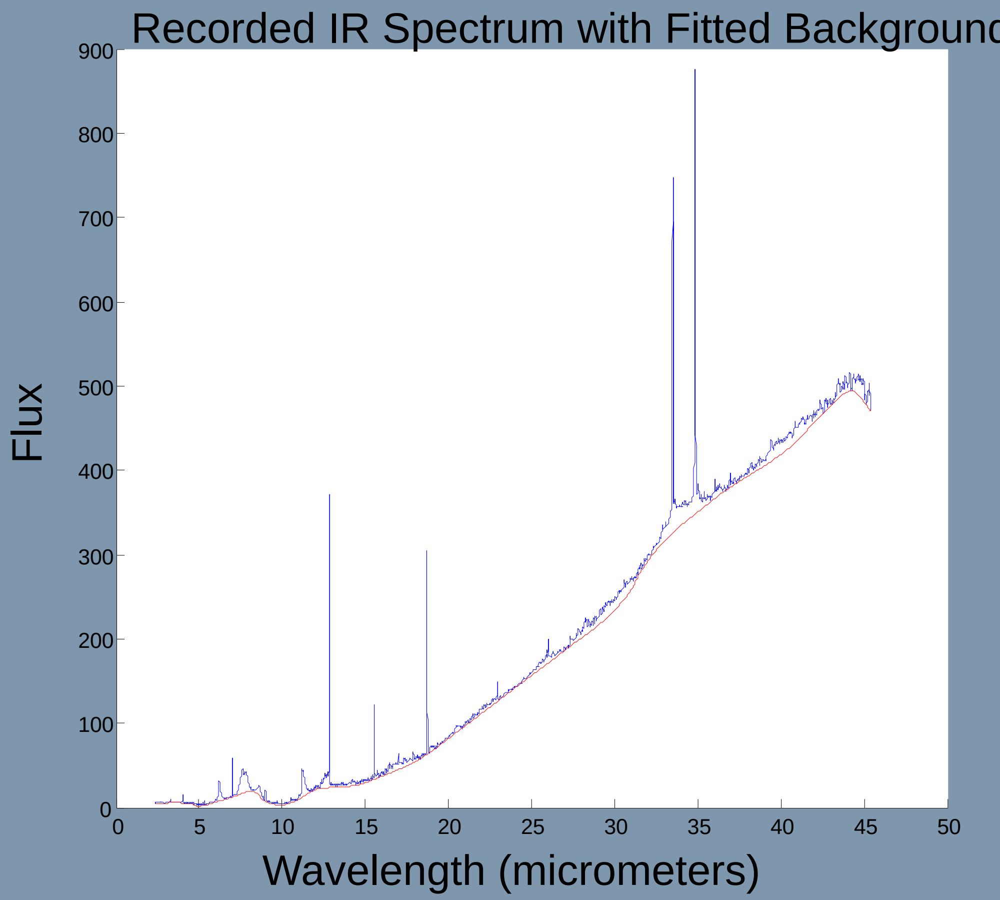
$$\text{Prior} \propto \exp\left(\frac{-(\int y''(\lambda)d\lambda)^2}{2\nu^2} \right)$$

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

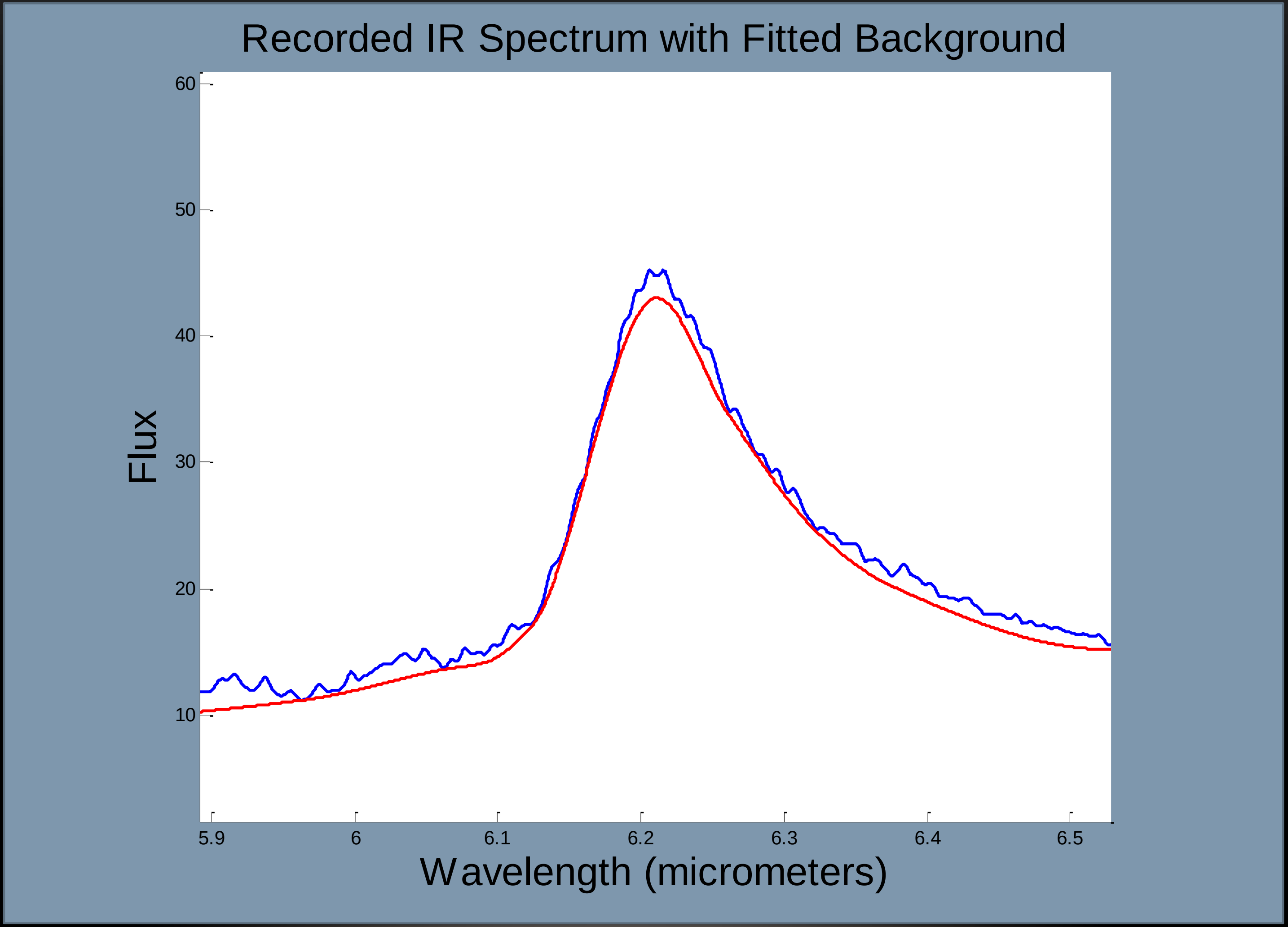
SYNTHETIC BACKGROUND REMOVAL



M82 STARBURST



PORTION OF THE ORION BAR



LIVE DEMO

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