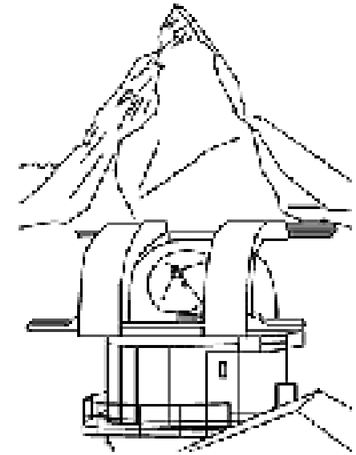
Les Houches

September 26, 2005



Observations and Molecular Spectroscopy

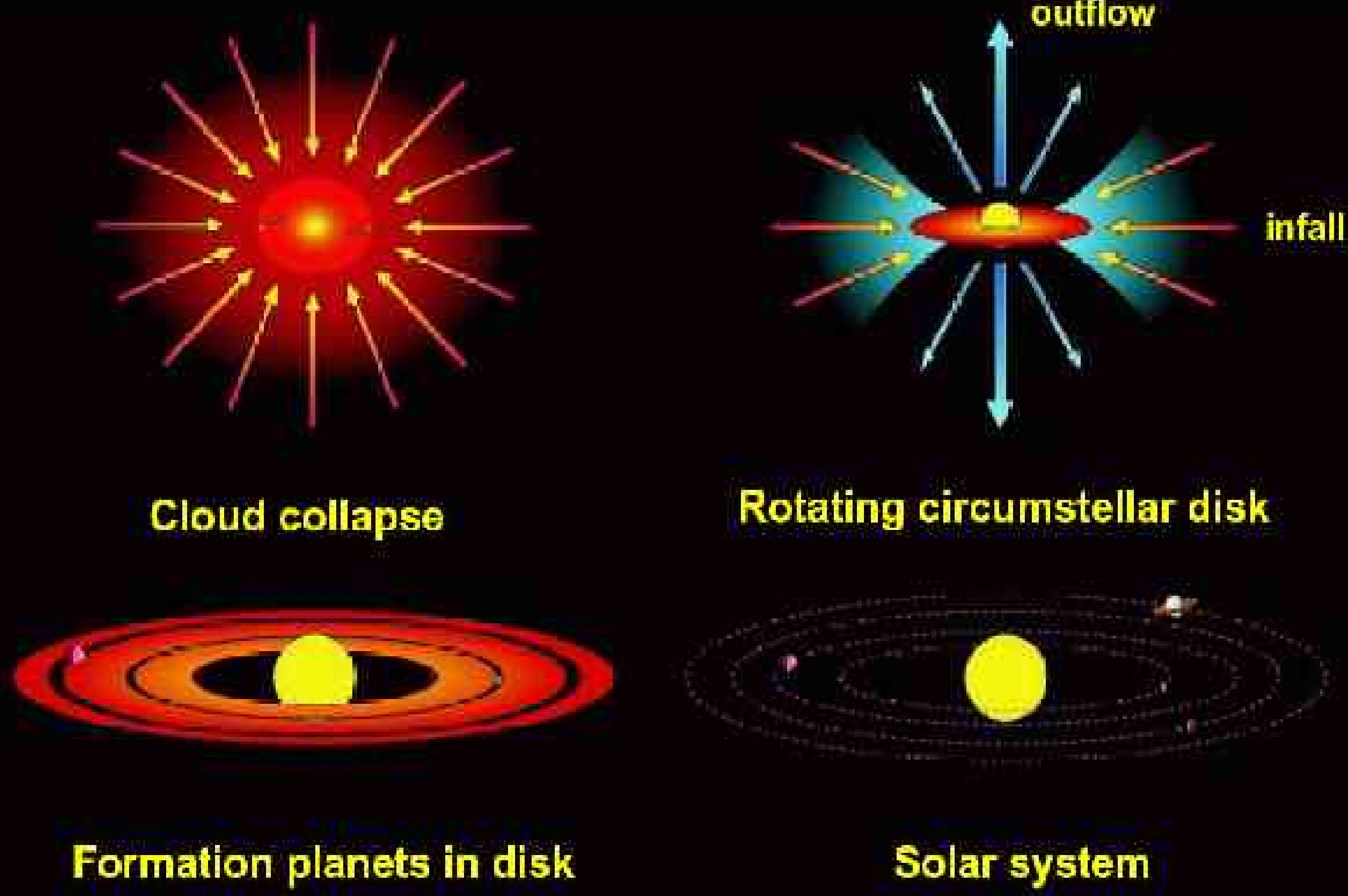
Stephan Schlemmer

WHAT? Observations and basic facts
Classification of spectral ranges

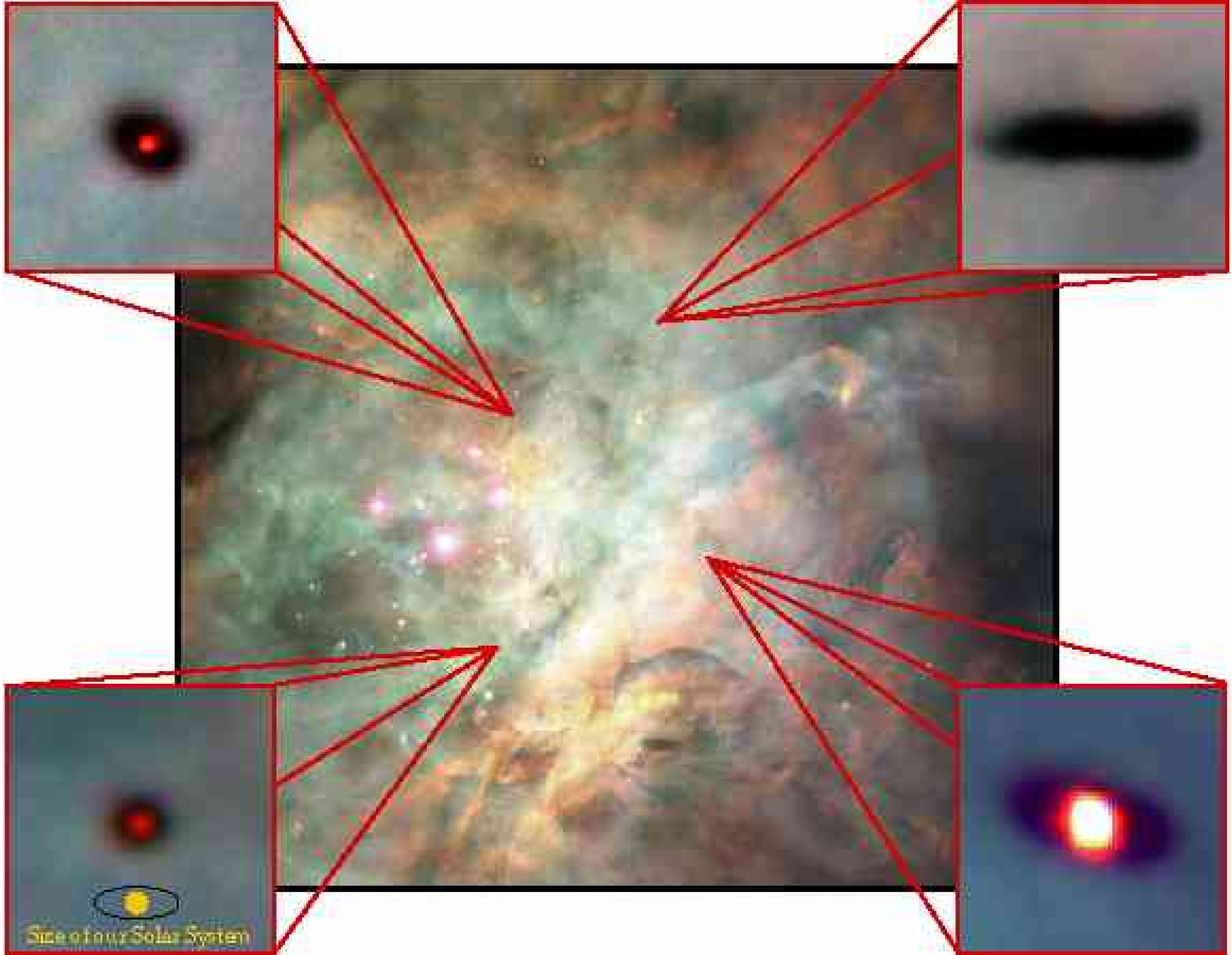
WHY? Identification of Species
Column Densities
Formation and Destruction?
De-/Excitation Mechanisms

HOW? Experimental Techniques (Laboratory work)

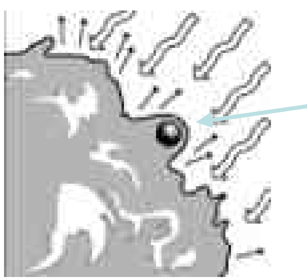
Scenario for star- and planet formation

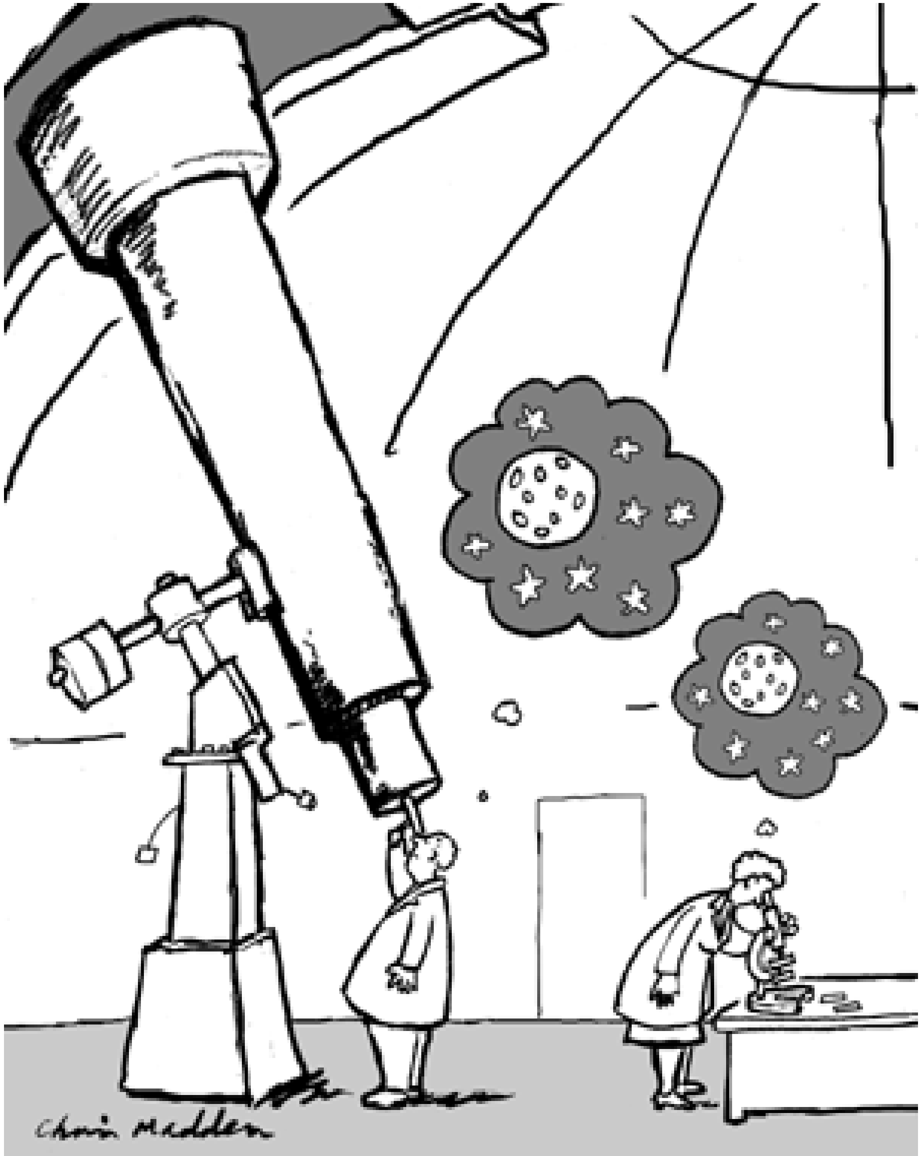


M. McCaughrean 2000


Size of our Solar System

Stellar Nursery in the Eagle Nebula



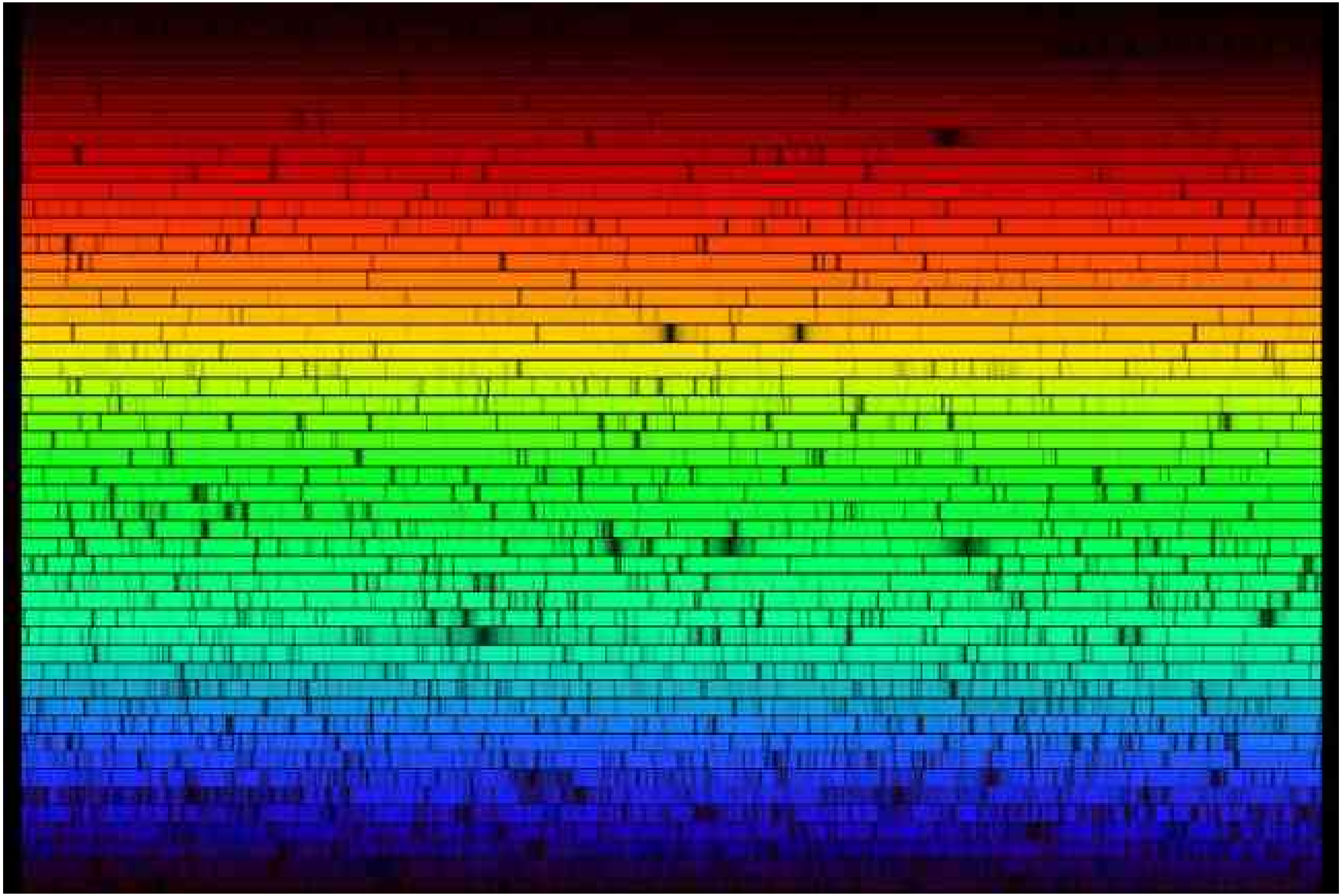


WHY spectroscopy?

