Molecular Evolution from AGB Stars to Planetary Nebulae

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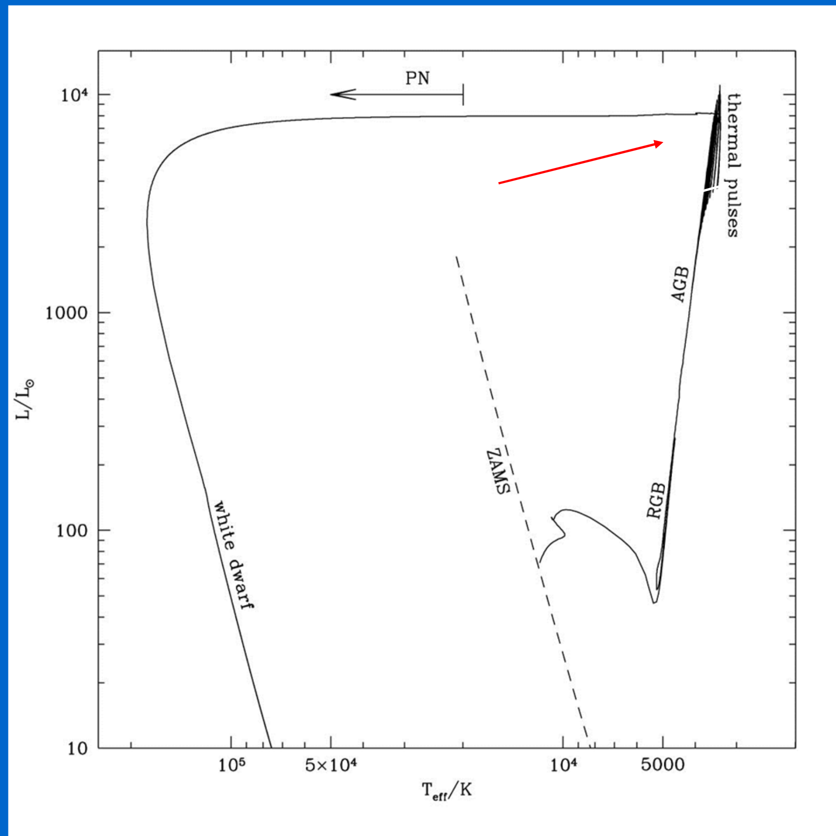
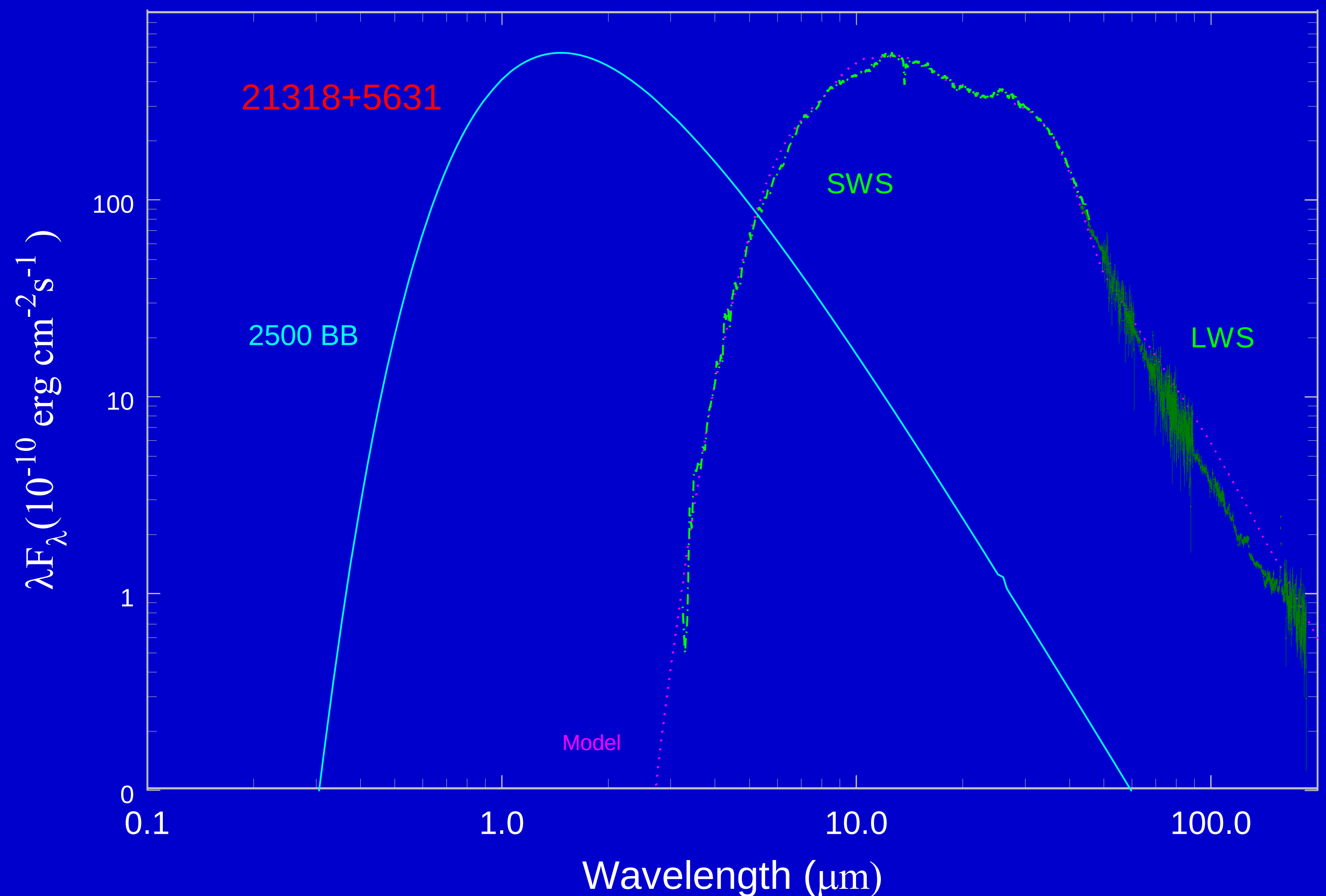
Evolution of intermediate mass (1-8 $M_\odot$) stars

- Triple-α reaction (He→C)
- Slow neutron capture (s-process) (Y, Zr, Ba, La, Ce, Pr, Nd, Sm, Eu, etc)
- Thermal pulse and dredge up
- Mass loss manifested in both IR continuum and molecular emissions



3 $M_\odot$ track

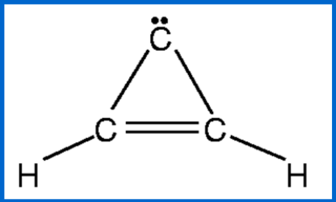
Cirucmstellar dust envelope completely obscures the central star



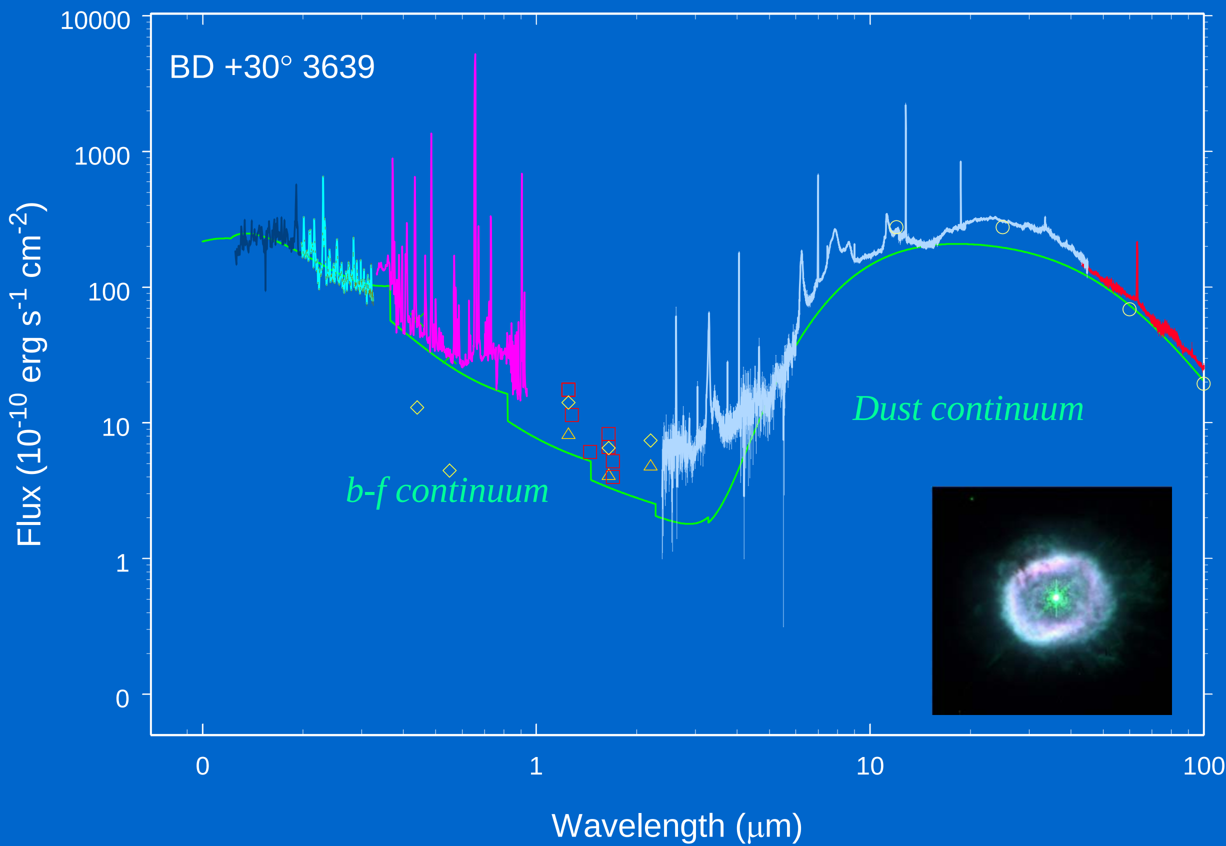
Molecules in the gas phase

- Rotational transitions of over 60 molecules have been detected in the circumstellar envelopes of AGB stars
- Inorganics: CO, SiO, SiS, NH_3, $AlCl$, ..
- Organics: C_2H_2, CH_4, H_2CO, CH_3CN, ..
- Radicals: CN, C_2H, C_3, HCO^+
- Rings (C_3H_2), chains (HC_9N)

AGB stars are prolific molecular factories



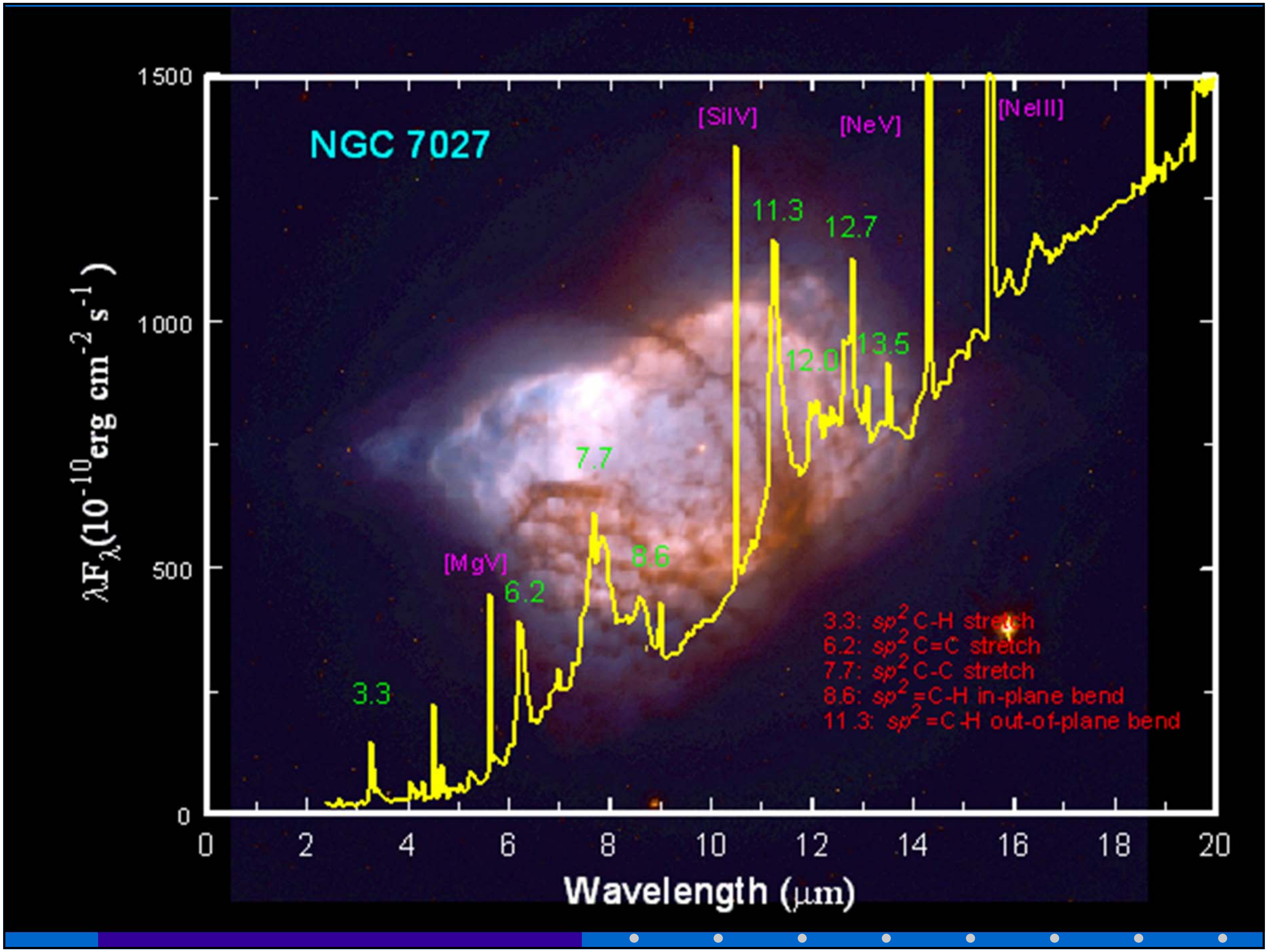
Remnant AGB dust envelope in PN



However, the chemical composition of the dust is not the same

The dust continuum

- Strong continuum emission from a few μm to mm wavelengths
- Cold component (T~50-100 K): remnant of AGB dust envelope
- Warm component (T~200 K): dust formed in post-AGB evolution

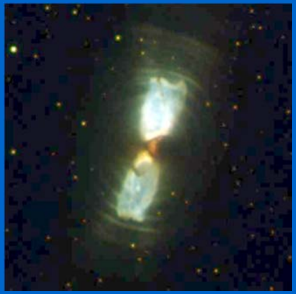

NGC 7027
1500
1000
500
0
0
2
4
6
8
10
12
14
16
18
20
Wavelength (μm)
λFλ(10⁻¹⁰erg cm⁻² s⁻¹)
3.3
[MgV]
6.2
7.7
8.6
[SiIV]
11.3
12.0
12.7
13.5
[NeV]
[NeIII]
3.3: sp2 C-H stretch
6.2: sp2 C=C stretch
7.7: sp2 C-C stretch
8.6: sp2 =C-H in-plane bend
11.3: sp2 =C-H out-of-plane bend

When are the aromatic compounds synthesized?

