Fullerenes in circumstellar and interstellar environments

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Presence of C_{60} and C_{70} in space firmly established

Diverse sources

Unexpected: Neutral and cool

Unclear: Formation
state (solid/gas)
excitation mechanism

Cami, Bernard-Salas, Peeters, Malek, 2010, Science 329, 1180.

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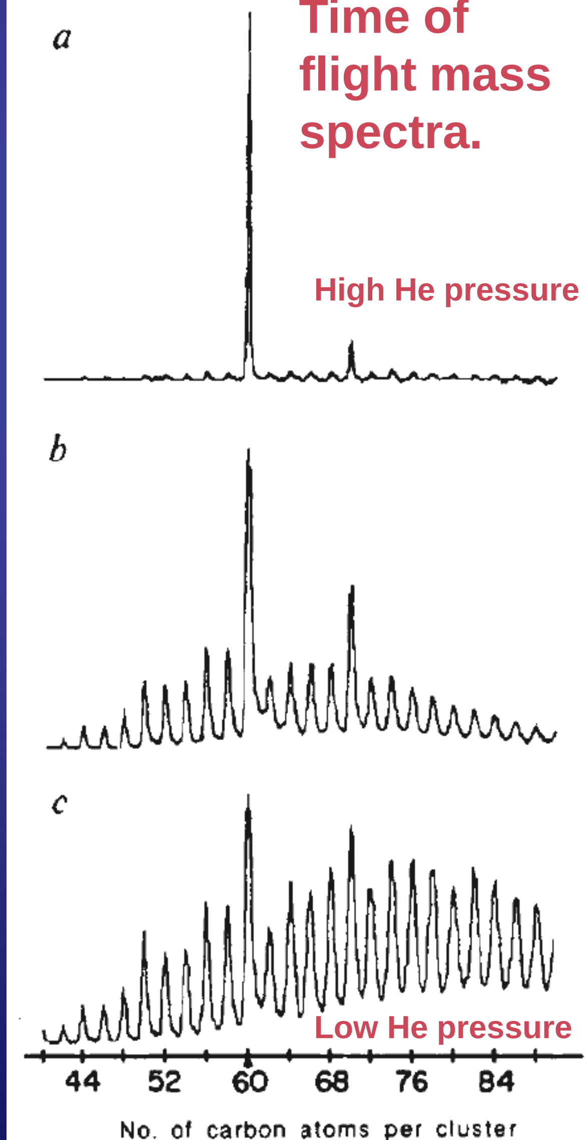
Fig. 1 A football (in the United States, a soccerball) on Texas grass. The C_{60} molecule featured in this letter is suggested to have the truncated icosahedral structure formed by replacing each vertex on the seams of such a ball by a carbon atom.

The discovery of C_{60} and C_{70}

Kroto et al. 1985

Time of flight mass spectra.



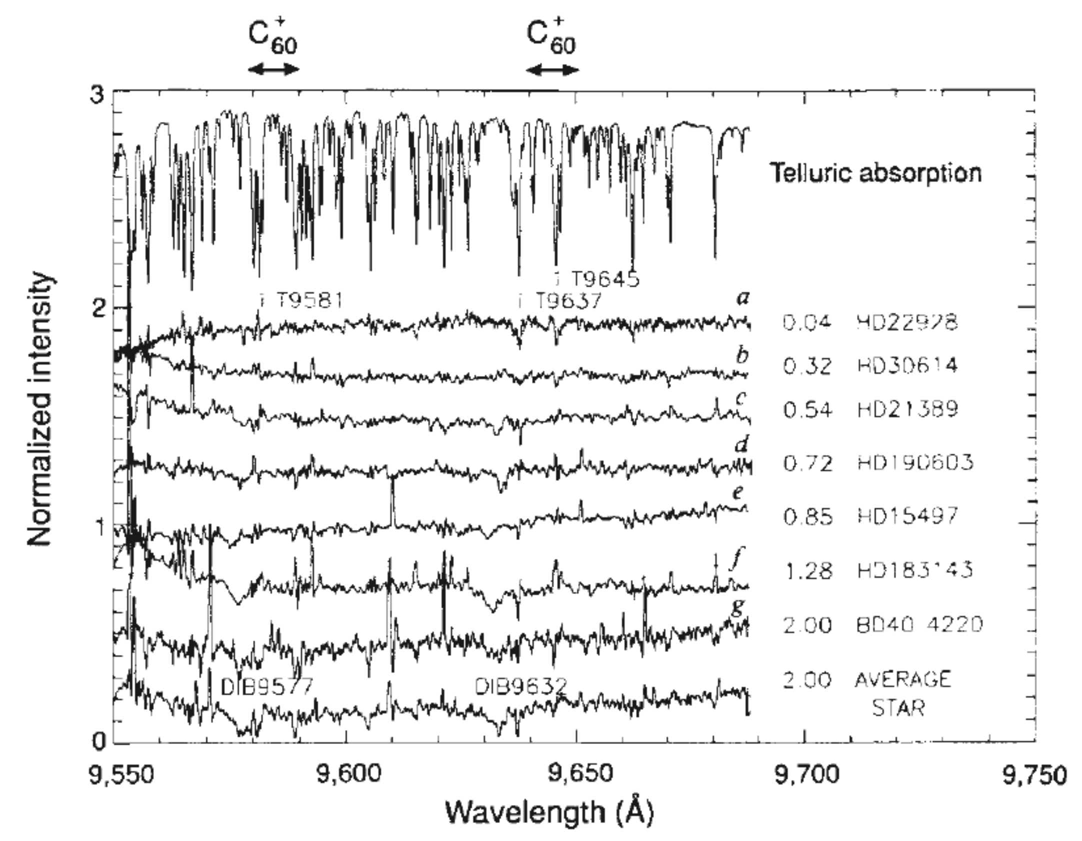
Graphite vaporization in H-poor atmosphere, using He as buffer gas.

Increasing He pressure -> increasing collisions -> most stable species survive: C_{60} and C_{70}.

Widespread and abundant in space?

Astro Searches

- Electronic bands of *neutral* C_{60} in interstellar medium: not found (Herbig, 2000), but not surprising.
- Electronic bands of C_{60}^{+}: promising case , awaiting laboratory confirmation (Foing&Ehrenfreund, 1994)

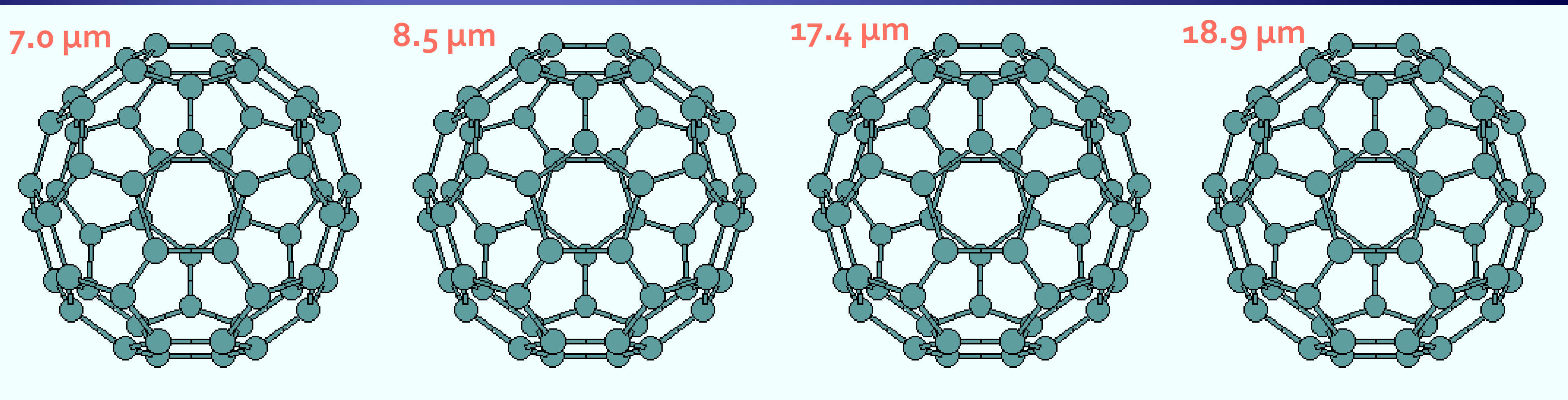


C_{60} & C_{70} vibrational modes

- Neutral C_{60}: 174 fundamental vibrational modes, but only 4 are IR active: 7.0, 8.5, 17.4, 18.9 µm.
- Neutral C_{70}: 204 fundamental vibrational modes; 32 are IR active.

- Note: cation spectra quite different.

