EVOLVED STARS
THE ALMA ERA

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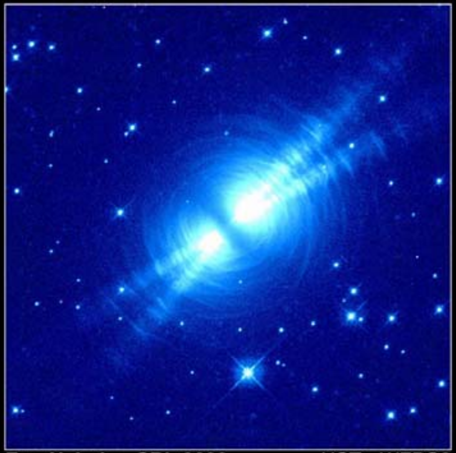
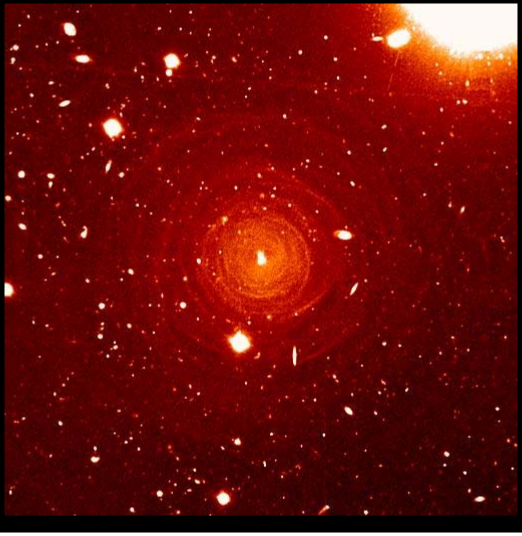
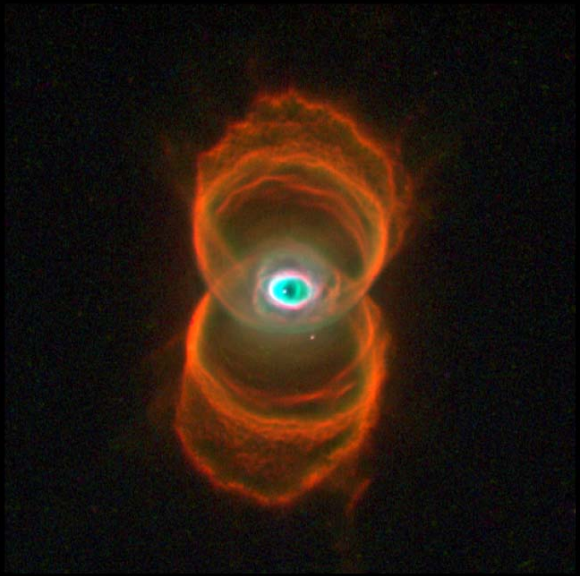
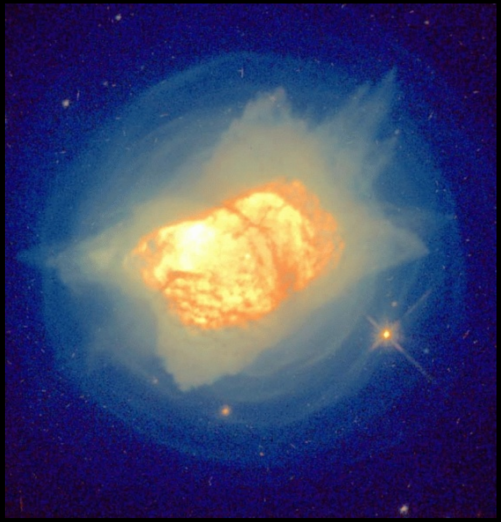


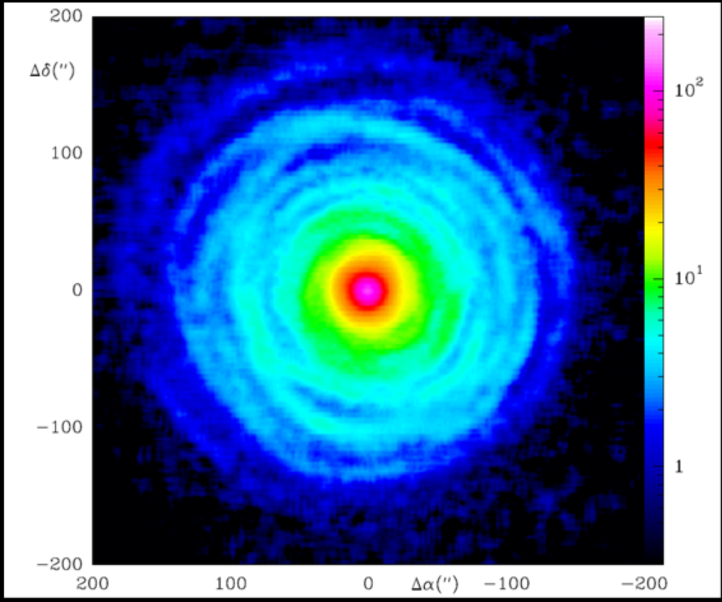
Egg Nebula · CRL 2688 HST · WFPC2
PRC96-03 · ST ScI OPO · January 16, 1996
R. Sahai and J. Trauger (JPL), the WFPC2 Science Team and NASA





Hourglass Nebula · MyCn18 HST · WFPC2
PRC96-07 · ST ScI OPO · January 16, 1996
R. Sahai and J. Trauger (JPL), the WFPC2 Science Team and NASA





AGBs and Astrochemistry

Why Molecular Astrophysics in AGBs ?

50% of known molecular species in space detected in AGBs (most of them in IRC+10216, but also VyCMa)

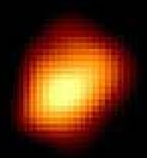
Determination of the physical conditions of the gas

Determination of the molecular abundances => Chemical evolution=> Chemical Complexity=>feedback to the ISM

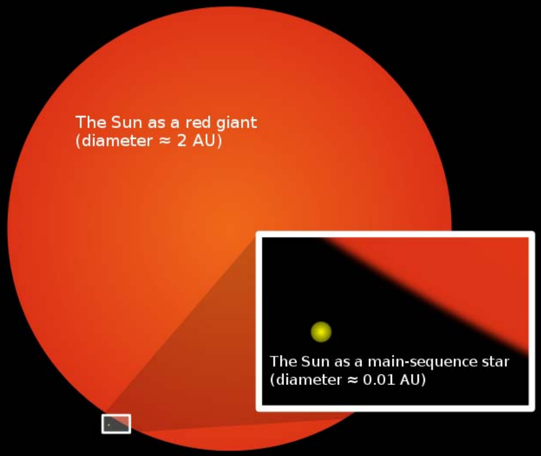
Determination of the dynamical evolution of circumstellar clouds

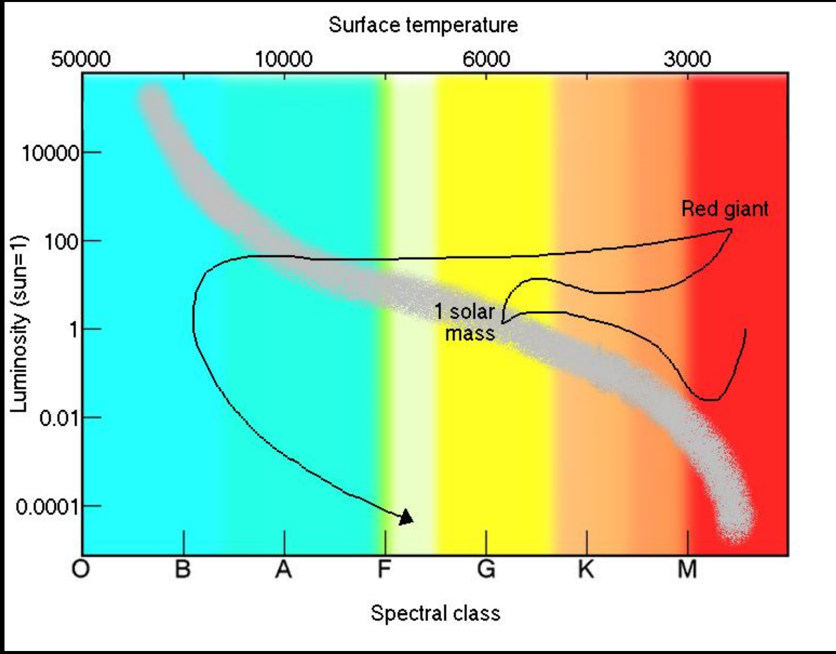
Main source of dust grains production in space

Water has been found in C- and O-rich CSM.



Mira Star





A BRIEF INTRODUCTION TO THE STRUCTURE AND EVOLUTION OF AGB STARS

CHEMISTRY UNDER THERMODYNAMICAL EQUILIBRIUM

DUST GRAIN FORMATION

CHEMISTRY IN THE EXTERNAL SHELLS

THE PROBLEM OF H_2O, C-rich or O-rich, that is the question !

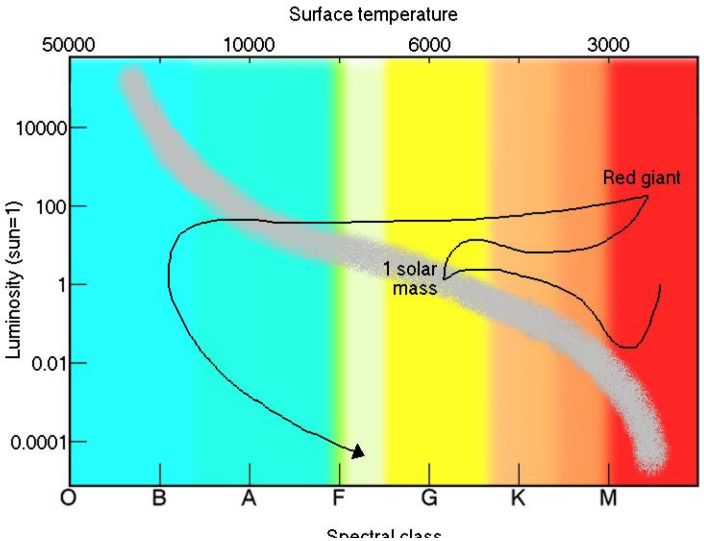
THE CHEMICAL EVOLUTION OF THE ENVELOPE:
FROM AGBs TO PLANETARY NEBULA

WHAT ALMA CAN DO IN THE FIELD OF EVOLVED STARS ?

Low-Mass Star = $M < 4\ M_{sun}$

Stages of Evolution of a Low-Mass star:

Main Sequence star
Red Giant star
Horizontal Branch star
Asymptotic Giant Branch star
Planetary Nebula phase
White Dwarf star



Main Sequence Phase

Energy Source: Hydrogen fusion in the core

What happens to the He created by H fusion?

- Core is too cool to ignite He fusion
- Slowly builds up an inert He core

Main-Sequence (H-burning) Lifetime:

- ~10 Gyr for a 1 M_{sun} star (e.g., Sun)
- ~10 Tyr for a 0.1 M_{sun} star (red dwarf)

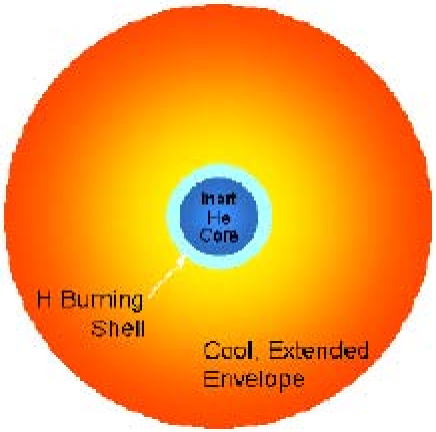
Core Hydrogen Exhaustion

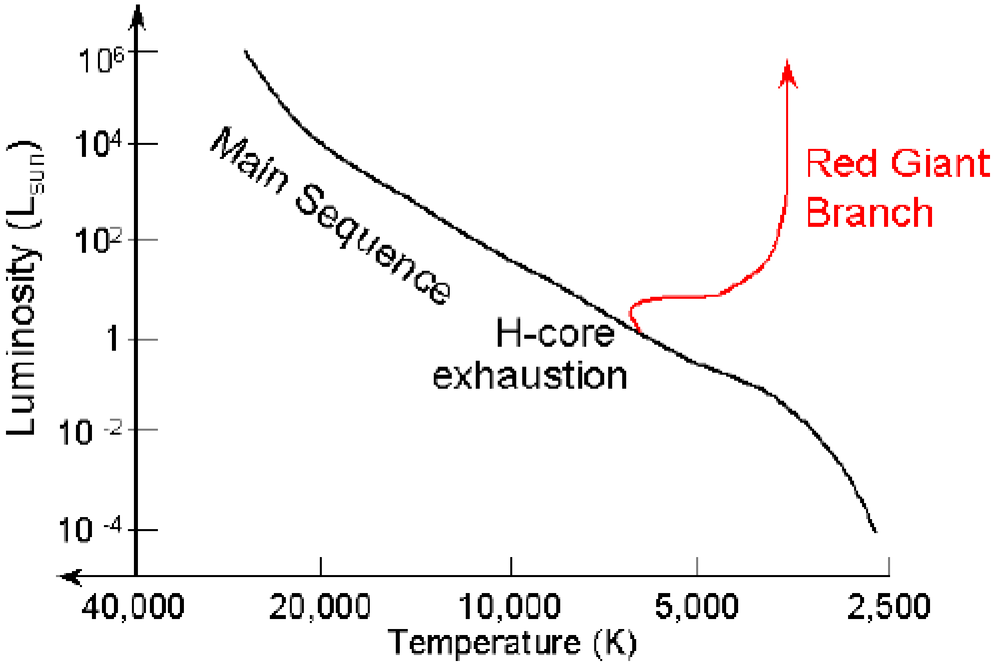
Inside:

- He core collapses & starts to heat up.
- H burning zone moves into a thin **shell** surrounding the core
- Collapsing core heats the H shell above it, driving the fusion faster.
- More fusion = more heating, so that Pressure > Gravity

Outside:

- Envelope **expands** and **cools**
- Star gets **brighter** and **redder** & climbs up the Giant Branch.





Climbing the Red Giant Branch

It takes a star about 1 Gyr to climb the Red Giant Branch

- He core contracting & heating, but no fusion
- H burning to He in a shell around the core
- Huge, puffy envelope ~ size of orbit of Venus

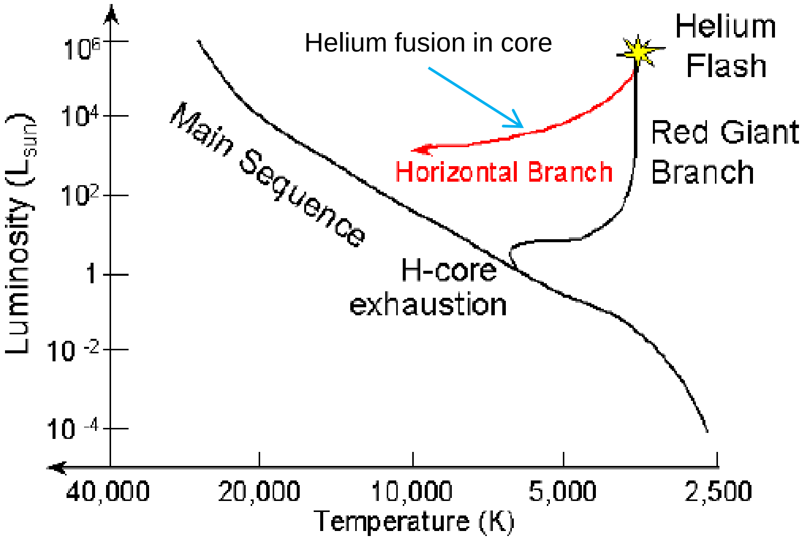
At the Tip of the Red Giant Branch:

- T_{core} reaches 100 Million K
- Ignite He burning in the core in a **flash**.

Helium Flash

At 100 Million K, a new fusion source ignites: the **Triple-alpha Process**.

This is the fusion of three ^{4}He nuclei into one ^{12}C (carbon) nucleus:



When this occurs, the star leaves the Giant Branch.

Inside:

- Starts generating primary energy from He burning in the **core**.
- Gets additional energy from an H burning **shell** surrounding the core.

Outside:

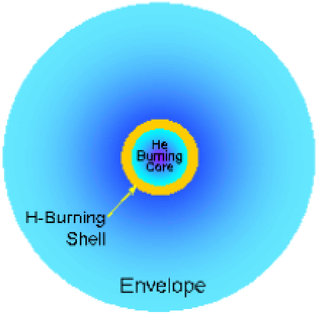
- Gets **hotter** and **bluer**.
- Star **shrinks** in radius, getting **fainter**.

The new energy source helps the star begin to regain Hydrostatic and Thermal Equilibrium. As it does so, it moves onto the **Horizontal Branch**.

Horizontal Branch Phase

Structure:

- He-burning core
- H-burning shell



The Triple-alpha Process is very inefficient at producing energy, so it can only last for about 100 Myr.