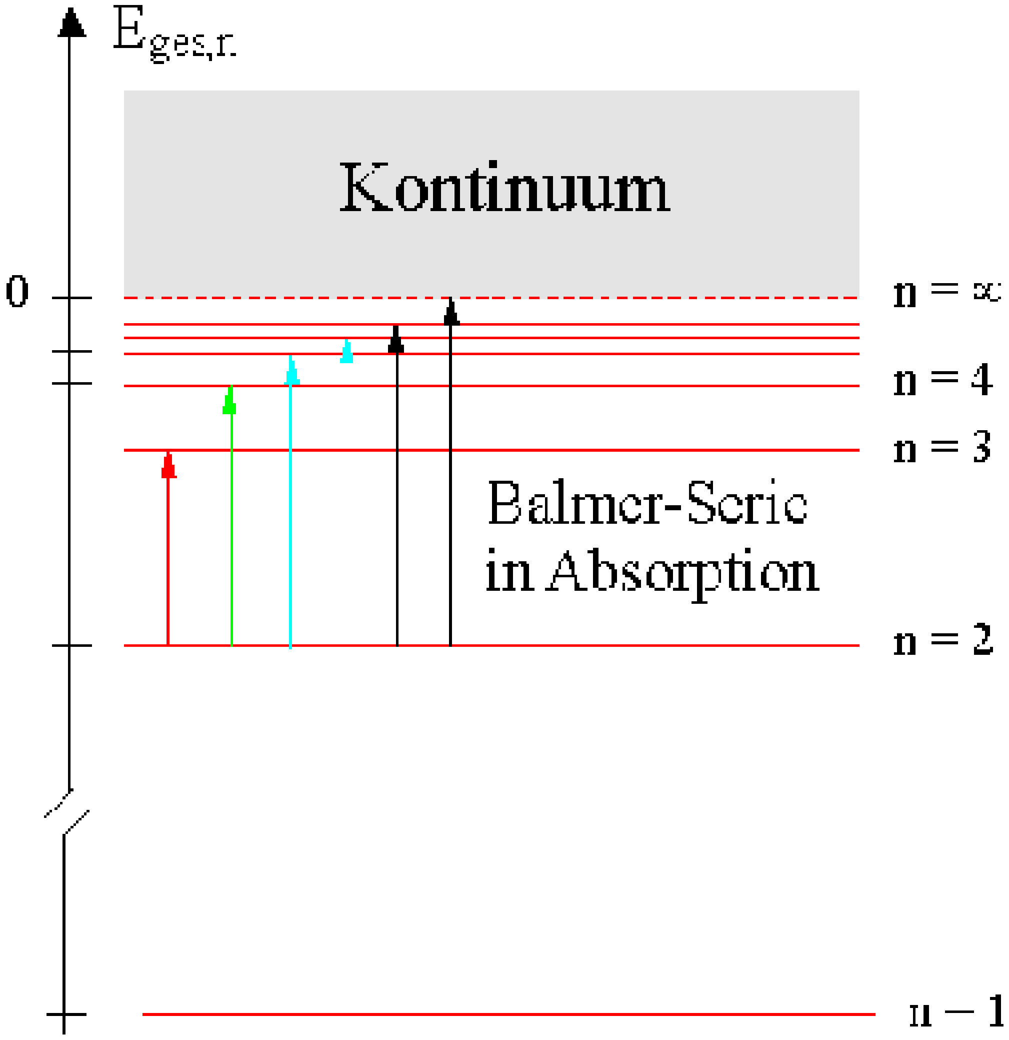
- ► Identification of species
- ► Abundances of species

Fraunhofer lines of the sun

Joseph von Fraunhofer katalogisierte 1815 mehr als 500 dunkle Linie



Fraunhofer lines of the sun

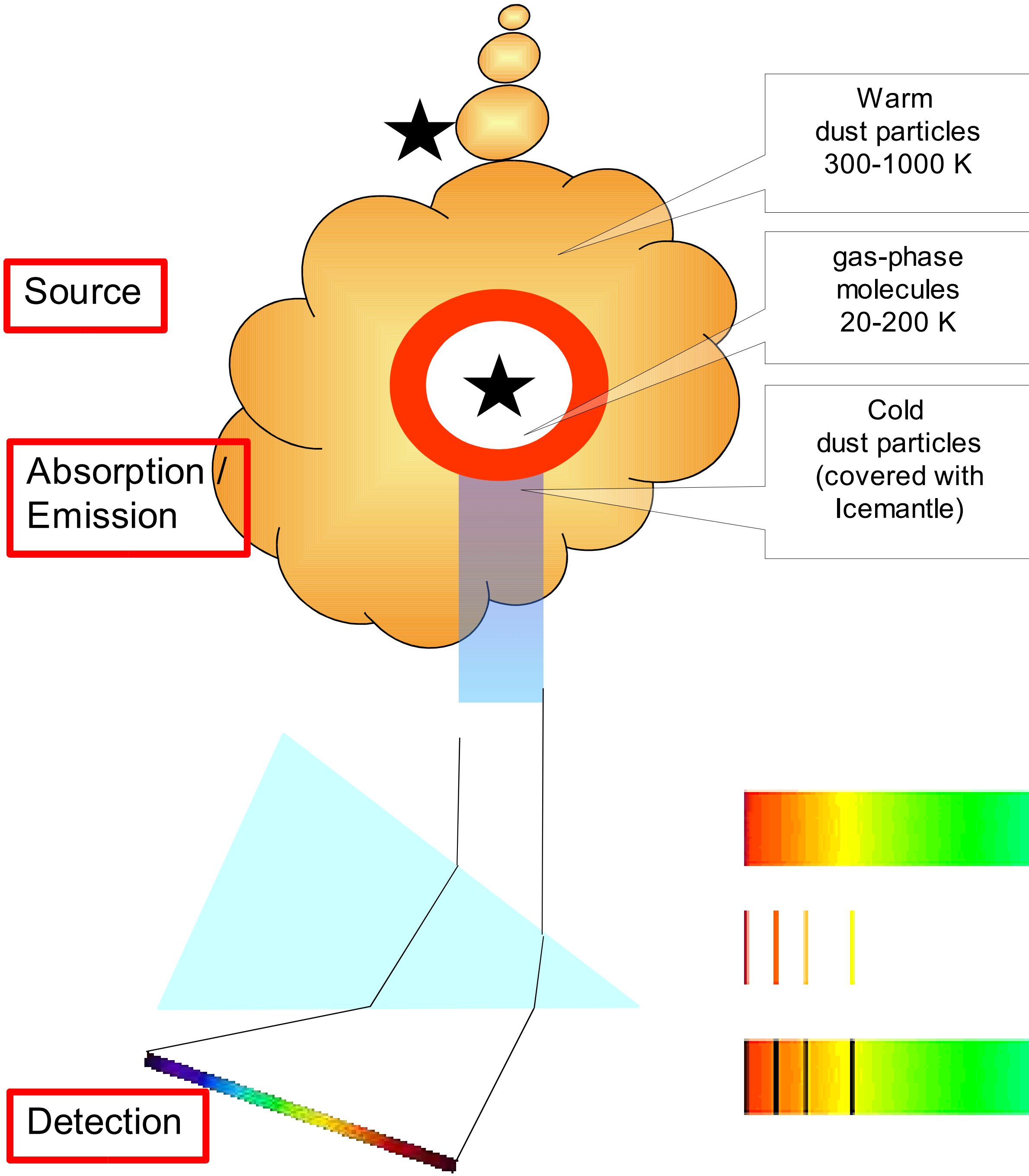


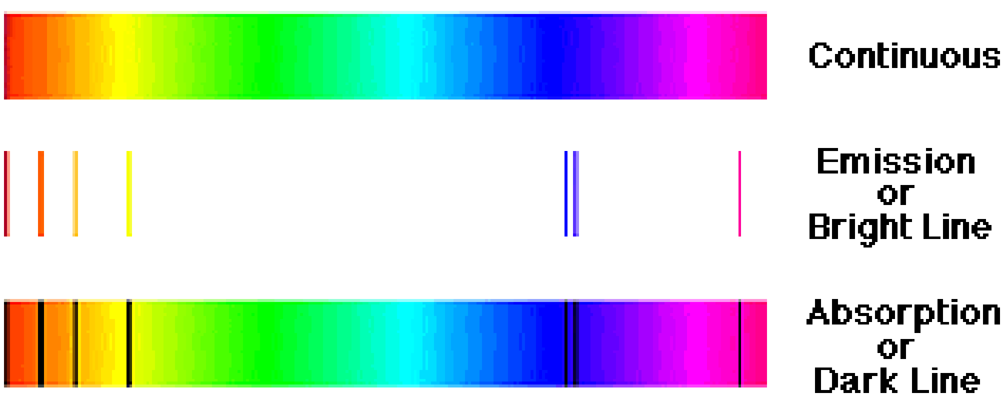
Kirchhoff

Bunsen

Need for Spectroscopy

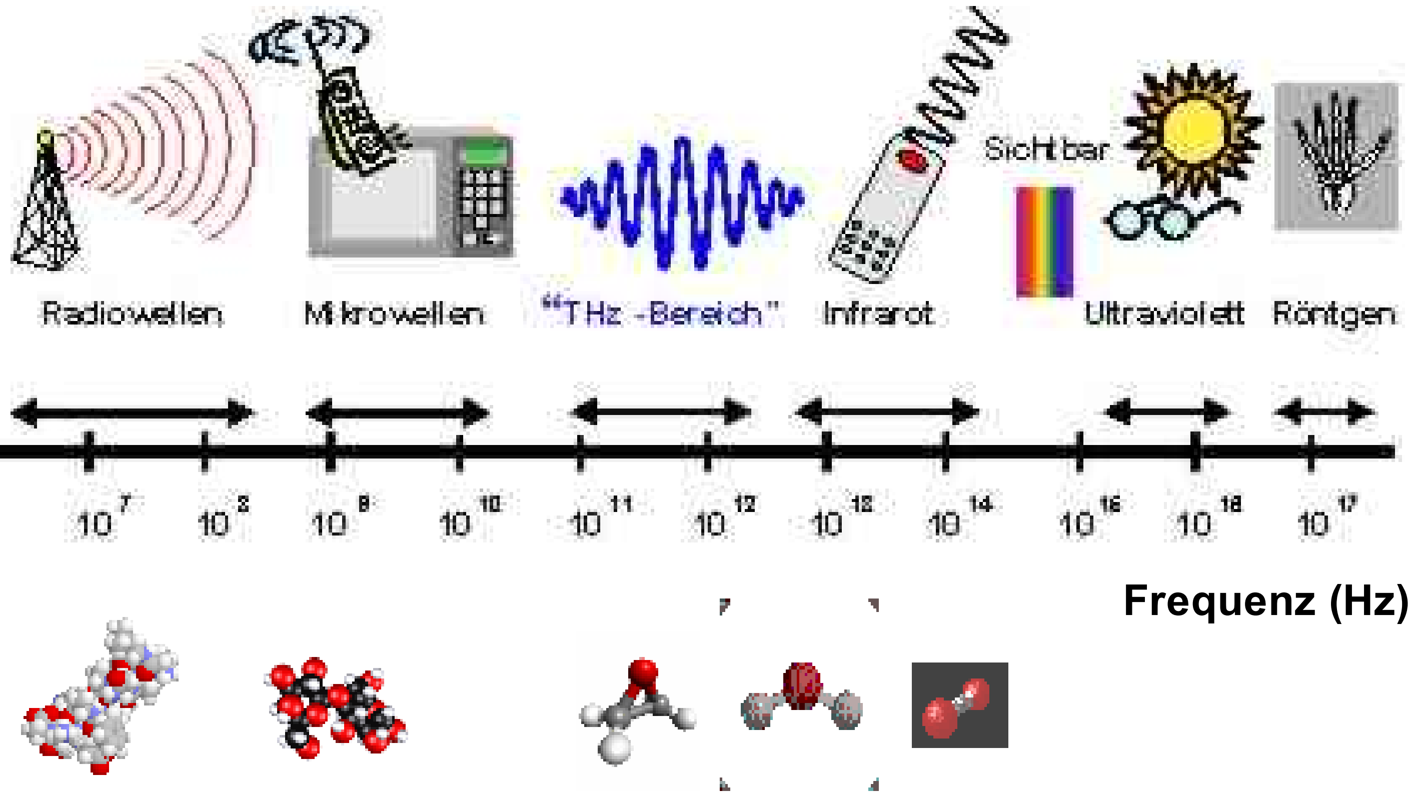
Bunsen & Kirchhoff
150 years ago





Idea for a laboratory experiment

Radiosources and their electromagnetic Spectrum



Radiosignals are very weak:

A Jansky is an intensity of 10^{-26} Watt/Meter^2 Hz

= 0,00000000000000000000000001W/m^2 Hz

100 m
dish
Effelsberg

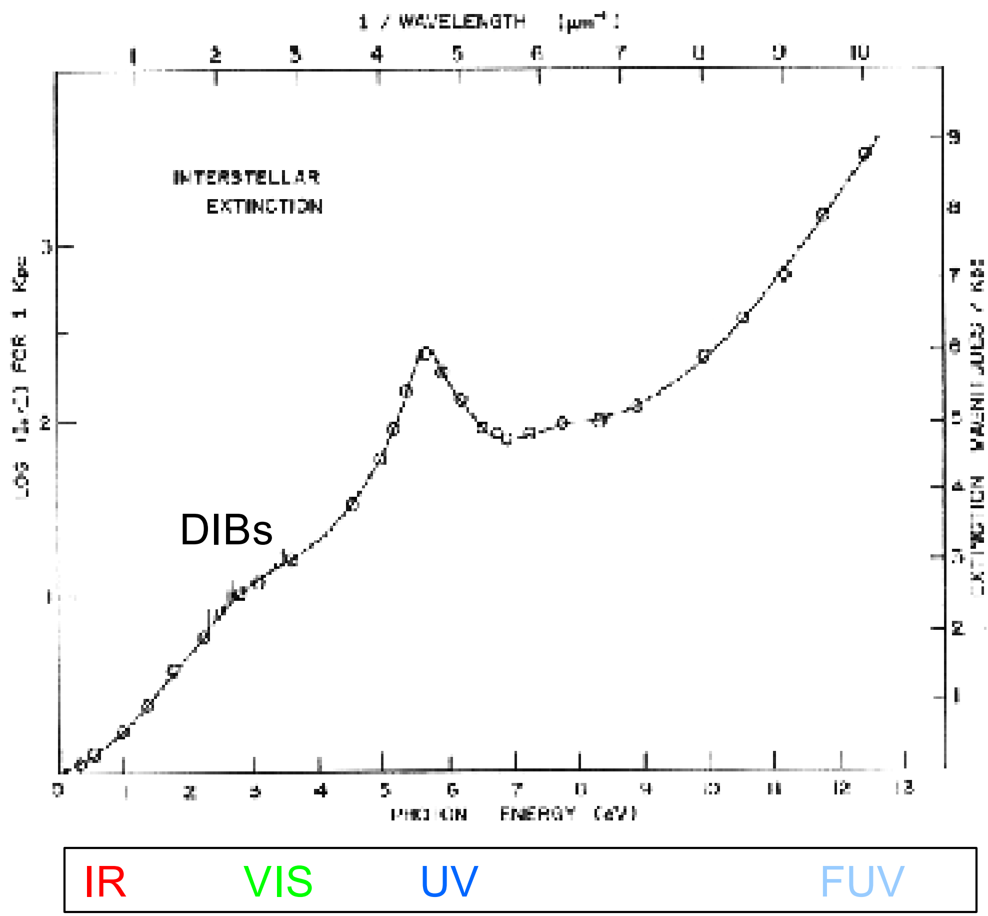
Interstellar Extinction

Extinction =
Absorption + Scattering

Spectral Overview

Average Interstellar Extinction

Extinction = Scattering + Absorption



<u>Optical Depth:</u> 1 kpc column of dust 0.2 μm homogeneous Solid

(1 kpc = 3 10^3 light years)

How do you know there is DUST?

Why are your backlights RED?