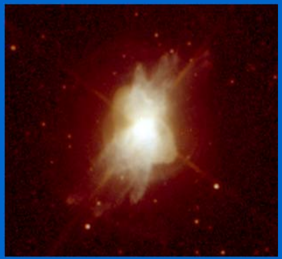
- Aromatic infrared bands (AIB) not seen in AGB stars
- AIBs are strong in young planetary nebulae
- Must have emerged during the evolution between AGB and PN phases

Proto-planetary nebulae

- Objects in transition between AGB and PN stages
- ~30 PPN are known, most discovered as the result of follow up of the IRAS survey (Kwok 1993, *Ann. Rev. Astr. Ap.*, 31, 63)

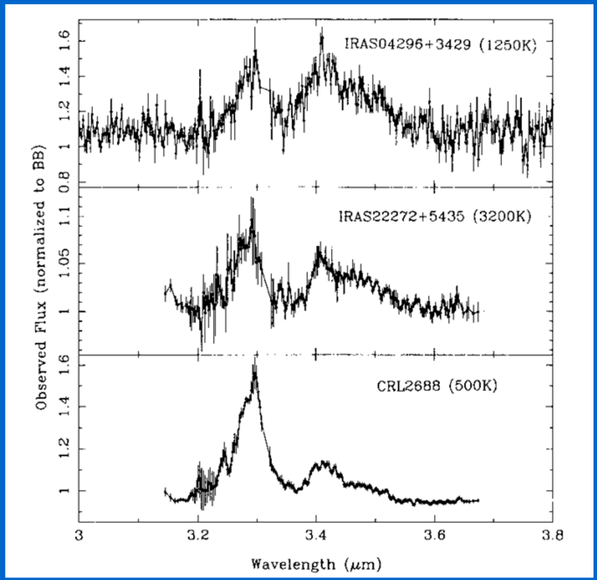


No UV radiation, visible image due to scattered starlight

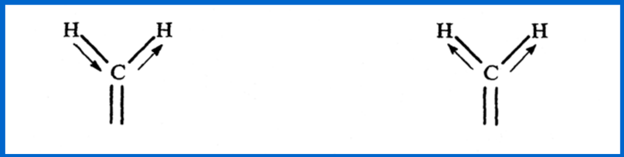


3.4 μm aliphatic C-H stretch

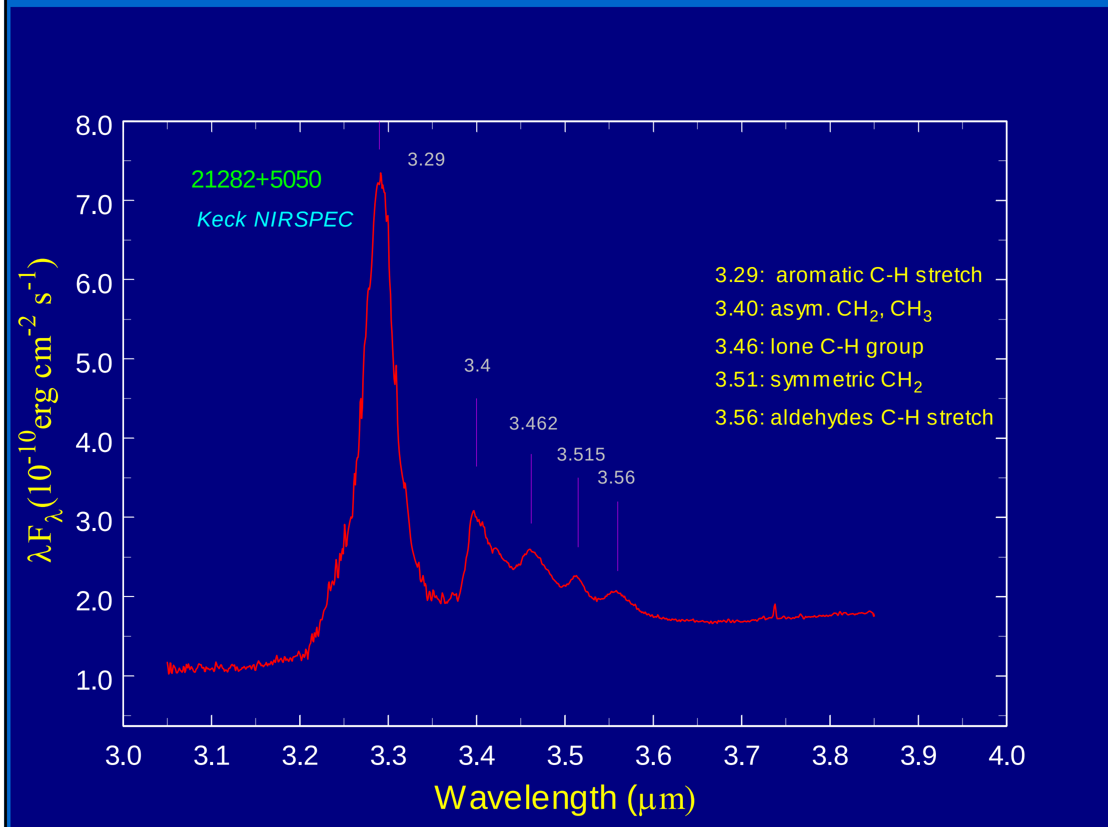
- 3.38 μm: asymmetric CH_3
- 3.42 μm: asymmetric CH_2
- 3.46 μm: lone C-H group
- 3.49 μm: symmetric CH_3
- 3.51 μm: asymmetric CH_2

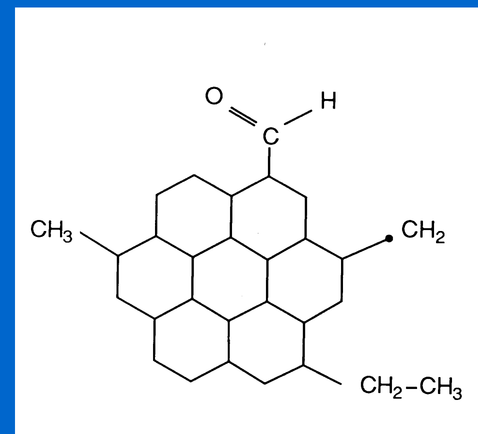


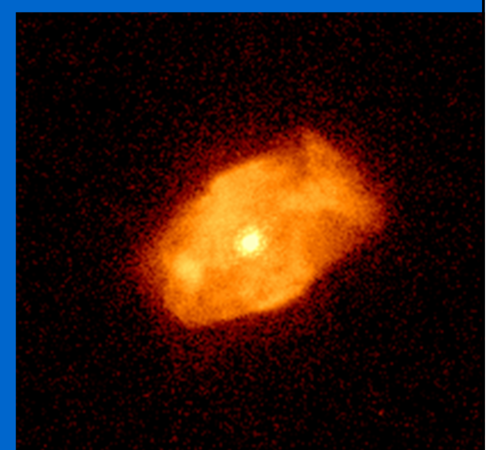
The 3.4 μm feature just as strong as the 3.3 μm feature



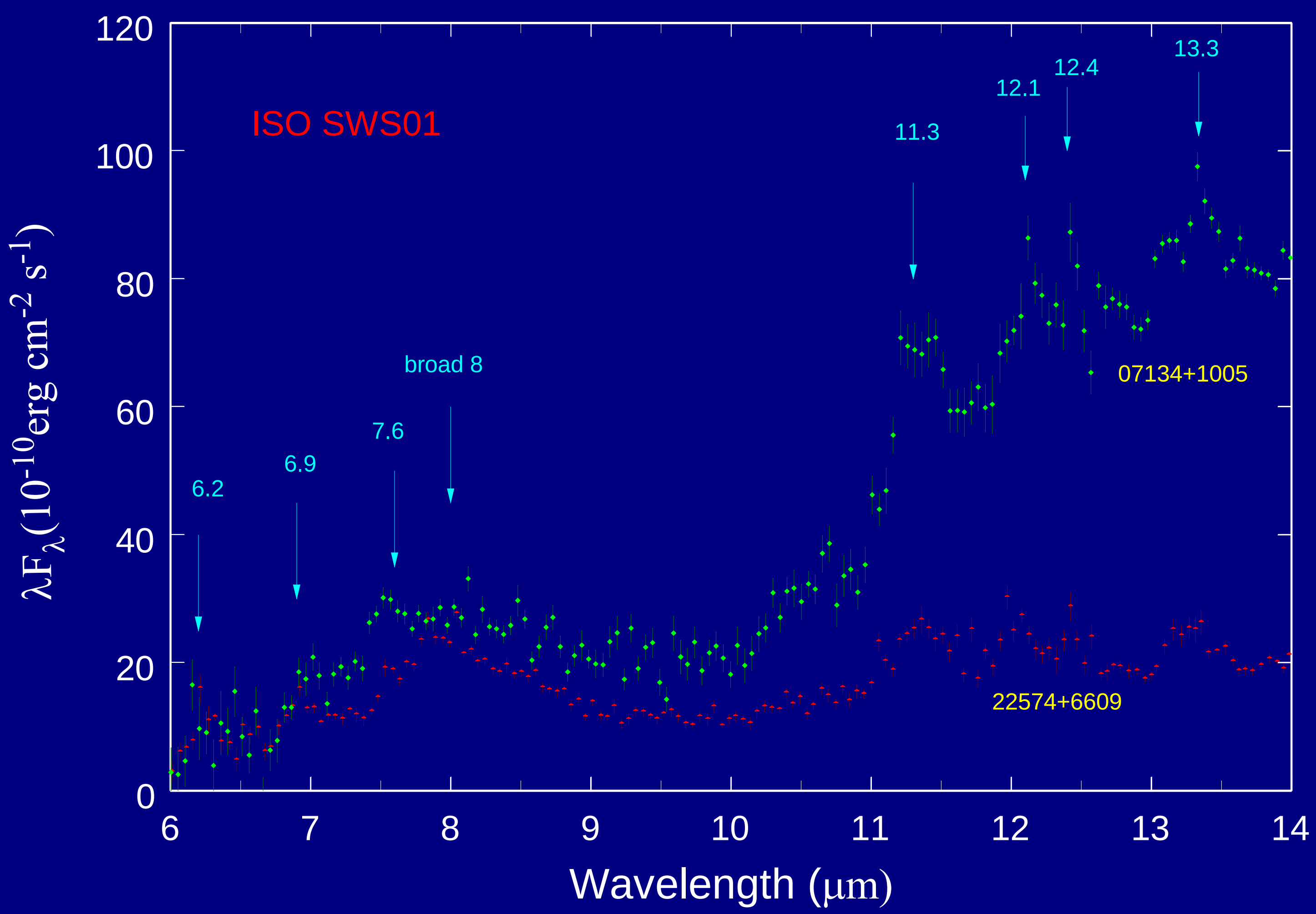
Aliphatic sidegroups in young PN







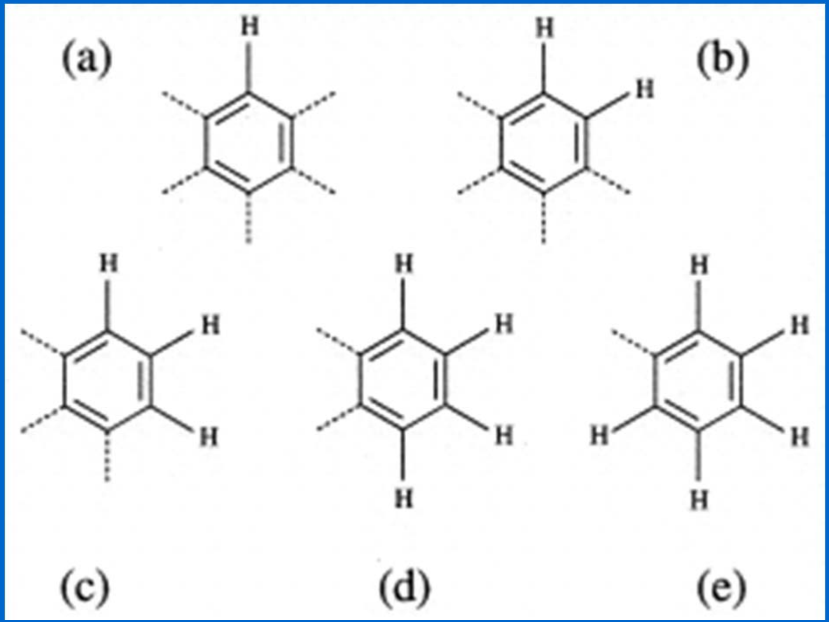
6.9 μm aliphatic C-H bending mode in PPN spectra