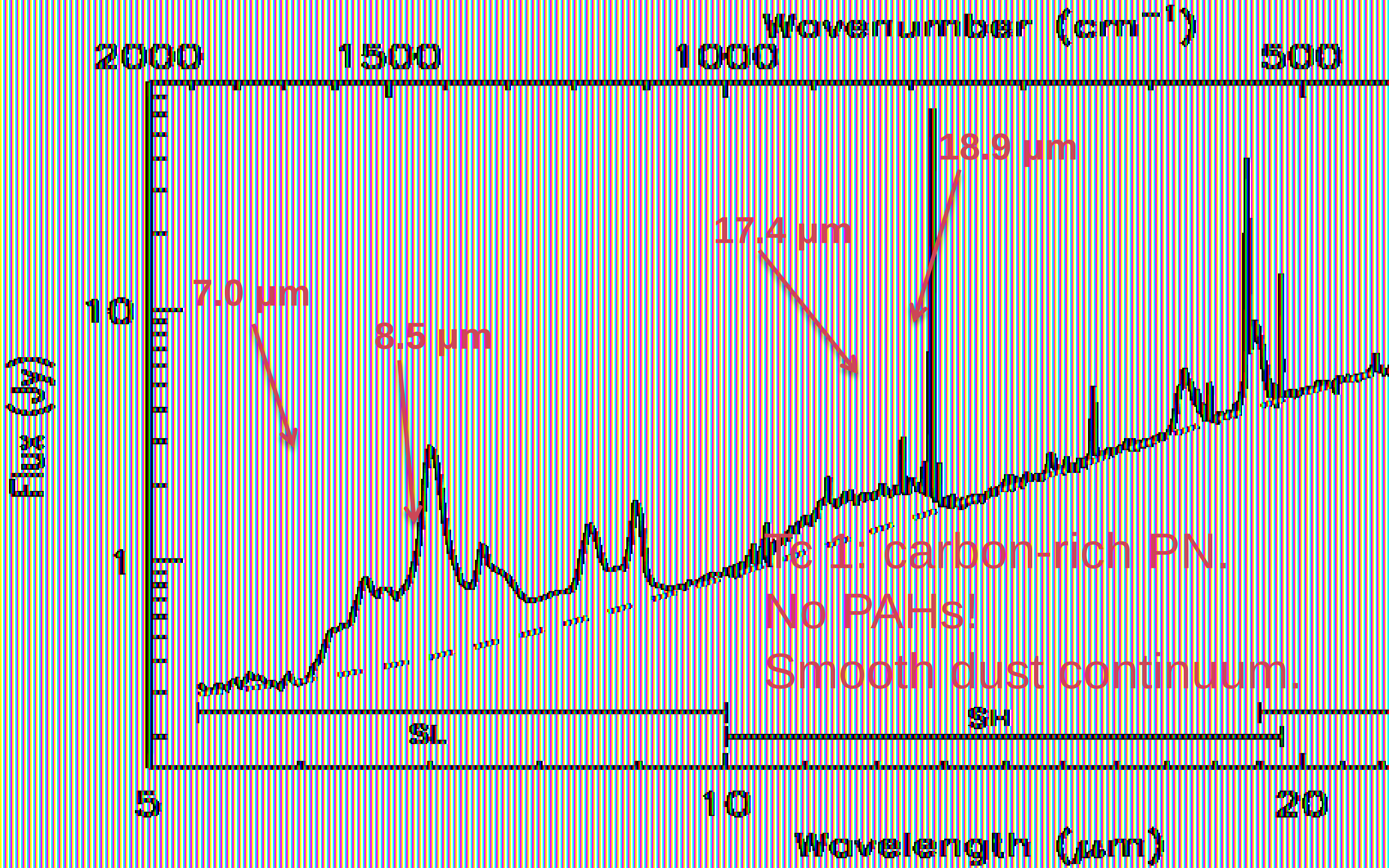
Menéndez& Page



IR Bands: observational studies

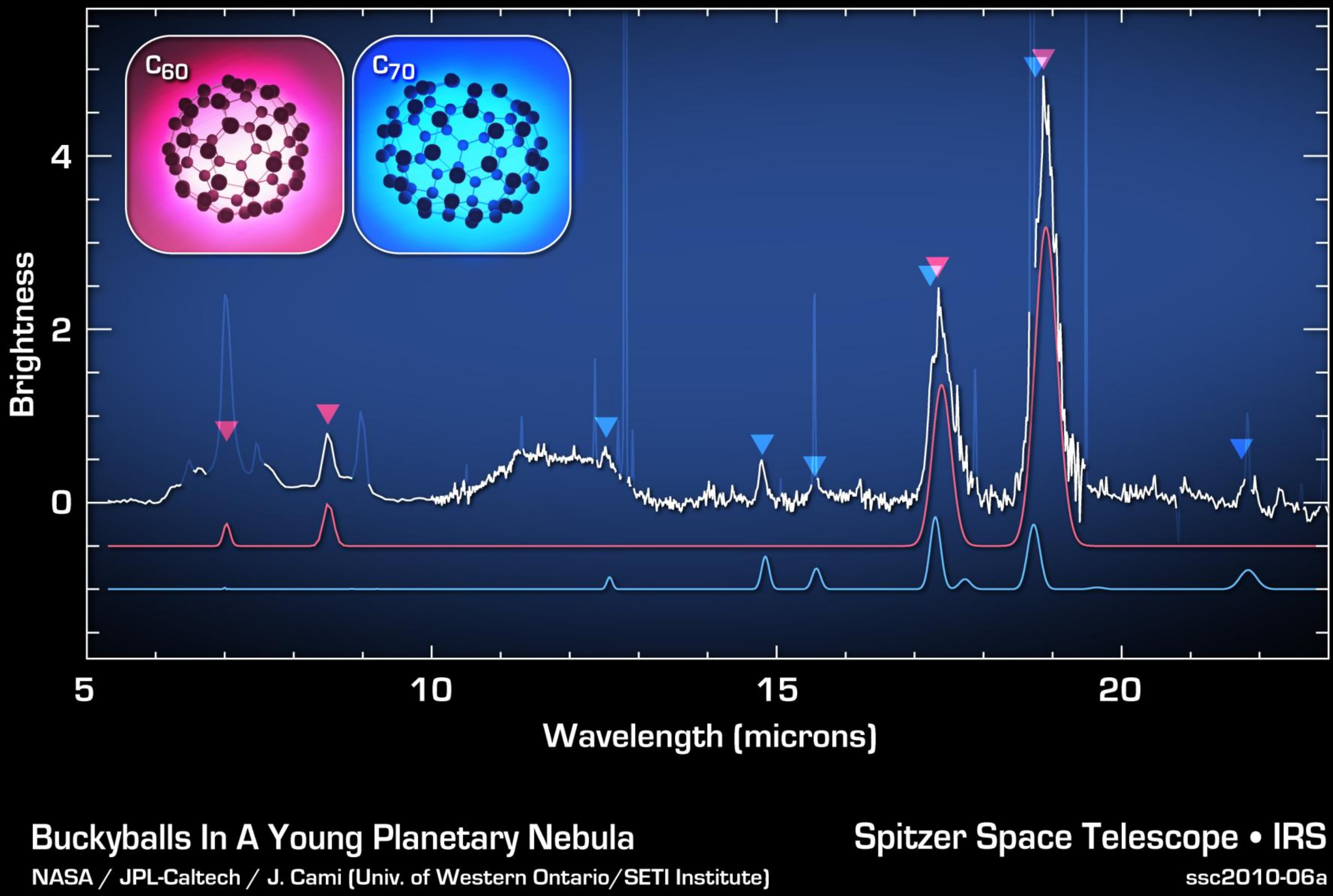
- Dedicated IR searches: no C_{60} was detected. (Clayton et al., 1995; Moutou et al., 1999).
- C_{60} suggested as a good candidate to explain features at 17.4 and 18.9 µm in Reflection Nebula NGC 7023 (Sellgren et al., 2007).

Spitzer-IRS observations of Tc 1



Tc 1: carbon-rich PN.
No PAHs!
Smooth dust continuum.

Observed Mar 21, 2005 with IRS in both Low-Resolution and High-Resolution modules.



Laboratory data: wavelengths & widths depend on T!