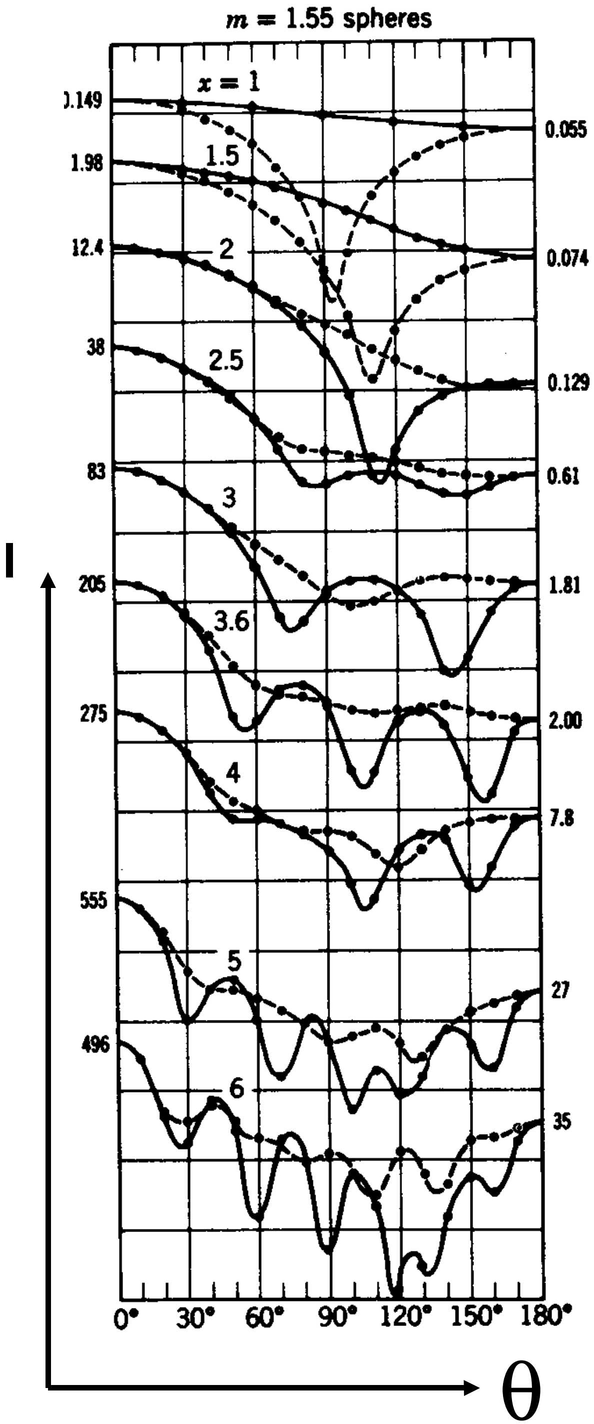
Why is the sky blue?


a = 250 nm
x (λ=600nm) = 2.6


a = 250 nm
x (λ=600nm) = 2.6

Control experiment


Finest Polishing
Powder
Optics School Leiden
25 nm < a < μm

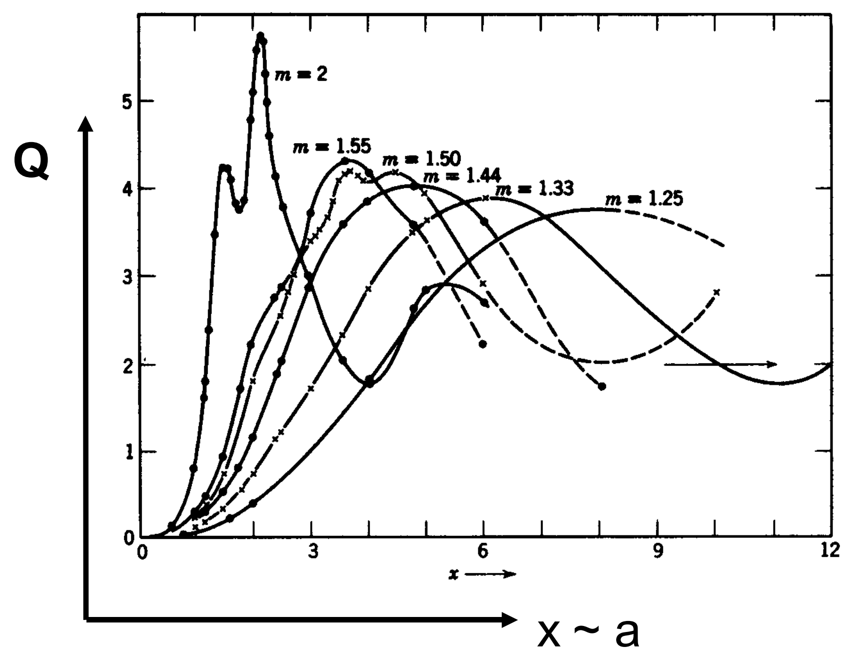


H.C. van de Hulst (Leiden 1957)
Light Scattering by small particles

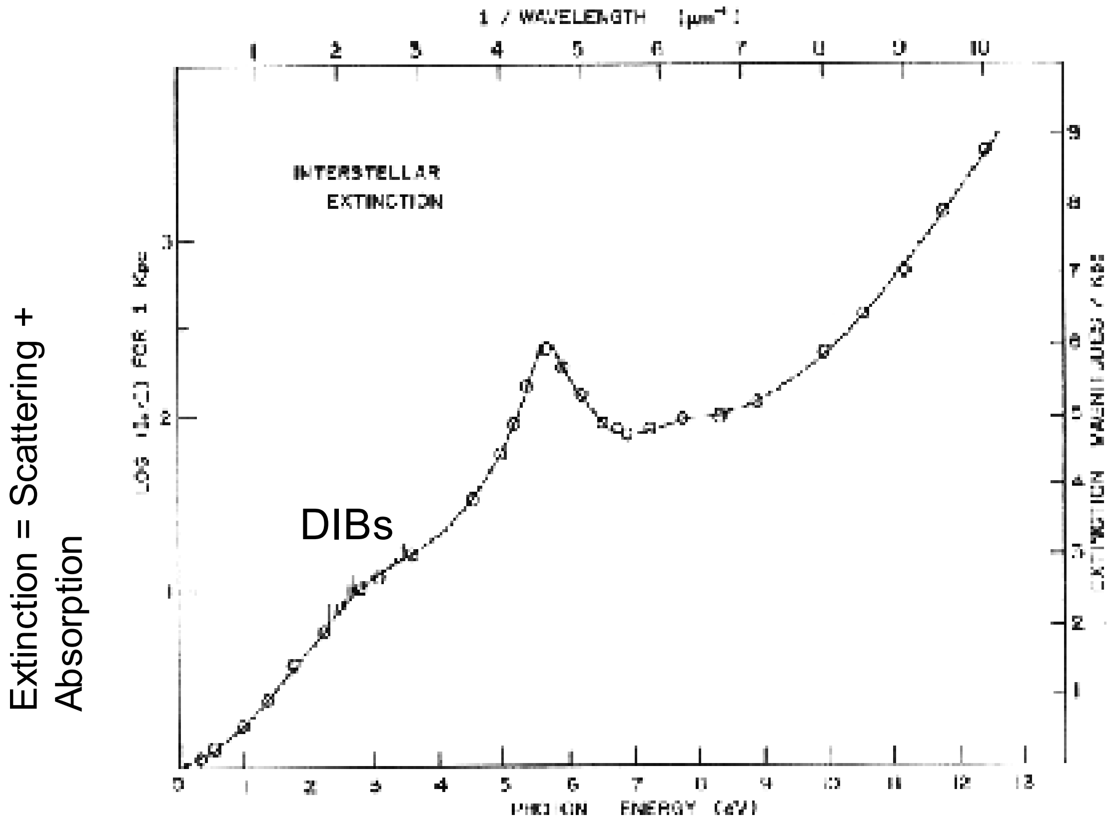
m: refractive index
x=2πa/λ: Mie-Parameter

Mie-Scattering: a ~ λ
Extinction Q ~ λ^{-2}

Rayleigh-Scattering: a << λ
Extinction Q ~ λ^{-4}



Average Interstellar Extinction



IR VIS UV FUV

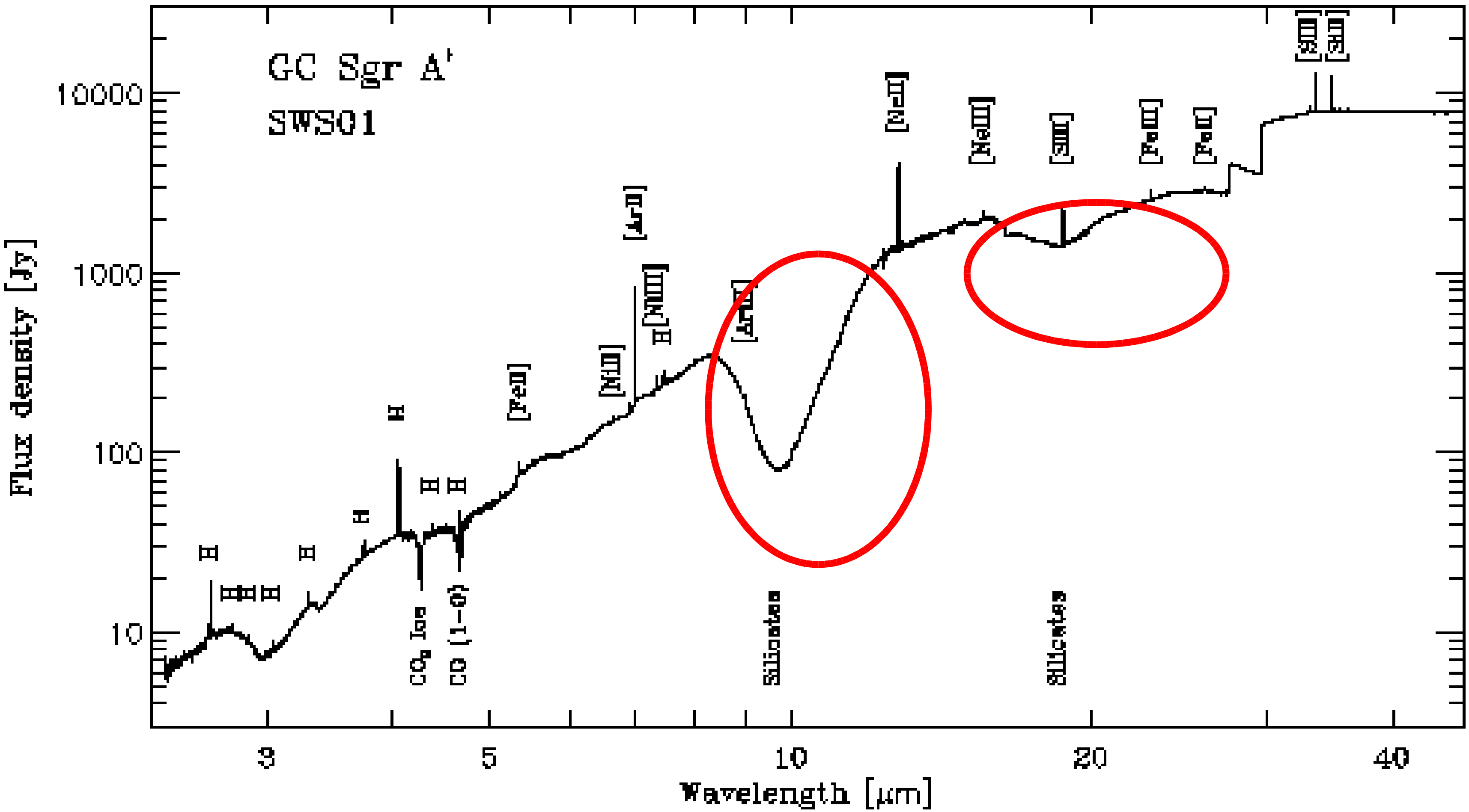
Optical Depth: 1 kpc column of dust 0.2 µm homogeneous Solid

(1 kpc = 3 10^3 light years)

Interstellar Extinction

Dust Absorption Features

Solid State Features from ISO



Comparing ISO Observations with Laboratory Results

TiC

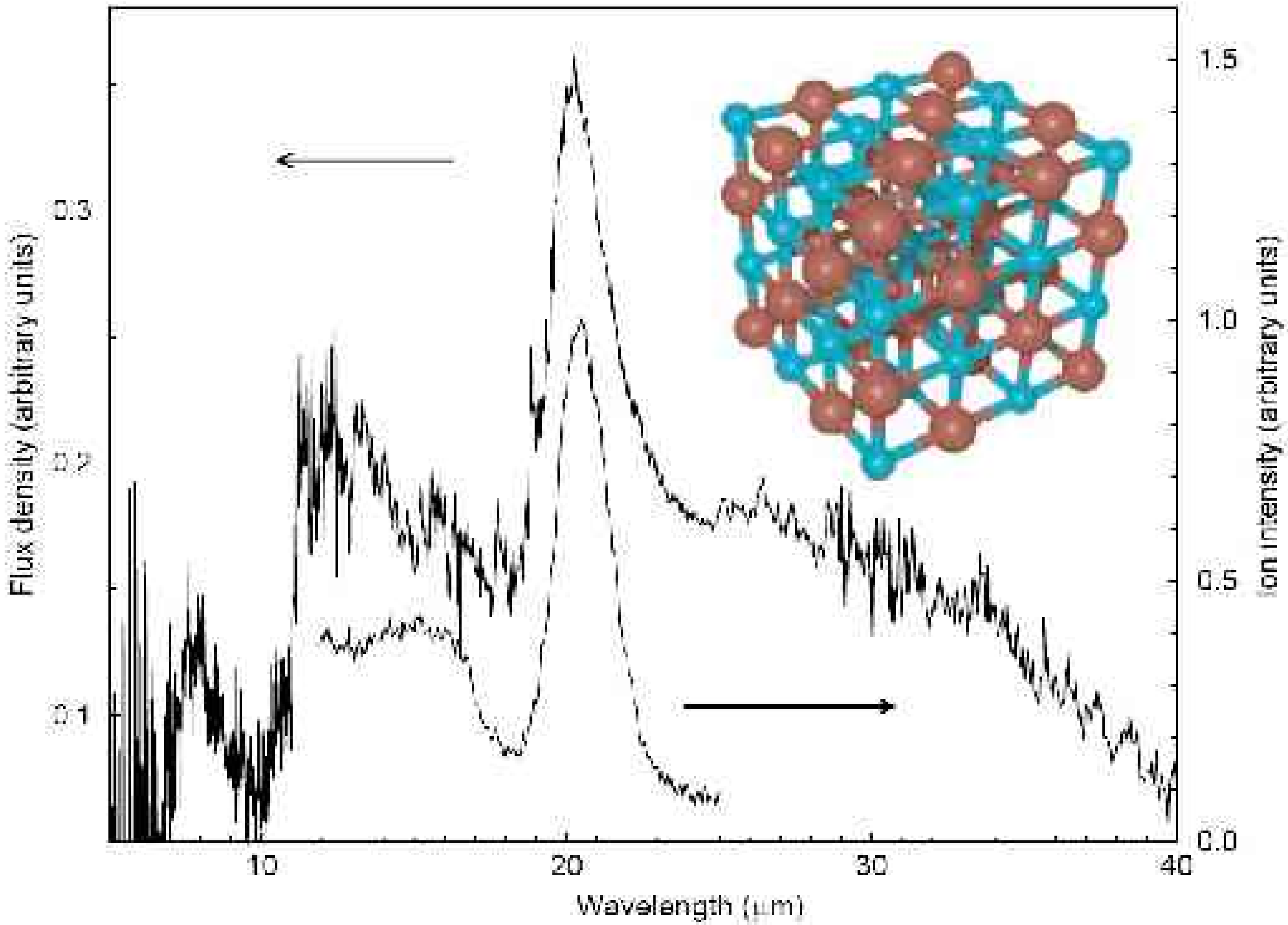
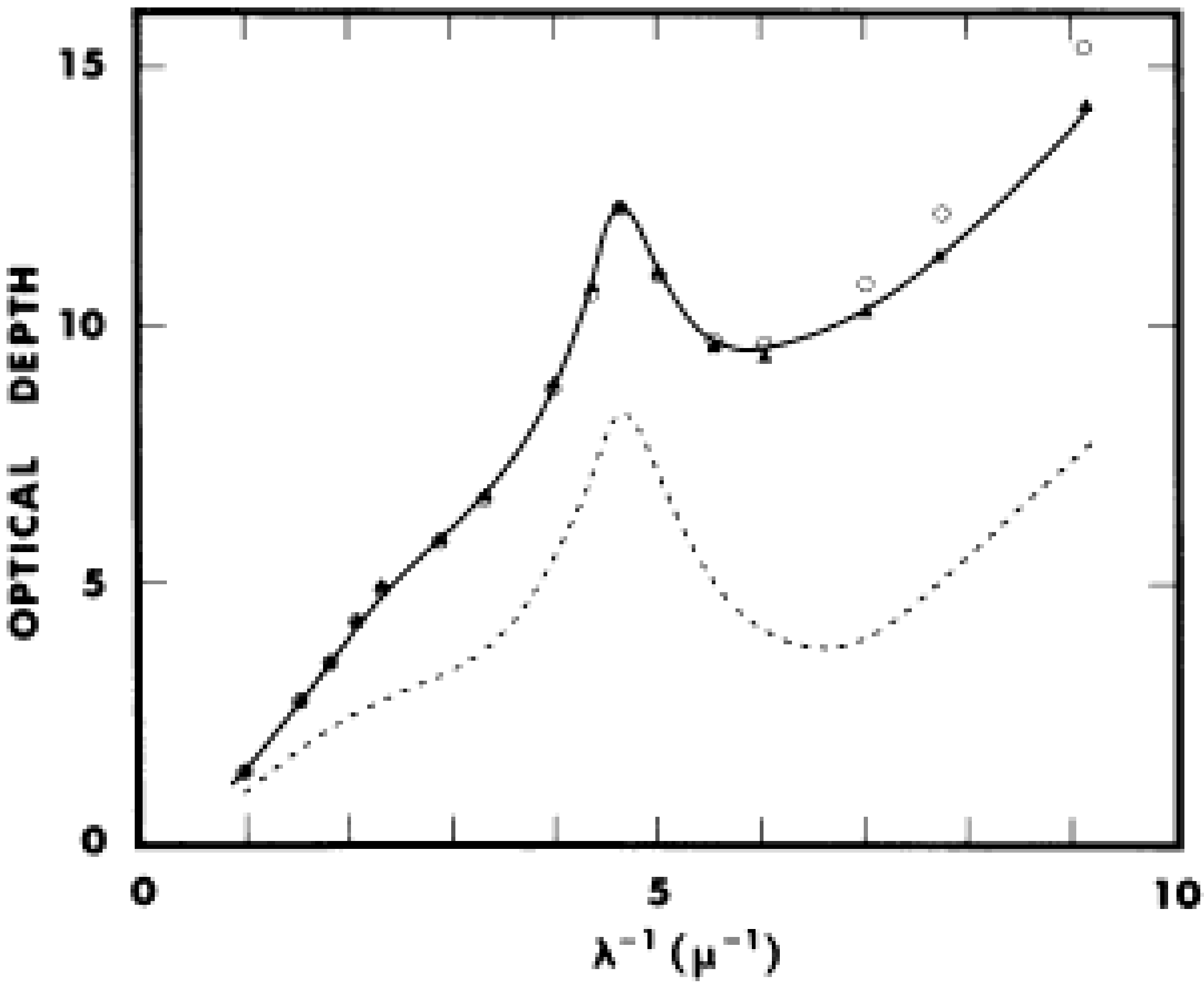