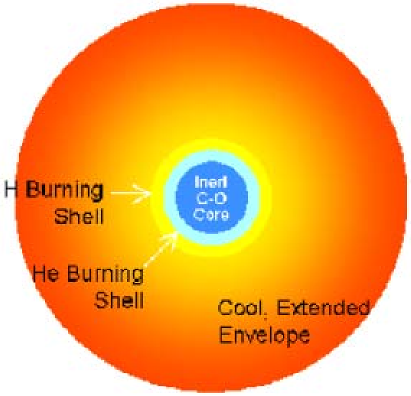
While it goes on, the star steadily builds up a C-O core, but it is still too cool to ignite Carbon fusion

Asymptotic Giant Branch Phase

After 100 Myr, the core runs out of Helium for Triple-Alpha fusion.

Inside:

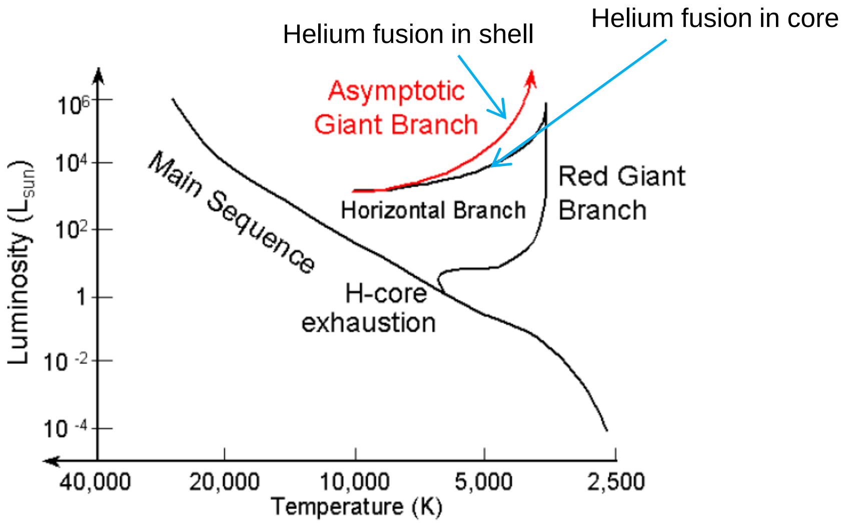
- C-O core collapses and heats up
- He burning shell outside the C-O core
- H burning shell outside the He burning shell



Outside:

- Star grows rapidly in radius and cools

Climbs the Giant Branch again, but at a higher effective Temperature than the Giant Branch, so it ascends with a bluer color, putting it slightly to the left of the original Giant Branch on the H-R Diagram:



He burning is very temperature sensitive: Triple-alpha fusion rate ~ T^{40}!

Consequences:

- Small changes in T lead to
- Large changes in fusion energy output

Star experiences huge **Thermal Pulses** that destabilize the outer envelope.

Core-Envelope Separation

Rapid Process: takes ~10^5 years

Outer envelope gets slowly ejected (fast wind)

C-O core continues to contract:

- With the weight of envelope taken off, the core heats up less
- It never reaches the Carbon fusion ignition temperature of 600 Million K

Core and Envelope separate physically.

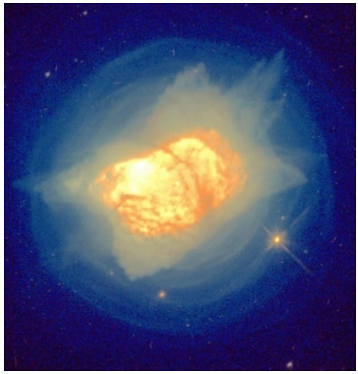
Planetary Nebula Phase

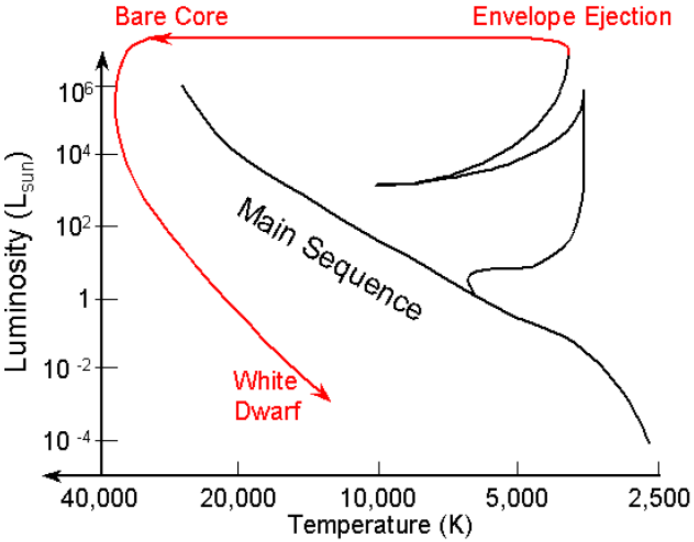
Expanding envelope forms a **nebula** around the contracting C-O core:

- Ionized and heated by the hot central core.
- Expands away to nothing in ~10^4 years.

The star briefly becomes host to a **Planetary Nebula**

The hot C-O core is exposed, and moves quickly to the left on the H-R Diagram at nearly constant luminosity and increasing temperature.





Core Collapse to White Dwarf

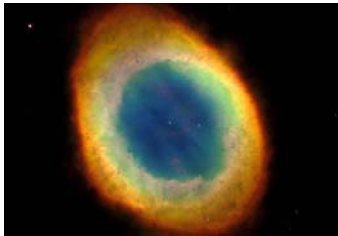
The contracting C-O core becomes so dense that a new gas law takes over...

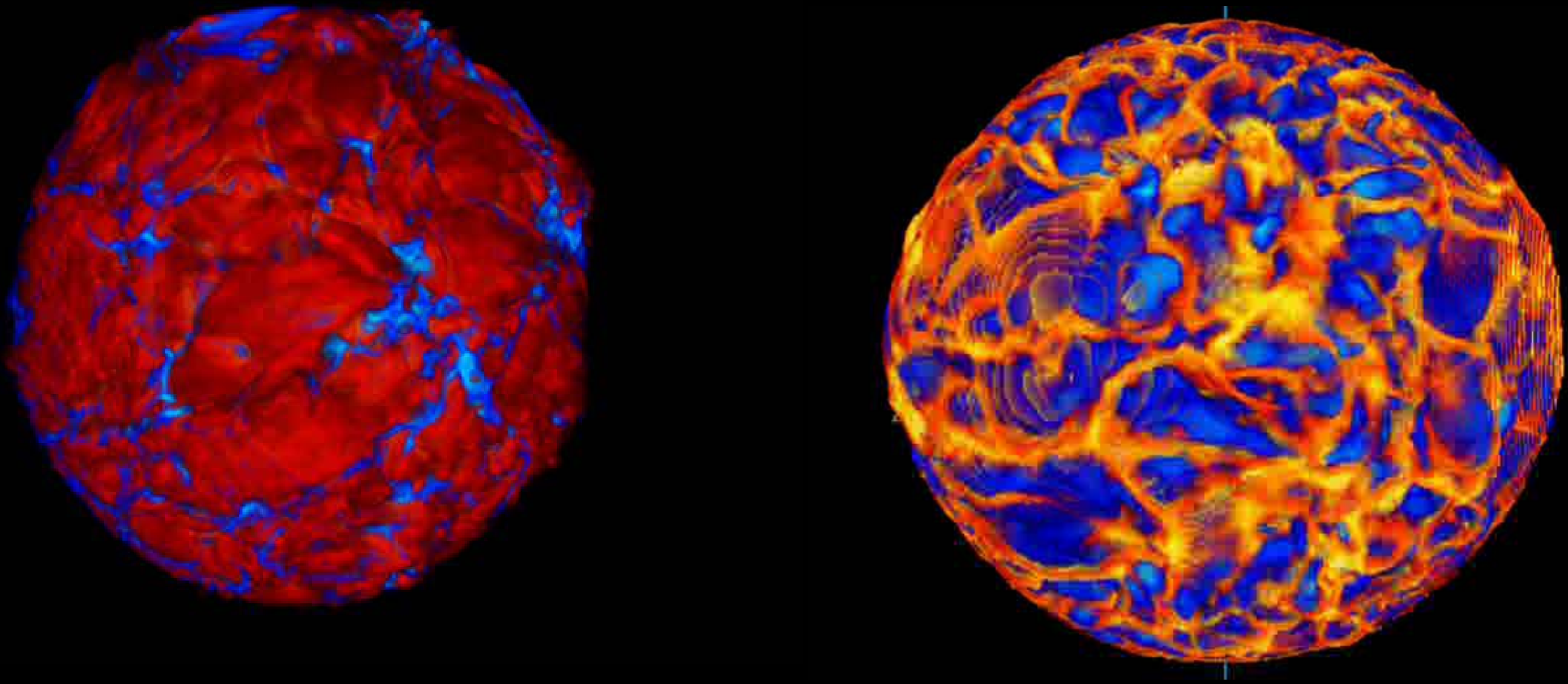
Degenerate Electron Gas:

- Pressure becomes independent of Temperature
- P grows rapidly & soon counteracts Gravity

Collapse halts when $R \sim 0.01 R_{sun}$ (~ R_{earth})

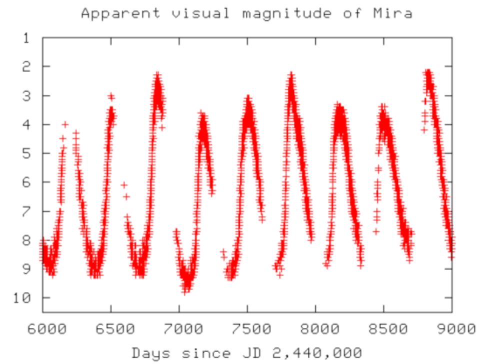
Degenerate core becomes a *White Dwarf*

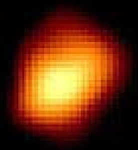




Porter et al. http://www.lcse.umn.edu/research/RedGiant/

Parameters for some well known AGB stars	Max Magnitud	Min Magnitud	Period days
Mira (o Ceti)	2	10,1	331,996
χ Cygni	3,3	14,2	408,5
R Hydrae	3,5	10,9	388,87
R Carianae	3,9	10,5	308,71
R Leonis	4,4	11,3	309,95
S Carinae	4,5	9,9	149,9
R Cassiopeiae	4,7	13,5	430,46
R Horologii	4,7	14,3	407,6
U Orionis	4,8	13	368,3
RR Scorpii	5,0	12,4	281,45
R Serpentis	5,16	14,4	356,41
R Centauri	5,3	11,8	546,2
R. Trianguli	5,4	12,6	266,9
R Leporis	5,5	11,7	427,1
R Aquilae	5,5	12	284,2
R Aquarii	5,8	12,4	386,96
U Cygni	5,9	12,1	463,24

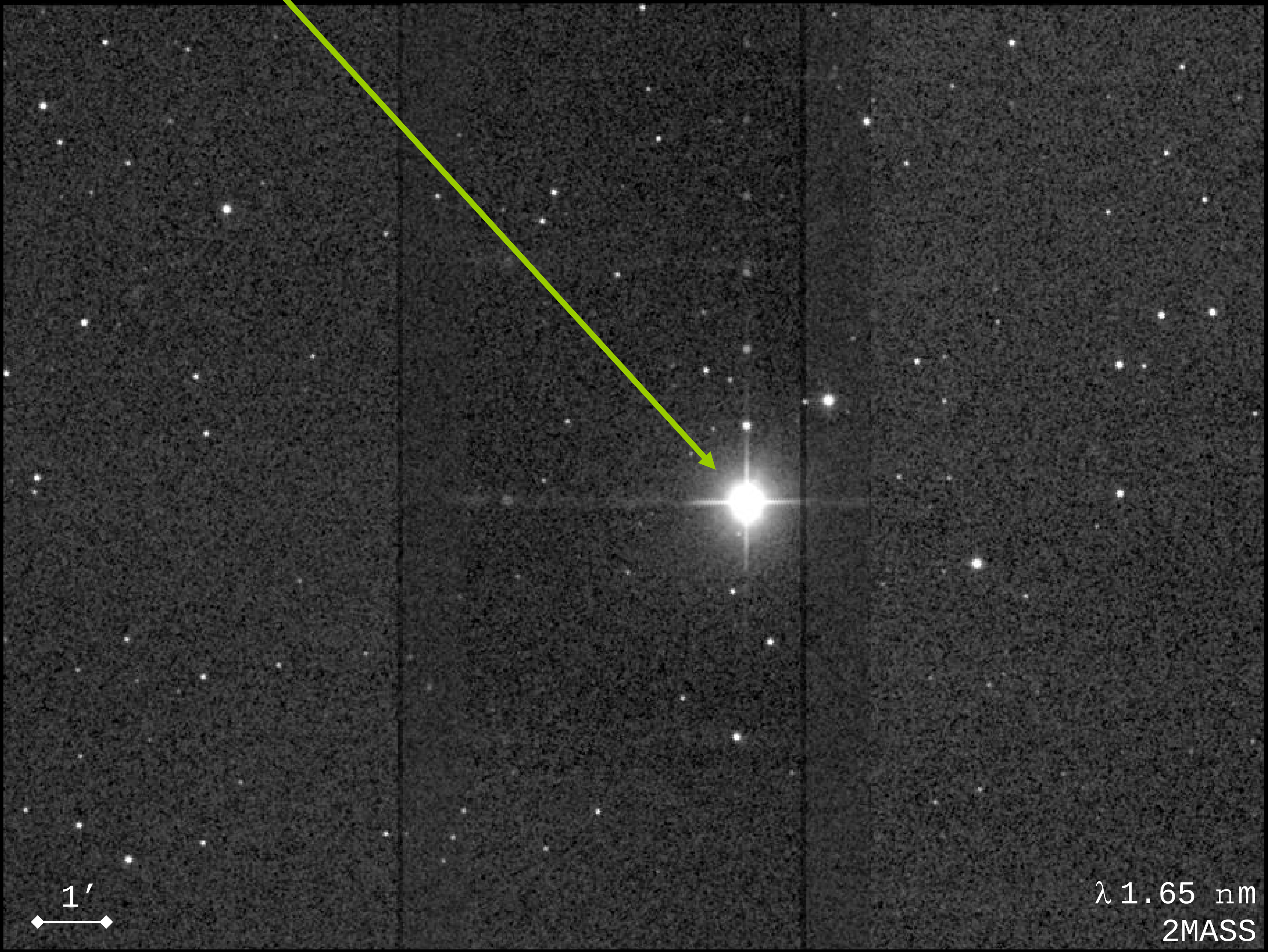




OUR LABORATORIES

NO FINE TUNING OF THE EXPERIMENT !!! WE HAVE TO DEAL WITH THE NATURE AS IT IS

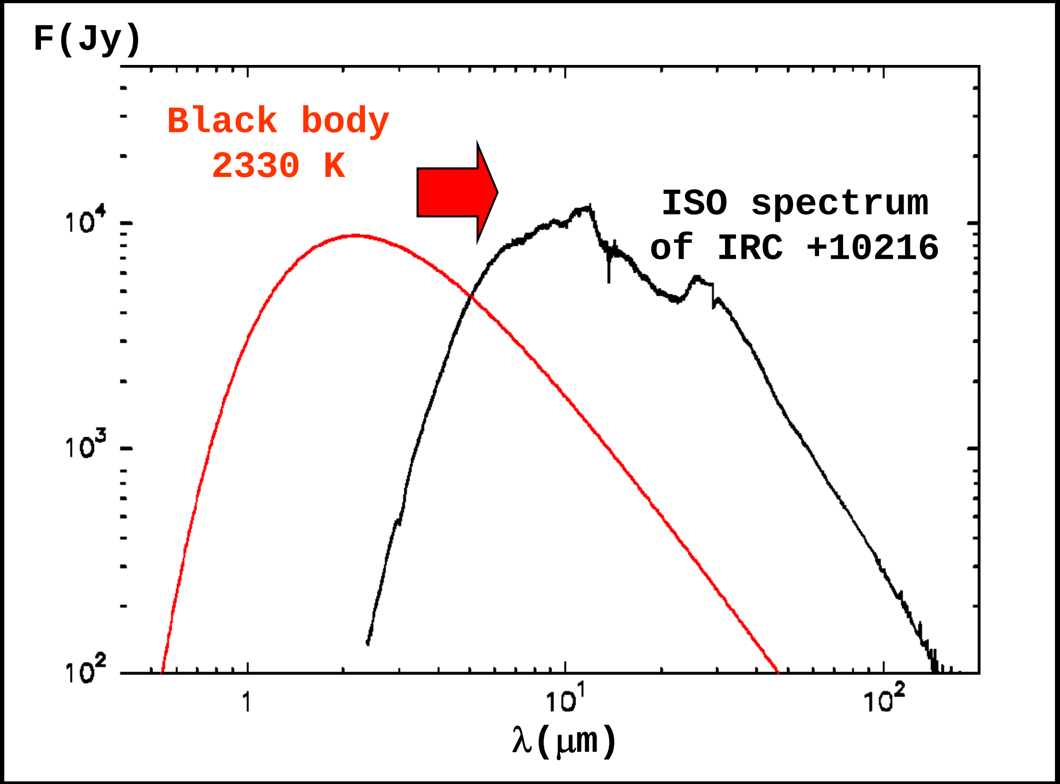
IRC +10216 or CW Leo

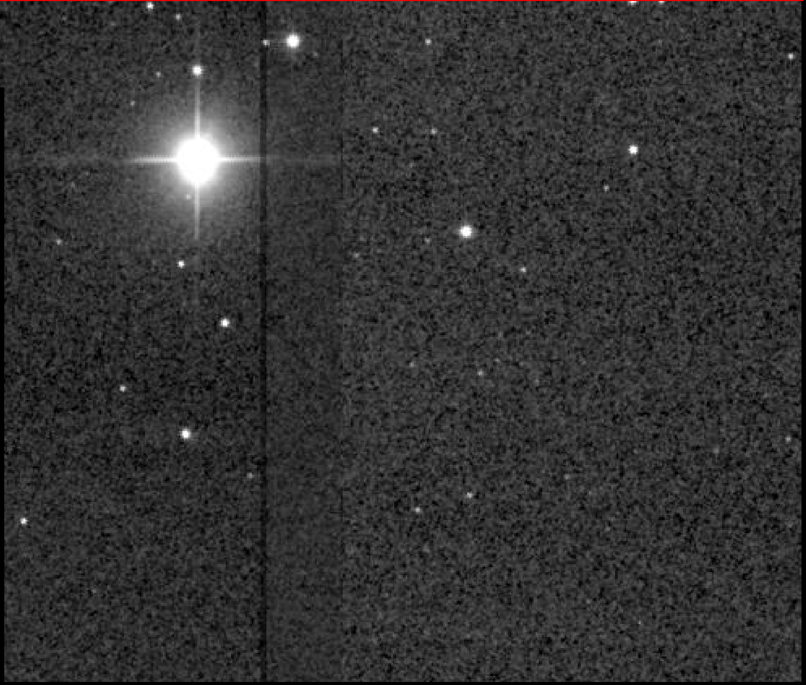


AGB stars loss mass through an isotropic wind

Extended dusty and molecular circumstellar envelope

- \# main source for the reclycing of the ISM
- \# strong absorption of the stellar light
- \# Mass loss rate varies between 10^{-3}-10^{-8}





IRC +10216:

- the carbon-rich star nearest to the Earth (~120 pc)
- brightest object in the sky at λ ~5-10 nm

λ@10 μnm; ESO/La Silla
B. Stecklum & H.-U. Kaüfl

Chemical study of the envelope

¿Why is so interesting the study of chemical composition of IRC +10216 ?