The Bottom Line

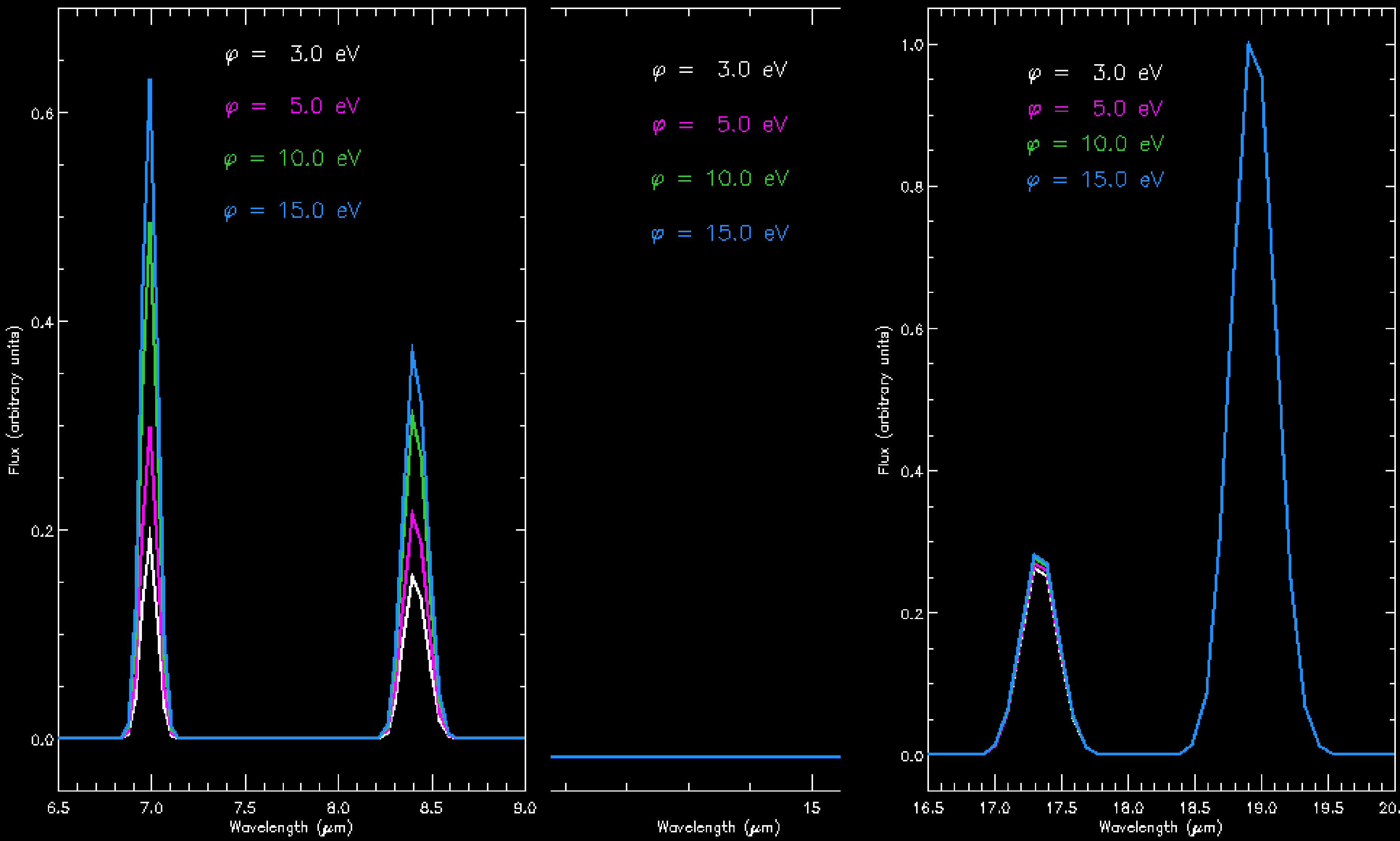
All measurable quantities (wavelengths, widths and strengths) are consistent with laboratory experiments carried out at temperatures comparable to what we derive.

C_{60} excitation

- Central star has a temperature of 30,000 K; thus average photon energies in the range 6—10 eV.
- Ionization potential is 7.6 eV; would expect C_{60} cation, not neutral C_{60}!

- Expected excitation: single-photon heating followed by fluorescent cooling in the IR.
- In that case, the 17.4 / 18.9 intensity ratio should be fairly insensitive to the photon energies.

Cooling Cascade

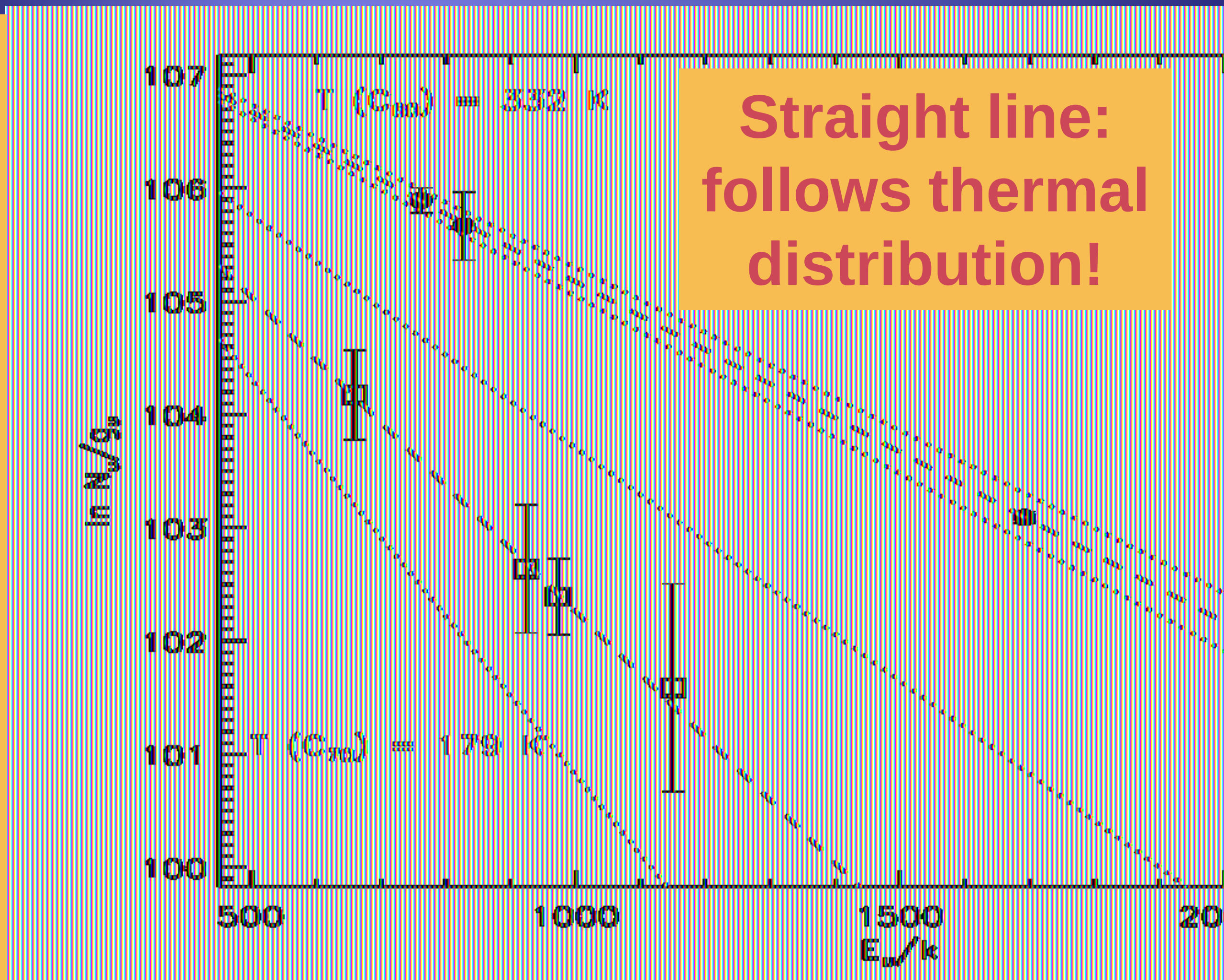


Band Ratios

	3 eV	5 eV	10 eV	15 eV	Tc 1
$I_{7.0}/I_{18.9}$	0.35	0.55	0.91	1.16	[Ar II] contam.
$I_{8.5}/I_{18.9}$	0.29	0.40	0.58	0.58	0.27
$I_{17.4}/I_{18.9}$	0.27	0.27	0.28	0.28	0.59

- Observed band ratios in Tc 1 are not compatible with fluorescent cooling; band ratios for 17.4 / 18.9 in different objects quite variable!