Fig. 1. The emission spectrum from the post-AGB object SAO 96709, taken by the ISO satellite (upper trace, left axis) and the wavelength spectra of TiC nanocrystal clusters recorded in the laboratory (lower trace, right axis). Also shown is a pictorial representation of a typical (4×4×4 atom) TiC nanocrystal. Carbon atoms are red; Ti atoms are blue.

Interstellar Extinction

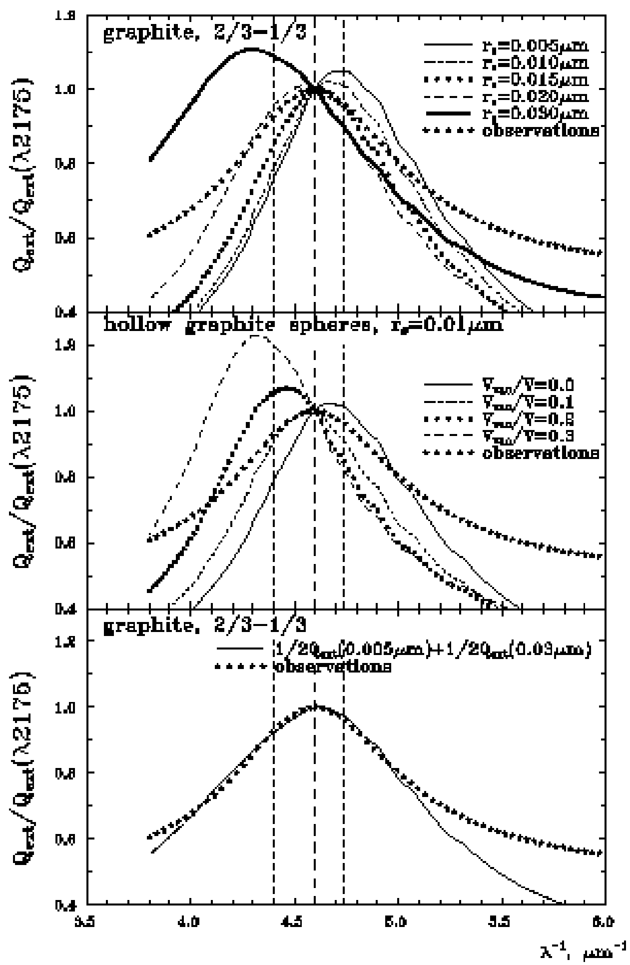
217 nm feature
UV - bump

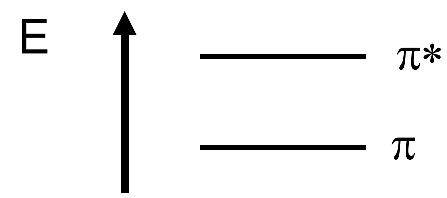


$P(a) \sim a^{-3.5}$

Mathis, Rumpl, and Nordsieck (1977)

π – π* Transition in Carbonaceous Material



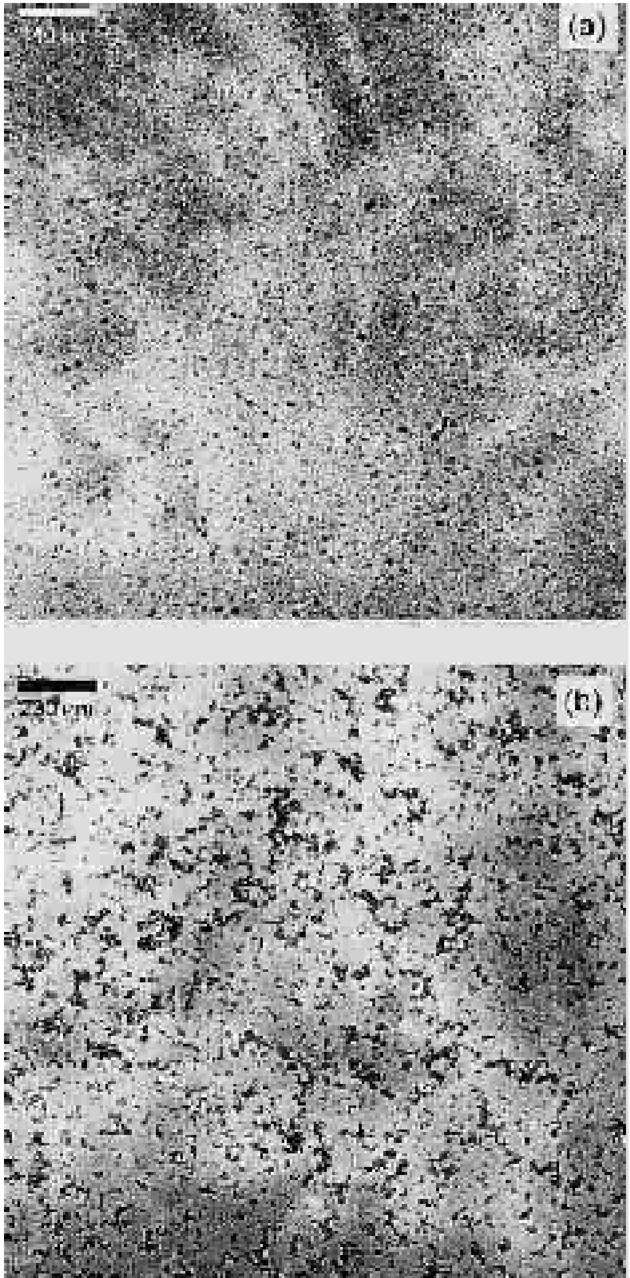


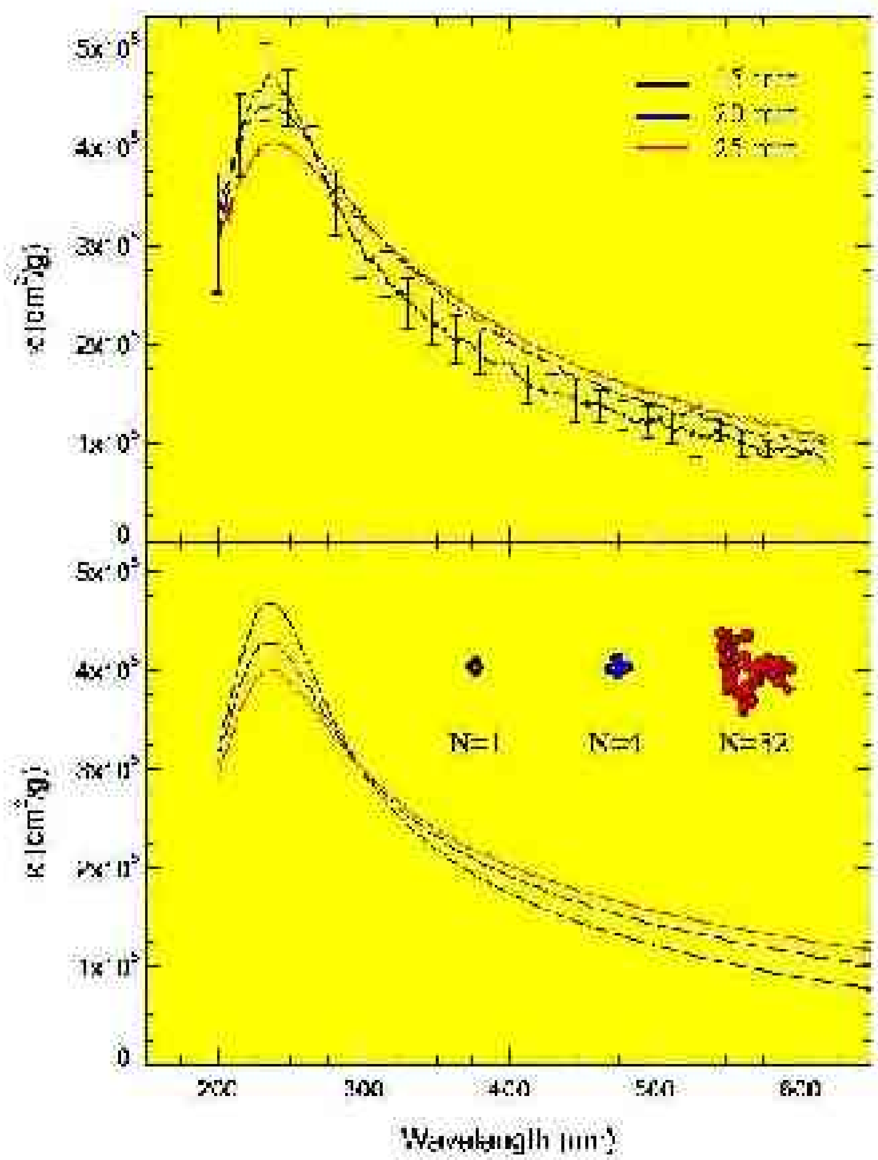
Normalized extinction efficiencies for **graphite spheres**. The calculations were made for homogeneous particles (upper panel) and hollow particles with a different fraction of vacuum (middle panel). The curve marked as ``observations'' corresponds to the wavelength dependence of the UV bump given by the mean galactic extinction curve (see,e.g., Sect. 3.1.2 in Voshchinnikov [2002]). The central position of the observed UV bump and its range of variations are marked. The lower panel shows the summary extinction of two graphite spheres with radii and (from upper panel) taken in equal proportions.

http://www.astro.spbu.ru/DOP/8-GLIB/ASTNOTES/node4.html

carbon: graphite, amorphous and graphitic carbons, coals, quenched carbonaceous composites, PAHs, carbonaceous (amorphous/glassy) particles

Electron Energy Loss Spectroscopy performed at the Fritz-Haber-Institut Berlin

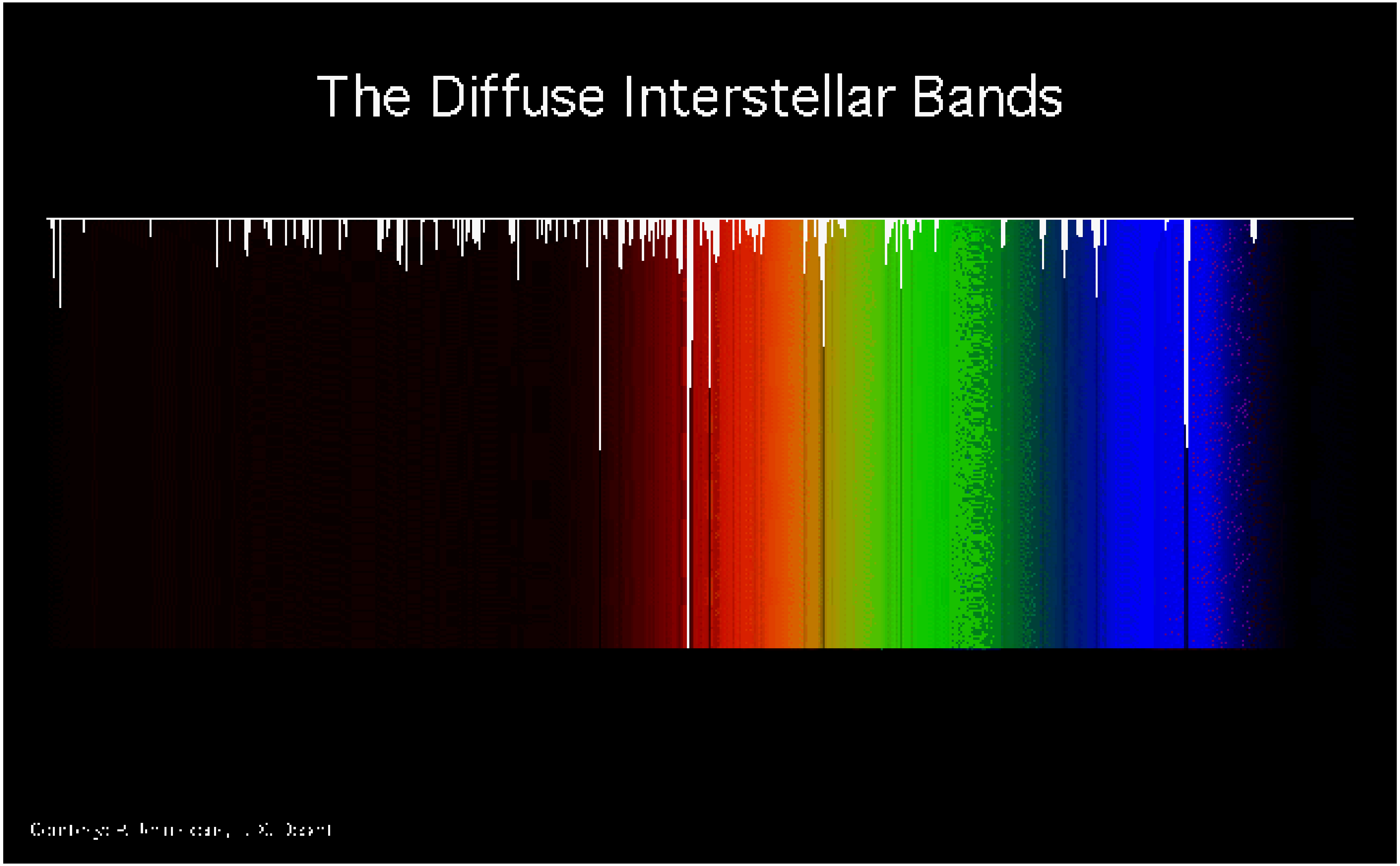




http://www.astro.uni-jena.de/Laboratory/Speclab/martin_results.html
http://www.astro.uni-jena.de/Laboratory/Database/carbon.html