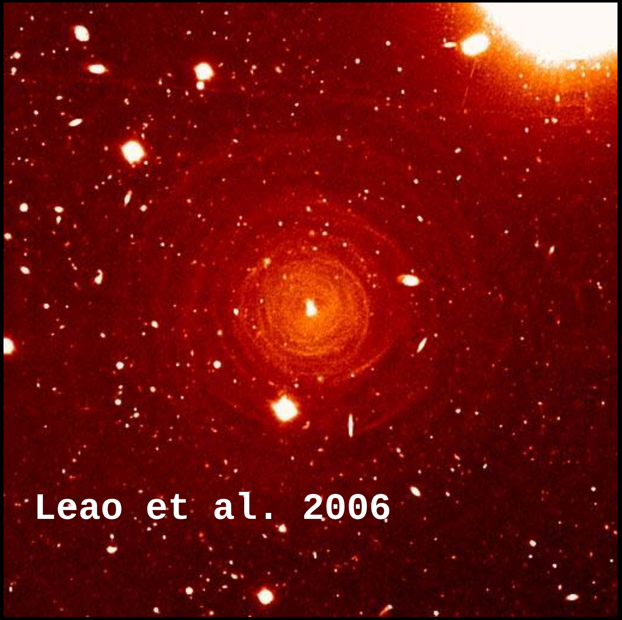
- IRC+10216 is a prototype of C-rich stars
- 50% of the molecules known in space have been detected in its CSE

The Extended Molecular envelope : The millimeter domain

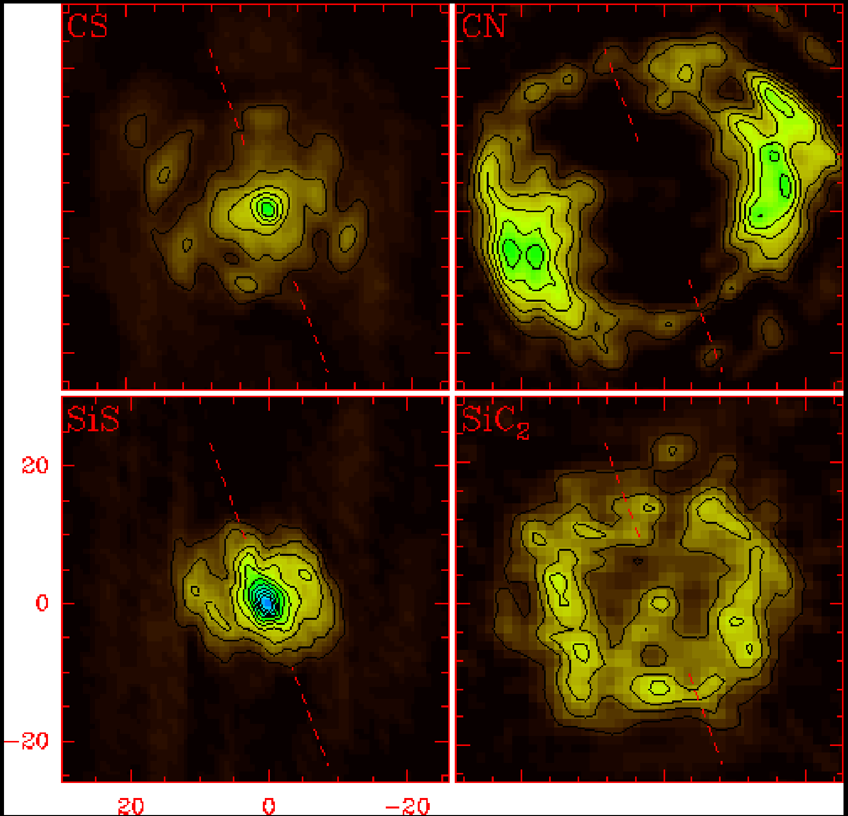
Two type of molecules:

I) Species formed under thermodynamical equilibrium near the photosphere

II) Species formed in the photodominated zone (the external shells of the envelope



Leao et al. 2006



EVOLVED STARS. BASIC CONCEPTS

* In the last stage of the star evolution stars are submitted to different processes of mass loss.

* The mass loss rate, dM/dt, can be as high as 10^{-4} M_O yr^{-1}.

* AGB stars inject into the ISM dust grains, molecules and heavy elements (^{12}C, ^{13}C, N, ^{17}O, ^{18}O,...)

*AGB stars inject momentum and energy into the ISM. O and B stars play a much more important role in this context but not in the chemical aspects.

* ¿ Which is the structure of an evolved star ?

The structure of the envelope depends on the distance to the star. The chemical composition will depend on the relative abundance of the atoms.

In the inner layers the abundance of C/O could be very different from the external layers because the gas is continuously enriched by the ejection of matter from the central object.

if C/O > 1 stars rich in Carbon
if C/O < 1 stars rich in Oxygen
if C/O ≈ 1 stars S

Photosphere : Temperature < 3000 K.
Very complex physical processes. Pulsation.

Theoretical values for isotropic mass loss rate :

Mass loss

$$\dot{M}(r) = n(r)\mu 4\pi r^2 V(r)$$

Density

$$\begin{aligned} n(r) &= \frac{C}{r^2}(V_\infty / v(r)) \qquad \mathrm{cm}^{-3} \\ C &= 3 \cdot 10^{37} \frac{\dot{M}_{-5}}{V_6} \qquad \mathrm{cm}^{-1} \end{aligned}$$

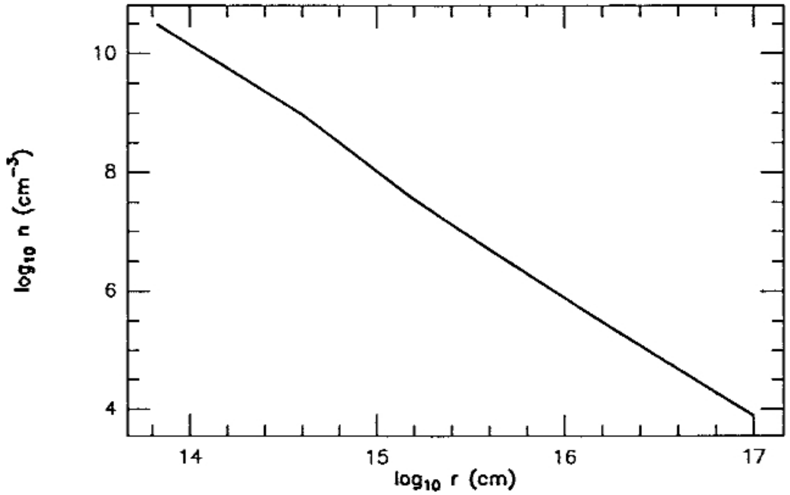
Temperature

$$T \sim 100 \left(\frac{r}{10^{16}} \right)^{-0.7} \mathrm{K}$$

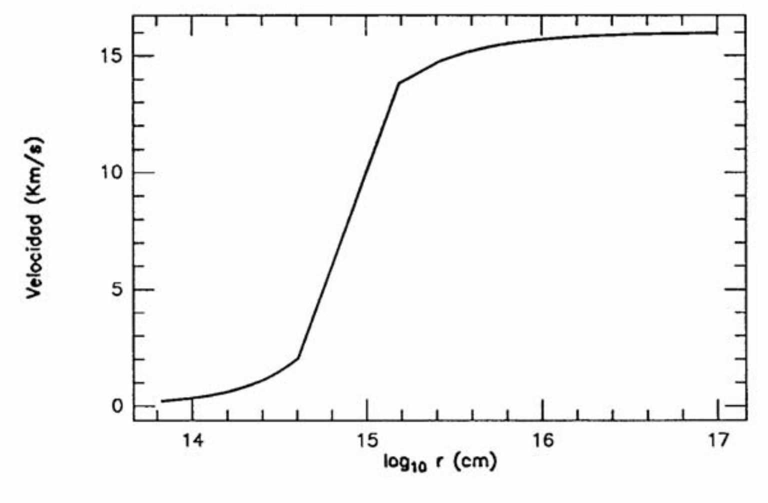
Velocity field

$$v(r) = V_\infty \left(1 - \frac{0.984 r_\circ}{r} \right)^{1/2}$$

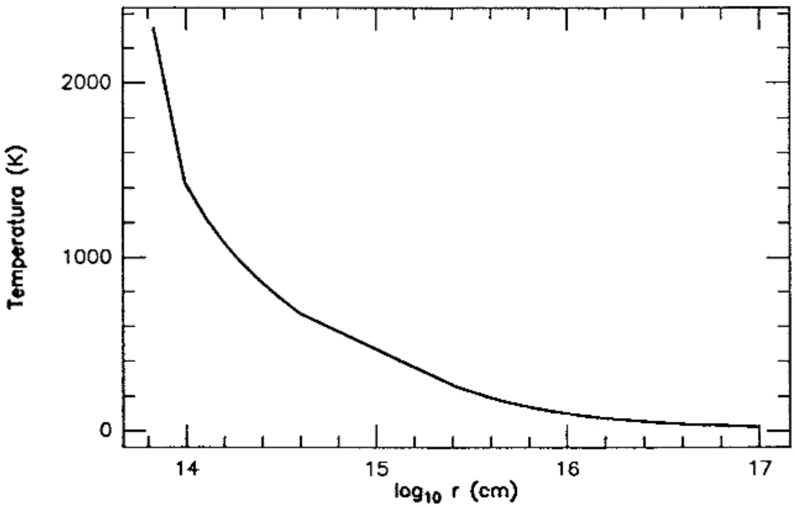
Physical Properties of an AGB Star



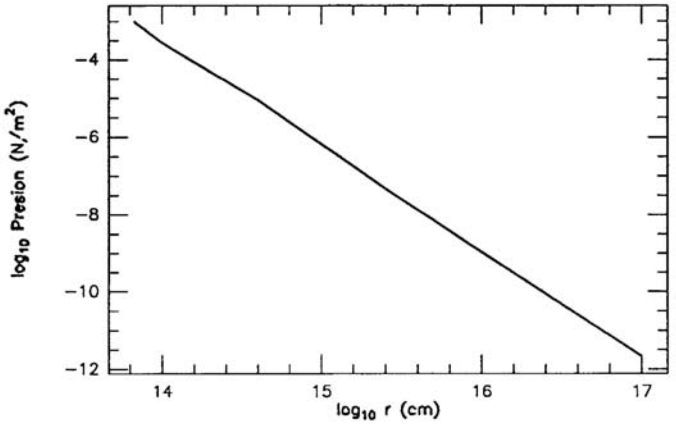
Density of H_2



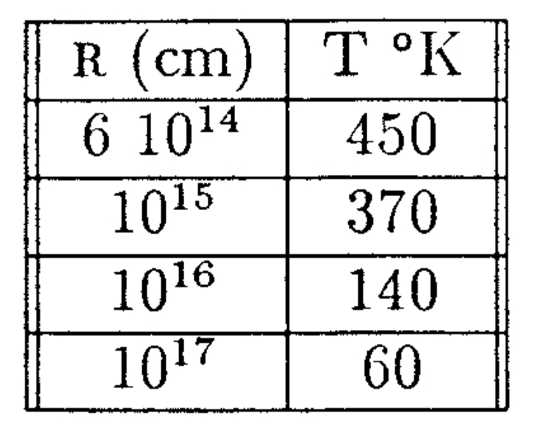
Velocity field



Temperature (K)



Pressure



R (cm)	T °K
$6\ 10^{14}$	450
10^{15}	370
10^{16}	140
10^{17}	60

At 10 stellar radii ($R_* \approx 6.7\ 10^{14}$ cm) the temperature is 450 K while in the zone of 1-2 stellar radii the gas must be at a temperature close to 1500 K. The density in innermost zone is of the order of 10^{10-12} cm^{-3}.

However, at 10 stellar radii is only of 10^{8-9} cm^{-3} and at 100 stellar radii of 10^{6} cm^{-3}.

The evolution time scale for the envelope is given by

$$\tau_{din} = r/v = 10^9 \left(\frac{r_{15}}{V_6}\right)$$

r_{15} and V_6 are the distance and velocity (units of 10^{15} cm, 10^{6} cm/s) For r_{15} = 1-100 and V_6 = 1 the dynamic time scale varies between 30 and 3000 years

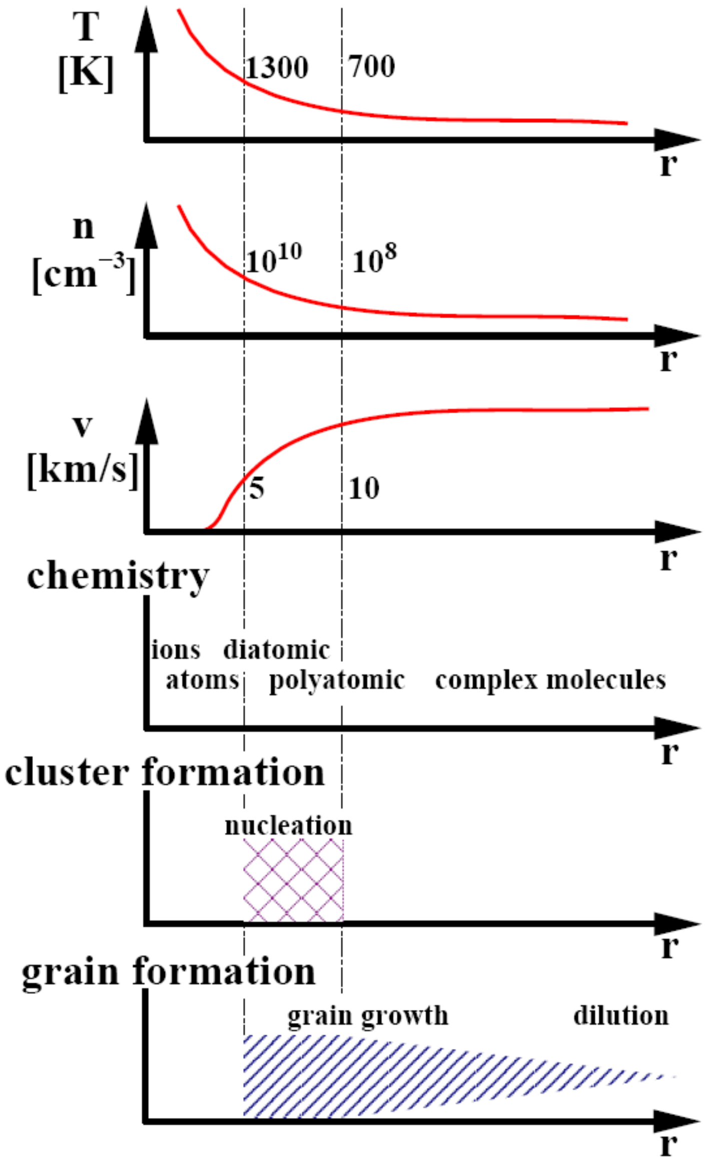


Figure 1. Schematic structure of a dust forming circumstellar shell. Dust nucleation is well confined to a region approximately between 1300 K and 700 K while the region of dust growth extends much farther outwards.