Sizes of the aromatic units

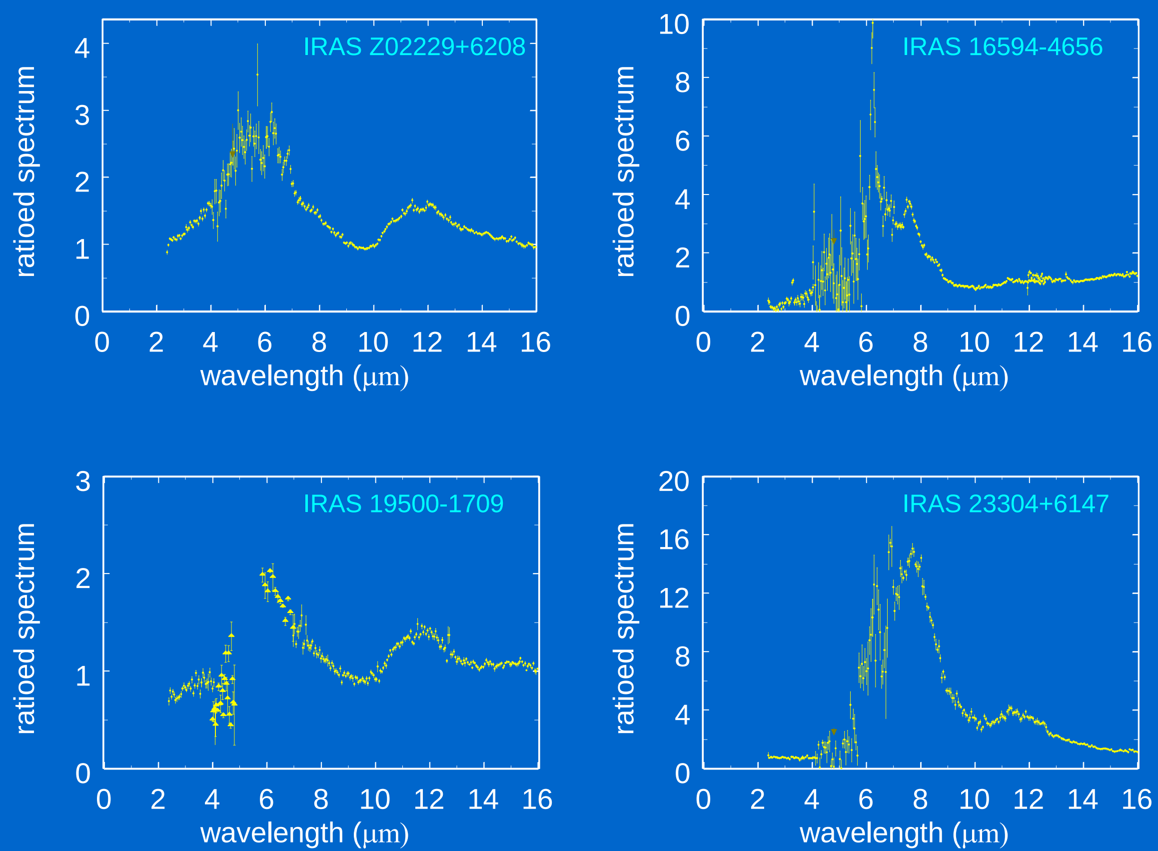
- Solo: 11.1-11.6 μm
- Duo: 11.6-12.5 μm
- Trio:12.4-13.3 μm
- Quarto: 13-13.6 μm

Frequencies of out-of-plane bending modes depend on the number of exposed edges

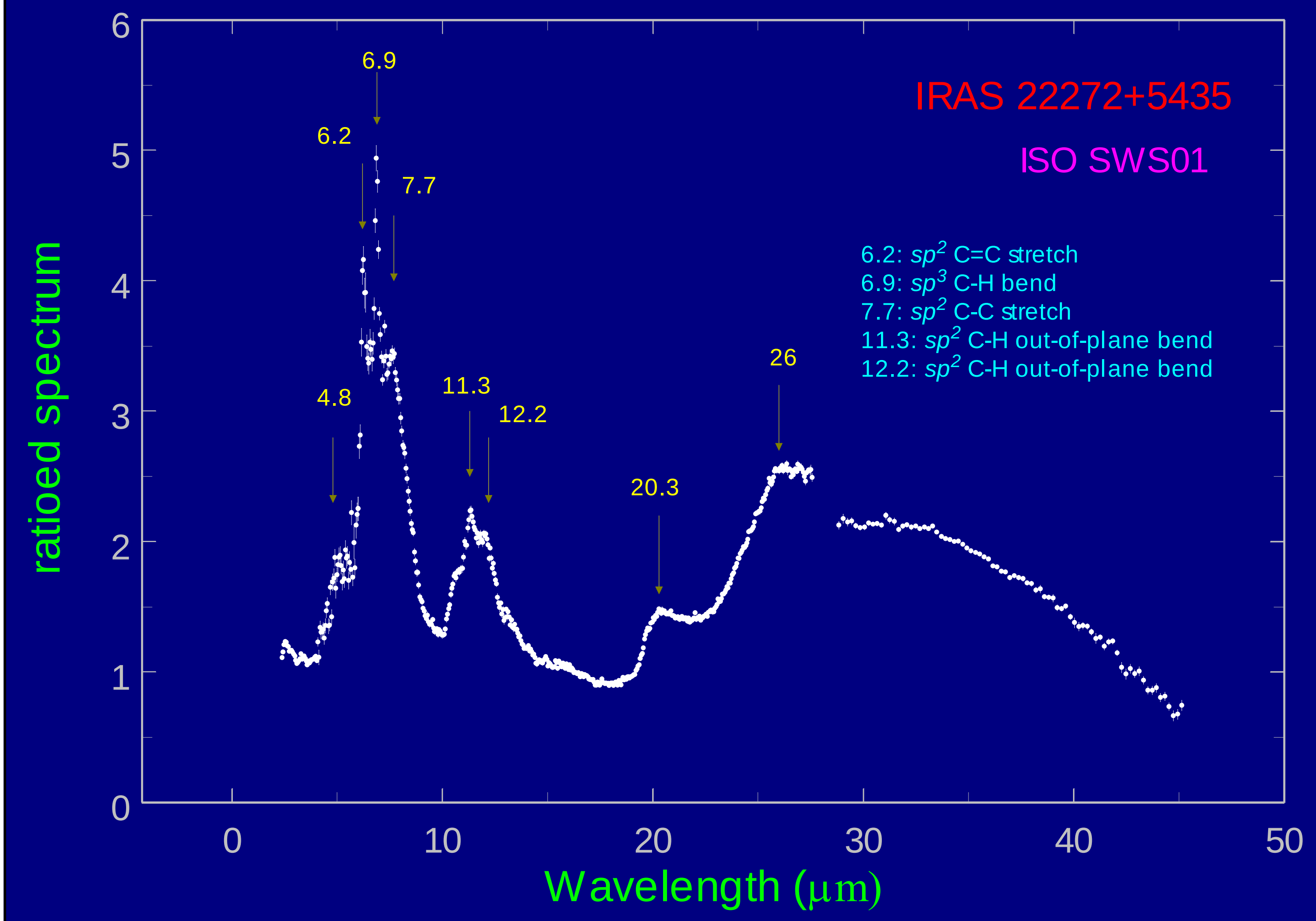


Hugdins and Allamandola 1999

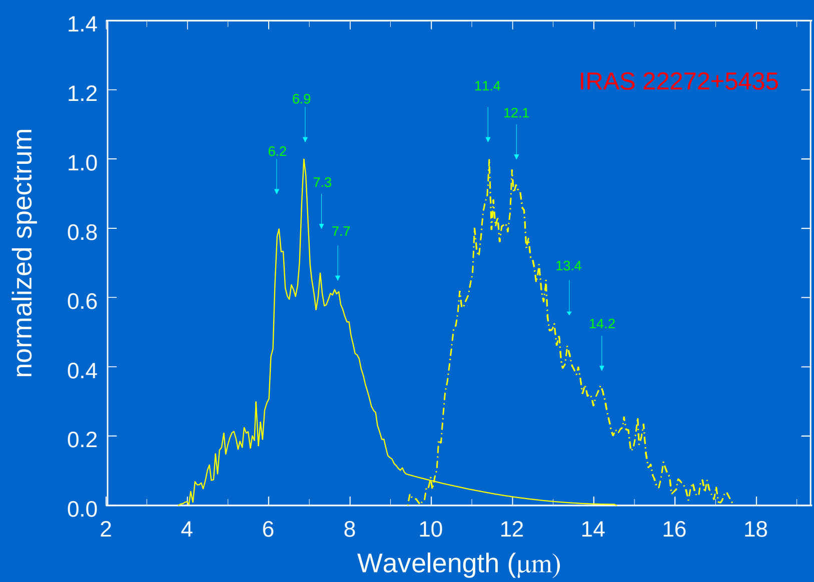
Broad emission plateaus

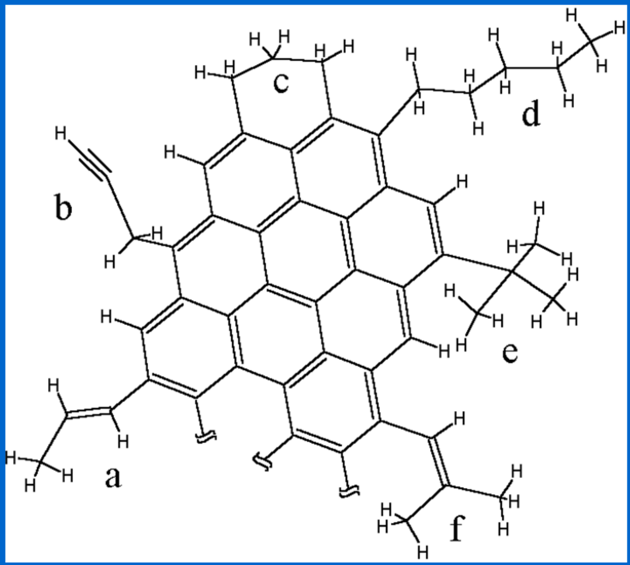


8 and 12 μm plateau features



Aliphatic bending modes



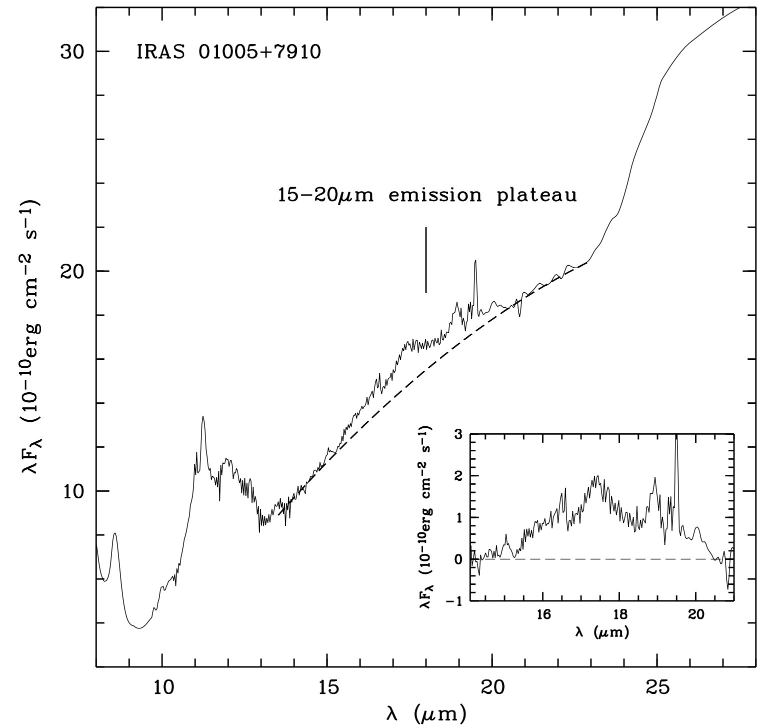


Kwok et al. 2001

- 8μm plateau: $-CH_3$ (7.25 μm), $-C(CH_3)_3$ (8.16 μm, “e”), $=(CH_3)_2$ (8.6 μm, “f”)
- 12 μm plateau: C-H out-of-plane bending modes of alkene (“a”, “b”), cyclic alkanes (9.5-11.5 μm, “c”), long chains of $-CH_2-$ groups (13.9 μm, “d”).