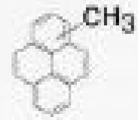
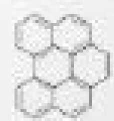
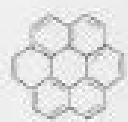
Interstellar Extinction

Diffuse Interstellar Bands
A long standing hunt for interstellar molecules



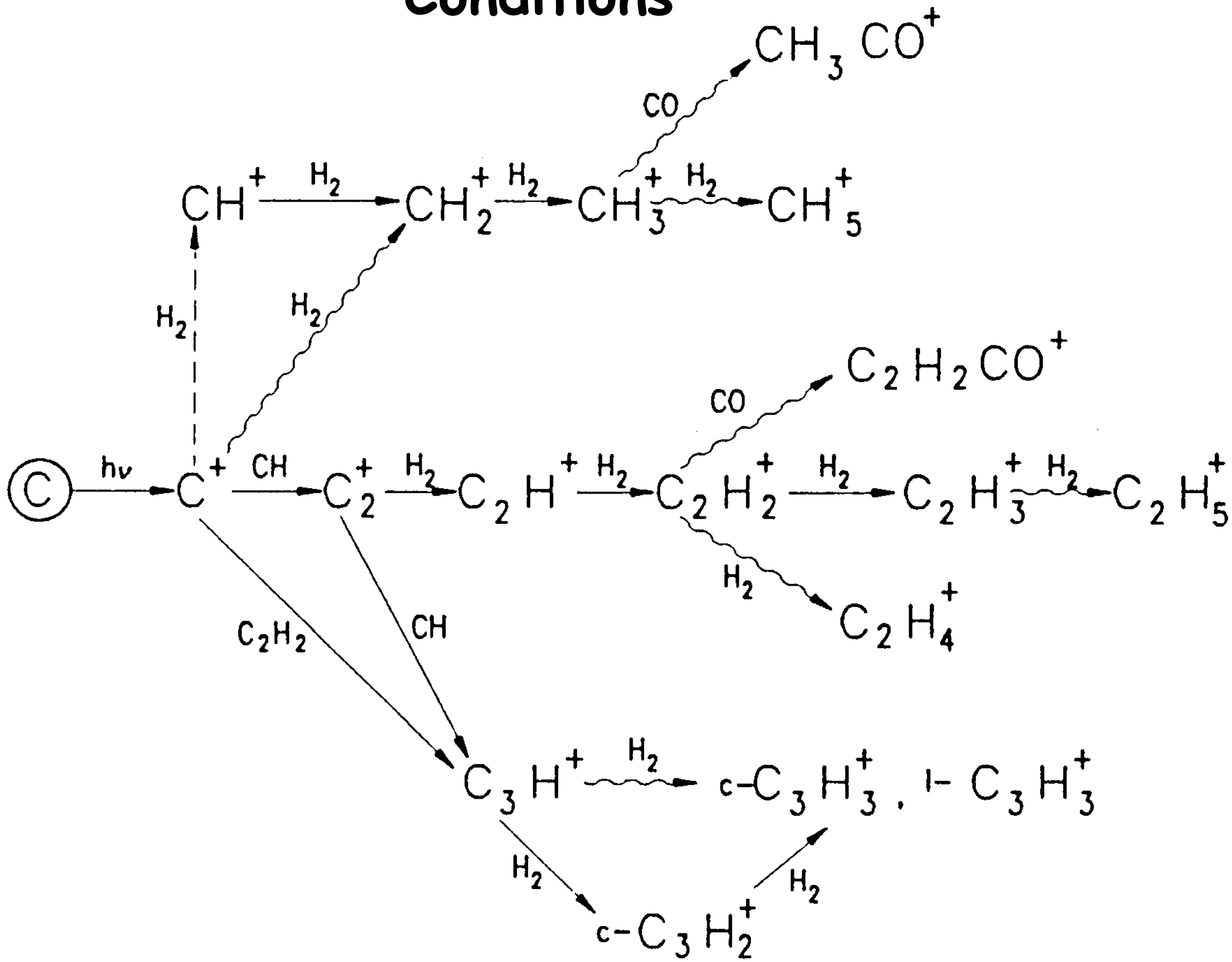
The first DIBs observed were those at wavelengths 5780 and 5797 Å.
Other strong DIBs are seen at 6284, 6614 and 4430 Å. The 4430 Å DIB is particularly broad at about 60 Å across - typical intrinsic stellar absorption features are 1Å or less across.

Comparison of DIBs with PAH Cation Bands.
PAHs Isolated in Neon Matrices

PAH^+		λ_{peak} (nm)	DIBs (nm)
Pyrene ($C_{16}H_{10}^+$)		439.5 (443.0 in Ar)	442.9
1-Methylpyrene ($CH_3 - C_{16}H_9^+$)		444.2	442.9
4-Methylpyrene ($CH_3 - C_{16}H_9^+$)		(457.7) 482.8 757.6	 482.4 758.1
Naphthalene ($C_{10}H_8^+$)		674.2 652.0	674.1 652.0
Phenanthrene ($C_{14}H_{10}^+$)		898.3 856.8	 857.2
Tetracene ($C_{18}H_{12}^+$)		864.7	864.8
Benzo(ghi)perylene ($C_{22}H_{12}^+$)		502.2 758.4 755.2 794.3	503.9 (?) 758.1; 758.6 755.8 (?); 756.2 793.5 (prob.)
Coronene ($C_{24}H_{12}^+$)		459.0 946.5	459.5 946.6

NASA Ames group: Louis Allamandola et al.

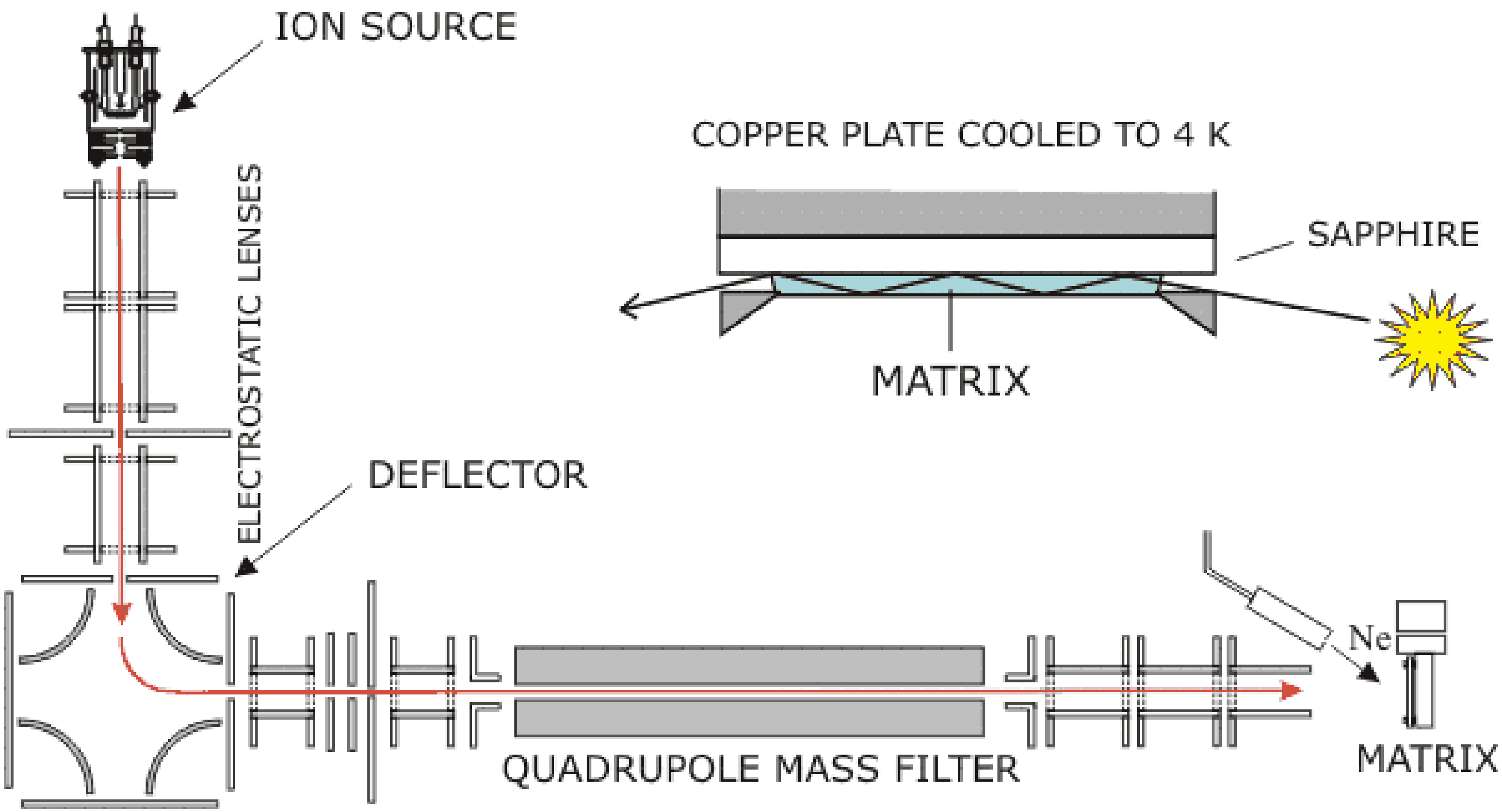
Formation of Small Hydrocarbons under Interstellar Conditions



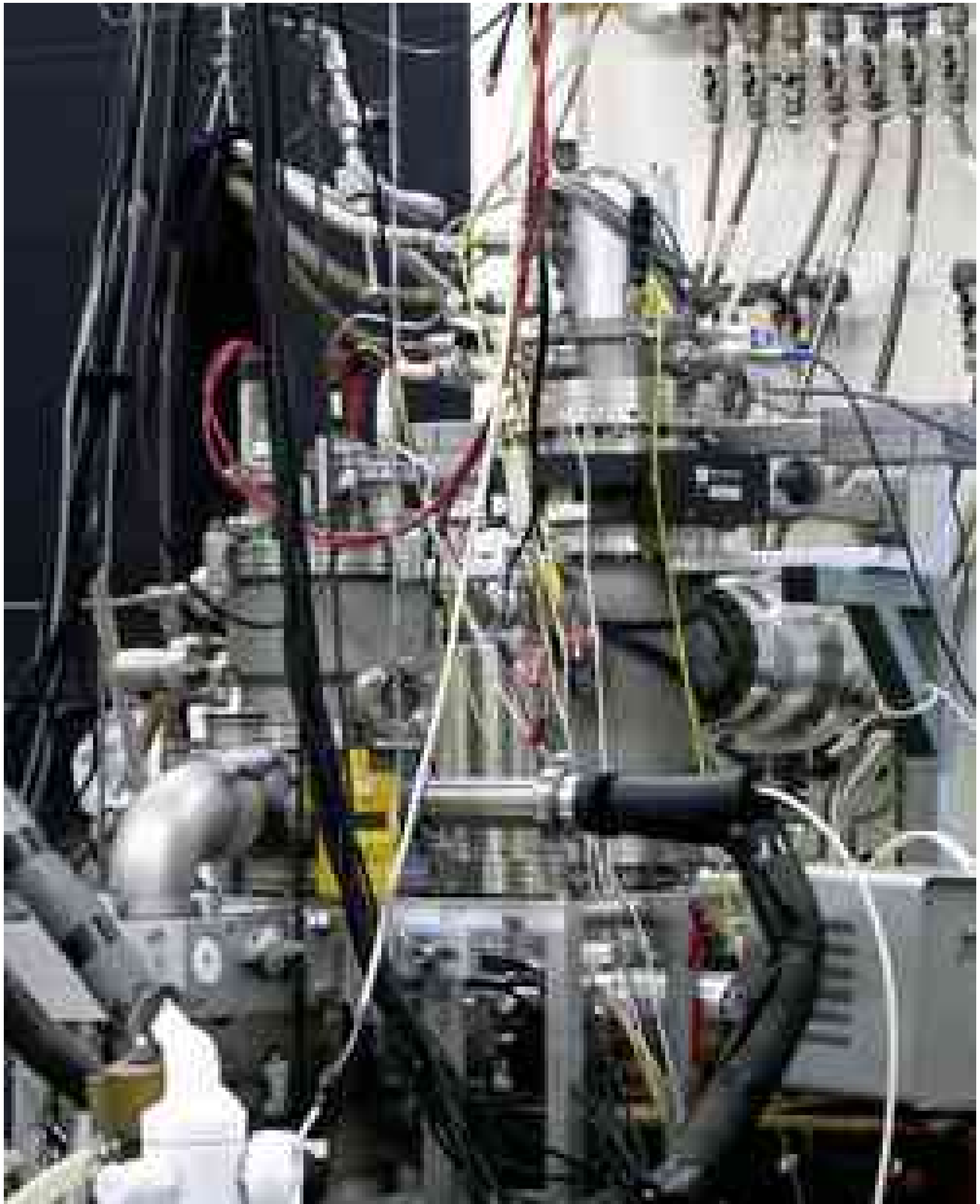
D. Gerlich and S. Horning, Chem. Rev. 92, (1992) 1509

Production and Detection of Transient Species

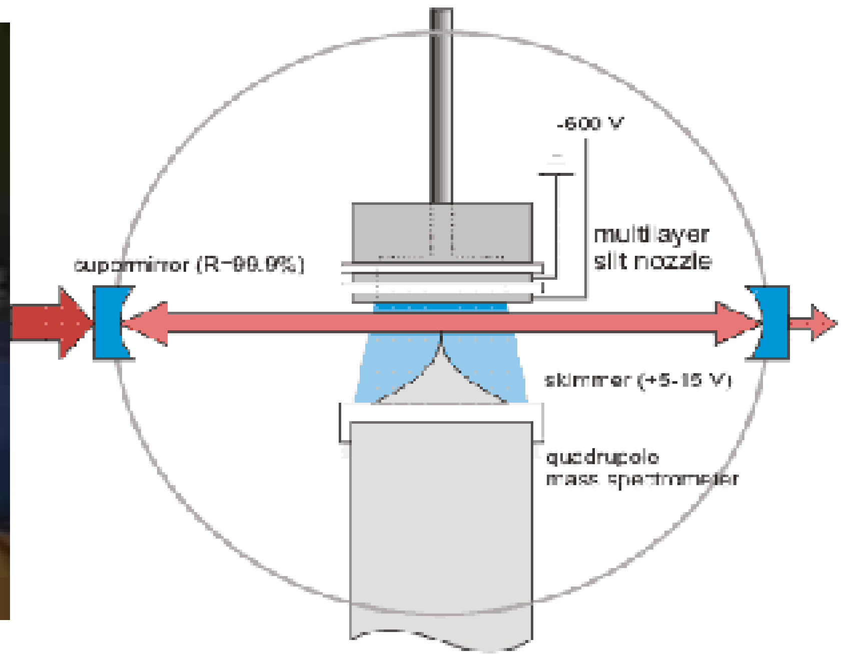
Martix-isolation Technique in Basel (John Maier)

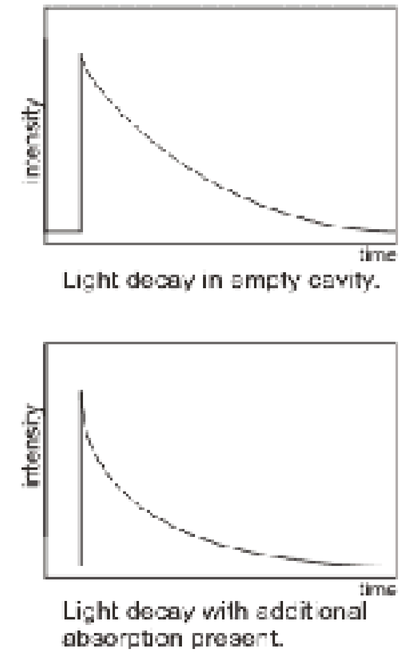


Martix-isolation Technique in Basel (John Maier)



Cavity Ring Down Spectroscopy CRDS in Basel





Rotationally resolved electronic spectrum of propadienylidene

Petre Birza, Andrei Chirokolava, Mitsunori Araki, Przemyslaw Kolek, John P. Maier*