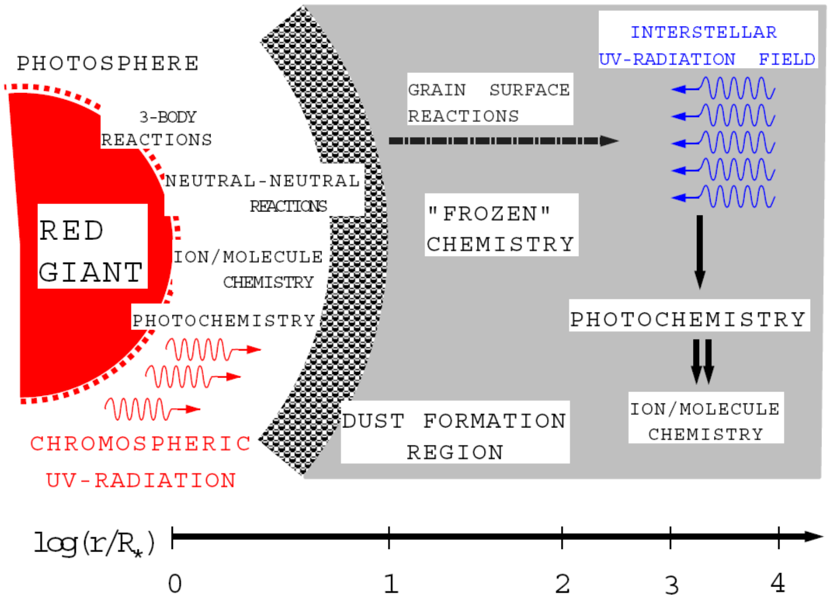
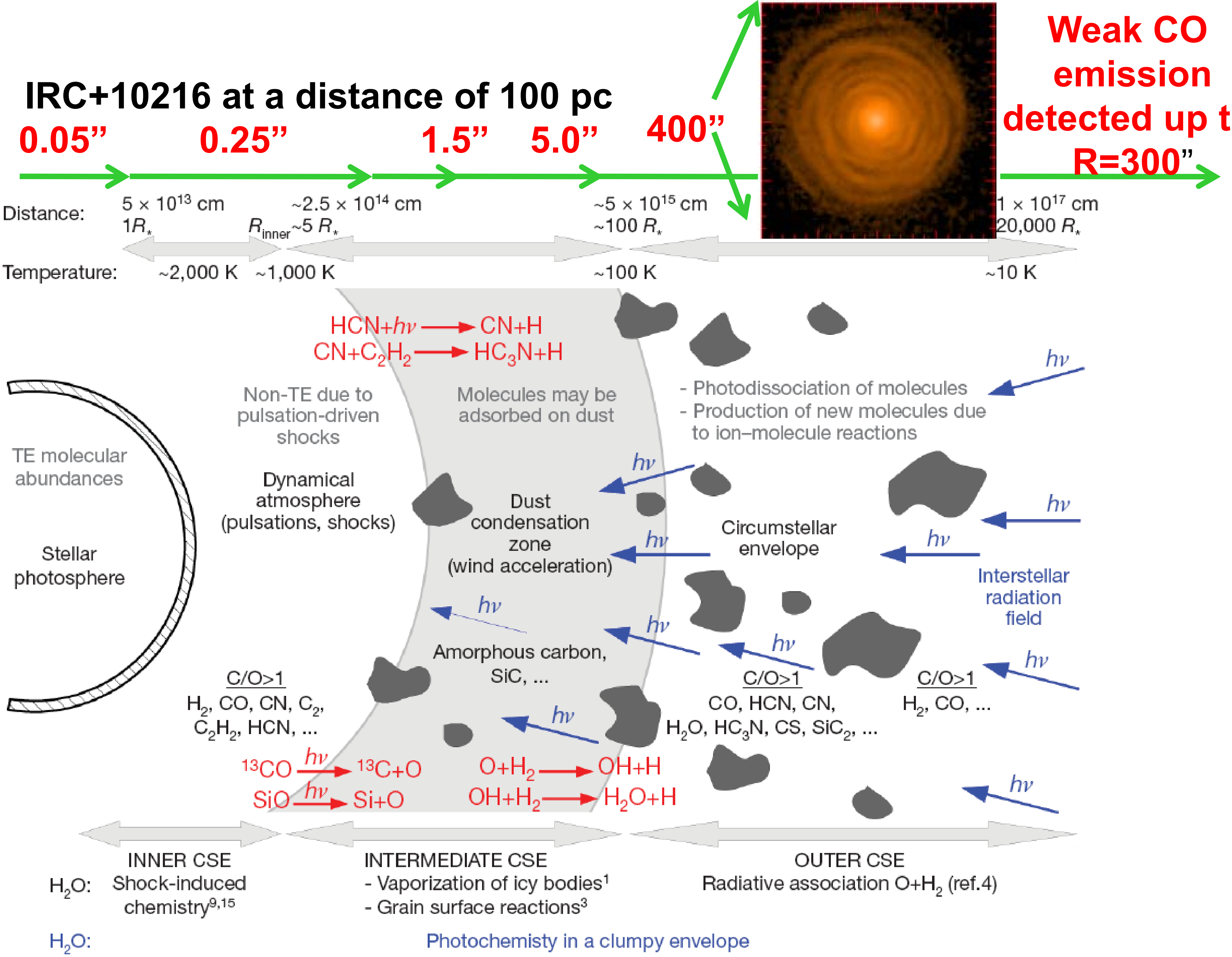


Figure 2. Chemical processes in different regions of the circumstellar shells around re
giants (adopted from Patzer (1996))

From Sedlmayr and coworkers

IRC+10216 at a distance of 100 pc



From Decin et al., 2010, Nature

MODELS UNDER THERMAL EQUILIBRIUM

Reaction rates and the path to form molecules are not important. Molecular abundances are determined by their value at thermo-dinamical equilibrium.

That means that two and three body reactions must be much faster that the time scale for dinamic evolution.

Of course, these models will provide reasonable results only for the most dense and warm regions. In the external layers of the envelope molecular abundances will be strongly dependent on the chemical kinetics and on the UV photons entering the envelope.

First studies for cold stars under the hyphotesis of ET :
Russell (1934)
Fujita (1939, 1940, 1941)

These models were able to predict the abundances of the most conspicous diatomic molecules detected in red giant stars (VO, TiO, CN, CH,…). These models also predicted the presence of some Polyatomic molecules that were detected 50 years later.

The models (Fujita) clearly indicated the role of the atomic abundances H:C:N:O in the abundances of diatomic species determined in ET. Russell was even able to apply his models to the Sun and to predict the presence of CO, CN and C2 for temperatures below 4000 K.

Tsuji 1973 :
Very detailed study of the chemistry under ET in cold stars. He considered 36 elementos and hundreds of molecules

McCabe in 1979 introduces the concept of molecular freezing.

* Molecules are formed in the innermost region of the envelope.

* Refractory species condensate and form dust grains.

* Radiation pression over dust grains and the star pulsation initiate the expansion of the envelope

* When the density and temperature of the gas decrease due to the expansion chemical reactions become very slow. The time scale for dinamic evolution is faster that the formation rate of molecules.

* The molecular abundances in the external layers reflect the abundances produced under ET in the innermost region.

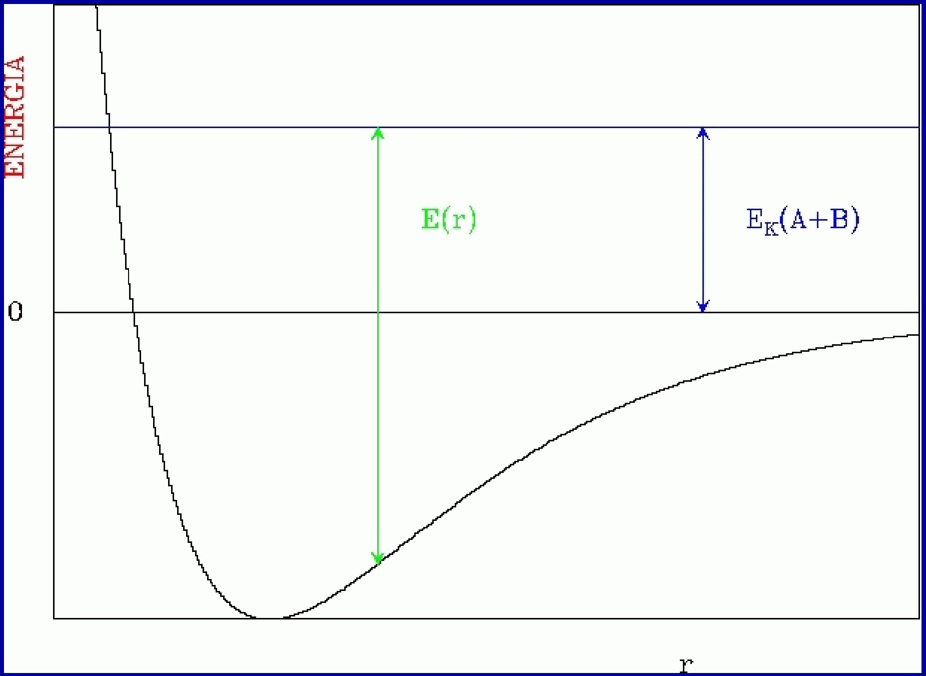
* OK for many species but of very difficult justification for radicals and large carbon-chains.

THREE BODY REACTIONS

Let us consider the reaction

$A + B \rightarrow AB^{*} \quad (k_1)$

It may happens that AB^{*} interacts with a third body (catalizer) to remove the energy excess produced in the formation of the activated complex. However, also AB^{*} could dissociate into the initial particles A and B



$AB^{*} + M \rightarrow AB + M \quad (k_2)$

$AB^{*} \rightarrow A + B \quad (k_3)$

The formation rate of the molecule AB, assuming that the activated complex reaches an equilibrium between formation and destruction is given by

$$dn(AB)/dt = n(AB^*) \times n(M)k_2$$
$$dn(AB^*)/dt = n(A) \times n(B) \times k_1 - n(AB^*) \times n(M) \times k_2 - n(AB^*) \times k_3$$

$$dn(AB^*)/dt = 0$$

$$n(AB^*) = \frac{n(A)\ \ n(B)\ \ k_1}{(\,k_3+k_2\ n(M)\,)}$$

and

$$dn(AB)/dt = \frac{k_1\ k_2\ n(A)\ \ n(B)\ \ n(M)}{k_3 + k_2\ \ n(M)}$$

If A, B y M are neutral species then $k_1 \approx 10^{-11}$ cm^3s^{-1} and $k_2 \approx 10^{-10}$ cm^3s^{-1} , but k_3 10^{+11} s^{-1}, and

$$dn(AB)/dt \approx 10^{-32}\ n(A)\ \ n(B)\ \ \ n(M)\ \ cm^{-3}s^{-1}$$

The best case in the ISM occurs for A=B=M= H

$$H + H + H \Leftrightarrow H_2 + H$$

For hydrides (BH) the optimal case will correspond to A=H, M=H and $B \in (C,N,O)$, i.e., $n(B) \approx 10^{-4}\ n(H)$ and

$$dn(BH)/dt \approx 10^{-36}\ n^3(H)\ cm^{-3}\ s^{-1} \quad B \in (C,N,O)$$

EXAMPLE:

Let us consider an atomic cloud without dust grains and without radiation field. For t=0 the density of atomic hydrogen is n and that of molecular hydrogen is 0. The formation of H_2 occurs through the reaction

$$H + H + H = H_2 + H$$

with a rate $K = 10^{-32}$ $cm^6\ s^{-1}$

The formation rate of H_2 is given by

$$\frac{dn(H_2)}{dt} = K\, n^3_H(t); \qquad f(t) = \frac{2\, n_{H2}(t)}{n_H(t) + 2\, n_{H2}(t)} = \frac{2\, n_{H2}(t)}{n}$$

$$\frac{df(t)}{dt} = K\, n^2\, (1 - f(t))^3$$

$f(t) = 0.5$ for which time ?

EXAMPLE

$f(t)=0.5$

$n(cm^{-3})$	10^5	10^{10}	10^{12}	10^{15}	10^{16}	10^{18}
t(years)	$6\ 10^{14}$	$6\ 10^4$	6	$6\ 10^{-6}$	$6\ 10^{-8}$	$6\ 10^{-10}$
				(600 s)	(6s)	(0.0006s)

The three body mechanisms is only efficient for densities larger than 10^{10} cm^{-3}. Even in this case, the density is not enough taken into account the dynamical time scale of evolution of the object.

For a density of 10^{14} cm^{-3}, i.e., the photosphere of an AGB star, the time necessary to transform H into H_2 is $6\ 10^{-4}$ yr = 5.3 hours !!!!

What chemistry under TE means ?

The main parameter is the total pressure of the gas (density and temperature). Let us define a fictious total pressure for H as

$$P_T = P_{\mathrm{H}} + P_{\mathrm{H^+}} + P_{\mathrm{H^-}} + P_{\mathrm{H_2}} + P_{\mathrm{He}} + P_{e^-}$$

It is possible to stablished a series of equations for each element

$$\begin{aligned}
\mathrm{P(H)} &= P_{\mathrm{H}} + P_{\mathrm{H^+}} + P_{\mathrm{H^-}} + 2P_{\mathrm{H_2}} \\
P_{\mathrm{He}} &= a(\mathrm{He})\mathrm{P(H)} \\
&= a(\mathrm{He})[P_{\mathrm{H}} + P_{\mathrm{H^+}} + P_{\mathrm{H^-}} + 2P_{\mathrm{H_2}}] \\
P_{e^-} &= P_{\mathrm{H^+}} - P_{\mathrm{H^-}}
\end{aligned}$$

The total pressure is given by

$$P_T = (a+1)P_{\mathrm{H}} + (2+a)P_{\mathrm{H}^+} + (2a+1)P_{\mathrm{H}_2} + aP_{\mathrm{H}^-}$$

For a molecule $A_aB_bC_c$, the constant of its dissociative process is given by

$$A_aB_bC_c \Longleftrightarrow aA + bB + cC$$

$$K_p(T) = \frac{P_A^a P_B^b P_C^c}{P_{ABC}}$$

Where P_i is the partial pressure of the component *i* and $K_p(T)$, the equilibrium constant, depends strongly on T.

For molecular hydrogen we have

$$K_{H_2} = \frac{P_H^2}{P_{H_2}}$$

And some thing similar can be written for the ionization processes

$$\begin{aligned} \mathrm{H} &\Longleftrightarrow \mathrm{H}^+ + e^- \\ \mathrm{H} + e^- &\Longleftrightarrow \mathrm{H}^- \end{aligned}$$

$$\begin{aligned} K_{\mathrm{H}+} &= \frac{P_{\mathrm{H}+} P_{e-}}{P_{\mathrm{H}}} \\ K_{\mathrm{H}-} &= \frac{P_{\mathrm{H}-}}{P_{e-} P_{\mathrm{H}}} \end{aligned}$$

We obtain three equations -non linear- for the fictious pressures

$$P_{\mathrm{H+}}^2 - P_{\mathrm{H-}}P_{\mathrm{H+}} - K_{\mathrm{H+}}P_{\mathrm{H}} = 0$$
$$P_{\mathrm{H-}} - K_{\mathrm{H-}}P_{\mathrm{H+}}P_{\mathrm{H}} + K_{\mathrm{H-}}P_{\mathrm{H-}}P_{\mathrm{H}} = 0$$
$$AP_{\mathrm{H}} + (A+1)P_{\mathrm{H+}} + \left(\frac{2A-1}{K_{\mathrm{H}2}}\right)P_{\mathrm{H}}^2 + (A-1)P_{\mathrm{H-}} - P_T = 0$$

where A = a(He)+1. The system can be solved easily through Newton-Raphson methods. When we have P_{H}, P_{H+} y P_{H-} the value of PH_2 can be obtained from

$$K_{\mathrm{H}_2} = \frac{P_{\mathrm{H}}^2}{P_{\mathrm{H}_2}}$$

And then we can derive P(H). For the other elements we obtain the partial pressures from the relation

$$\mathrm{P(i)} = a(\mathrm{i})\mathrm{P(H)}$$

Thermodinamical equilibrium

For each element we stablish a conservation law

$$\mathrm{P(i)} = P_i + P_{i^+} + P_{i^-} + \sum_k \omega_k^i P_k$$

where P_i, P_{i+}, P_{i-} are the partial pressures of *i*, i^+, *y* i^- and P_K is the partial pressure of molecule *K* in which the element *i* appears w^i_{K}. times

$$\mathrm{P(i)} = P_i + K_{i^+}\frac{P_i}{P_{e^-}} + K_{i^-} P_i P_{e^-} + \sum_k \omega_k^i \frac{P_i^{\omega_k^i} P_j^{\omega_k^j} \ldots P_l^{\omega_k^l}}{K_p^{(k)}(T)}$$

where $w^i_K+w^j_K+\ldots+w^l_K=n_K$, is the number of atoms in the molecule formed by the elements *i,j,..,l* and $K_p^{(K)}(T)$ is the dissociation constant

A similar expression can be written for the electrons

$$\begin{aligned} P_{e^-} &= \sum P_{\mathrm{iones}+} + \sum P_{\mathrm{moleculas}+} - \sum P_{\mathrm{iones}-} - \sum P_{\mathrm{moleculas}-} \\ &= \sum^{N+} \frac{K_{i+} P_i}{P_{e^-}} + \sum_k C_k P_i^{\omega_k^i} \cdots P_j^{\omega_k^j} \frac{P_l^{\omega_k^l + C_k} K_{l+}^{C_k}}{K_p^{(k)} P_{e^-}^{C_k}} - \\ &- \sum^{N-} K_{j-} P_j P_{e^-} - \sum_k C_k P_i^{\omega_k^i} \cdots P_j^{\omega_k^j} \frac{P_l^{\omega_k^l + C_k} K_{l-}^{C_k} P_{e^-}^{C_k}}{K_p^{(k)}} \end{aligned}$$

where N+ y N- are the number of positive and negative ions, etc..