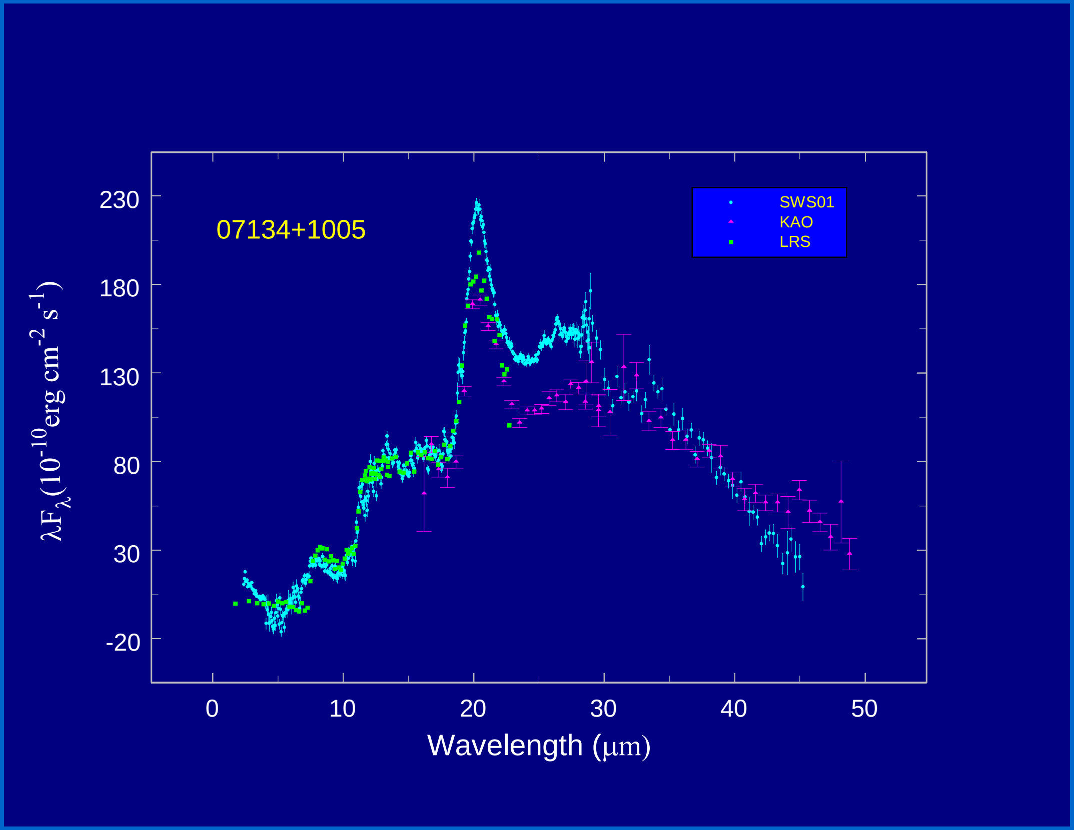
17 µm p

- Aromatic C-C-C in- and out-of-plane distortion? (Van Kerckhoven et al. 2000)



Zhang et al. 2010

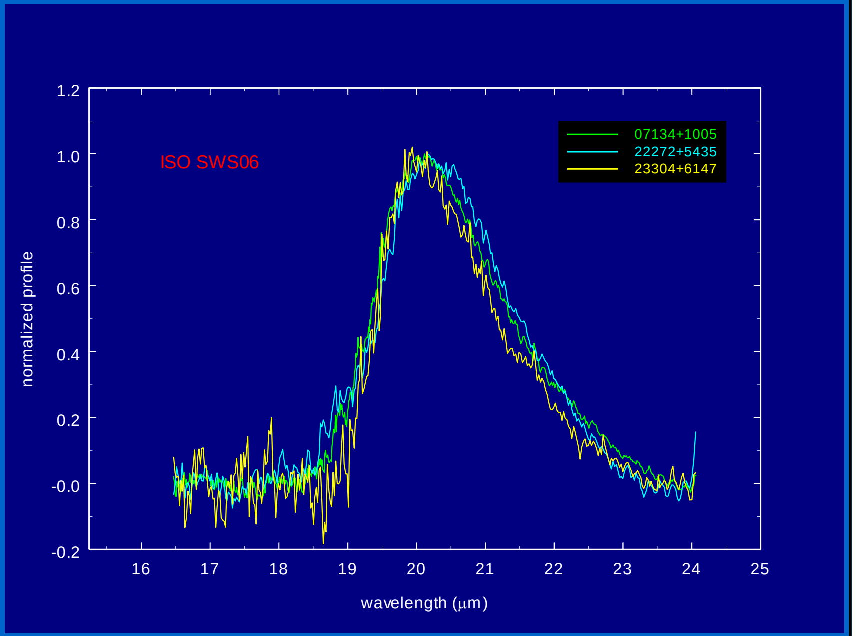
Unidentified 21 μm Feature



First detected by *IRAS LRS* in C-rich post-AGB stars (Kwok, Volk & Hrivnak 1989)

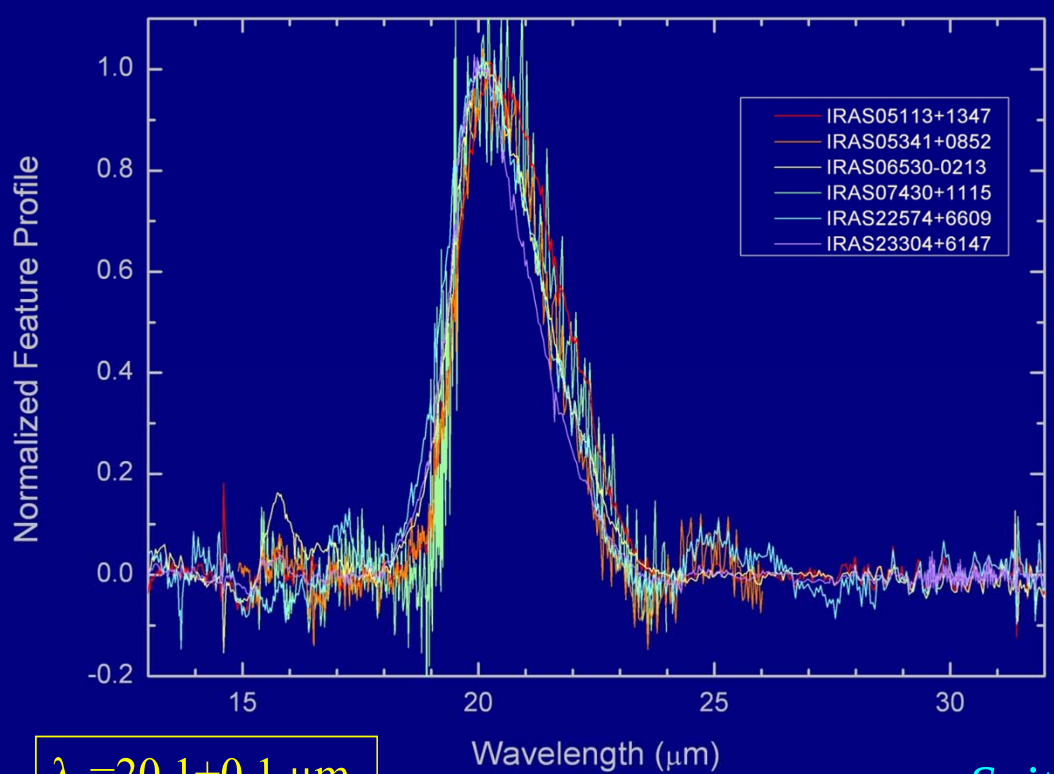
Asymmetric profiles

- *ISO SWS06* (λ/Δλ~2000)
- Uniform asymmetric shape after removal of cool continuum
- Consistent peak wavelength of 20.1 μm
- No sign of substructure⇒solid state



Volk et al. 1999

Consistent profiles

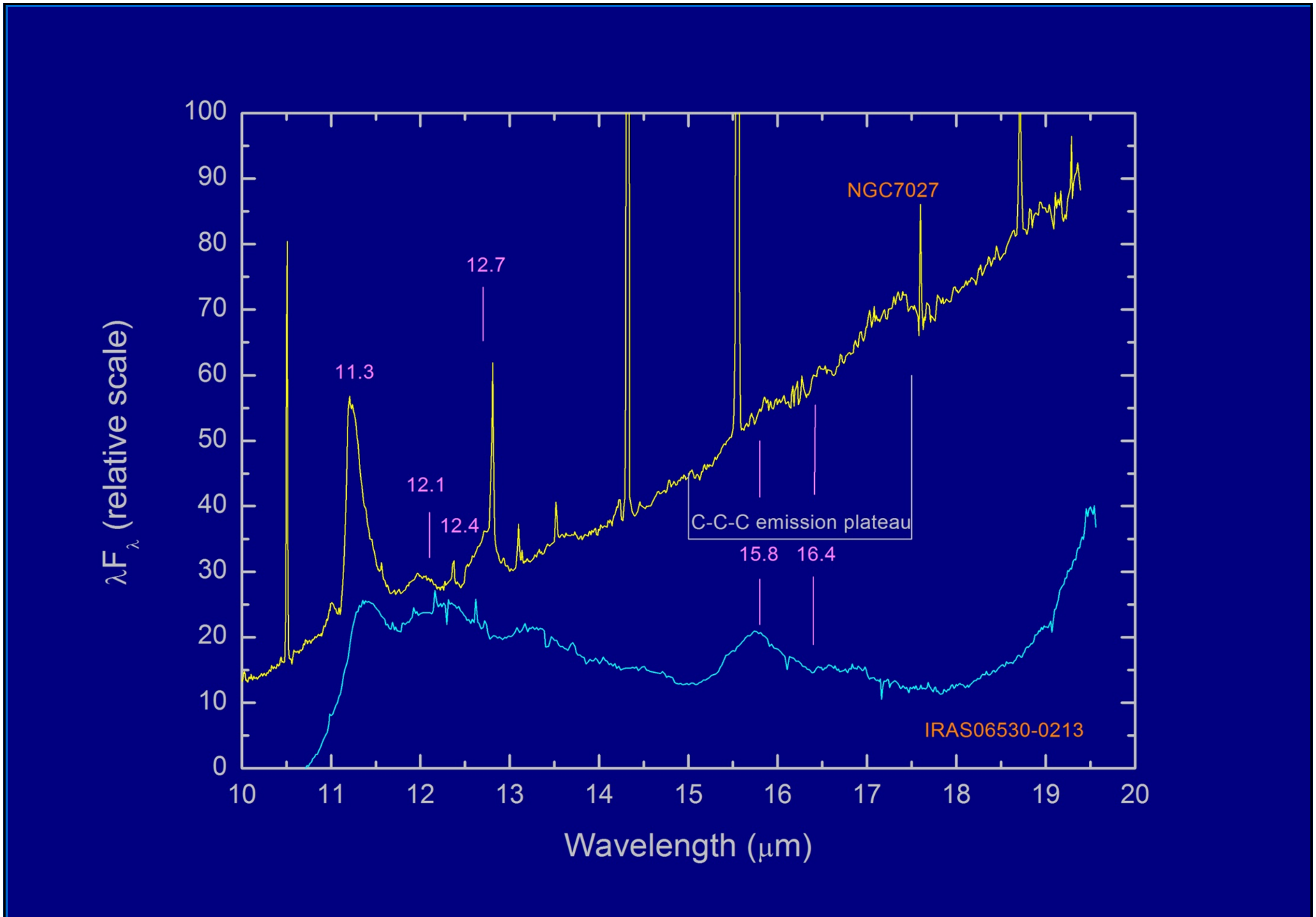


λ_0=20.1±0.1 μm

Spitzer IRS

Carrier of the 21 μm Feature

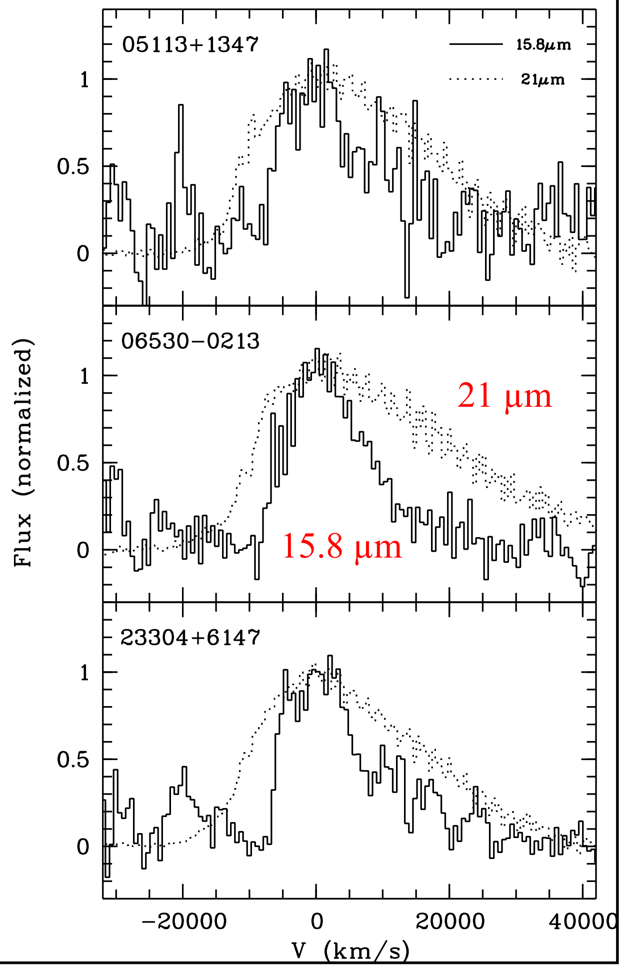
- Solid SiS_2: Goebel (1993), Begemann et al. (1996)
- Maghemite (Fe_2O_3) or magnetite (Fe_3O_4): Cox (1991)
- Amides (urea or thiourea): Courisseau et al. (1992), Papoular (2011)
- Hydrogenated amorphous carbon: Buss et al. (1990)
- Hydrogenated fullerenes ($C_{60}H_m$, m=1, 2…60) and their ions: Webster (1995)
- nanodiamonds (Hill et al. 1998)
- TiC nanoclusters (von Helden et al. 2000)
- O-substituted 5-member carbon rings (Papoular 2000)
- $^3\pi$-$^1\Sigma$ transition of C_2 (Gruen 2001)
- SiC (Speck & Hofmeister 2004)