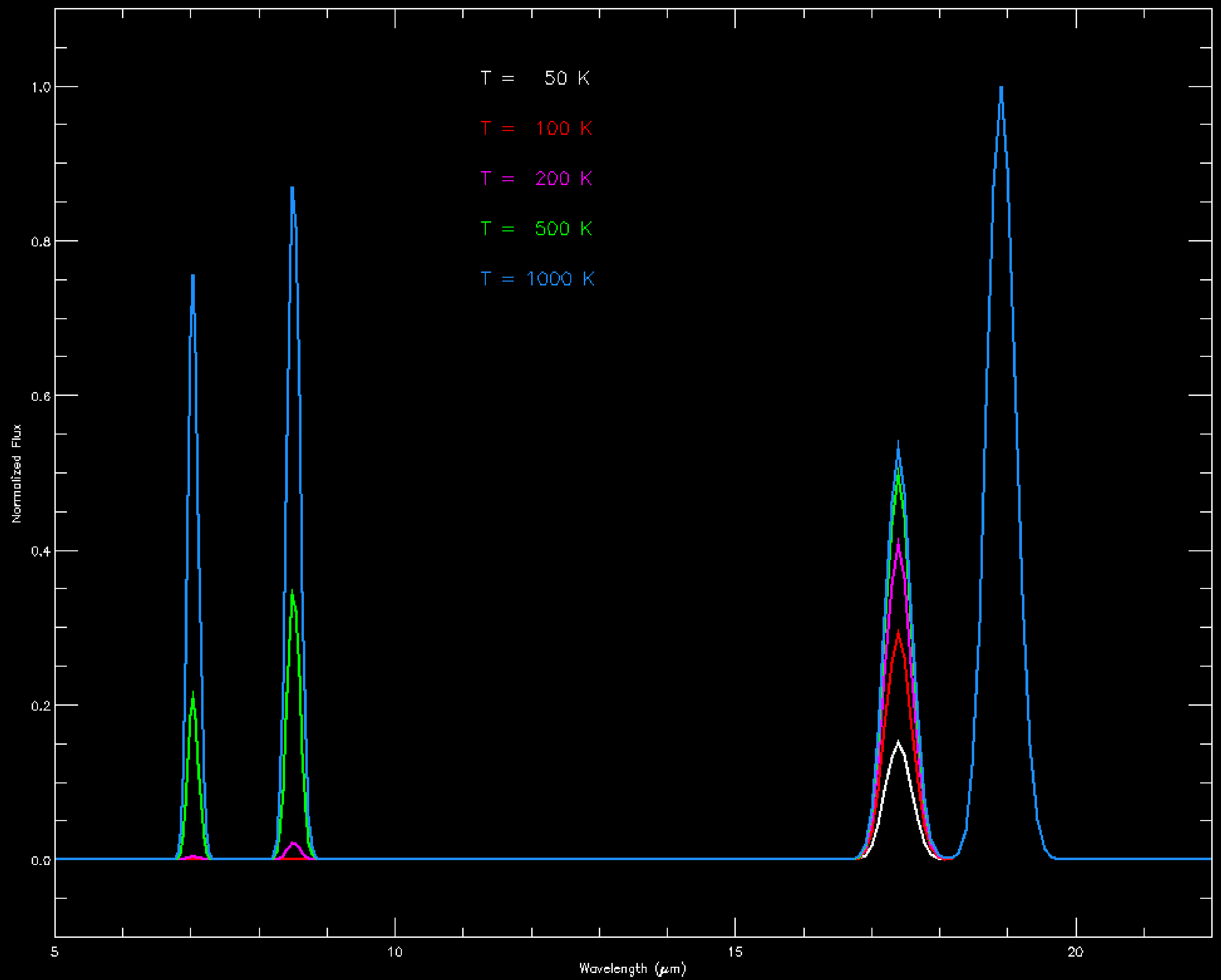
Excitation diagram



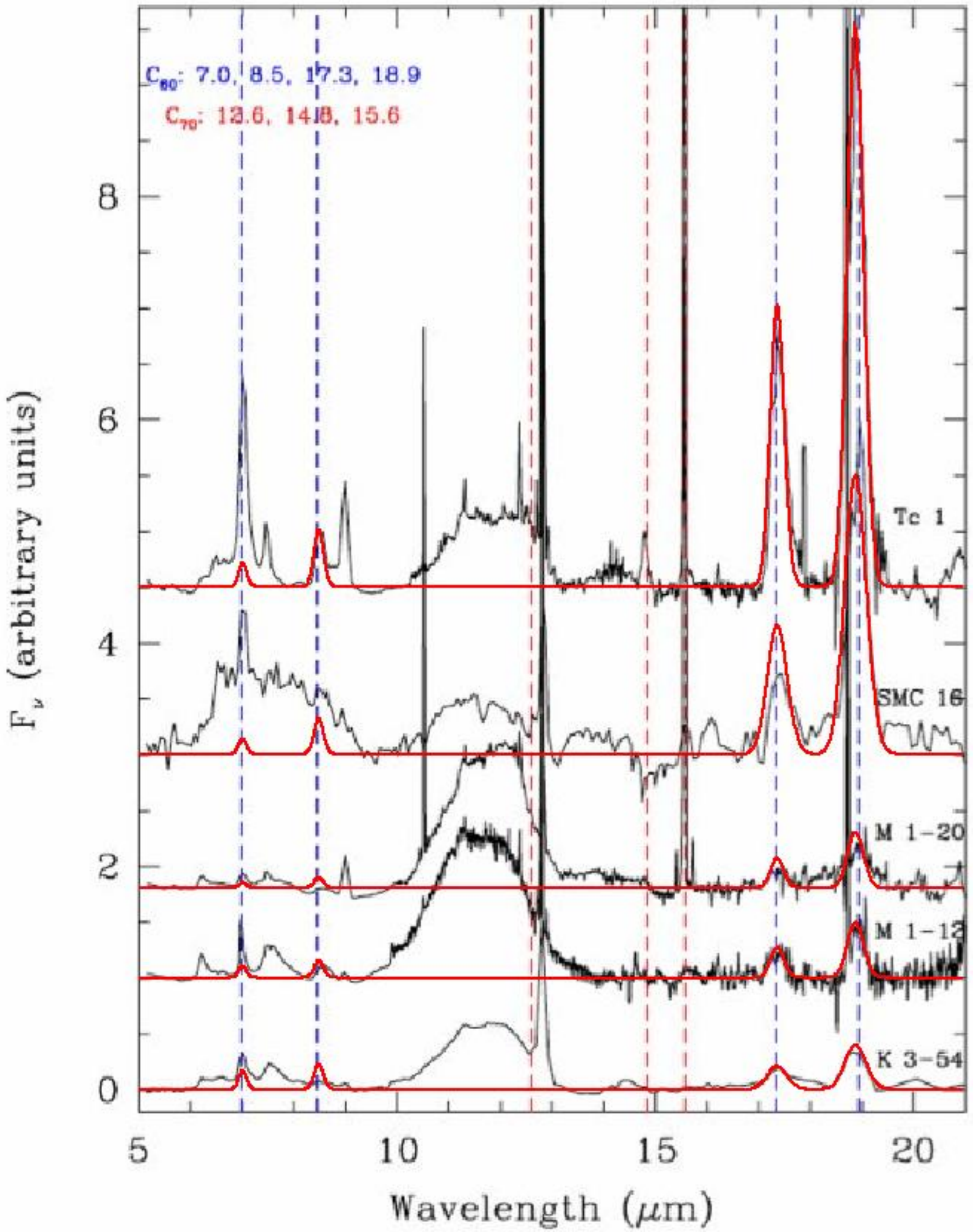
Population from emitted power

Energy of excited vibrational levels

Yields T and N; Use those parameters now to make model (especially useful to test other C_{70} bands).



T = 50 K
T = 100 K
T = 200 K
T = 500 K
T = 1000 K
Normalized Flux
0.0
0.2
0.4
0.6
0.8
1.0
5
10
15
20
Wavelength (μm)



More PNe with fullerenes (and some have PAHs). Including one in SMC!