From pure thermodinamic concepts it can be found that

$$-RT \ln K_p = \Delta G_T^o$$

It is easy to show that

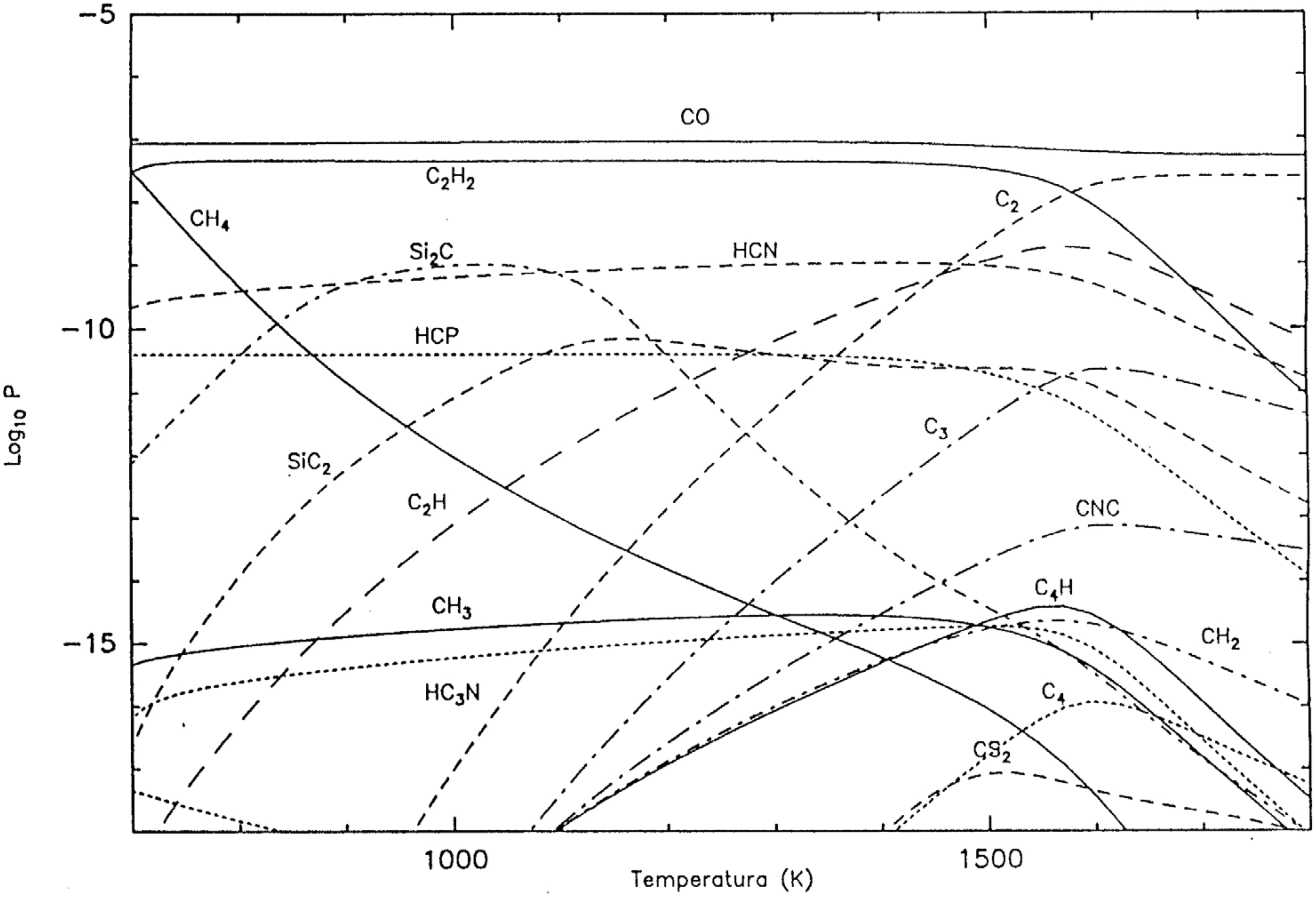
$$\begin{aligned} K_p(T) &= \frac{p_A^a p_B^b p_C^c}{P_{A_aB_bC_c}} \\ &= \left(\frac{kT}{V}\right)^{NA-1} \frac{\phi_A^a \phi_B^b \phi_C^c}{\phi_{ABC}} \exp\left[-(a\epsilon_{oA} + b\epsilon_{oB} + c\epsilon_{oC} - \epsilon_o^{ABC})/kT\right] \end{aligned}$$

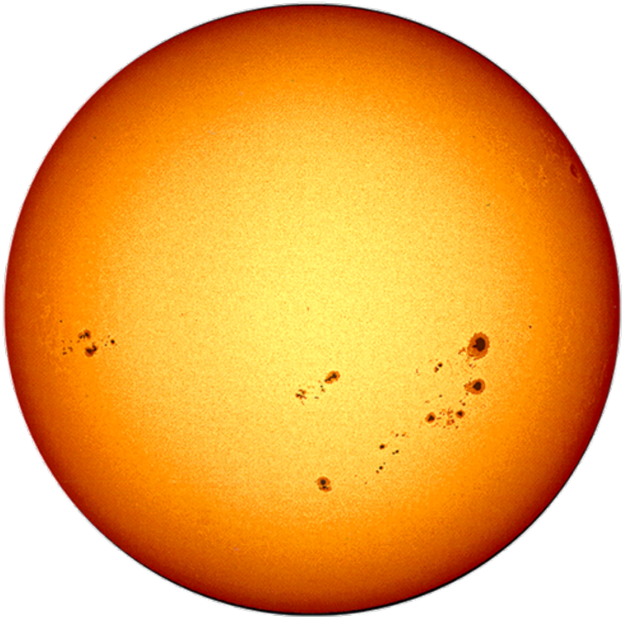
$$\begin{aligned} K_p(T) &= (kT)^{NA-1}(2\pi kT/h^2)^{\frac{3}{2}(NA-1)} \left(\frac{m_A^a m_B^b m_C^c}{m_{ABC}}\right)^{3/2} \\ &\quad \frac{\phi_A^a \phi_B^b \phi_C^c}{\phi_{ABC}} e^{-\Delta E_o^o/RT} \end{aligned}$$

$$\begin{aligned} \log K_p(T) &= \frac{5}{2}(NA-1)\log T + \frac{3}{2}\log \frac{m_A^a m_B^b m_C^c}{m_{ABC}} + \log \frac{\phi_A^a \phi_B^b \phi_C^c}{\phi_{ABC}} \\ &\quad + \frac{5}{2}(NA-1)\log k + \frac{3}{2}(NA-1)\log \frac{2\pi}{h^2} - \frac{\Delta E_o^o \log e}{RT} \end{aligned}$$

i.e., equilibrium constants can be derived from the partition functions of individual atoms and of the molecule !!!!

MOLECULAR ABUNDANCES AS A FUNCTION OF THE TEMPERATURE





Water in the Sun !!!!
Thermodynamical equilibrium works nicely

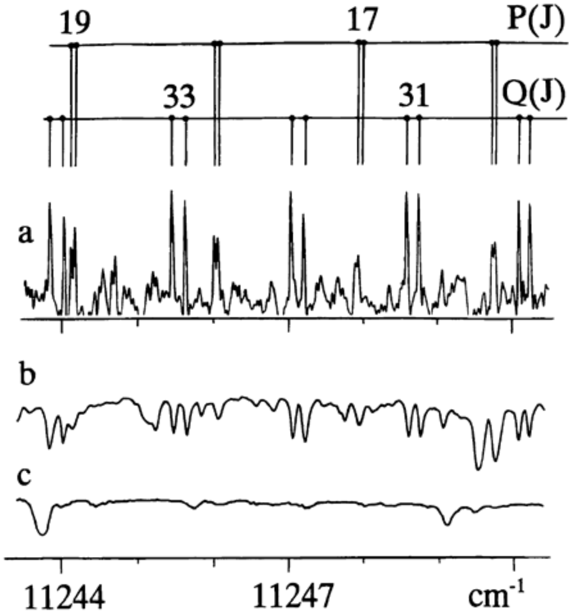


FIG. 1.—A part of the spectrum of the 0–0 band of the δ system ($b\,^1\Pi$–$a\,^1\Delta$) of TiO. (*a*) Laboratory spectrum; (*b*) sunspot spectrum; (*c*) photospheric spectrum.

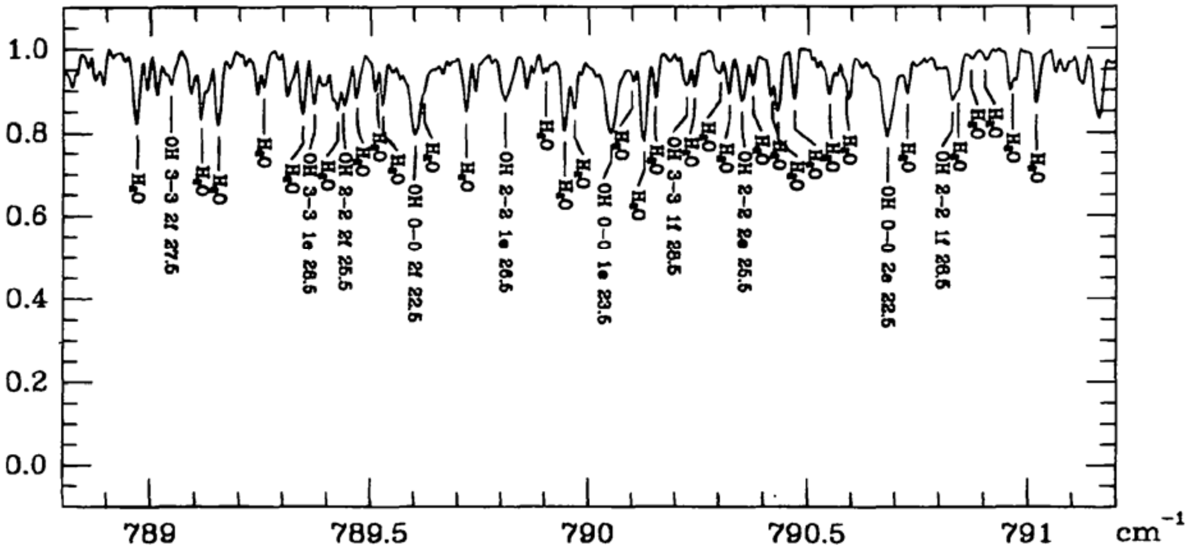
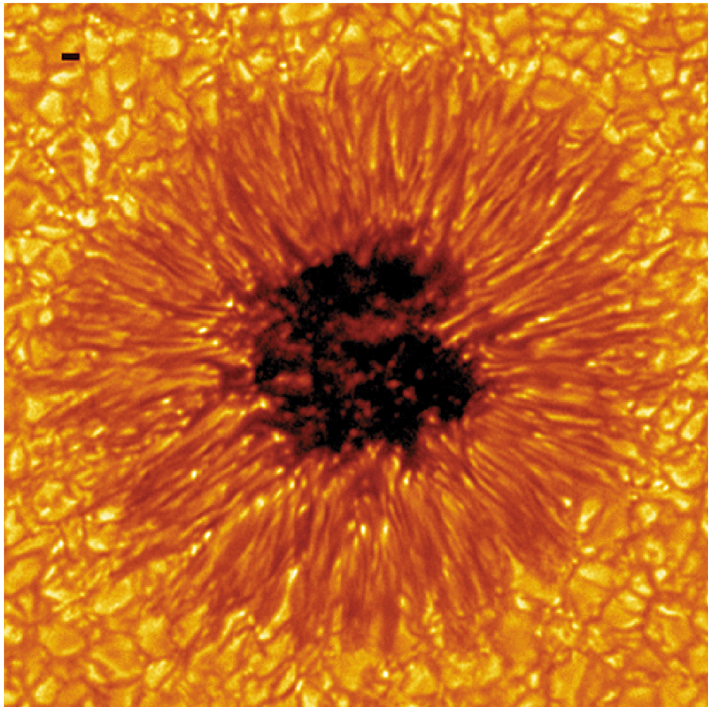
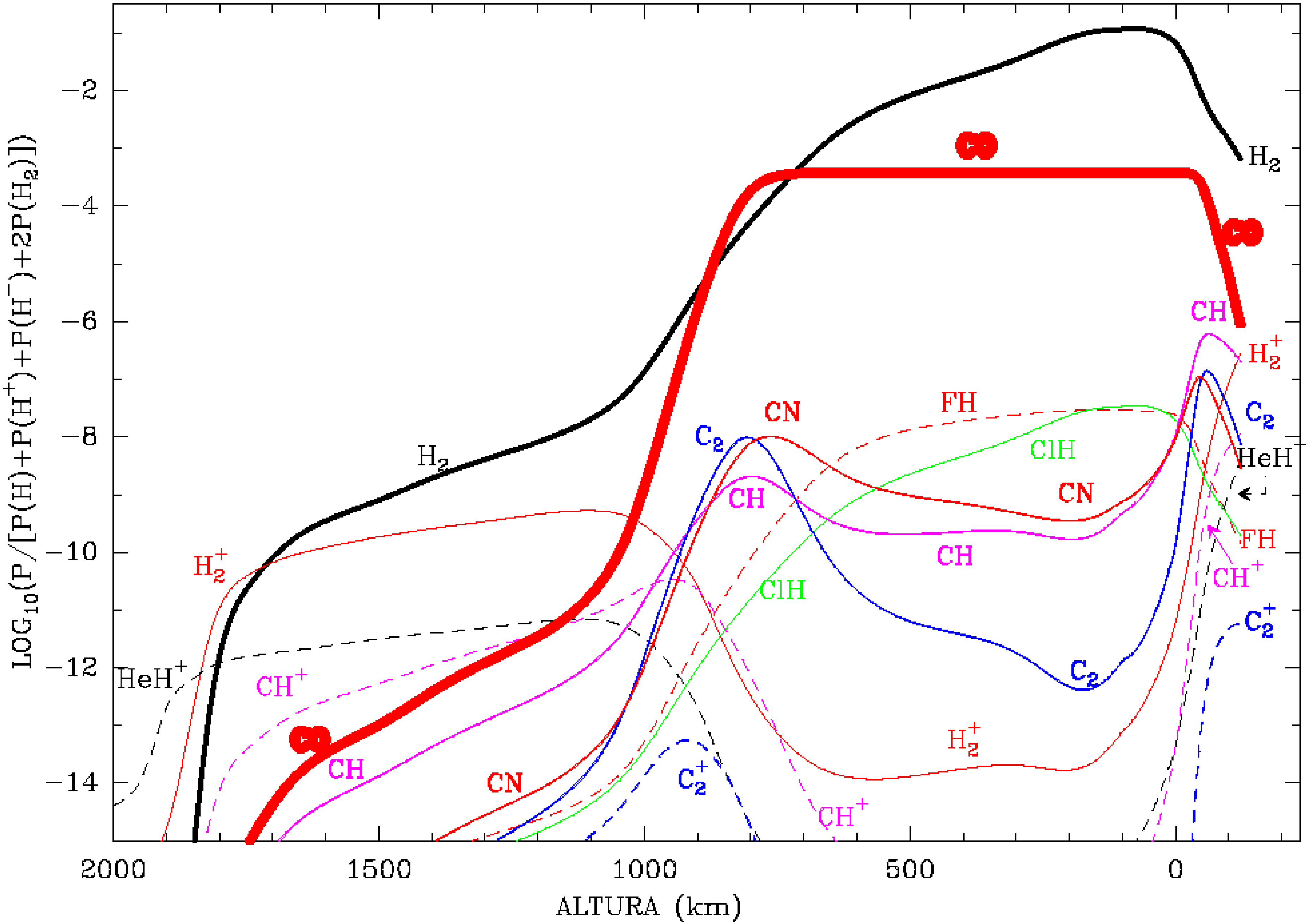
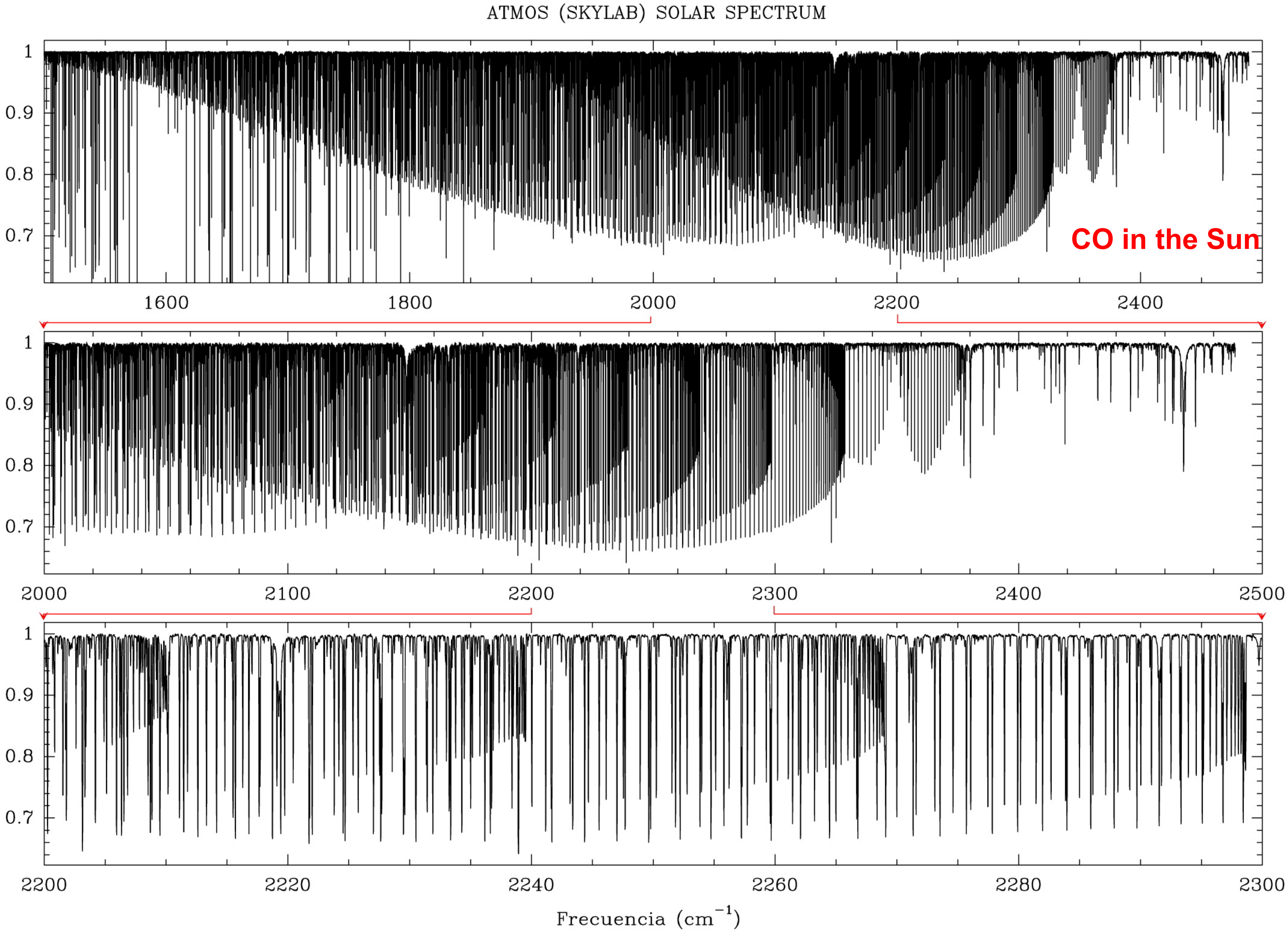