Features at 15.8 and 16.4 μm

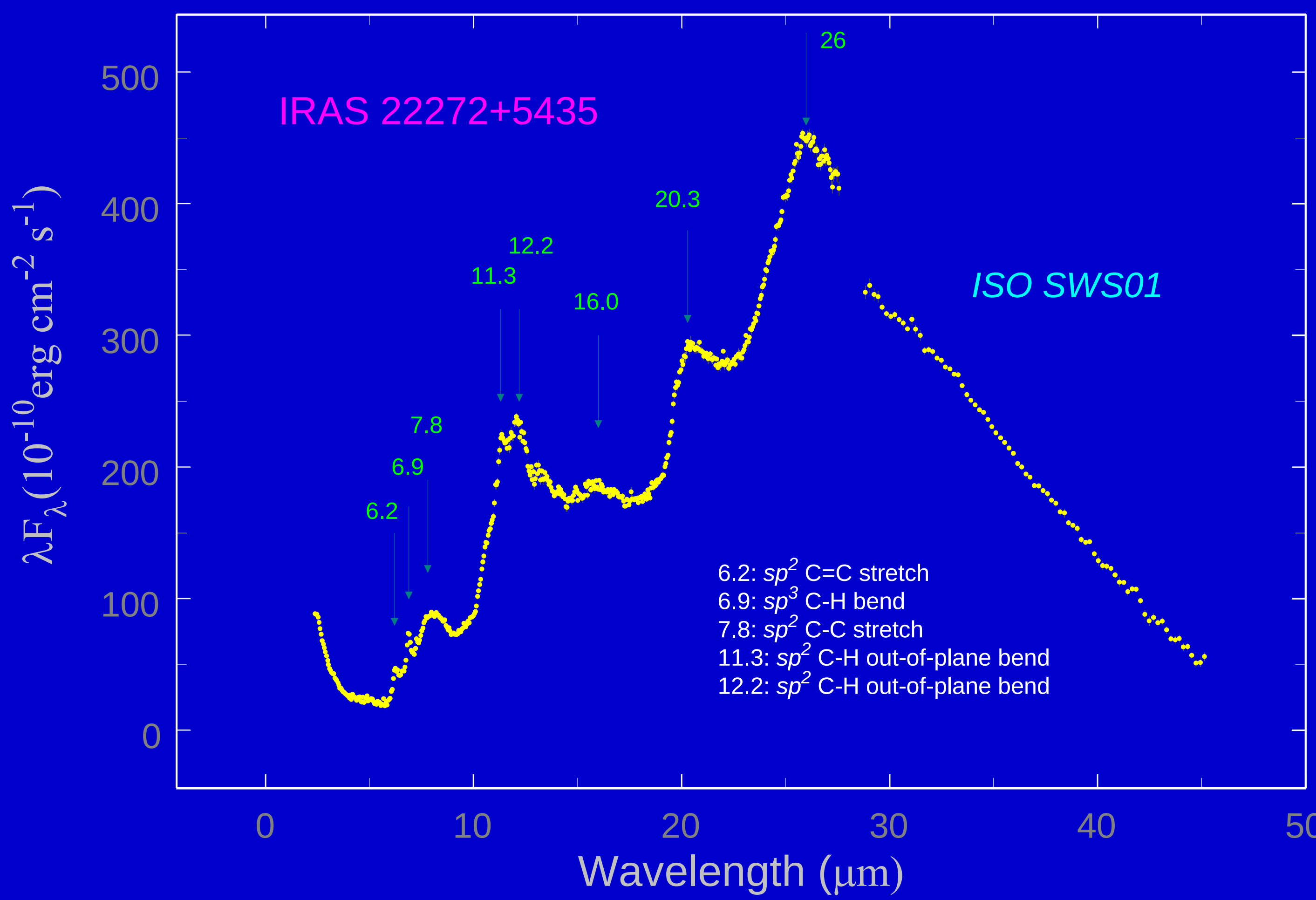
15.8 μm fe

- Δλ~1.3 μm
- Strong in 21 μm sources

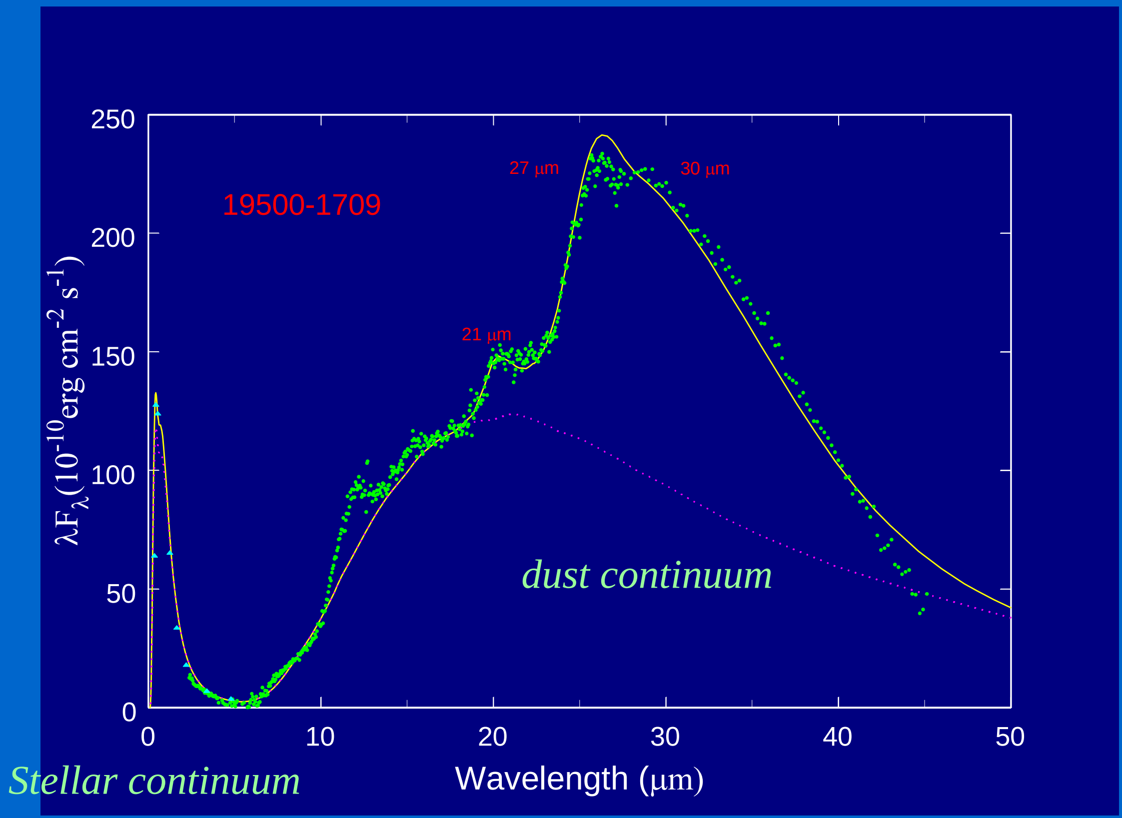


Hrivnak et al. 2009, Zhang et al. 2010

Unidentified 21 and 30 μm features



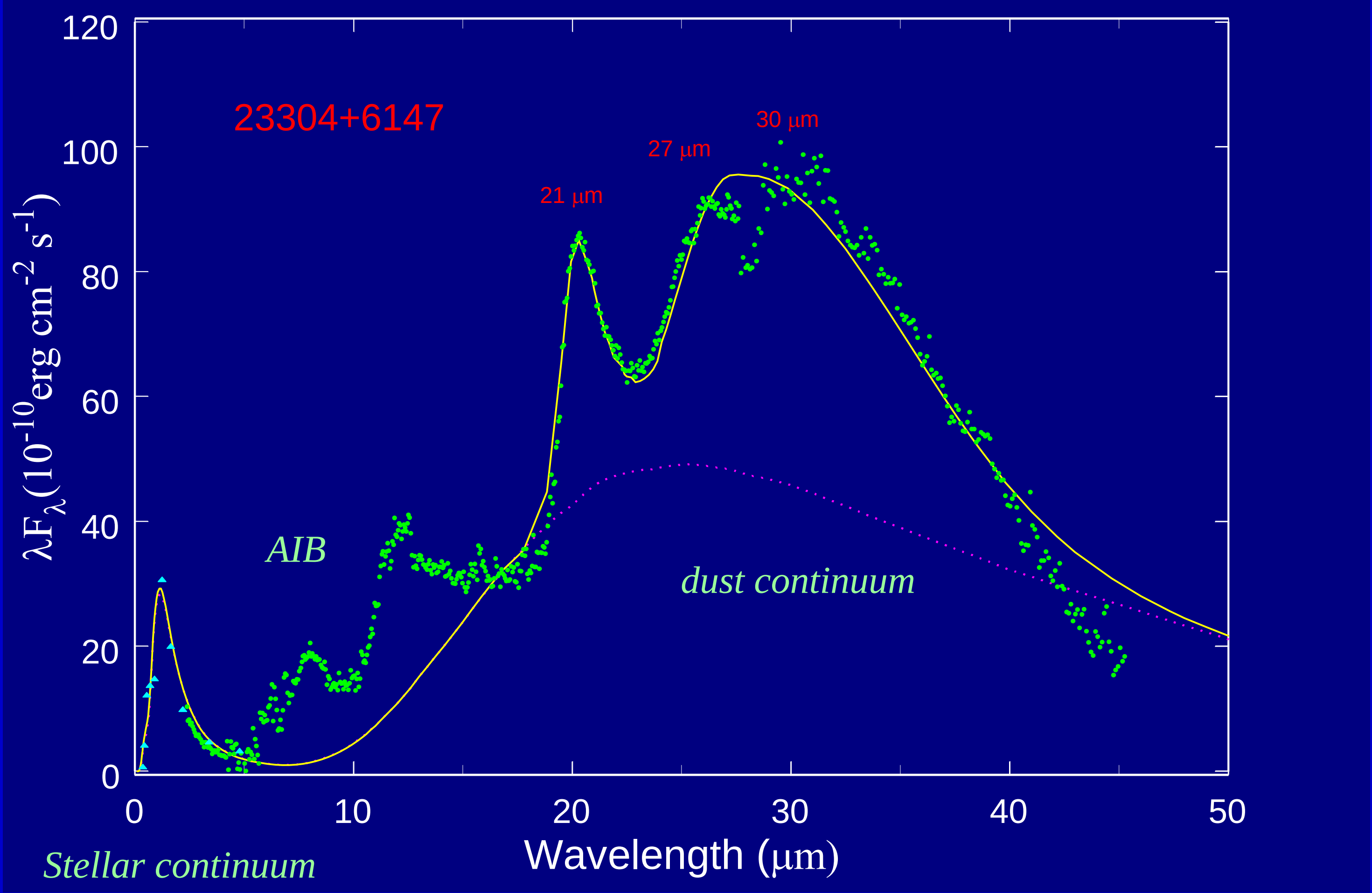
30 Micron Feature



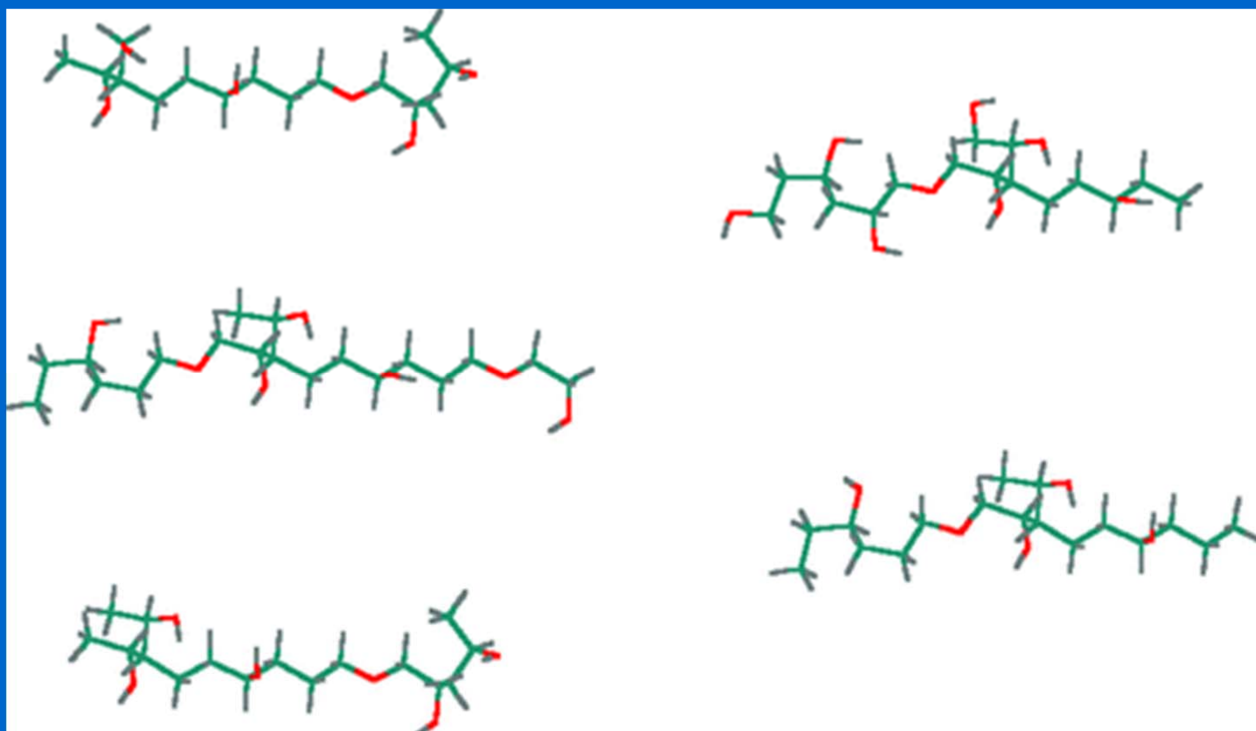
First detected in IRC+10216, AFGL 3068, IC 418, and NGC 6572 (Forrest et al. 1981)