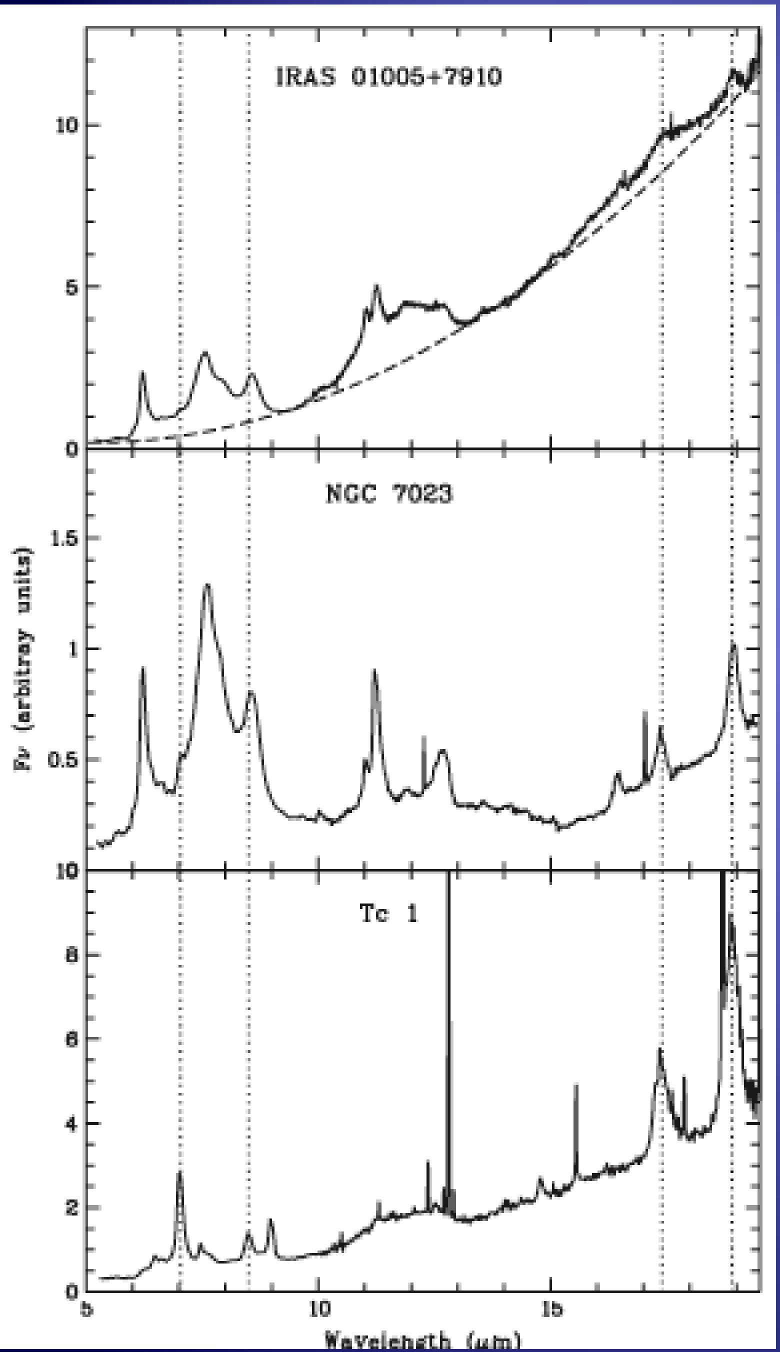
SMC 16: 326 K (?)

M1-20: 425 K (?)

M1-12: 546 K (?)

K3-54: 681 K (?)

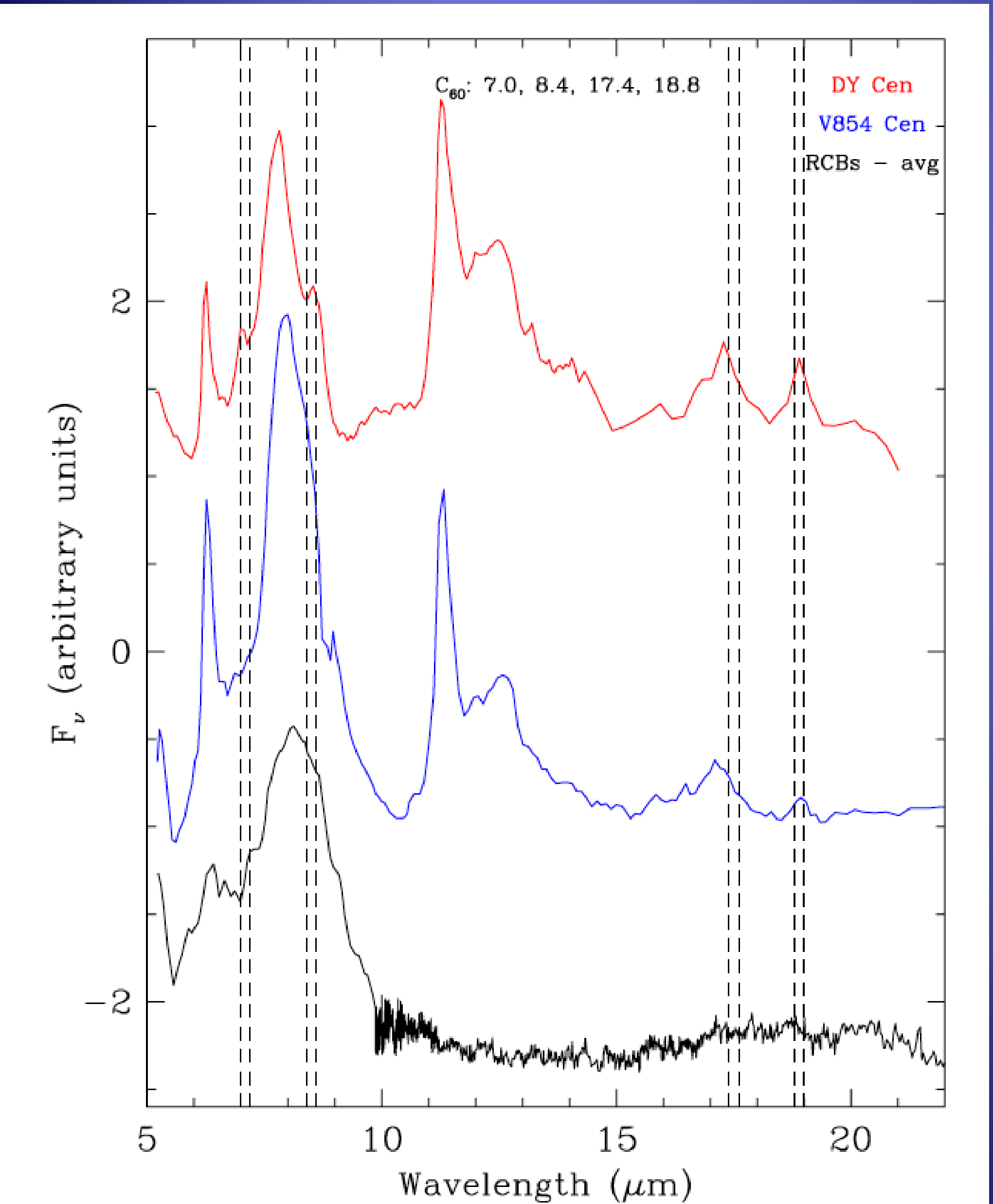
Garcia-Hernandez et al., 2010
Cami et al., 2011



Other sources

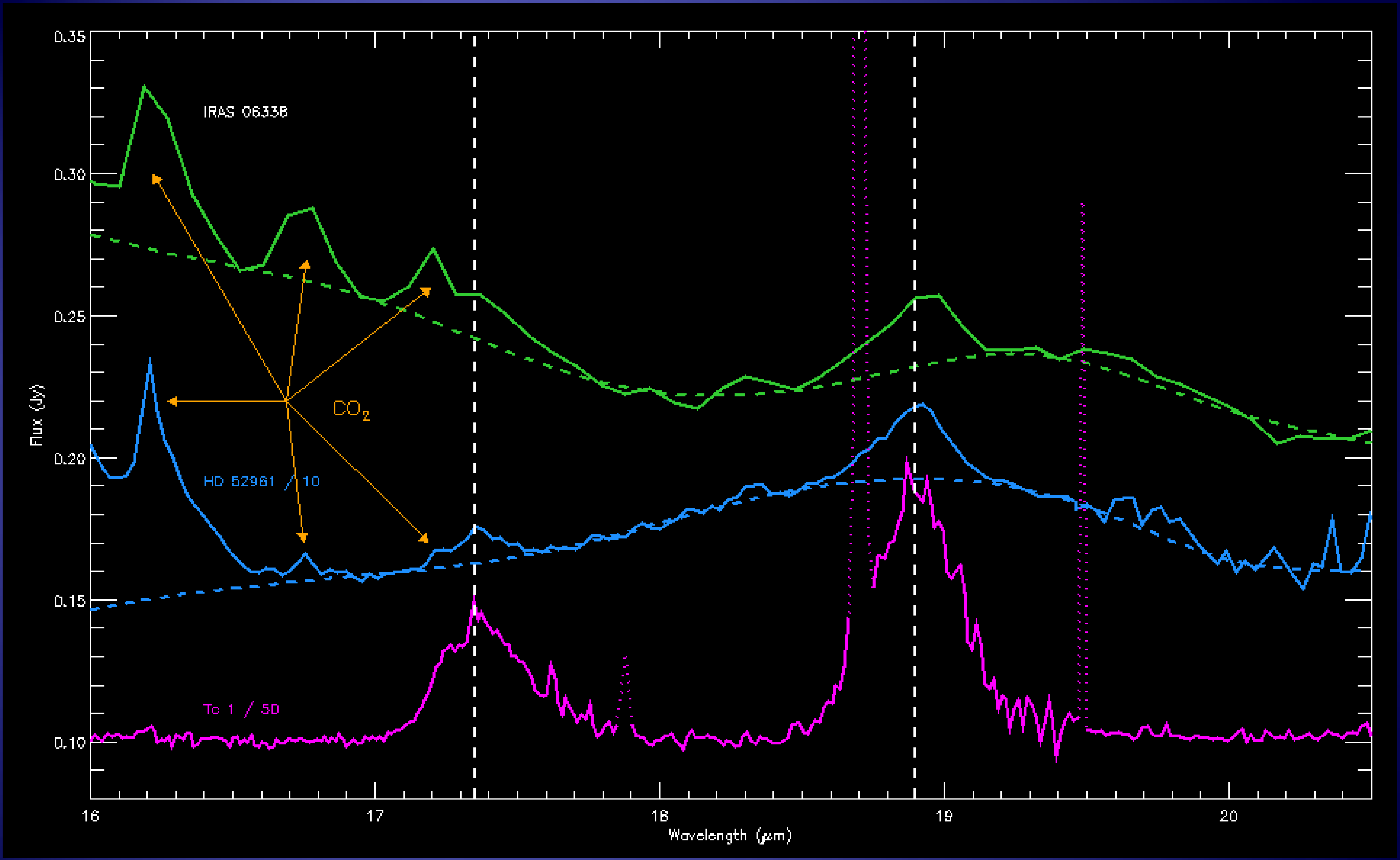
- PAHs and C_{60} in Proto-PN IRAS 01005+7910 (Zhang & Kwok, 2011).