FIG. 3.—A section of the umbral spectrum from 12.636 to 12.674 μm from atlas 4. The unidentified lines in this region are probably H_2O. The telluric lines were divided out with a penumbral reference spectrum similar to a photospheric spectrum.



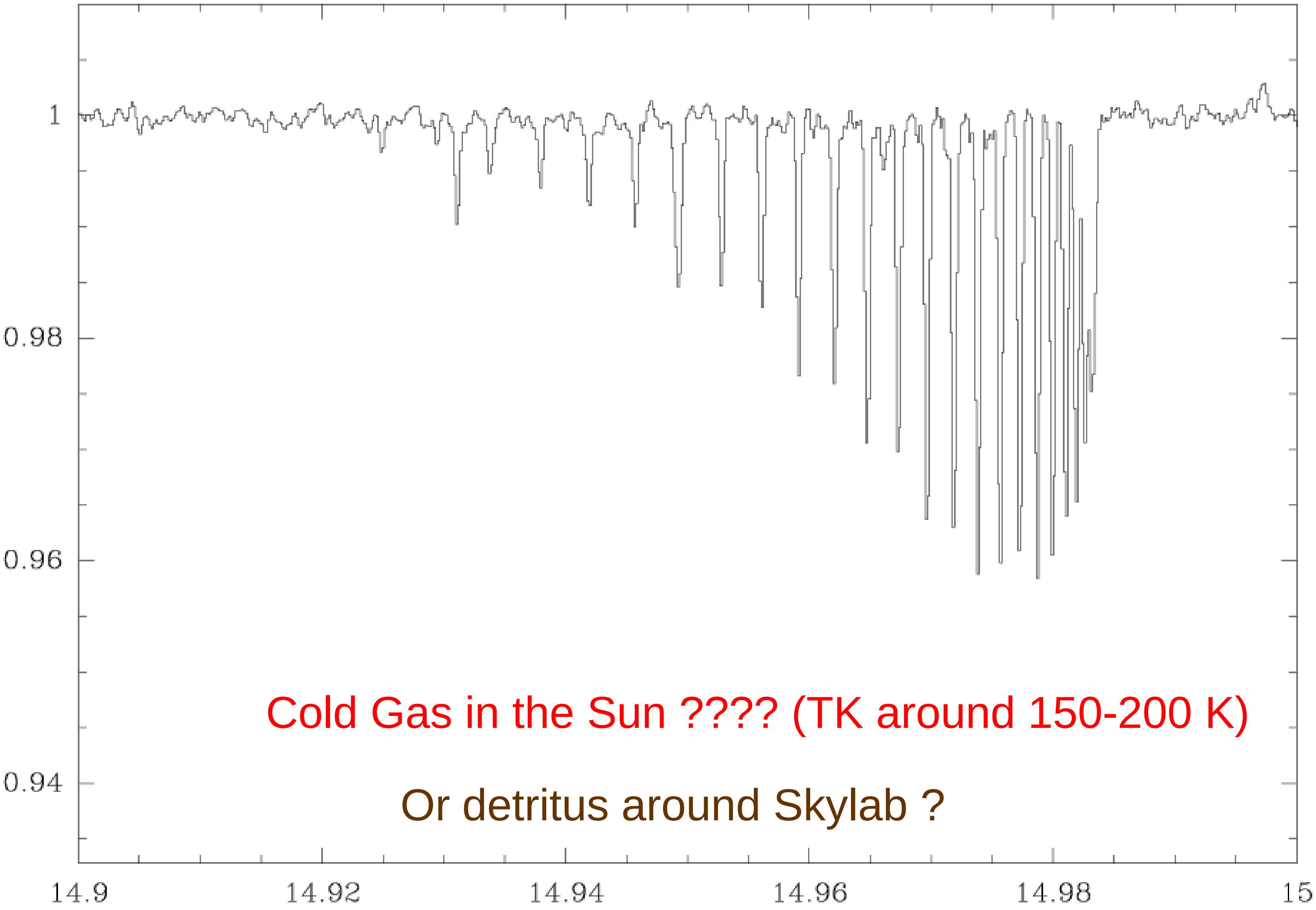


$LOG_{10}(P/[P(H)+P(H^+)+P(H^-)+2P(H_2)])$
−2
−4
−6
−8
−10
−12
−14
2000
1500
1000
500
0
ALTURA (km)
H_2
H_2
CO
CO
CO
CH
H_2^+
C_2
FH
CN
C_2
ClH
CN
CH
HeH^+
CH
FH
H_2^+
CH^+
ClH
C_2^+
HeH^+
CH^+
C_2
CH
CN
C_2^+
H_2^+
CH^+


ATMOS (SKYLAB) SOLAR SPECTRUM

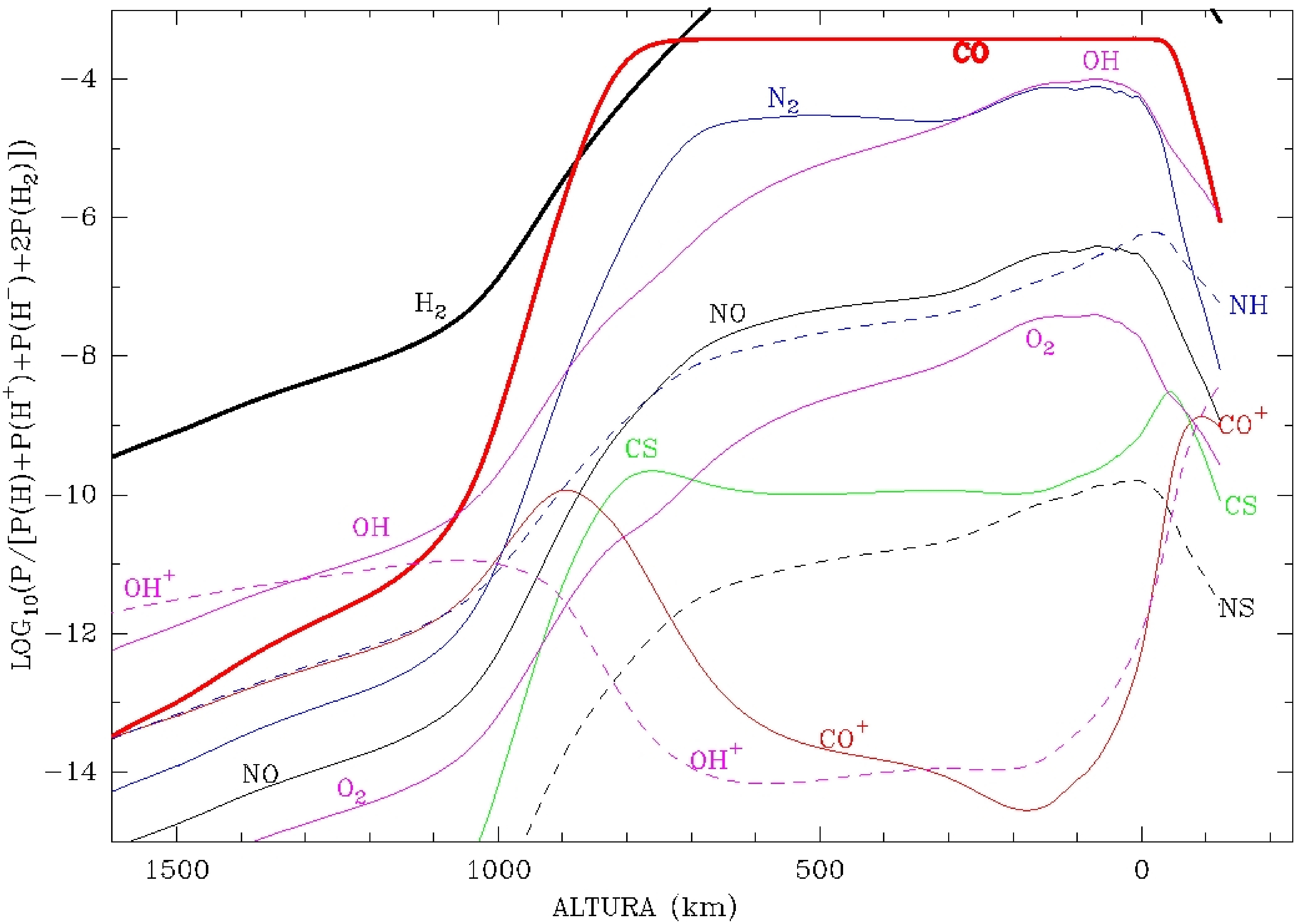
CO in the Sun

All frequencies can be computed with a few constants !



Cold Gas in the Sun ???? (TK around 150-200 K)

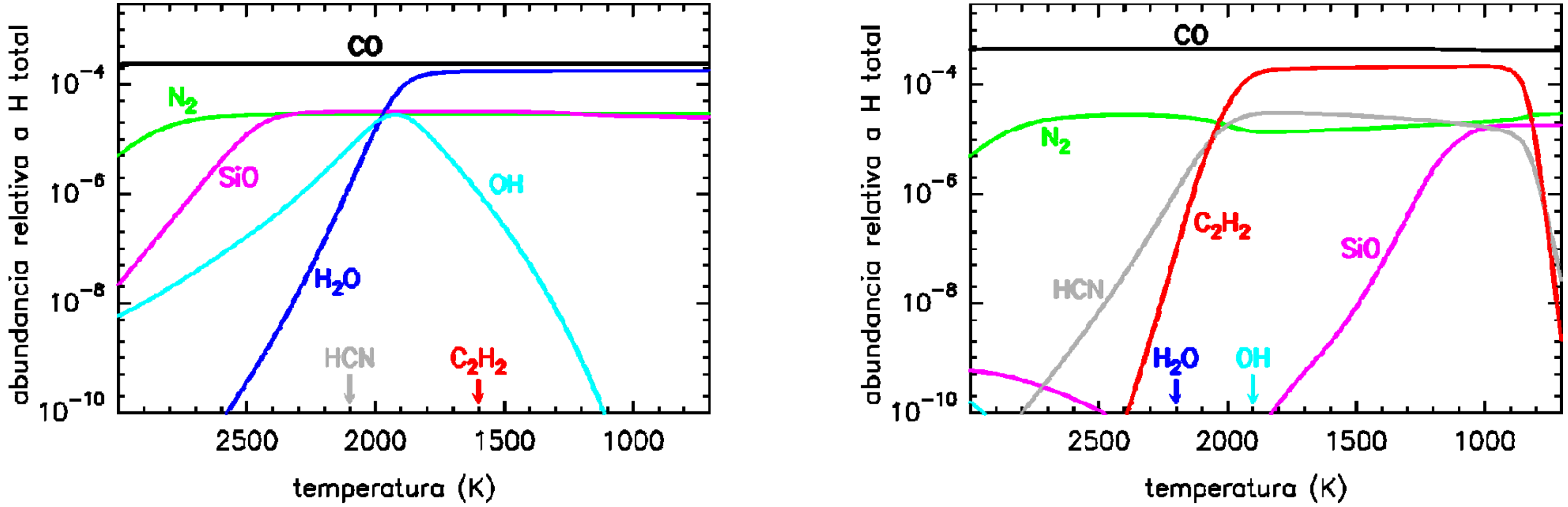
Or detritus around Skylab ?


CO
OH
N_2
H_2
NO
NH
O_2
CO^+
CS
CS
OH
OH^+
NS
CO^+
OH^+
NO
O_2
$\mathrm{LOG}_{10}(\mathrm{P}/[\mathrm{P(H)}+\mathrm{P(H^+)}+\mathrm{P(H^-)}+2\mathrm{P(H_2)}])$
−4
−6
−8
−10
−12
−14
1500
1000
500
0
ALTURA (km)