Now observed in a number of PPNs

AIB, 21, and 30 μm features in C-rich PPN



The roles of O, S, and N

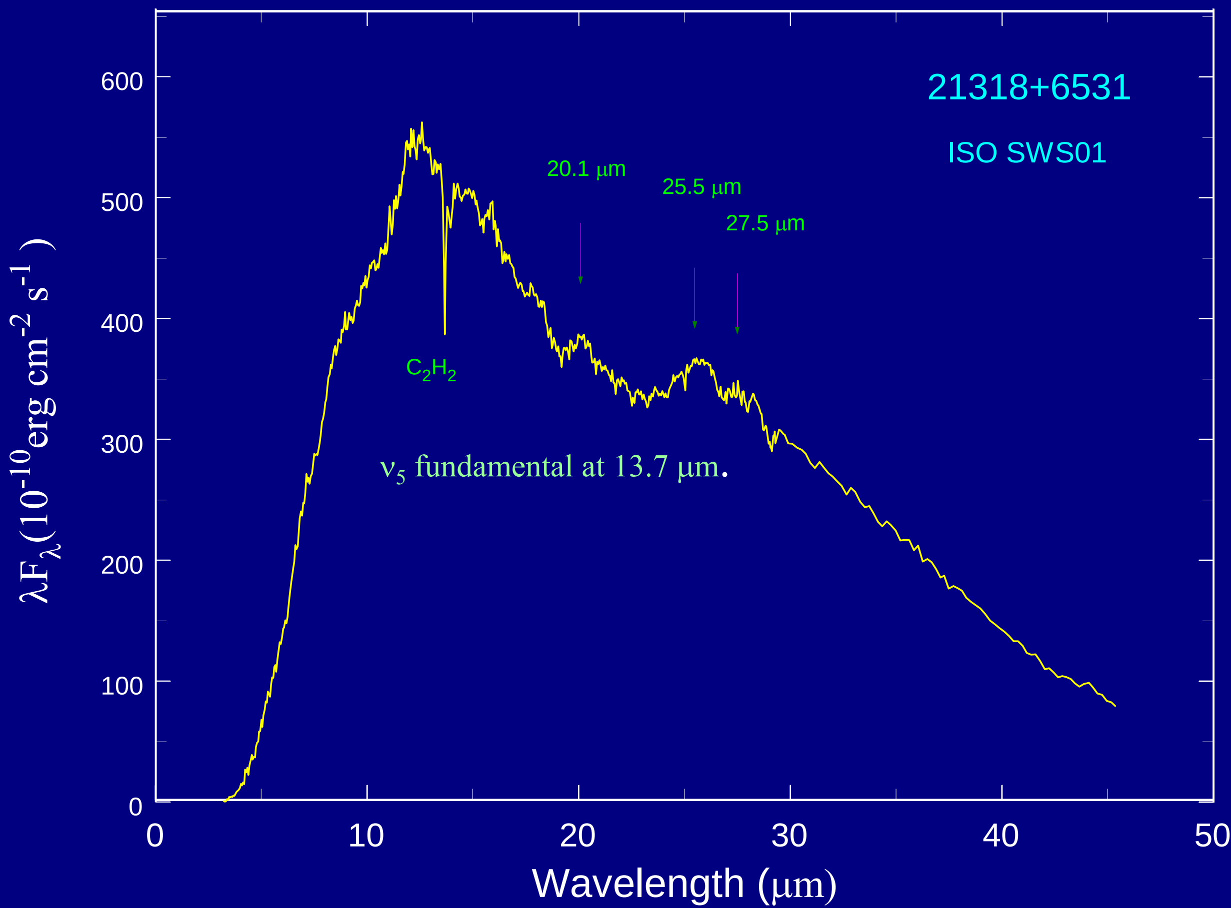


Red: O
Green: C
Grey: H

Aliphatic chains of CH_2 groups, oxygen bridges, and OH groups

Papoular 2011

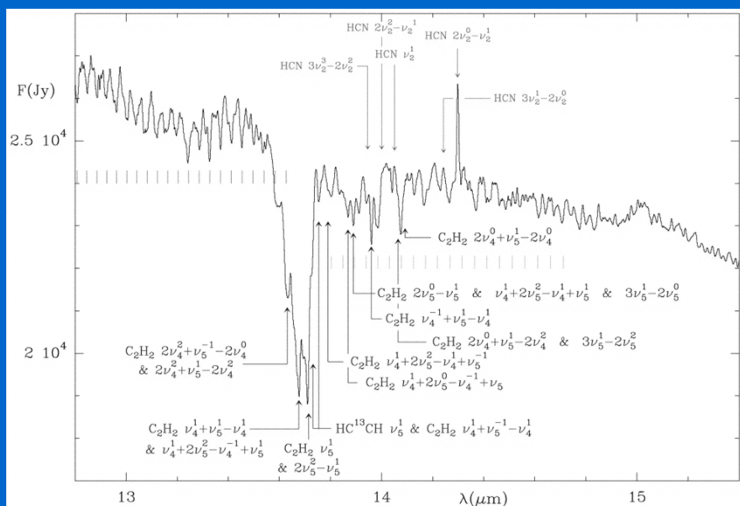
30 μm feature first appear in carbon stars



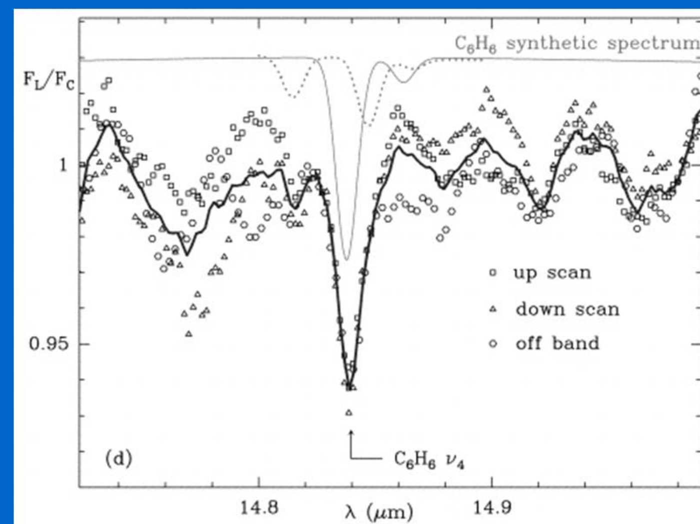
Extreme carbon stars with optically thick envelopes

Volk et al. 2000

From acetylene to benzene

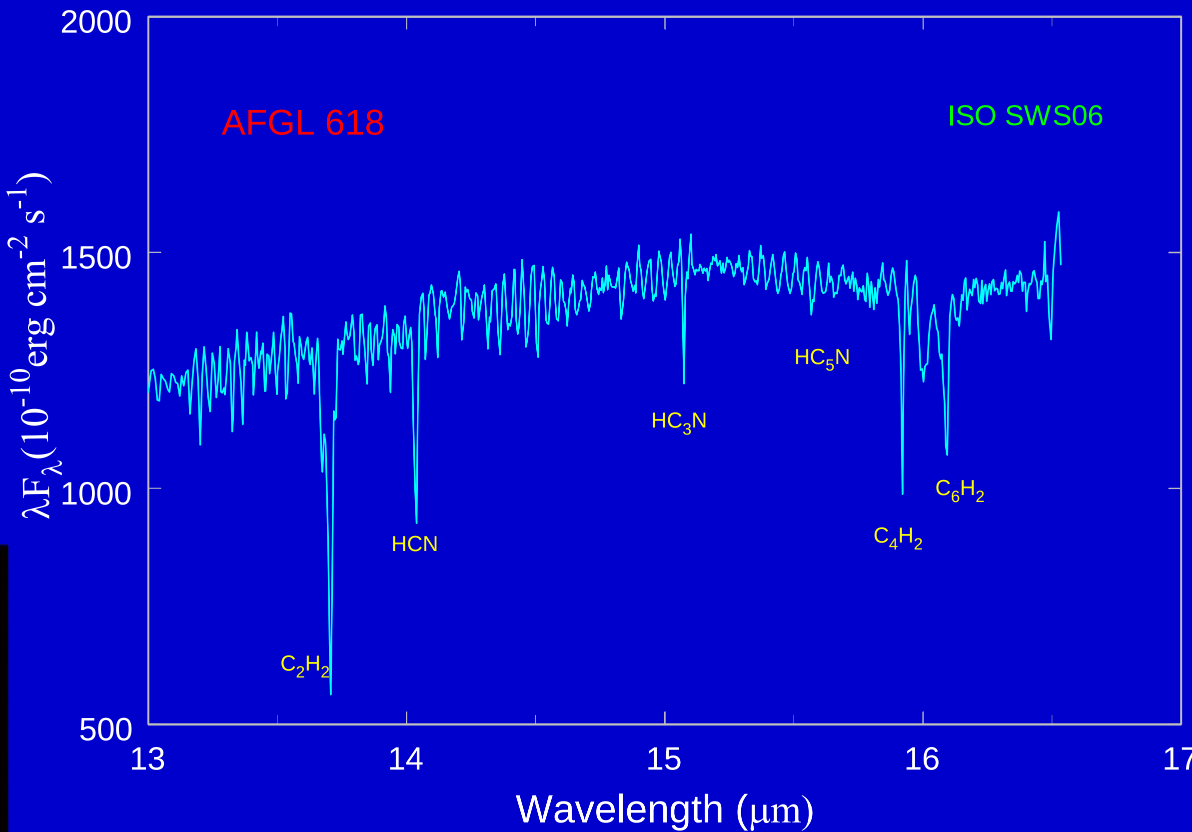


IRC+10216: bending modes of C_2H_2 (Cernicharo et al. 1999)



AFGL 618: C_4H_2, C_6H_2, C_6H_6 (Cernicharo et al. 2001)

Polymerization of C_2H_2 in Post-AGB evolution



Chemical evolution from AGB to PN

- Extreme carbon stars (t~10^4 yr): $C_2H_2 \Rightarrow C_6H_6$
- PPN (t~10^3 yr): clusters of aromatic rings with peripheral aliphatic bonds
- PN (t~10^4 yr): loss of H and a progressive formation of clusters of rings into more structured units

Photochemistry

- The 8 and 12 μm plateau features are due to a variety of alkane and alkene groups attached to hydrogenated aromatic rings.
- When exposed to UV light, the aliphatic side groups are modified, leading to larger aromatic rings.
- Isomerization, bond migrations, cyclization reactions.
- Ring closure and cycloaddition transform alkenes into ring systems.
- H loss leads to fully aromatic rings

Net result: UV transforms aliphatic to aromatic groups

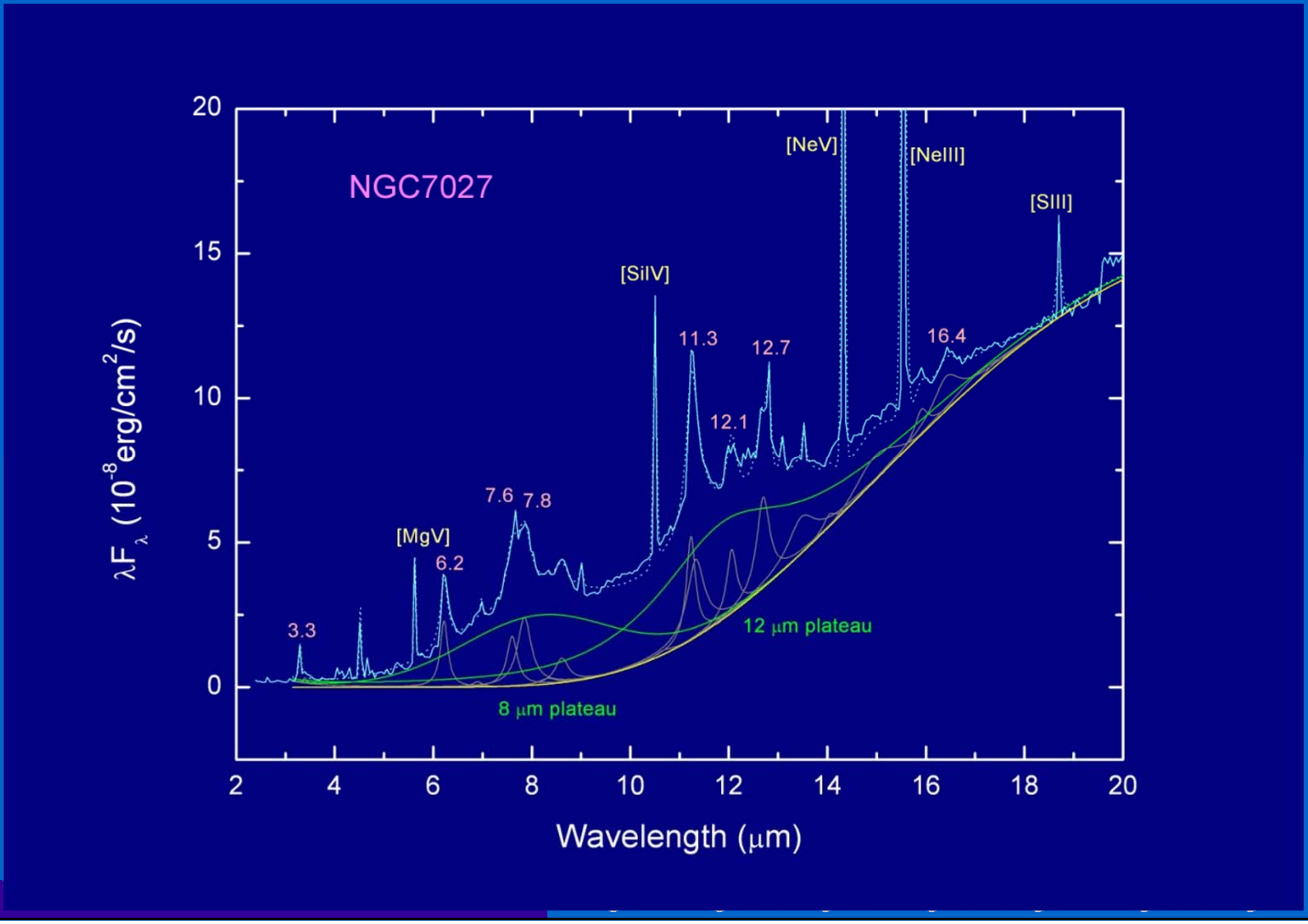
Advantages of circumstellar chemistry

- Single energy source
- Simple geometry
- Well-determined physical environment (density $\rho(r)$, temperature $T(r)$, radiation background $I(r)$)
- Chemical time scale defined by dynamical time scale (AGB: 10^4 yr, PPN: 10^3 yr, PN: 10^4 yr)