R CorBor stars



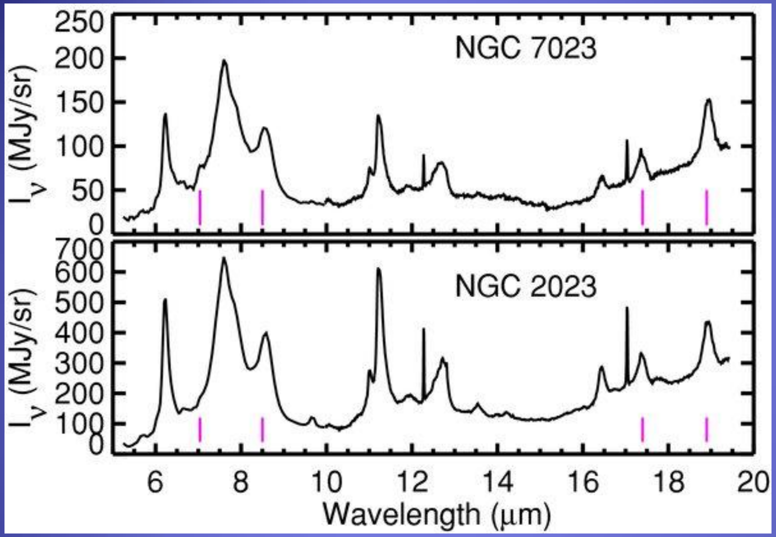
Only show up in the two most H-rich R CorBor stars.

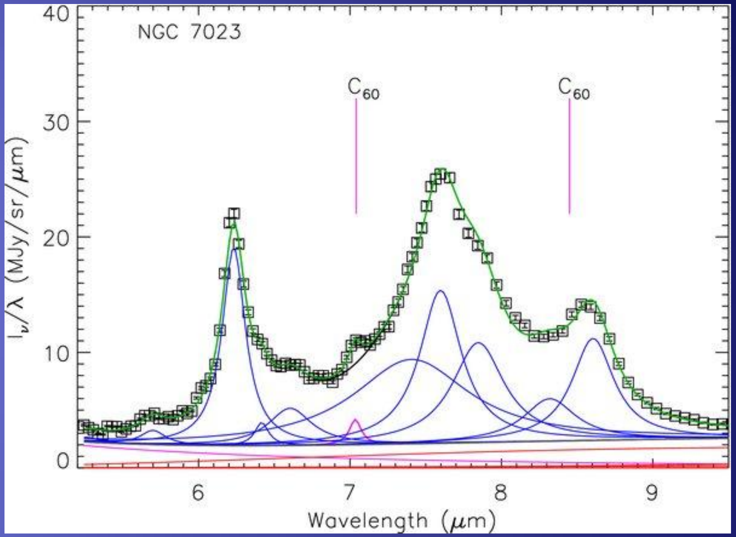
(Garcia-Hernandez et al., 2011)



O-rich binary post-AGB stars
(Gielen et al., 2011).

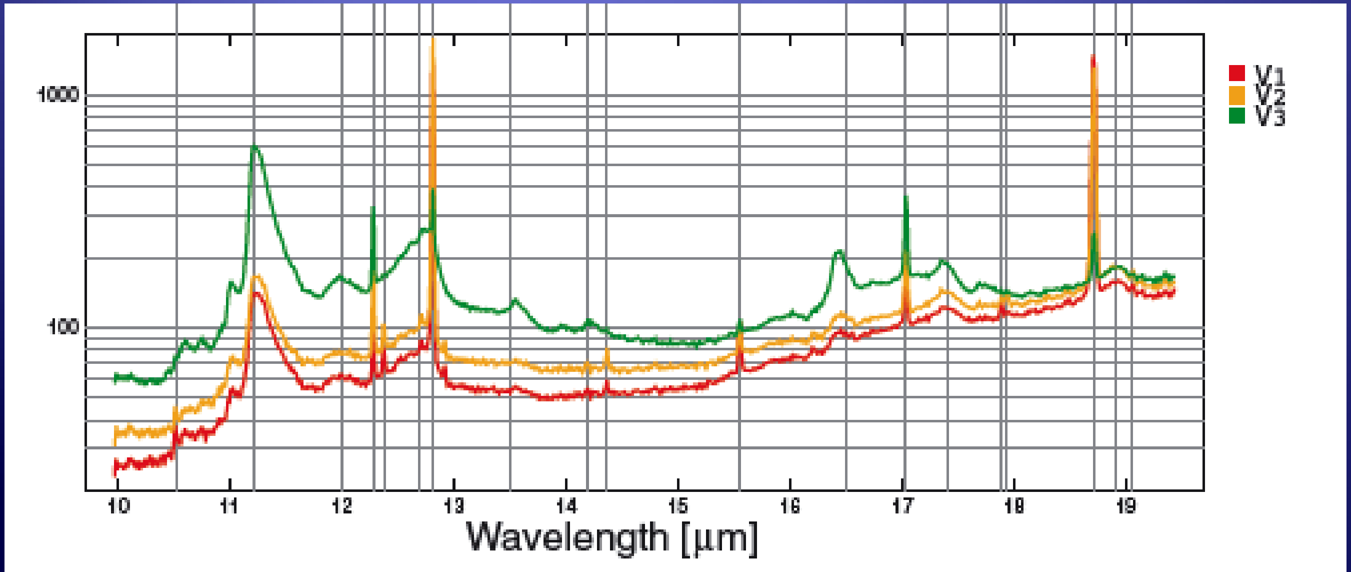
C_{60} in ISM





RNe

(Sellgren et al., 2010)



Orion Bar

(Rubin et al., 2011)

Fullerene Formation

- Observations suggest that fullerenes form in the circumstellar environments of evolved stars.
- At "moderate" temperatures (as expected for most circumstellar environments) and high enough densities, fullerenes self-assemble from carbon clusters….
- …but only in H-deficient gas!
  (de Vries et al., 1993; Wang et al. 1995)
- Process is efficient: ≈1% of C is turned into C_{60} – comparable to PNe abundance estimates.

Fullerene Formation (2)

- On first sight, appealing to explain Tc 1:
  - strong C_{60}
  - no PAHs
  - no other clear H-containing molecules.
- However, H ***is*** present at large in the nebula, and also in the photosphere!

- Why is there no trace of even the simplest H-containing carbonaceous molecules??