O-rich or C-rich, that is the question

O-rich star
[C]/[O] < 1

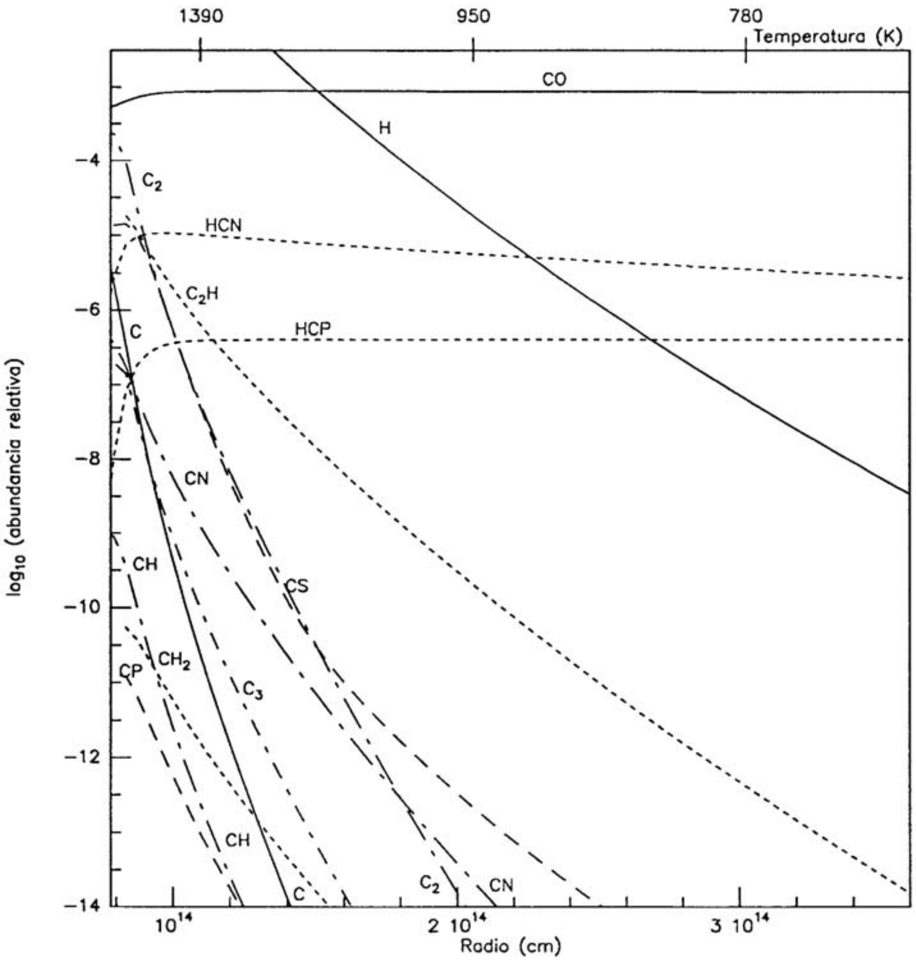
C-rich star
[C]/[O] > 1

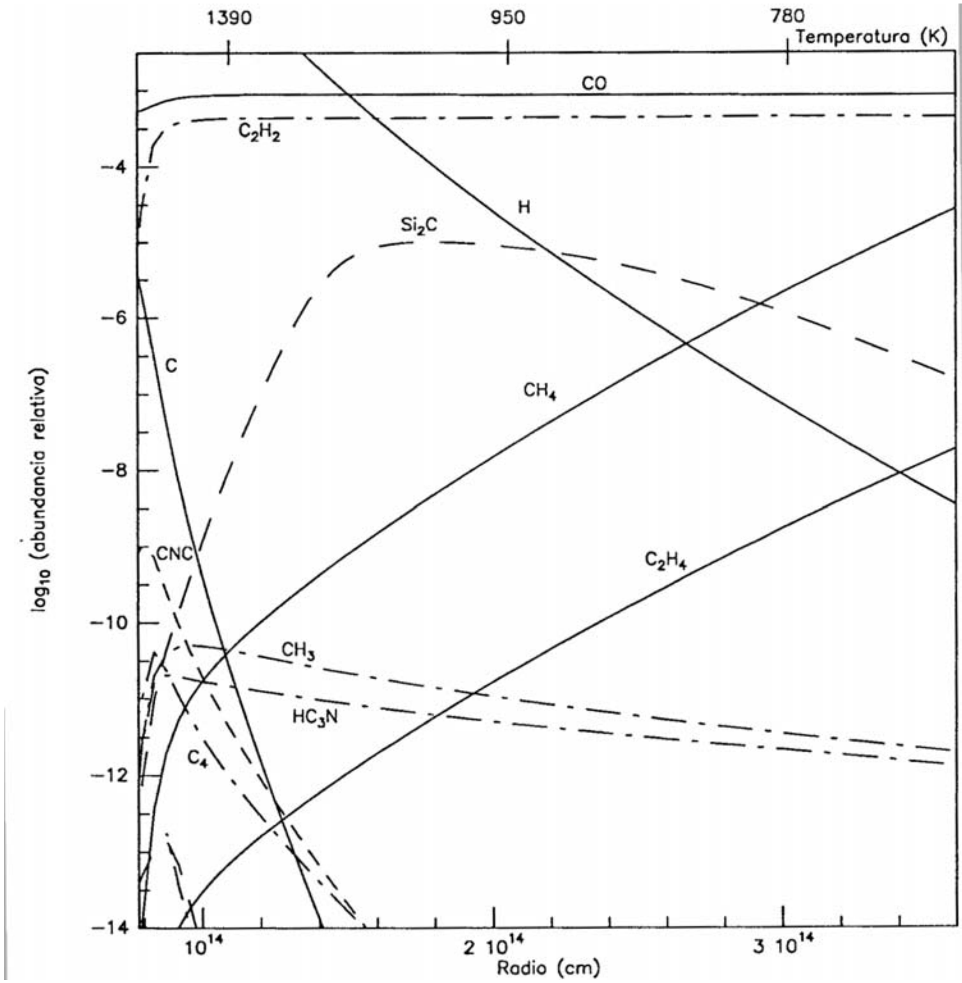


O-bearing molecules:
H_2O, SiO, OH, …

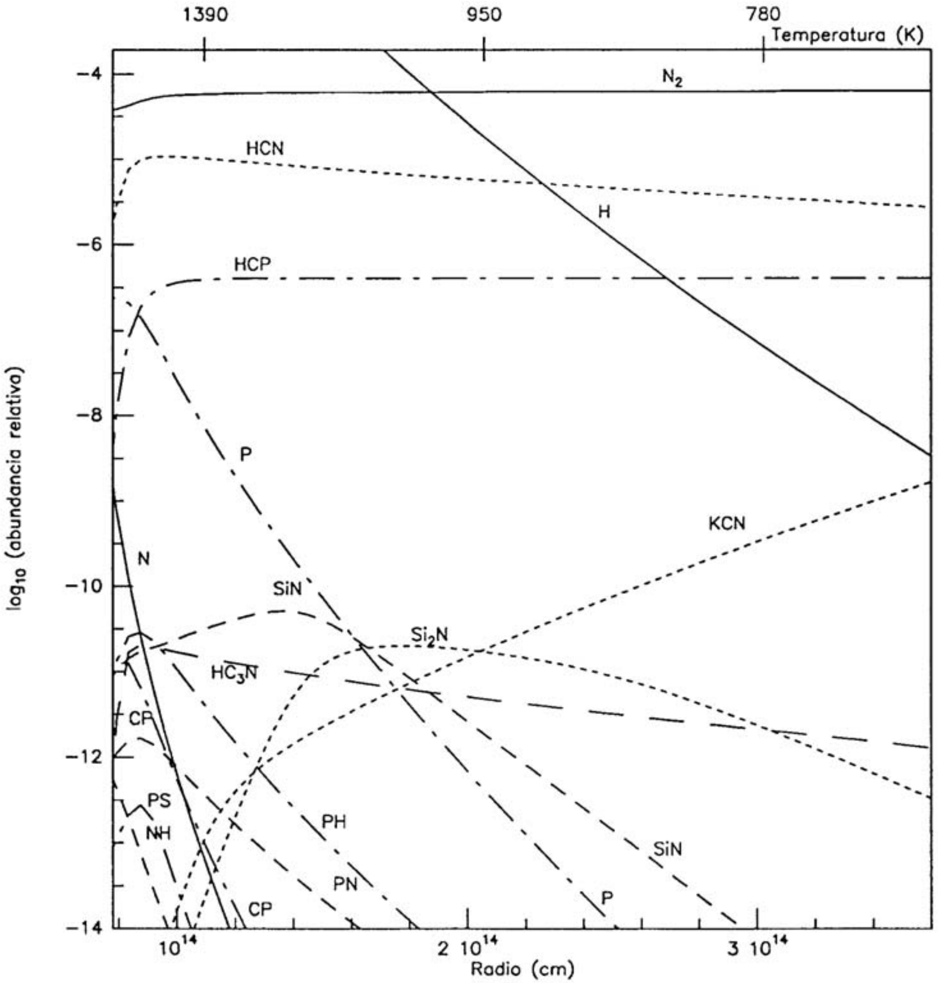
C-bearing molecules:
C_2H_2, HCN, CS, …

C-rich Stars (IRC+10216)

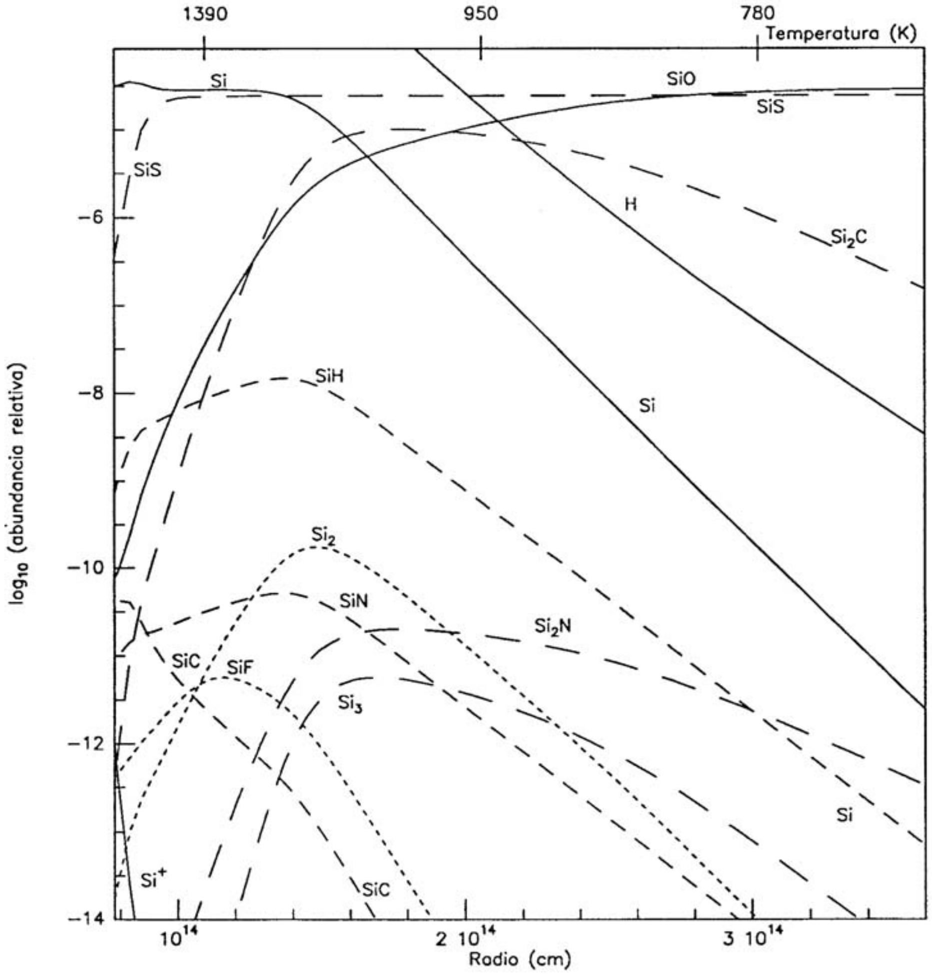




Carbon-bearing Molecules



Molecules with N and P



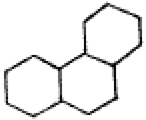
Molecules with Si

What happens if we consider big carbon-rich molecules?

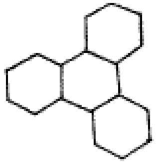
C_6H_6

$C_{10}H_8$ (naphthalene)

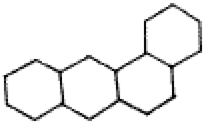
$C_{14}H_{10}$ (anthracene)



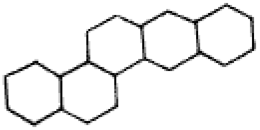
$C_{14}H_{10}$ (phenanthrene)



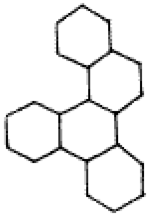
$C_{18}H_{12}$ (triphenylene)



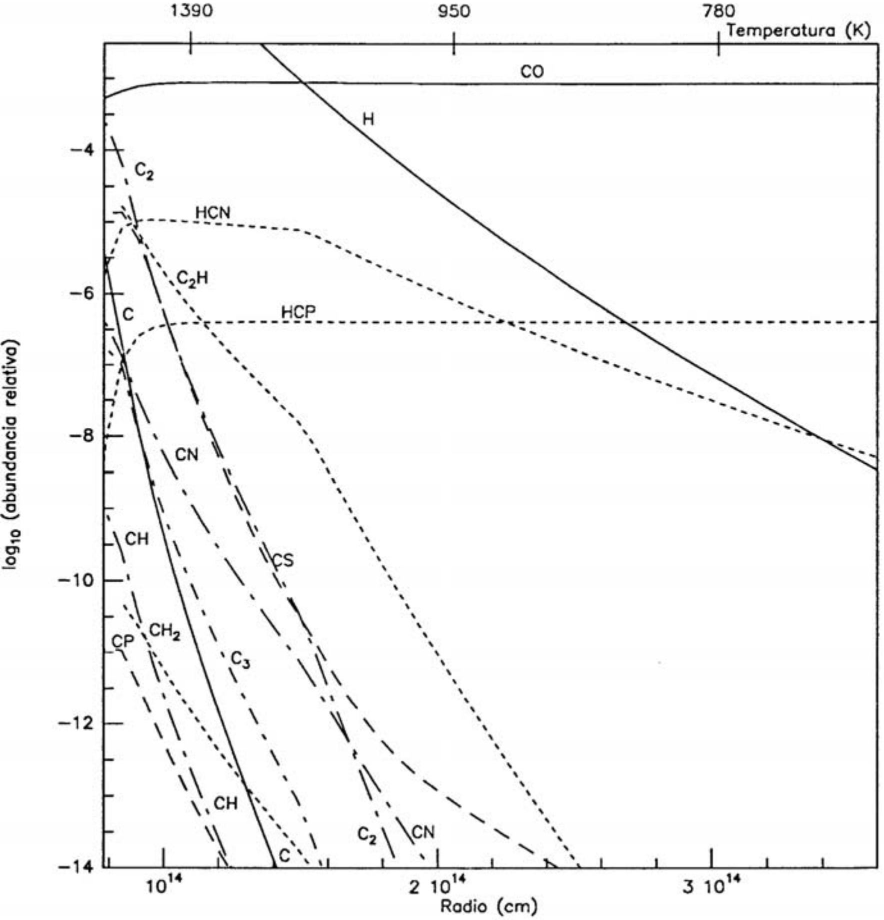
$C_{18}H_{12}$ (benzo(c)phenanthrene)



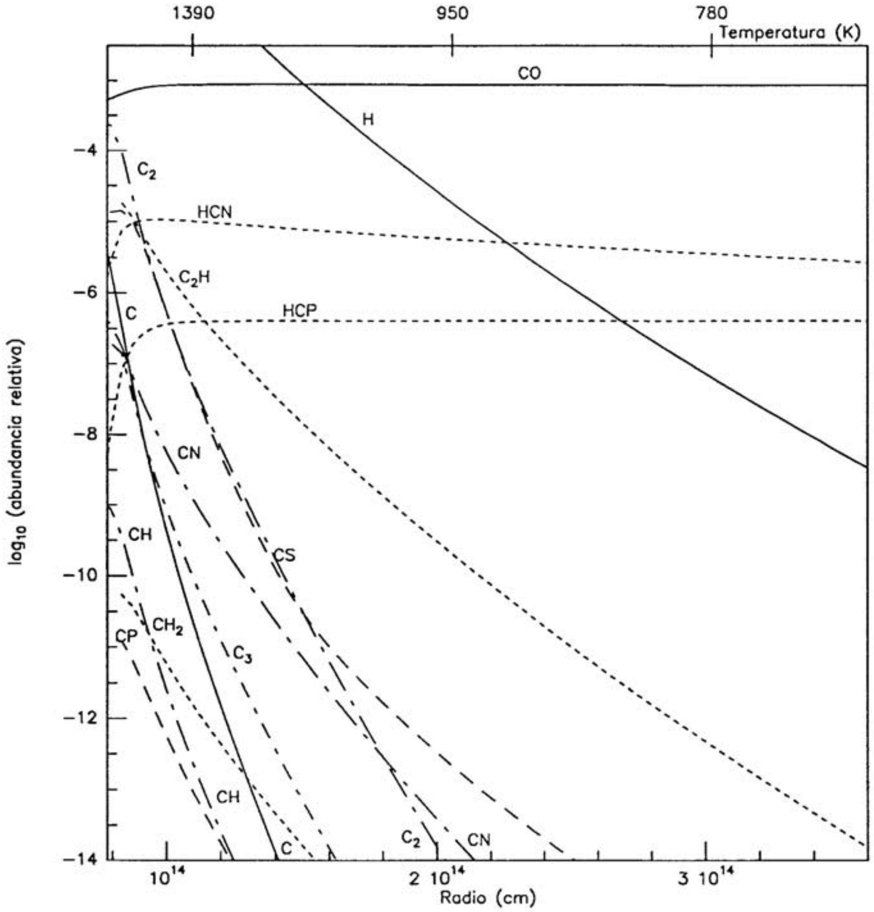
$C_{22}H_{14}$ (benzo(c)chrysene)



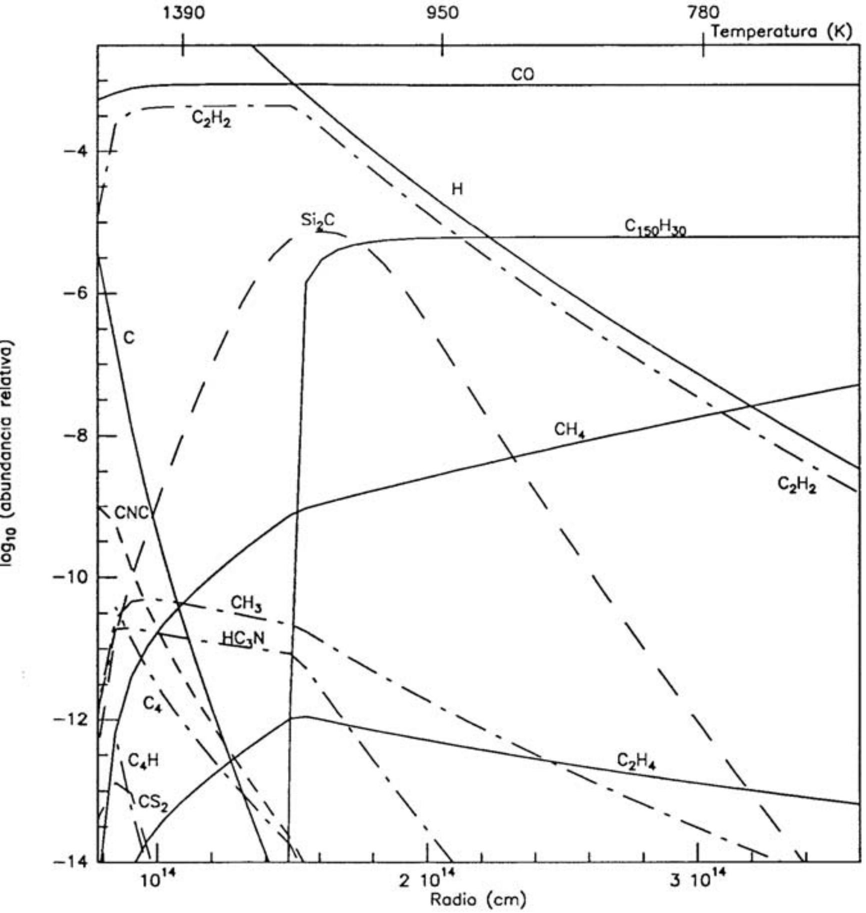
$C_{22}H_{14}$ (benzo(a)triphenylene)