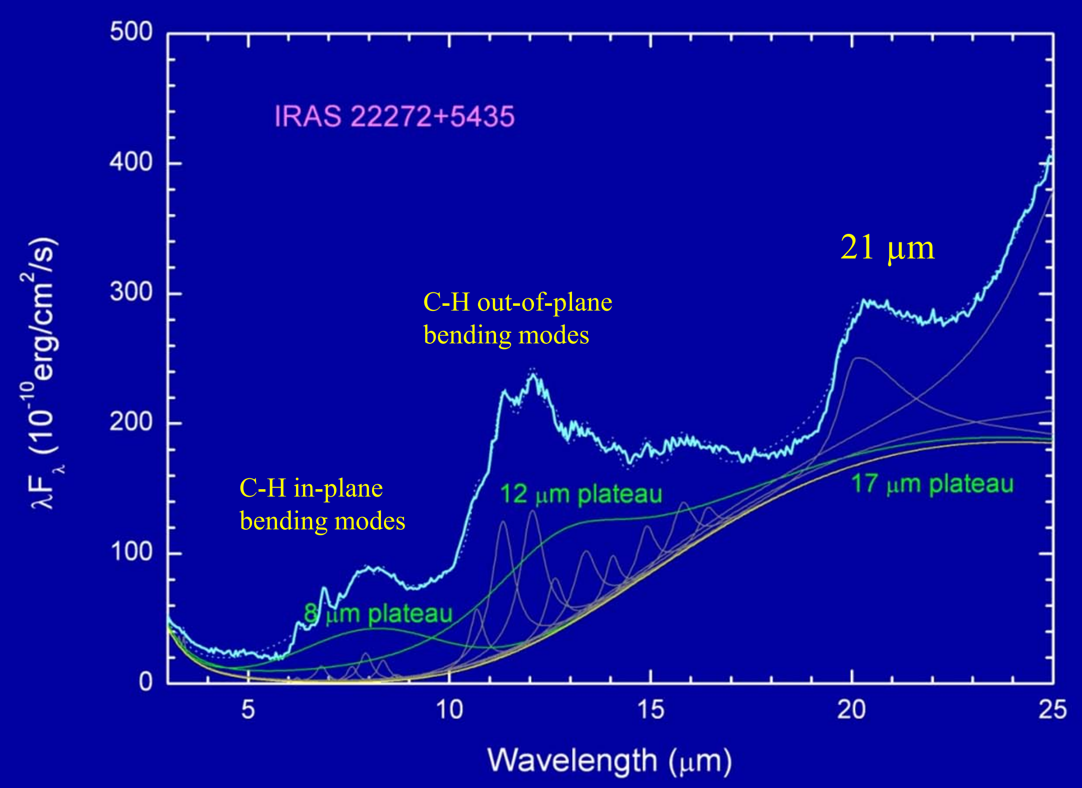
Spectroscopic properties

- A strong continuum from 3-200 μm
- Aromatic features at 3.3, 6.2, 7.7, 8.6, and 11.3 μm
- Aliphatic features at 3.4, 6.9 μm
- Other features at 15.8., 16.4, 17.4, 17.8, and 18.9 μm
- Plateau features at 8, 12, 17 μm

Spectral fitting



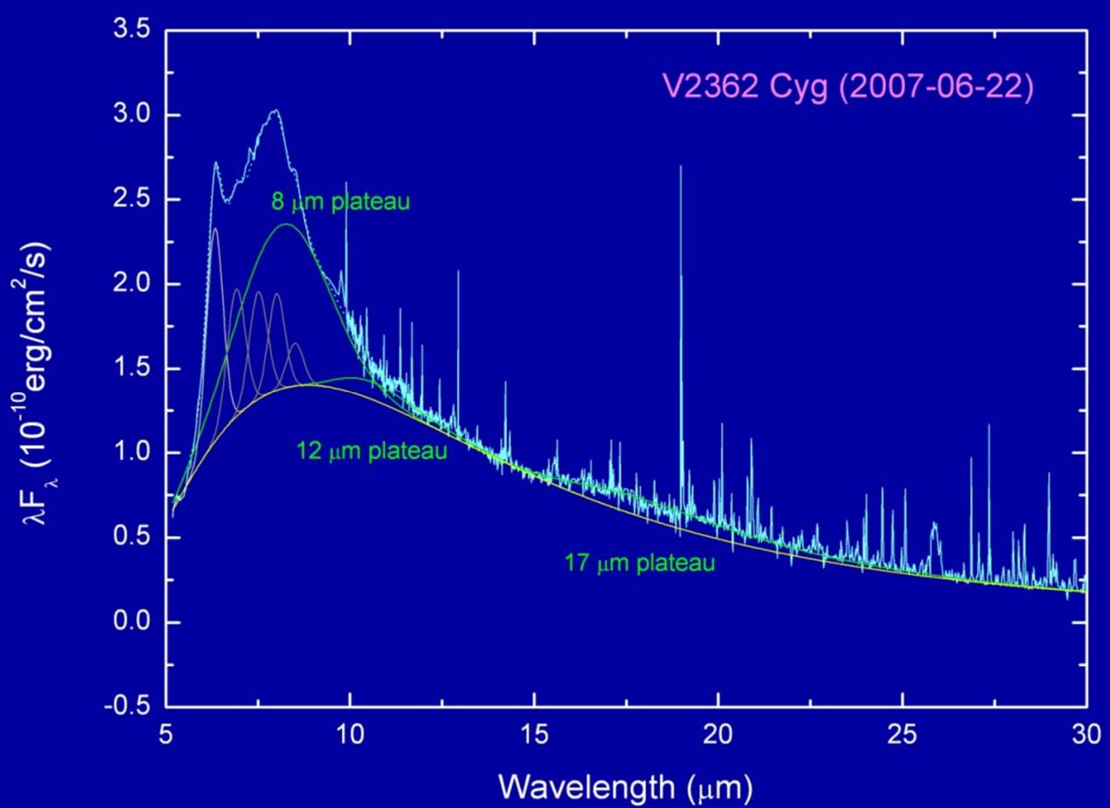
Proto-planetary nebulae



How do they form?

- Surface temperature of red giants: 3000 degrees
- Solid grains condensed from gas in the stellar wind under near vacuum conditions
- Theoretically impossible, especially during the PPN phase
- Observationally we see aliphatics and aromatics form in PPN on time scales as short as hundreds of years
- In novae, they form on a time scale of days

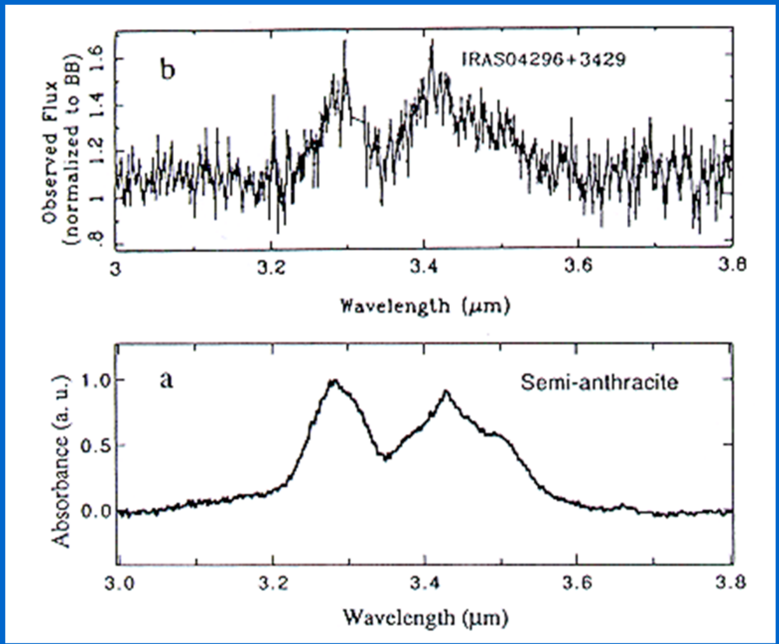
Organics in novae

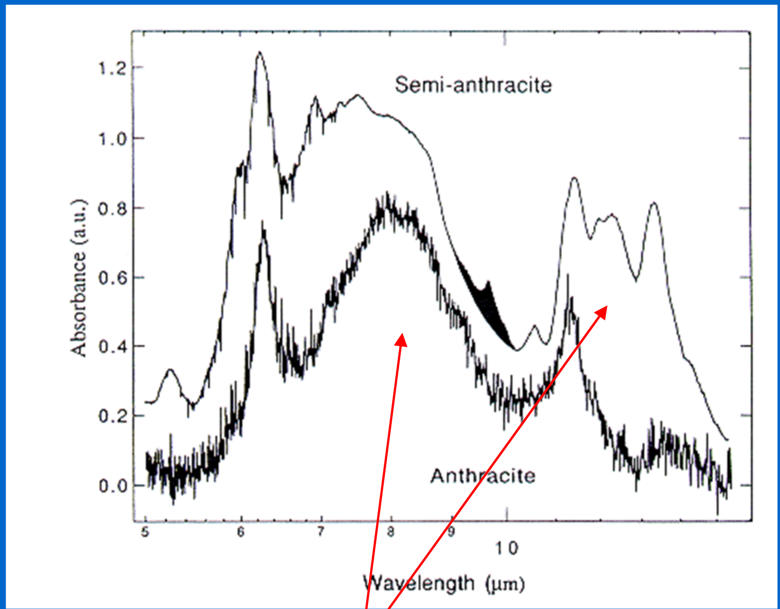


What is the chemical structure of the carrier?

- Natural substances: coal (Papoular et al. 1989), kerogen, petroleum fractions (Cataldo et al. 2002), soot
- Artificial substances: hydrogenated amorphous carbon (HAC, Jones et al. 1990), quenched carbonaceous composites (QCC, Sakata et al. 1987), carbon nanoparticles (Duley & Hu 2009, Jäger et al. 2009), tholins, HCN polymer