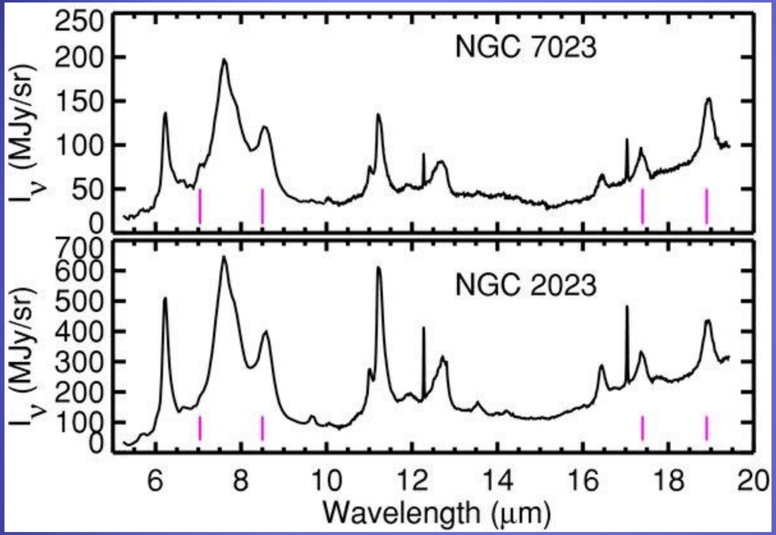
Fullerene Formation (3)

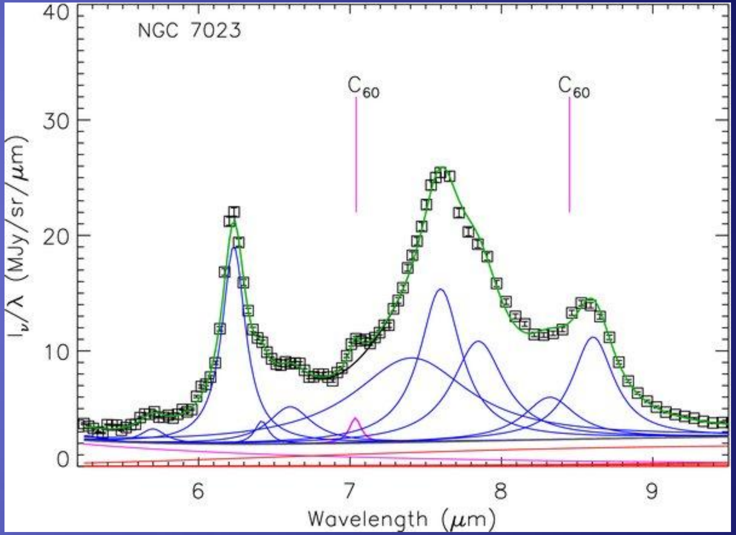
- Alternative: photo-processing of HAC yields simultaneous production of PAHs and fullerenes (e.g. Scott &Duley 1996).
- On first sight, appealing to explain those PNe that show both PAHs and C_{60}.
- Problems:
  - far less efficient (dominant species have 40 atoms)
  - produces many more small molecules and molecular fragments which are not seen in these objects….

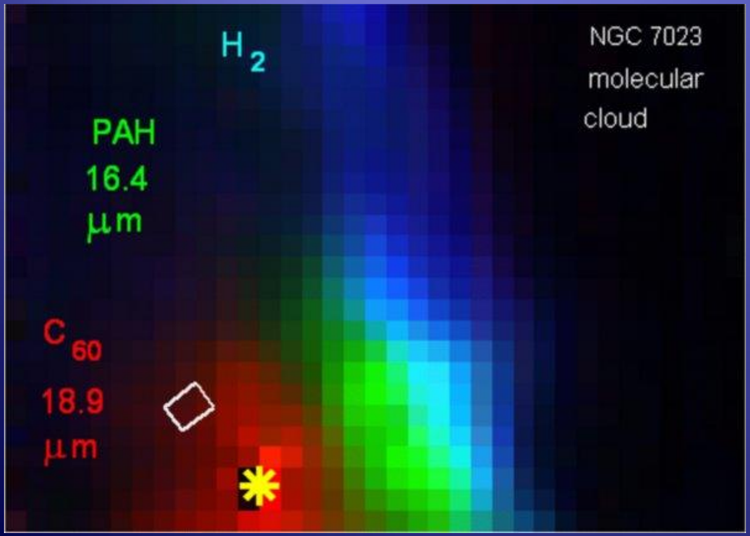
Fullerene Formation (4)

- Garcia-Hernandez (2010): most likely HAC photoprocessing: simultaneous appearance of PAHs and C_{60} clearly indicates that PAHs and fullerenes are co-existing….
- …but there is strong observational evidence at least in some sources that PAHs and C60 are in fact ***not*** co-located!

C_{60} in ISM (RNe)







Sellgren et al., 2010

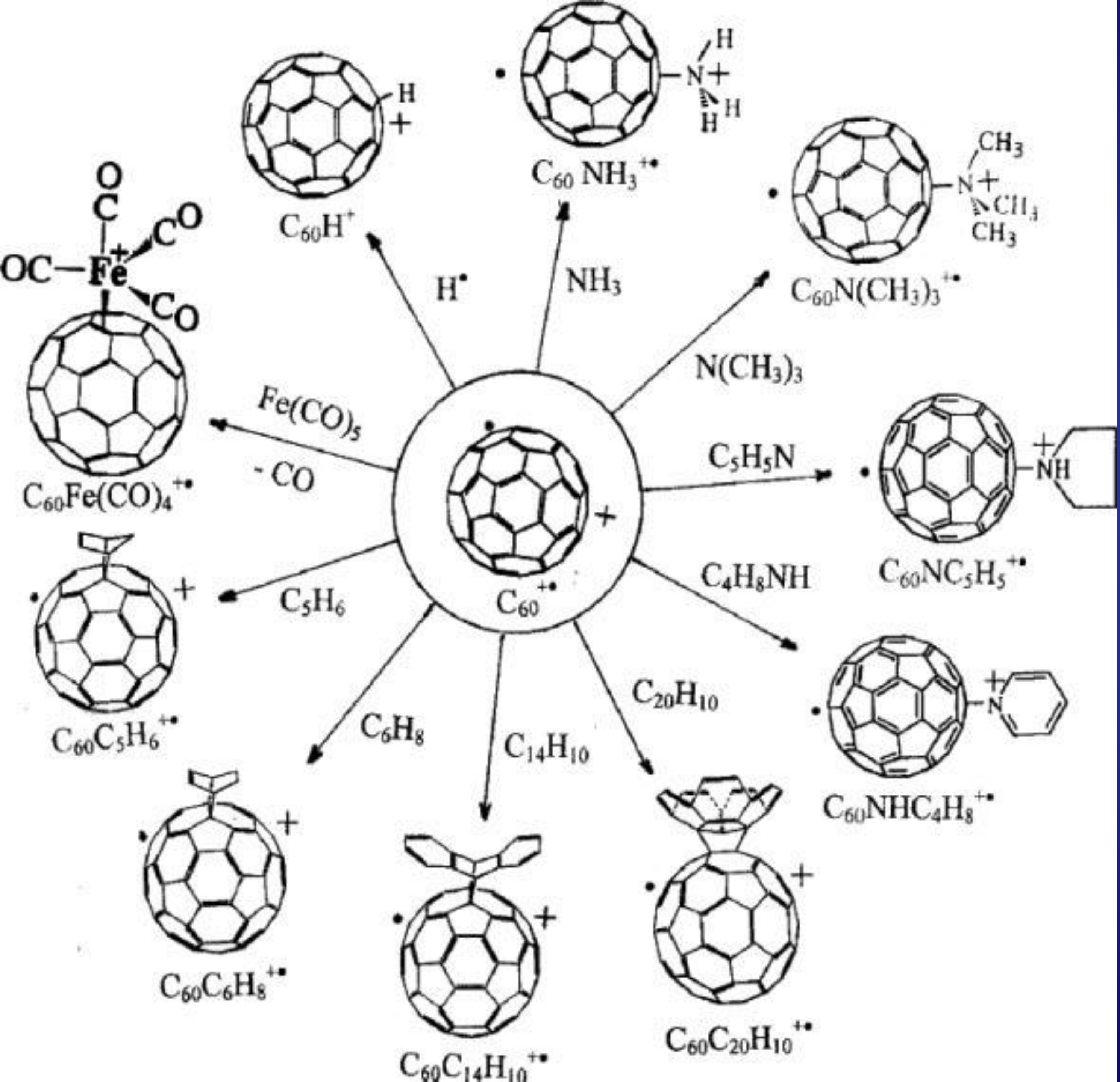
Fullerene Formation (6)

- Fullerenes can also form efficiently in H-rich environments at T > 3500 K (Jäger et al., 2009).
- Key is (once more) high density.

- Is this the route? Or is there yet another mechanism, e.g. to make fullerenes from PAHs?