The rotationally resolved electronic spectrum of a vibrational band in the $\tilde{A}^1A_2 \leftarrow \tilde{X}^1A_1$ transition of the cumulene carbon chain C_3H_2 was measured in the 625 nm region in a supersonic discharge using cw cavity ring down spectroscopy. The rotational structure was analysed using a conventional Hamiltonian for an asymmetric top molecule, and the constants A', B', and C' in the upper state were determined. The observed band is assigned to a combination of a_1 and b_2 vibrations with the frequency around 2000 cm^{-1}. The geometries in the $^1A_1$, $^1A_2$, $^1B_1$ states and the intersection point between the latter two were obtained using ab initio calculations. The effective structure in the measured vibrational level of the $^1A_2$ state was inferred from the determined constants

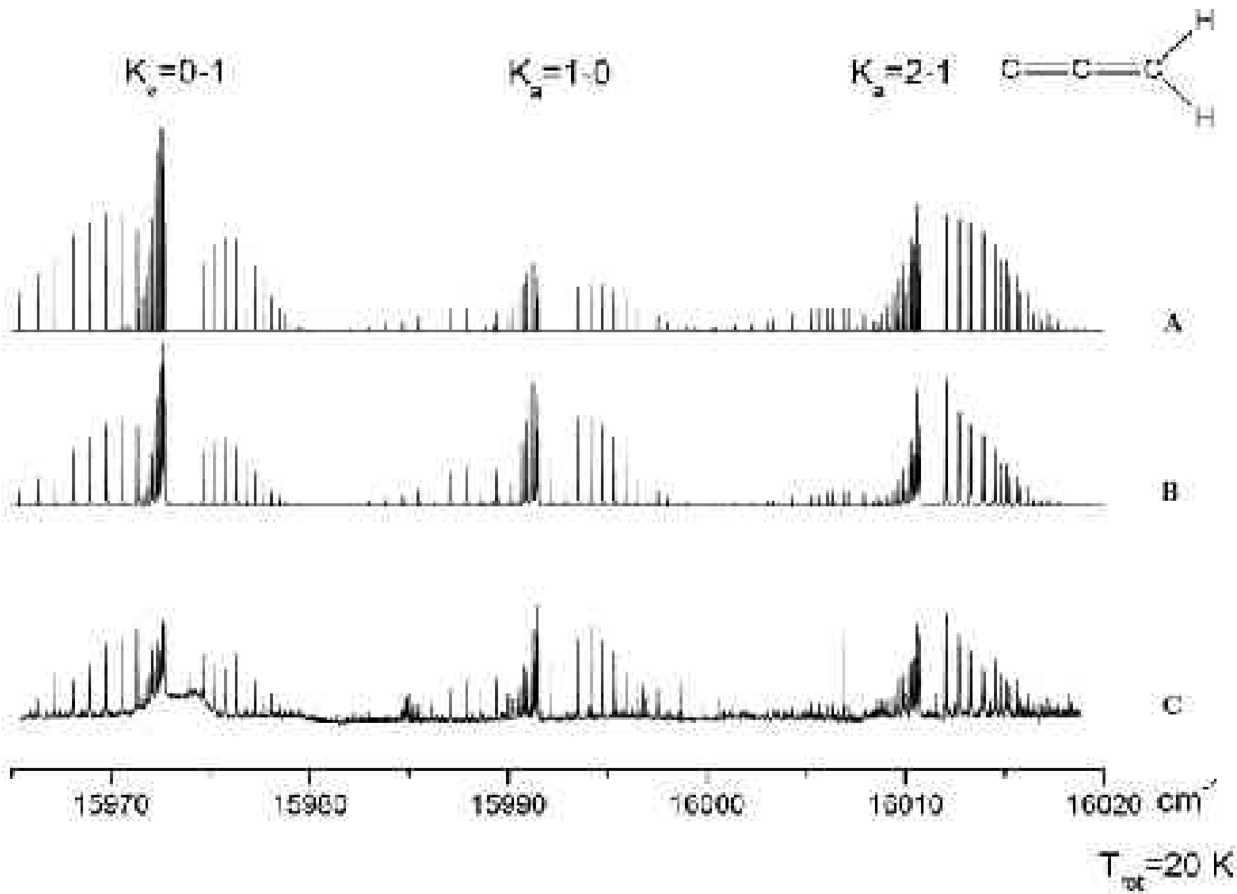
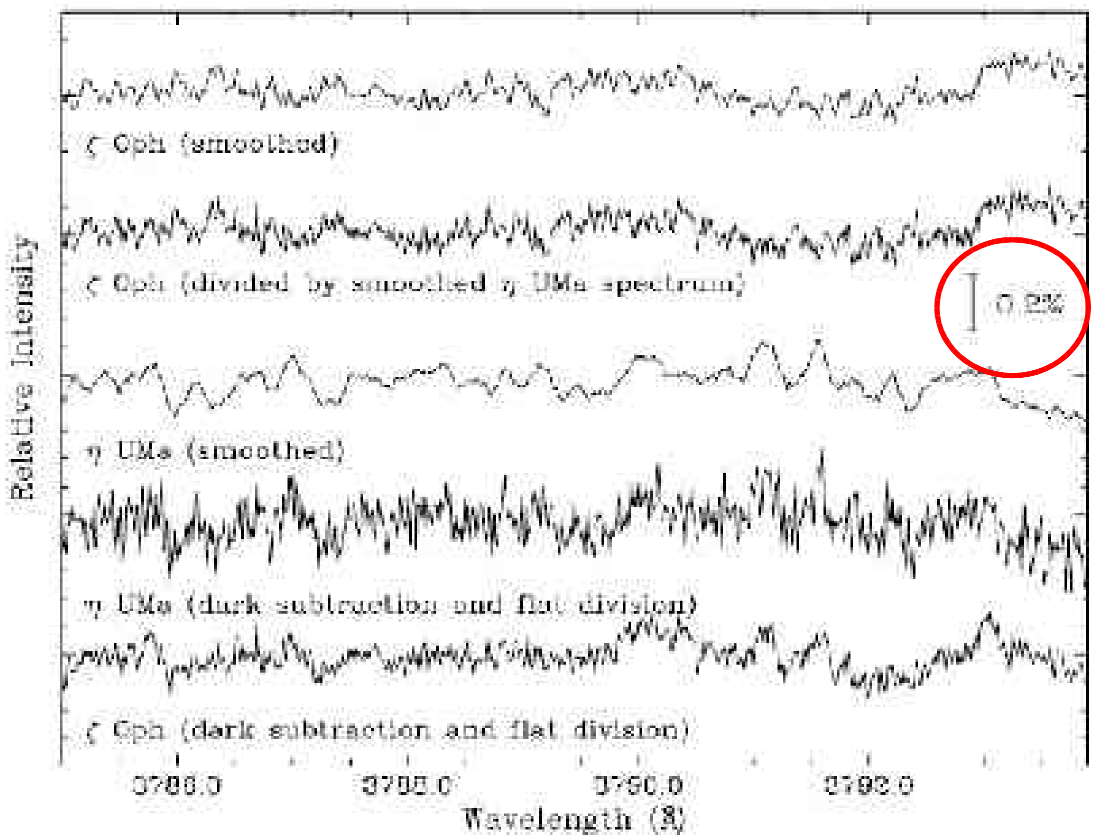


Fig. 1. Rotationally resolved spectrum of C_3H_2 (trace C) in comparison with the simulated ones: trace A using the independent Boltzmann population model, trace B a single Boltzmann population for the two nuclear spin isomers (spin statistical weight ee:eo:oe:oo = 1:1:3:3). The broad structure around 15970 cm^{-1} is the origin band of the $\tilde{B}^2\Pi_{1/2}-\tilde{X}^2\Pi_{1/2}$ transition of C_6H.

ISOCAM picture of the rho Ophiuchi cloud

LIMITS TO INTERSTELLAR C_4 AND C_5 TOWARD ζ OPHIUCHI

JOHN P. MAIER,[1]



We have made a sensitive search for the origin bands in the known electronic transitions of the linear carbon chains C_4 and C_5 at 3789 and 5109 Å toward ζ Oph ($A_v < 1$). The incentive was a recent detection of C_3 in this interstellar cloud with a column density of 1.6×10^{12} cm^{-2}, plus the availability of laboratory gas phase spectra of C_4 and C_5. Further, some models of diffuse interstellar clouds predict that the abundance of these latter species should be within an order of magnitude of C_3. Despite achieving a signal-to-noise ratio (S/N) of 2300 to 2600 per pixel at a resolution of ~110,000, the searches were negative, leading to 3 σ upper limits to the column density of $N(C_5) = 2 \times 10^{11}$ cm^{-2} and $N(C_4) = 4 \times 10^{12}$ to 10^{13} cm^{-2} where these values rely on theoretically calculated oscillator strengths. The implication of these limits is discussed along with the identification of molecules for study in future attempts to identify the carriers of the stronger diffuse interstellar bands.

JOHN P. MAIER,[1]

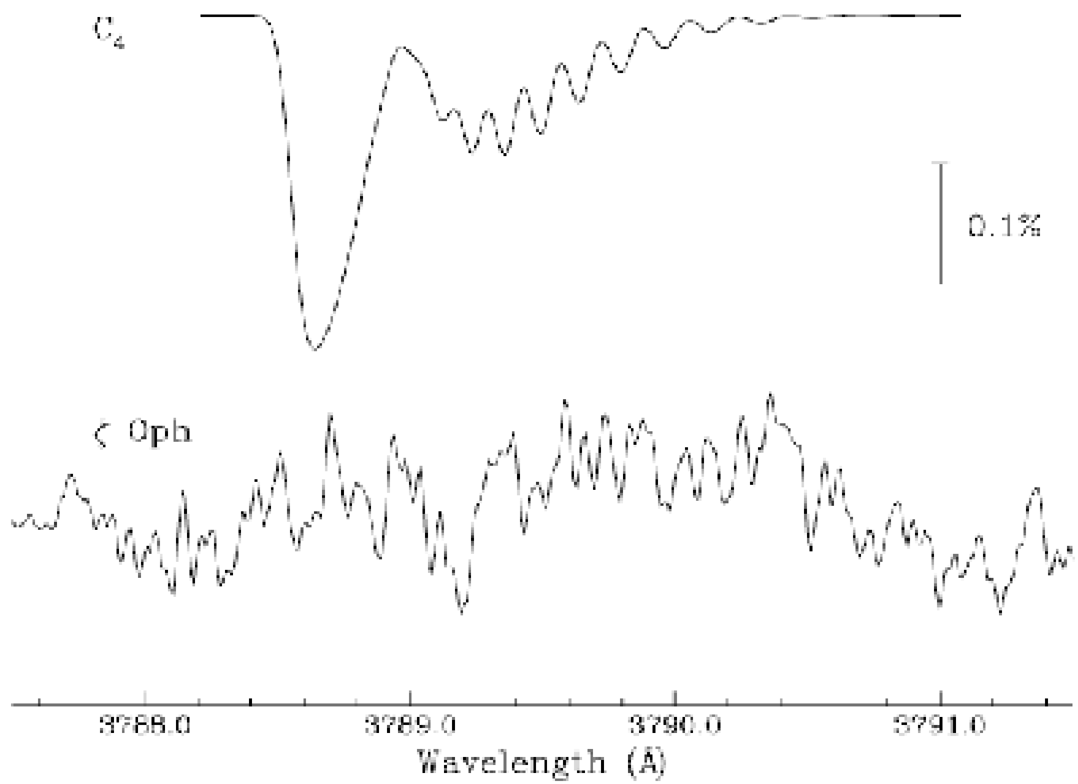


FIG. 2.—Comparison of a laboratory spectrum (*top*) of C_4 at 3788 Å from Linnartz et al. (2000) smoothed to a spectral resolution of 110,000 and compared to the observed spectrum (*lower*) of ζ Oph from Fig. 1.

JOHN P. MAIER,[1]

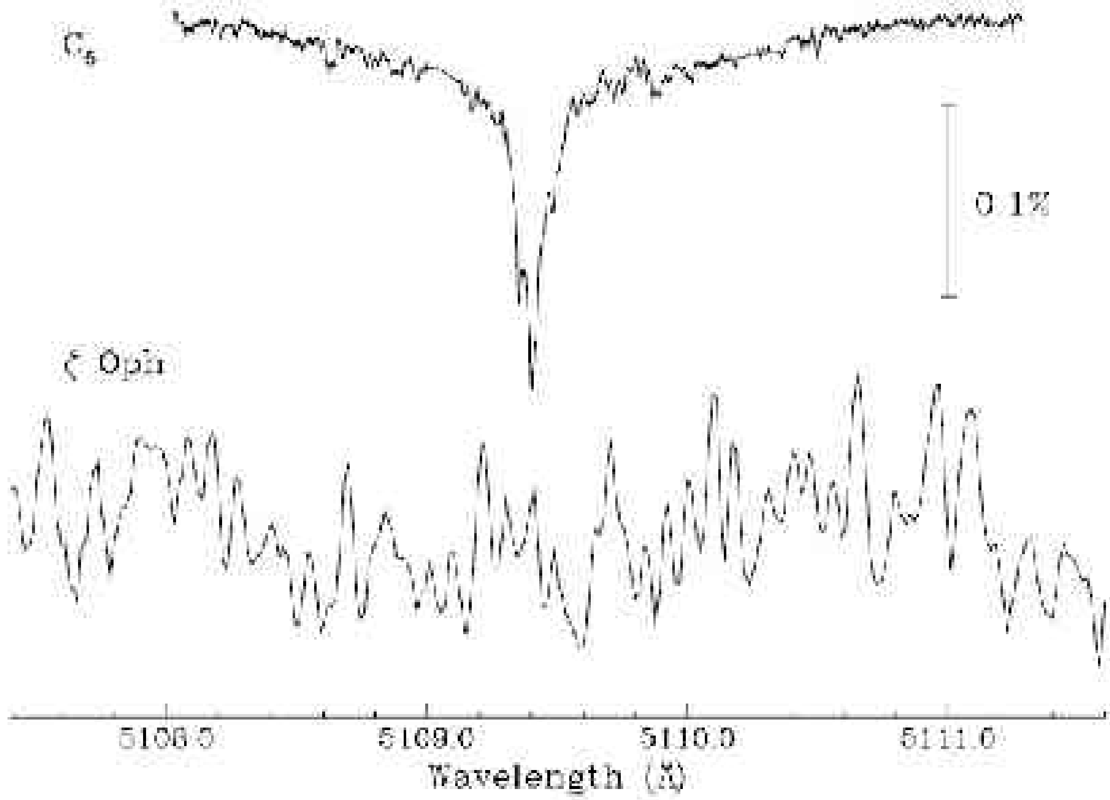
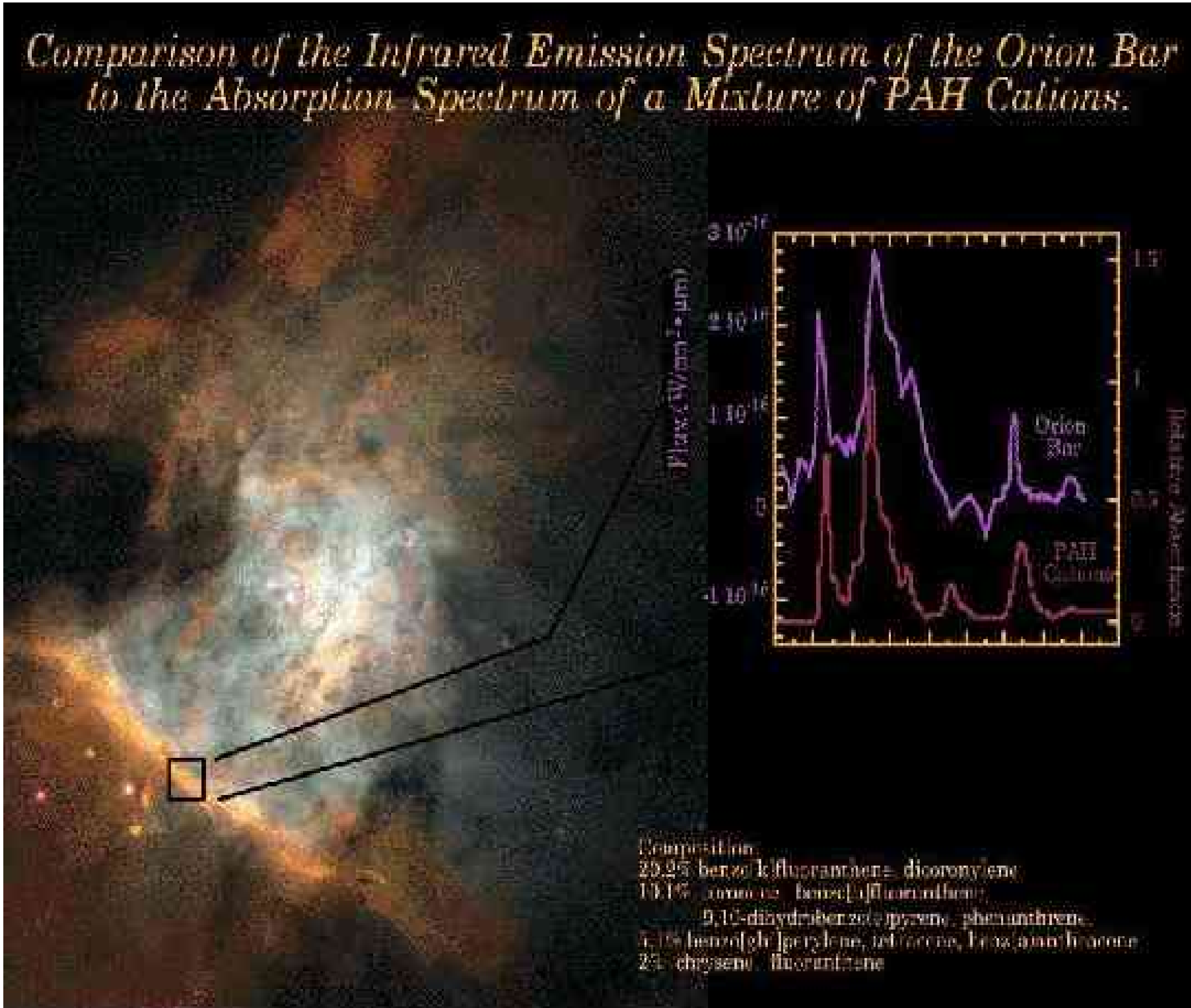