Infrared Spectrum of Coal



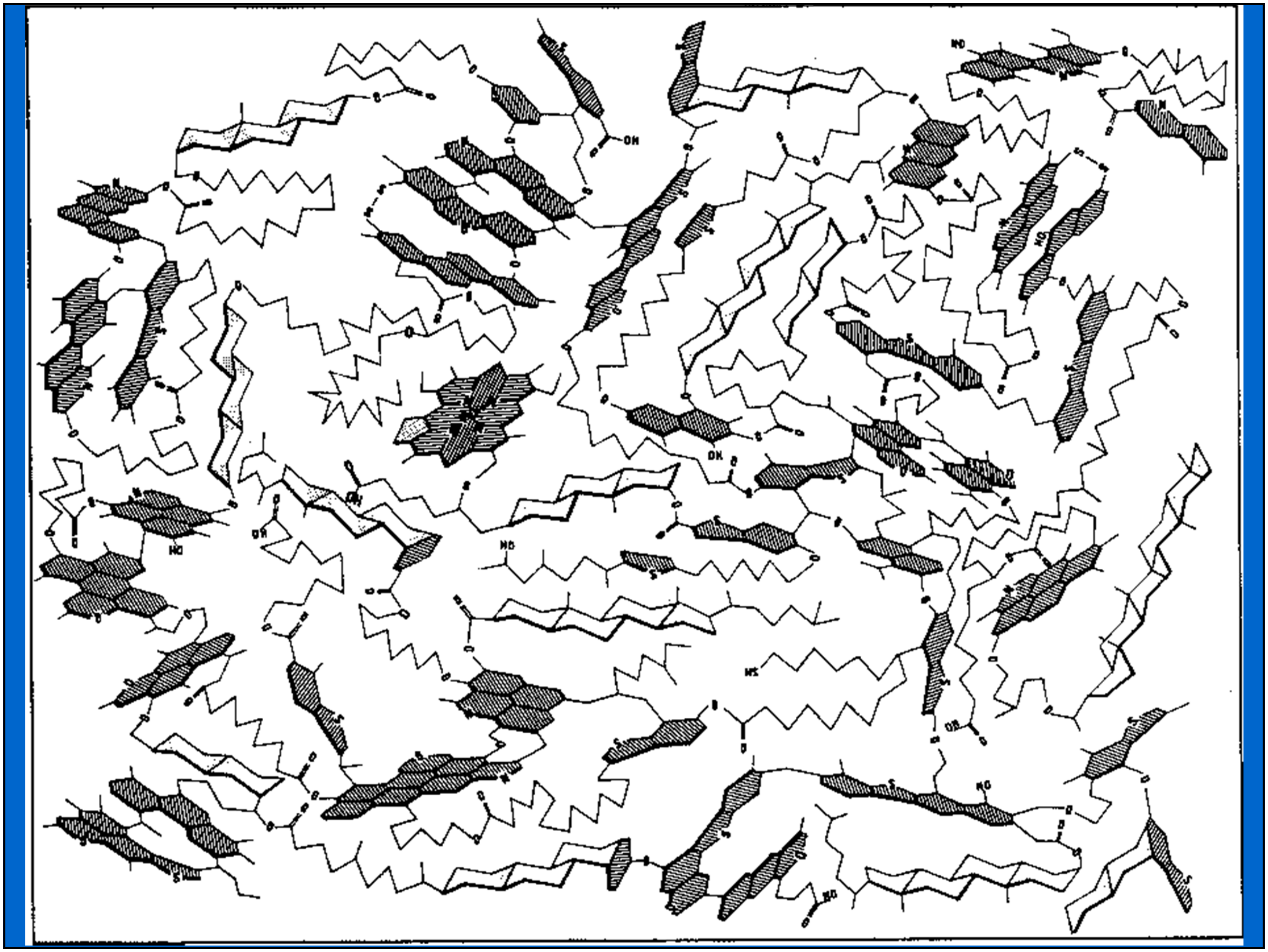


Emission plateaus

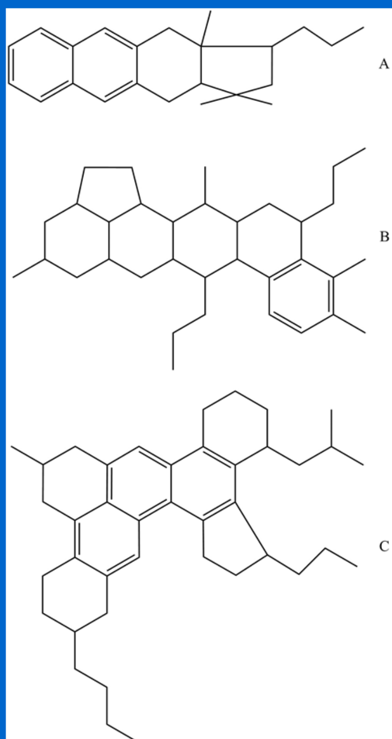
Guillois et al. 1996

Kerogen

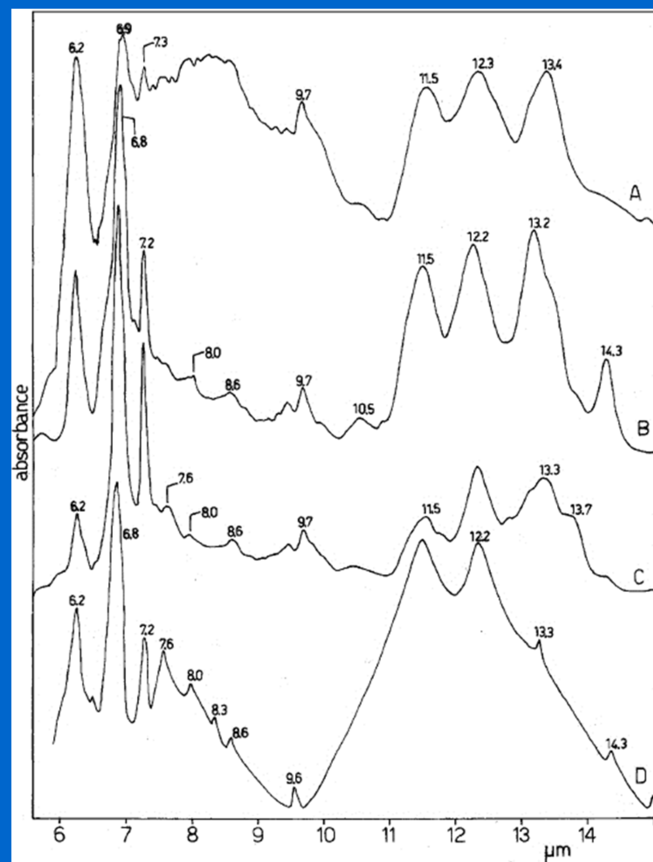
- random arrays of aromatic carbon sites, aliphatic chains $(-CH_2-)_n)$, and linear chains of benzenic rings with functional groups made up of H, O, N, and S attached
- a solid sedimentary, insoluble, organic material found in the upper crust of the Earth



Petroleum fractions



Cataldo et al. 2004



Anthracite coal

Modified fraccion 2

Distillate aromatic extract

PPN 22272+5435

Laboratory Simulations of Cosmic Dust

- Quenching of plasma of 4-torr methane (Sakata et al. 1987)
- Hydrocarbon flame or arc-discharge in a neutral of hydrogenated atmosphere (Colangeli et al. 1995)
- HAC films prepared by laser ablation of graphite in a hydrogen atmosphere (Scott and Duley 1996)
- Infrared laser pyrolysis of gas phase molecules (C_2H_4, C_4H_6)$\Rightarrow$C-based nanoparticles (Herlin et al. 1998)

Pure C & H or with N?

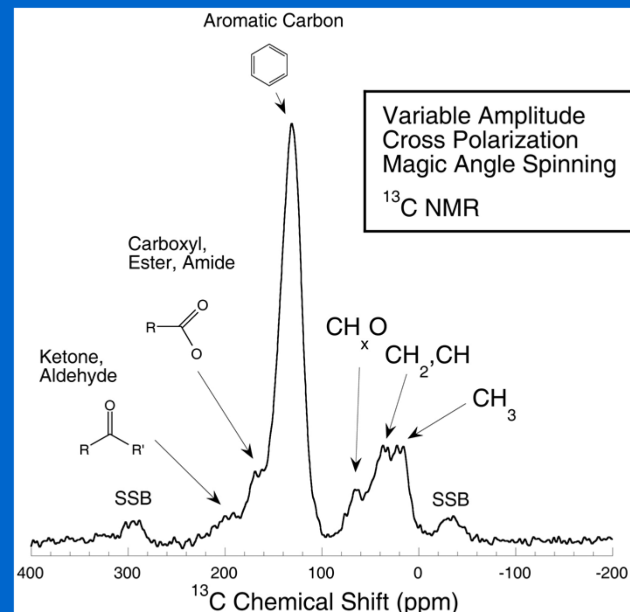
- QCC: hydrocarbon plasma deposition
- Tholins: refractory organic materials formed by UV photolysis of reduced gas mixtures (N_2, NH_3, CH_4, etc.)
- HCN polymers: amorphous hydrogenated carbon nitride, formed spontaneously from HCN

Organics in the Solar System

- Planets and their satellites, asteroids, comets, minor bodies in the outer Solar System
- Traditional picture: made up of minerals, metals, and ices
- Organics represent a major component of meteorites, comets, asteroids, and IDPs (talk by Alexander)

Carbonaceous Chondrite Meteorites

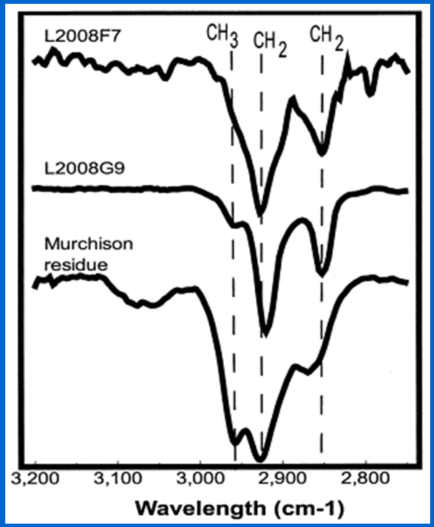
- Over 70% of the organic matter in meteorites is in the form of insoluble macromolecular material similar to kerogen (Kerridge 1999)
- possibly of interstellar origin due to excess of D, ^{13}C, ^{15}N, etc.

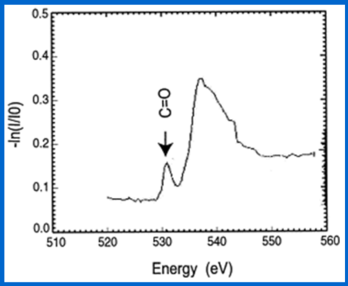


Functional groups identified in Murchison IOM (Cody et al. 2011)

Interplanetary Dust

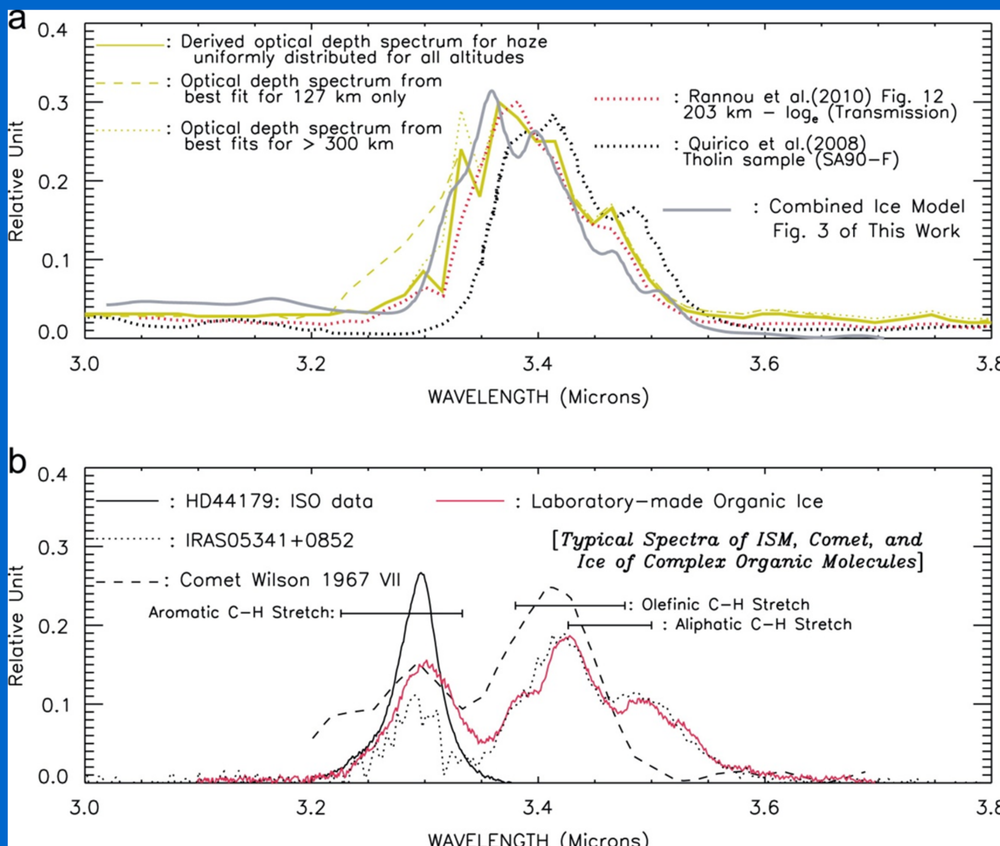
- Few microns to tens of microns in size (Brownlee 1978)
- Silicates (olivine & pyroxene)
- 10-12% carbon content
- 3.4 µm aliphatic feature and sometimes C=O group (Flynn et al. 2003, Keller et al. 2004)





O-XANES spectrum of IDP

Comparison between 3.4 μm features in Titan haze, comets, and PPNs

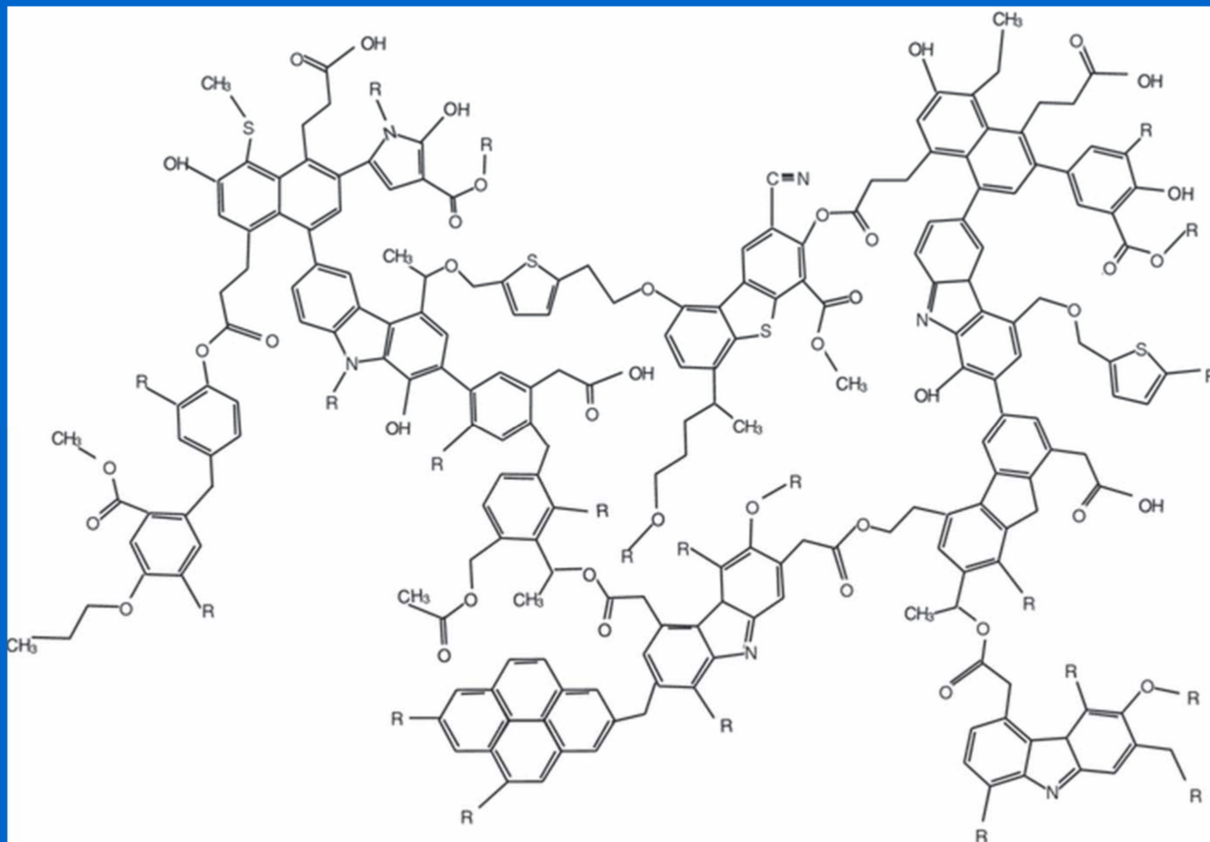


Kim et al. 2011

Kim et al. 2011

A model

- the organic matter in PN and PPN show a lot of similarities to IOM in meteorites and organic solids in comets and IDPs.
- An amorphous solid with mixed aromatic/aliphatic structure
- Contains impurities (O, N, S,) beyond C and H
- Small aromatic islands linked by aliphatic bridges
- Nanometer to micrometer in size



- *R: organic moiety*
- *Aromatic rings and aliphatic chains*
- *O, N, S impurities*

Derenne & Robert 2010

Summary

- Organic compounds are everywhere in the Universe (from solar system to ISM to galaxies)
- Hydrocarbons with linear, aromatic and aliphatic structures are detected in the circumstellar envelopes of evolved stars
- These carbonaceous materials undergo a change from aliphatic to aromatic structures during the transition from PPN to PN
- Chemical evolution leading to complex organic compounds can take place over only a few thousand years in the circumstellar environment

Summary (cont.)

- The detection of pre-solar grains suggests that grains from AGB stars can survive the journal through the ISM and reach the Solar System
- Macromolecular organics in meteorites, IDP, comets, and planetary satellites show similarities with organics produced by planetary nebulae
- To what extent was the Early Earth chemically enriched by the early bombardment?

A star-Earth connection