Future aspects

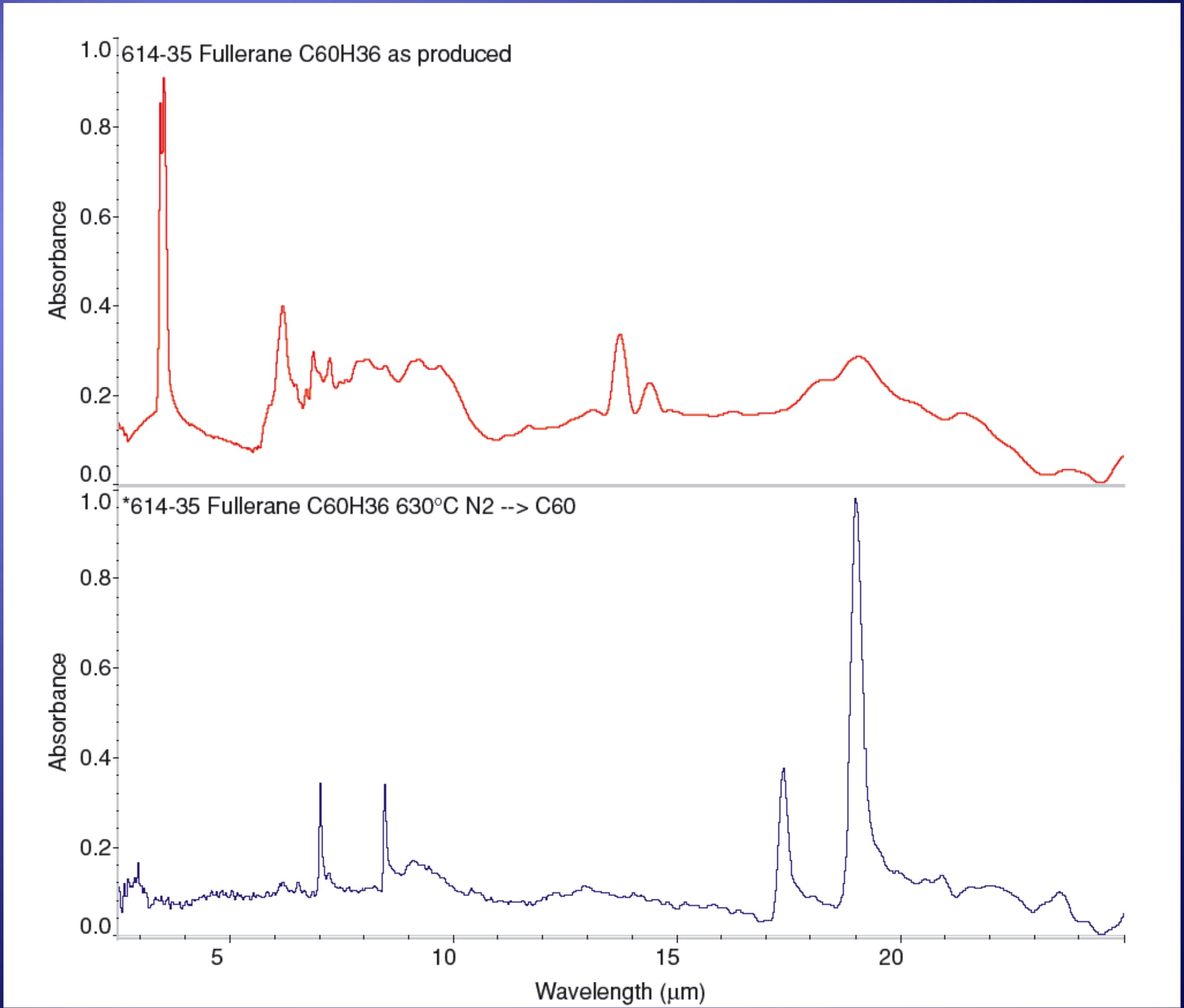
- What to do once you have made fullerenes?
- Make other stuff – could be important e.g. for the DIBs!



C60H+
C60 NH3+•
C60N(CH3)3+•
H•
NH3
N(CH3)3
Fe(CO)5
- CO
C60Fe(CO)4+•
C5H5N
C60NC5H5+•
C4H8NH
C60NHC4H8+•
C5H6
C60+•
C60C5H6+•
C6H8
C14H10
C20H10
C60C6H8+•
C60C14H10+•
C60C20H10+•

Bohme, 2009

Hydrogenated fullerenes?

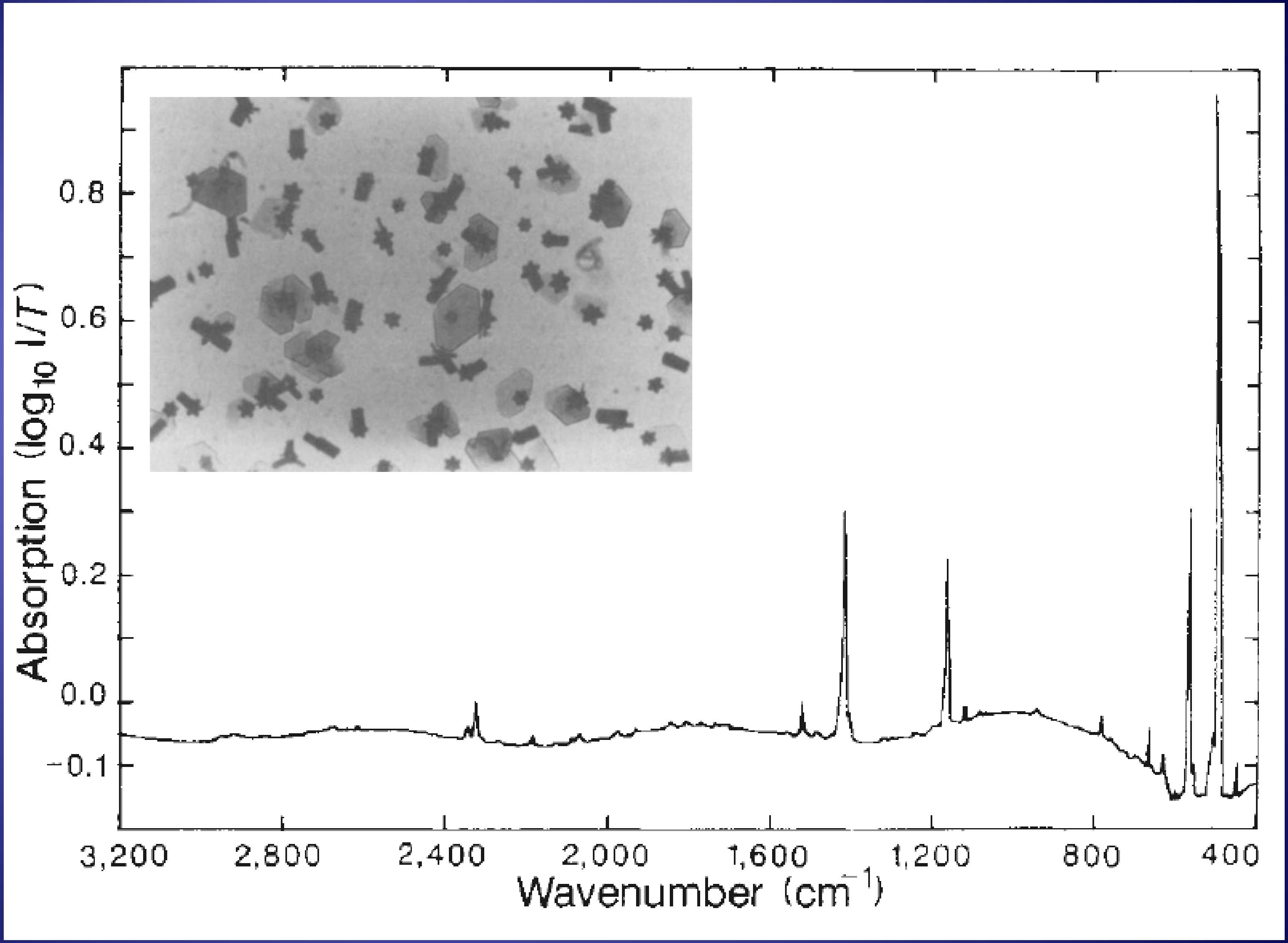


Cataldo& Iglesias-Groth, 2009.

Surprises & Issues

Fullerenes are neutral.	Ionization potential of C_{60} is 7.6 eV; T_{eff} of Tc 1 is 30,000 K.
Fullerenes are ‘cool’.	Stochastic heating: would expect stronger 7 & 8.5 μm.
Symmetric band profiles.	No contributions from hot bands? No anharmonicities?
LTE intensities.	Rare observation in gas phase species.

Solid state C_{60}?



Solid C_{60}, same vibrational modes!

Kraetschmer 1990

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