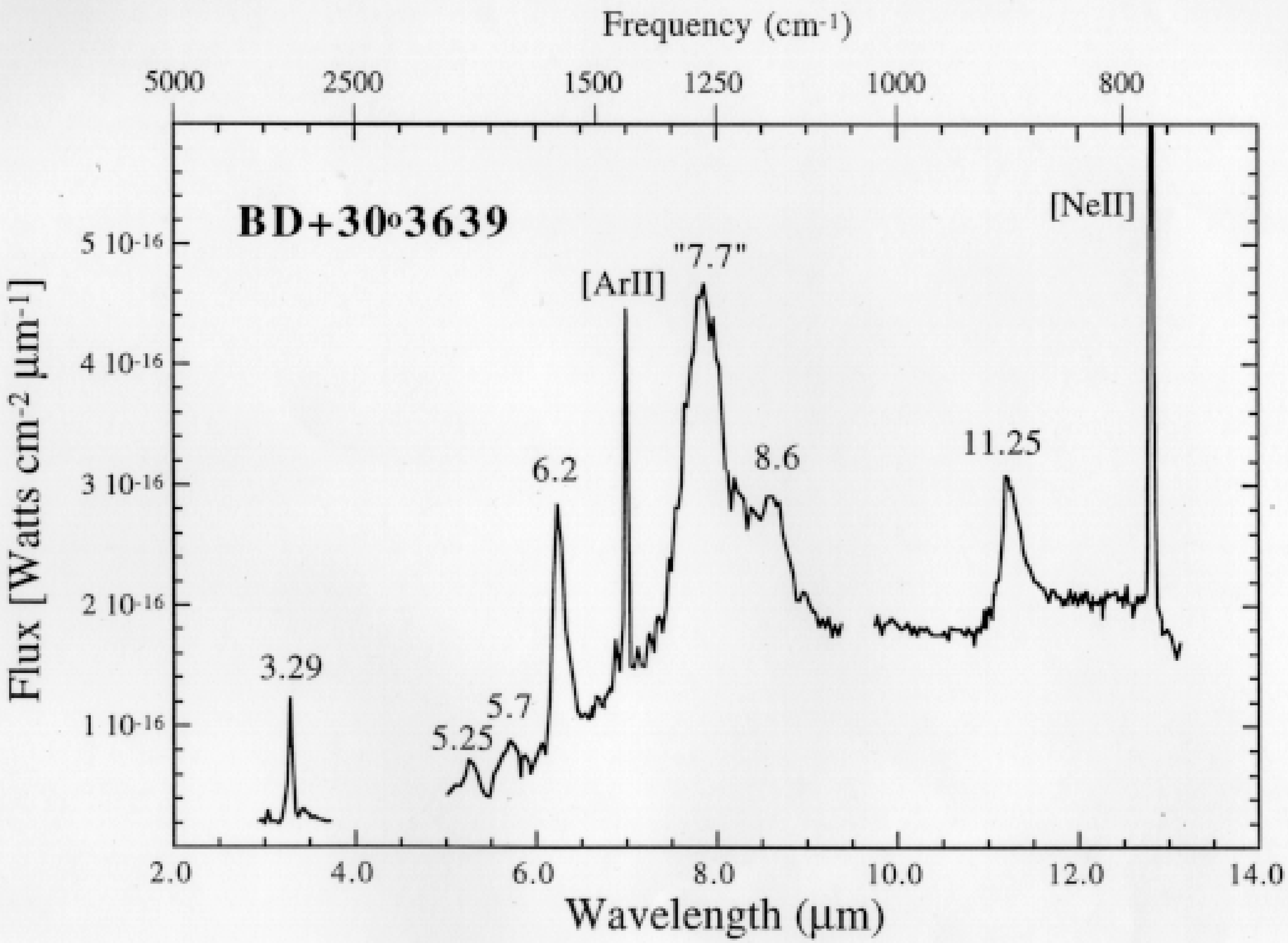
FIG. 3.—Comparison of a laboratory spectrum (*top*) of C_5 at 5109 Å from Motylewski et al. (1999) smoothed to a spectral resolution of 110,000 and compared to the observed spectrum (*lower*) of ζ Oph.

Interstellar Extinction

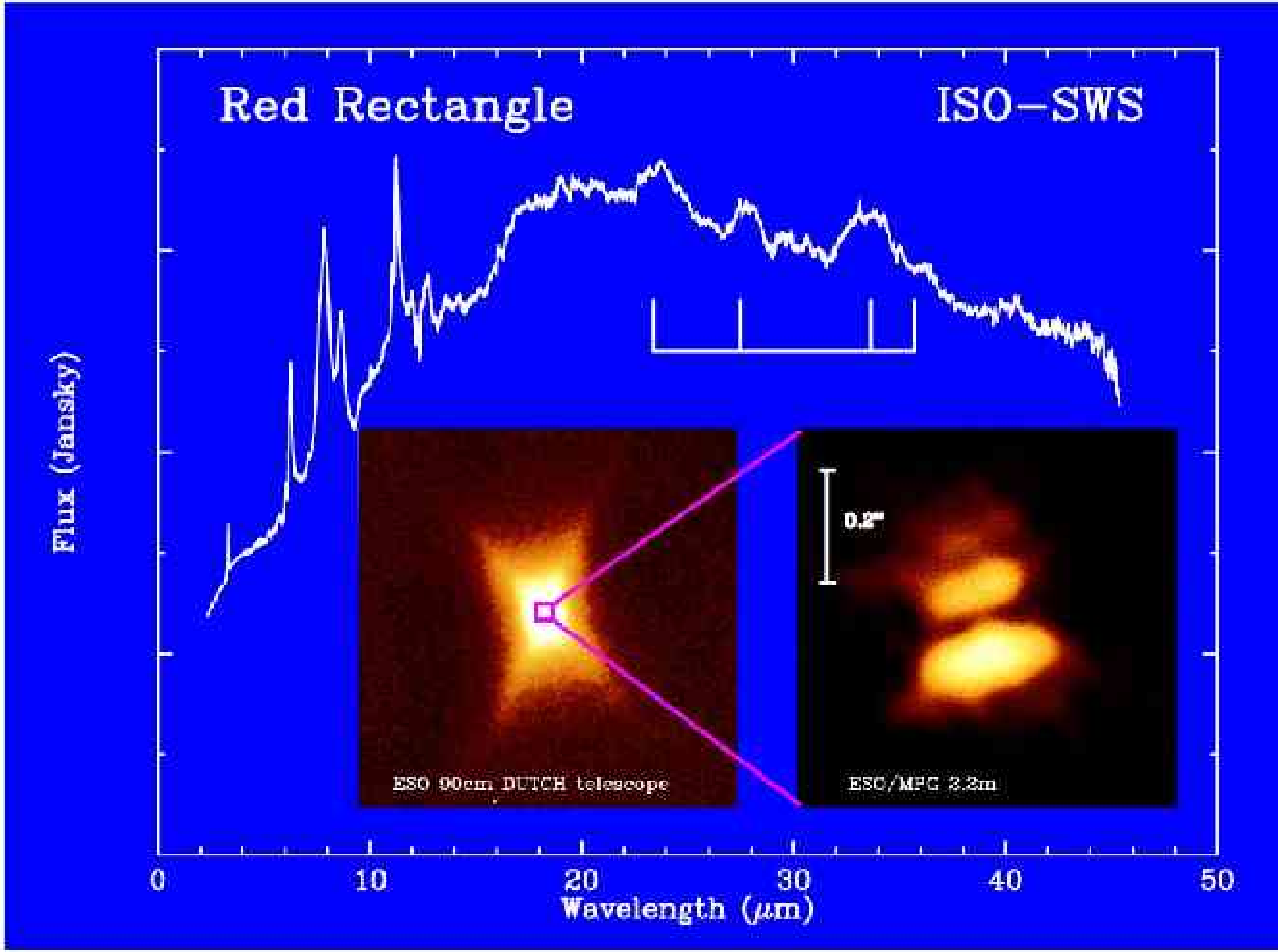
Unidentified Infrared Bands
and
PAH Hypothesis



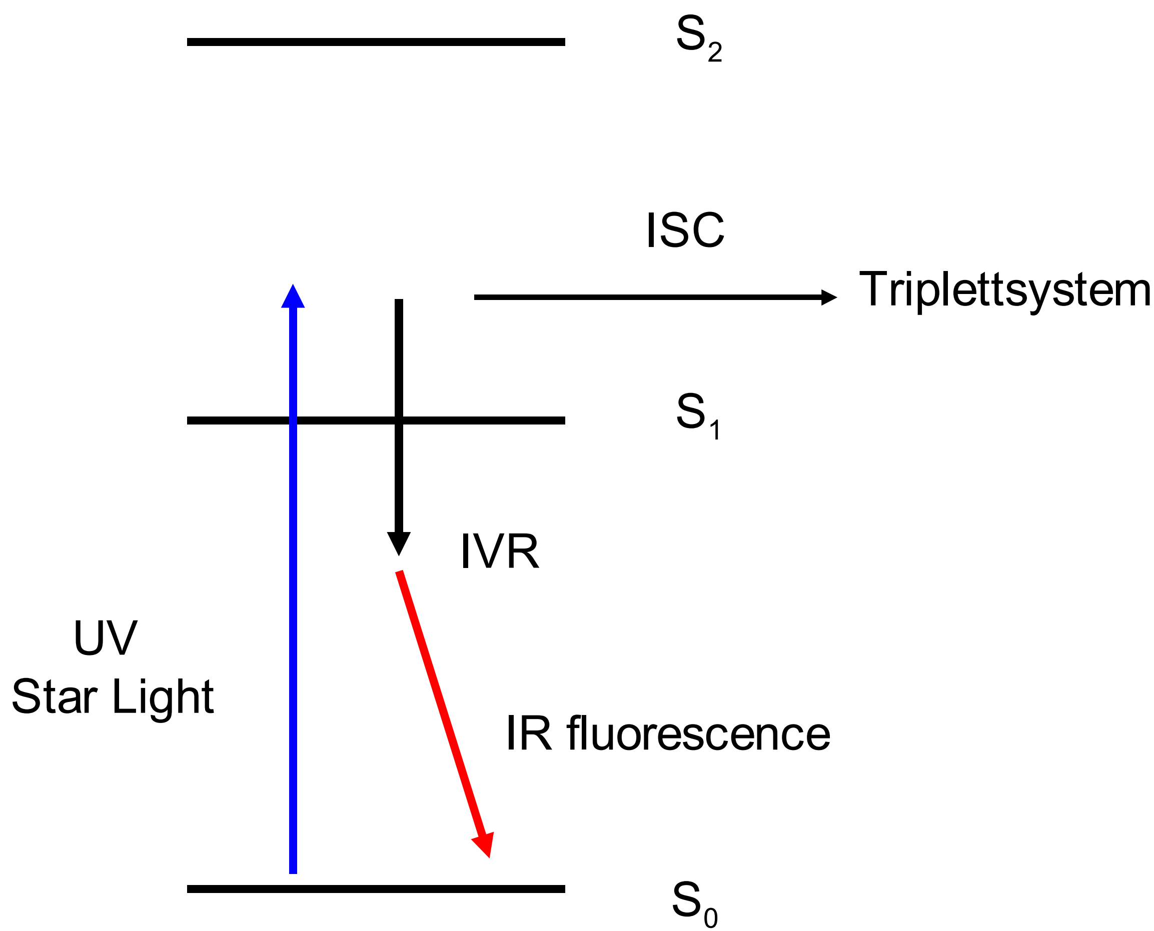
Comparison of the Infrared Emission Spectrum of the Orion Bar
to the Absorption Spectrum of a Mixture of PAH Cations.
Orion Bar
PAH Cations
Composition



Frequency (cm-1)
5000
2500
1500
1250
1000
800
BD+30o3639
[NeII]
"7.7"
[ArII]
6.2
8.6
11.25
3.29
5.7
5.25
5 10-16
4 10-16
3 10-16
2 10-16
1 10-16
Flux [Watts cm-2 µm-1]
2.0
4.0
6.0
8.0
10.0
12.0
14.0
Wavelength (µm)

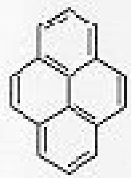

Red Rectangle
ISO–SWS
Flux (Jansky)
Wavelength (μm)
0
10
20
30
40
50
0.2"
ESO 90cm DUTCH telescope
ESO/MPG 2.2m

Polycyclic Aromatic Hydrocarbons
PAH – UIR Hypothesis

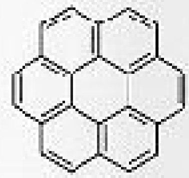


PAH Structures

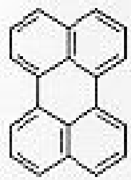
Pericondensed



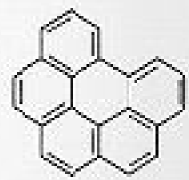
Pyrene
$C_{16}H_{10}$



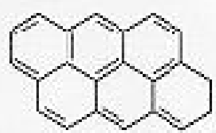
Coronene
$C_{24}H_{12}$



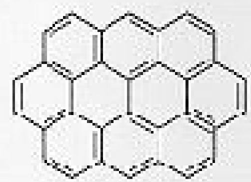
Perylene
$C_{20}H_{12}$



Benzo[ghi]perylene
$C_{22}H_{12}$

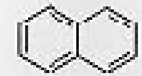


Antanthrene
$C_{22}H_{12}$

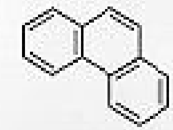


Ovalene
$C_{32}H_{14}$

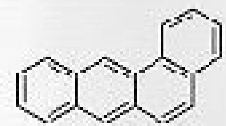
Catacondensed



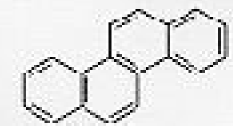
Naphthalene
$C_{10}H_8$



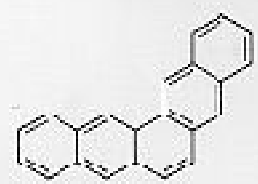
Phenanthrene
$C_{14}H_{10}$



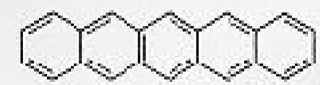
Tetraphene
$C_{18}H_{12}$



Chrysene
$C_{18}H_{12}$

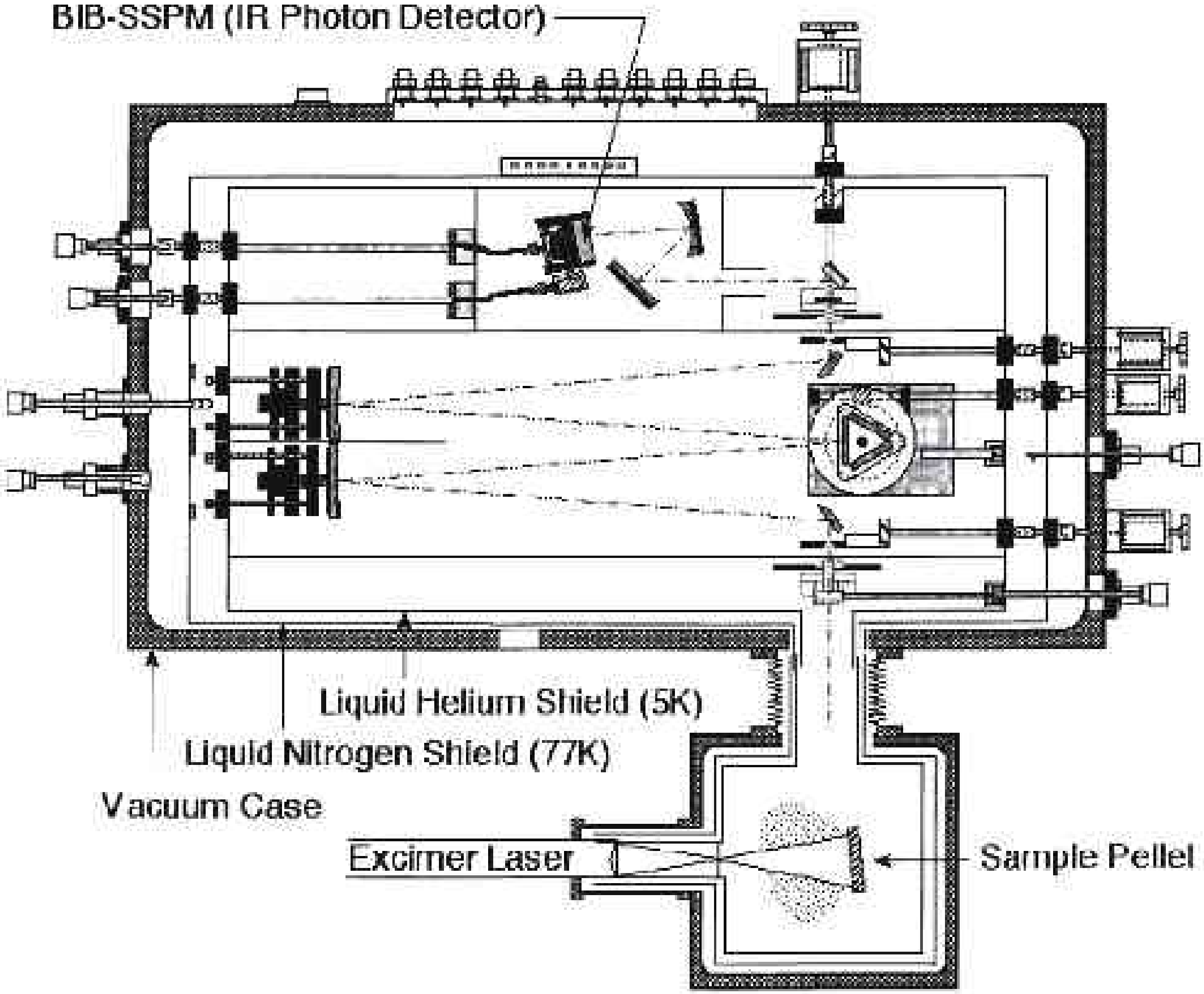


Pentaphene
$C_{22}H_{14}$

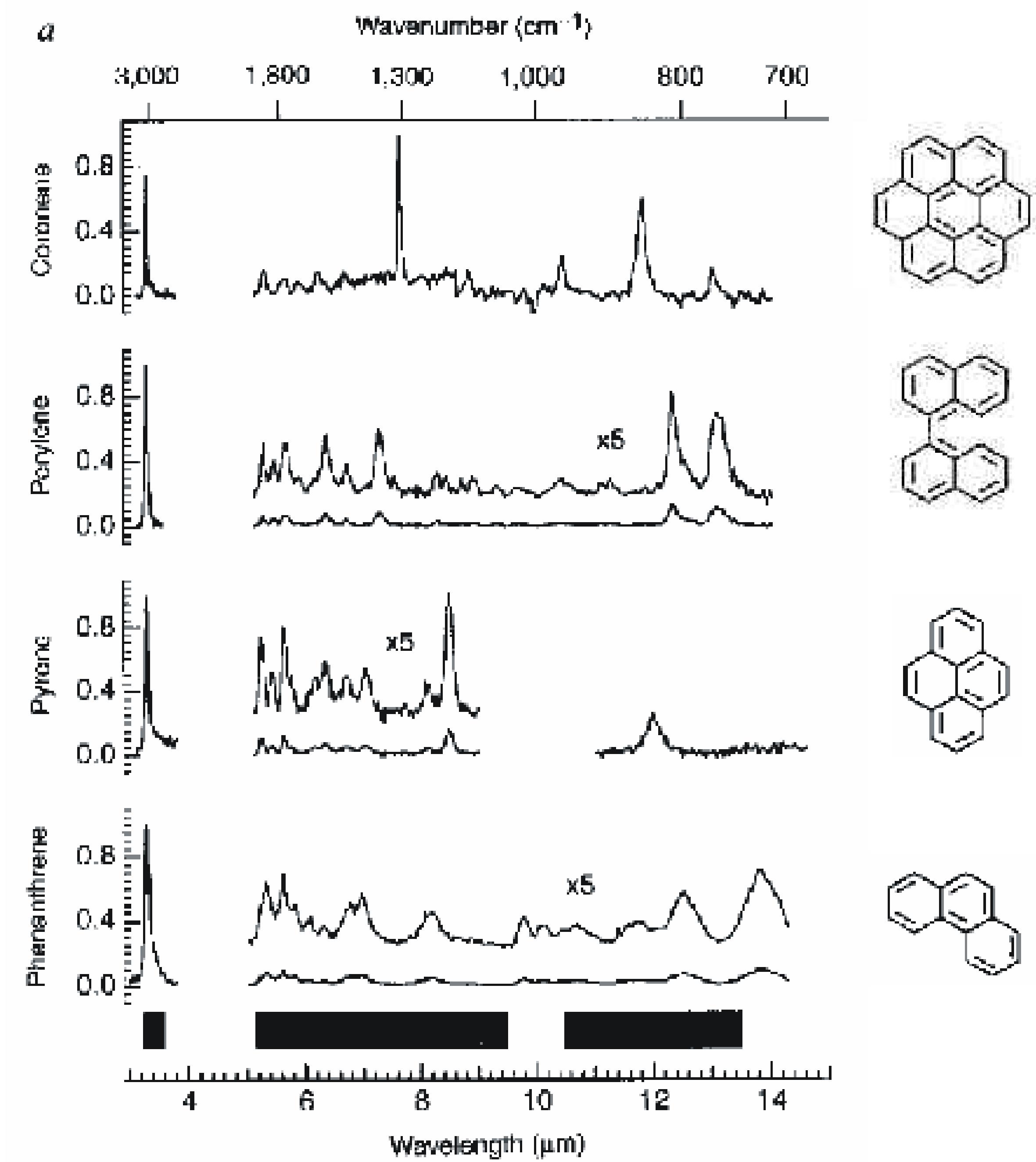


Pentacene
$C_{22}H_{14}$

UIR wavelength (μm)	3.3	6.2	7.7	8.7	11.2
UIR bandwidth FWHM (cm^{-1})	30	30	70 to 200*		30
Characteristic PAH vibrations (see text)	C–H stretch	C–C stretch	C–C stretch	C–H in-plane bend	C–H out-of-plane bend†



BIB-SSPM (IR Photon Detector)
Liquid Helium Shield (5K)
Liquid Nitrogen Shield (77K)
Vacuum Case
Excimer Laser
Sample Pellet

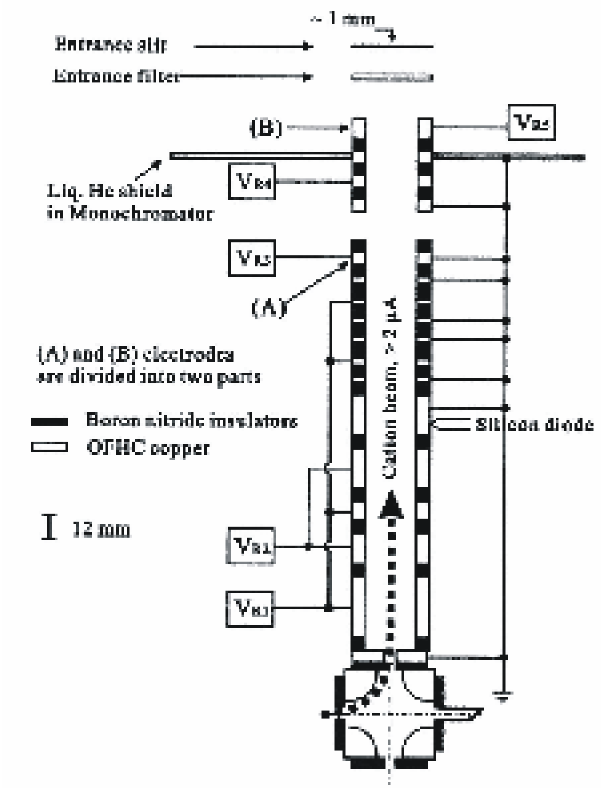


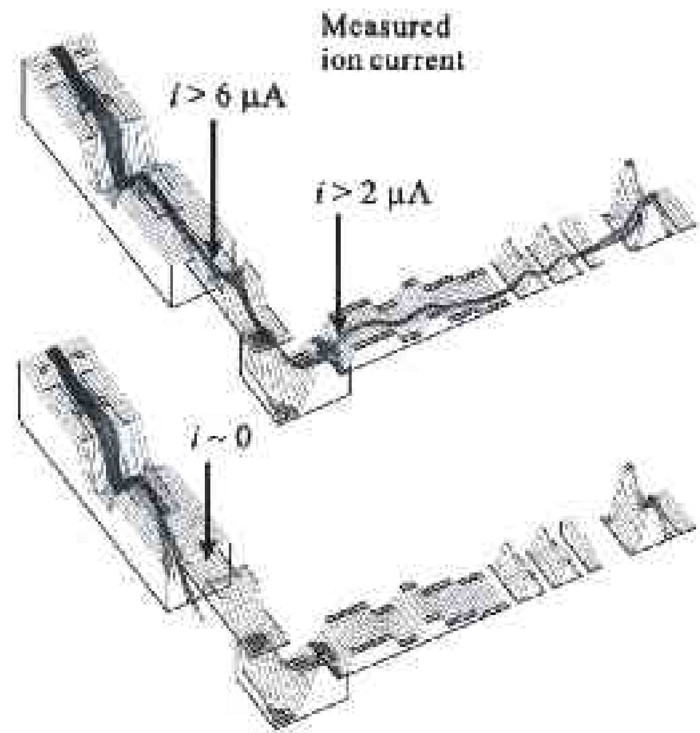
Problems

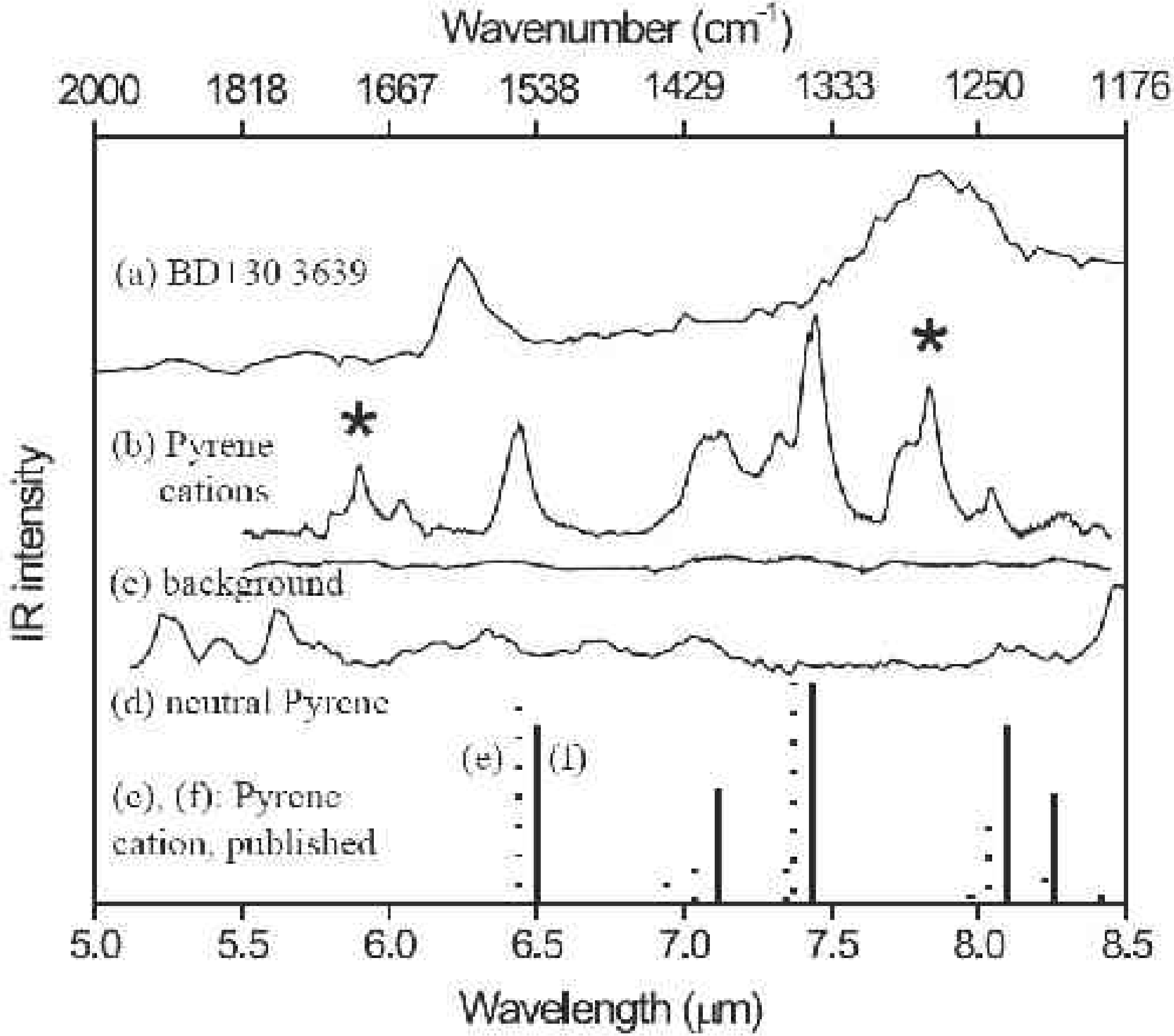
3. Fluorescence outside UIR bands

2. Inverse intensity ratio 3.3 vs. 6.7 μm

The search for PAH Ions







Problems

No mass selection

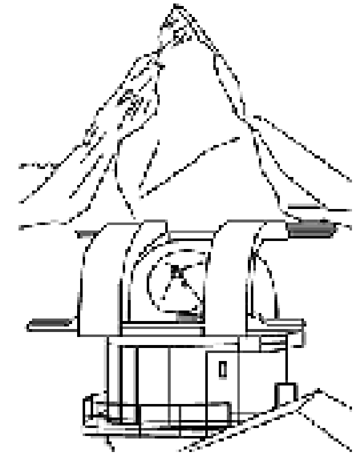
signal from

Parent,
hydrogenated
Dehydrogenated,
Cluster?

Les Houches *September 26, 2005*

Observations and Molecular Spectroscopy

Stephan Schlemmer



WHAT? Observations and basic facts
Classification of spectral ranges

WHY? Identification of Species
Column Densities
Formation and Destruction?
De-/Excitation Mechanisms

HOW? Experimental Techniques (Laboratory work)