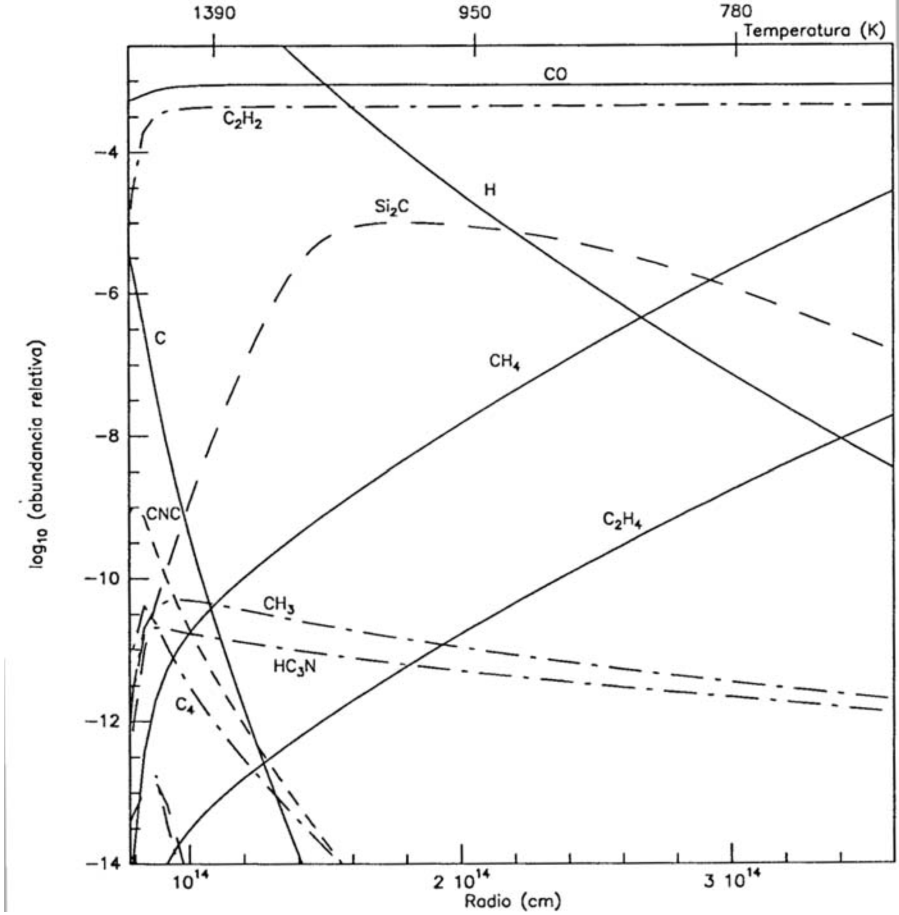
With PAHs



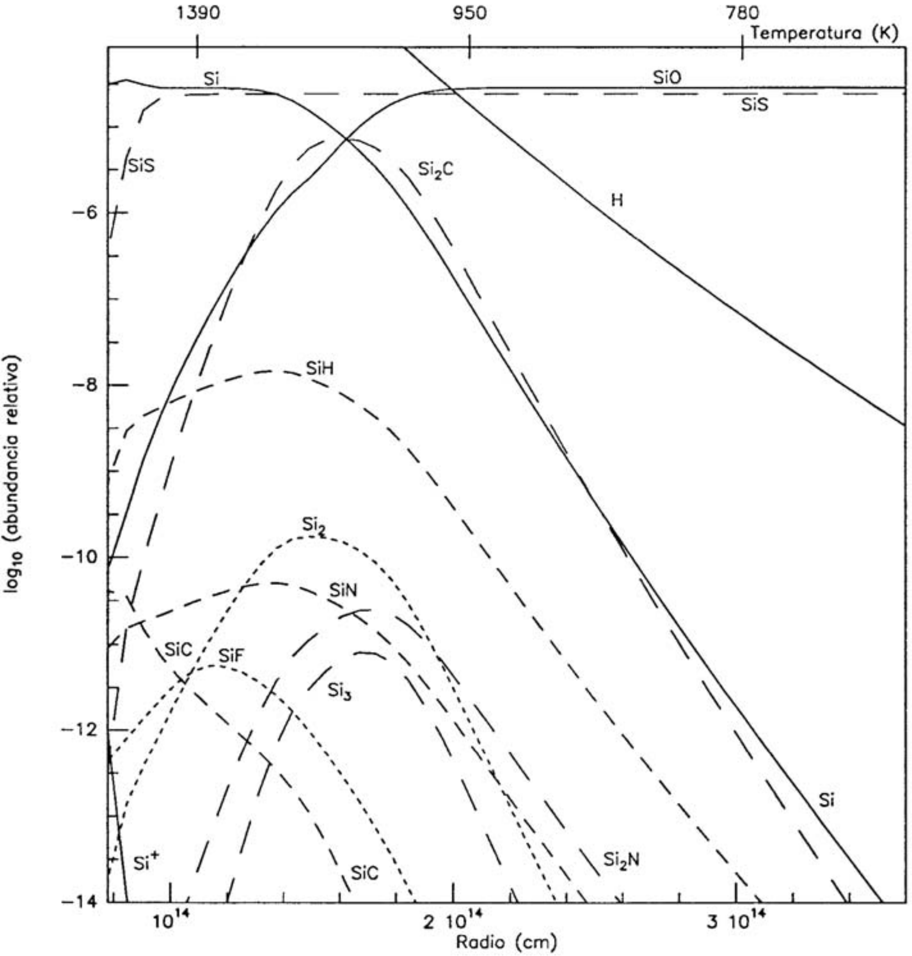
Without PAHs



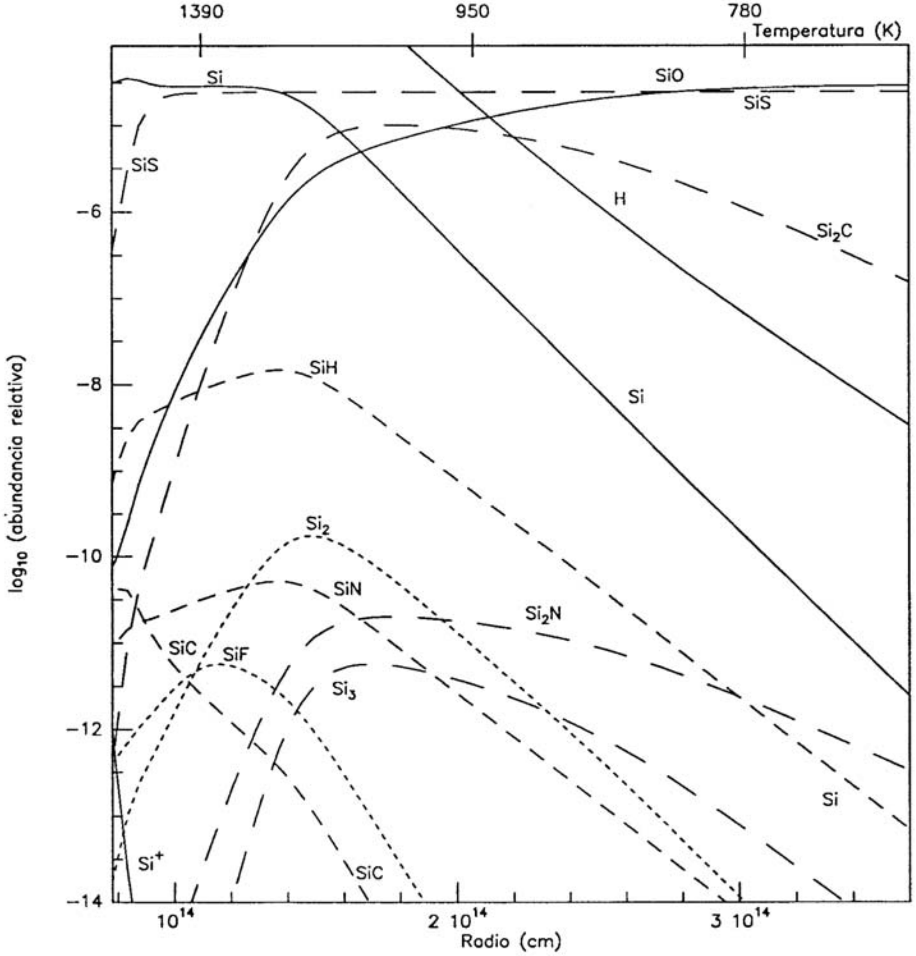
With PAHs



Without PAHs



With PAHs



Without PAHs

THE ASTROPHYSICAL JOURNAL, 401:269–287, 1992 December 10

POLYCYCLIC AROMATIC HYDROCARBON FORMATION IN CARBON-RICH STELLAR ENVELOPES

ISABELLE CHERCHNEFF,[1,2] JOHN R. BARKER,[1,4] AND ALEXANDER G. G. M. TIELENS[3]

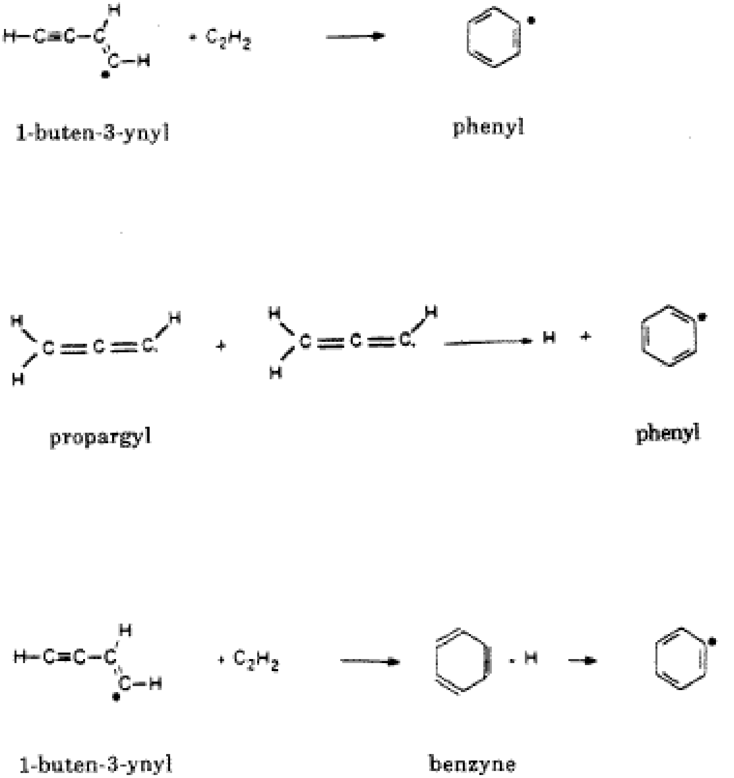


FIG. 3.—Dominant routes for the first-ring closure: 1-buten-3-ynyl route from Frenklach & Warnatz (1987); Propargyl route from Miller & Melius (1990); Benzyne route from Frenklach & Feigelson (1989).

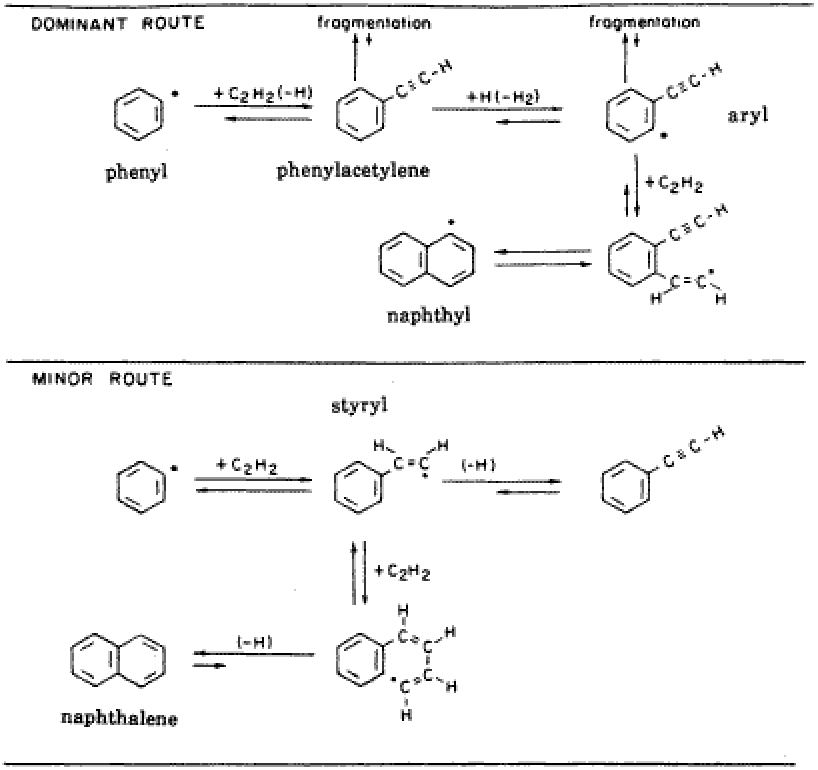


FIG. 4.—Second-ring cyclization routes: napthalene formation pathway from Frenklach et al. (1984) (dominant route), and from Bittner & Howard (1981) (minor route).

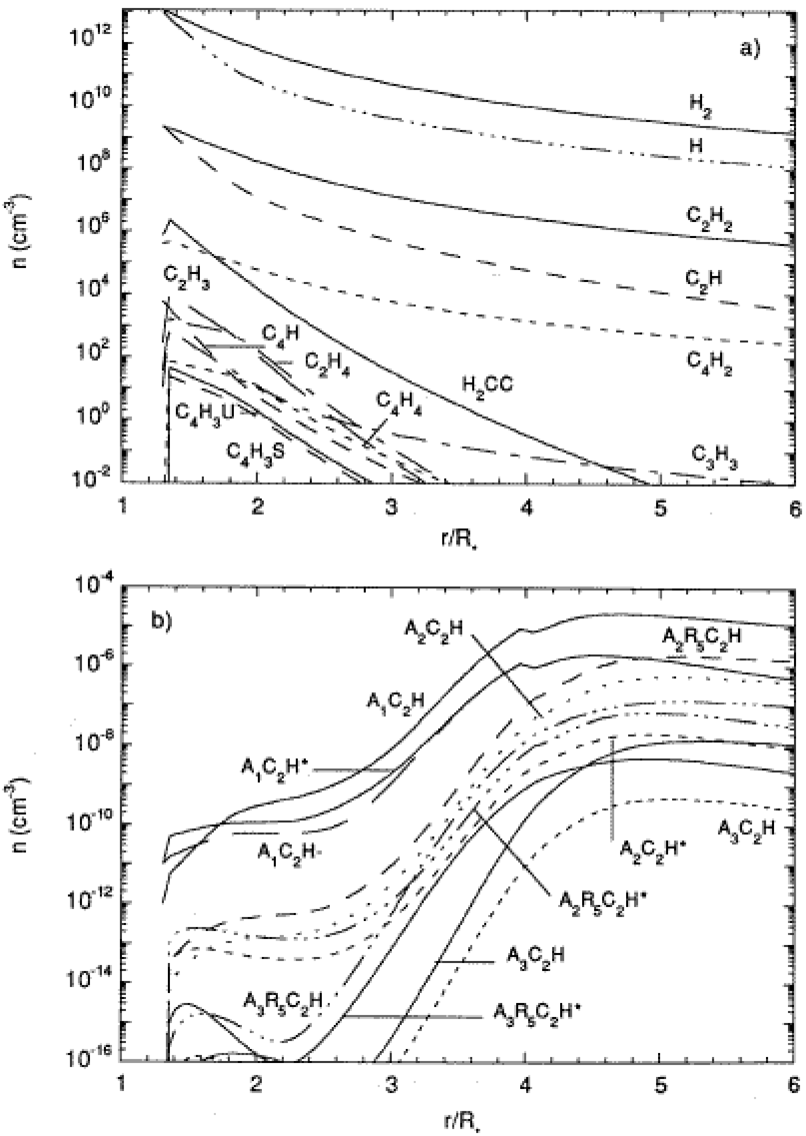


FIG. 5.—Concentration profiles for case 1: (*a*) main hydrocarbon molecules; (*b*) aromatic radicals and molecules (for notation, see Appendix A).

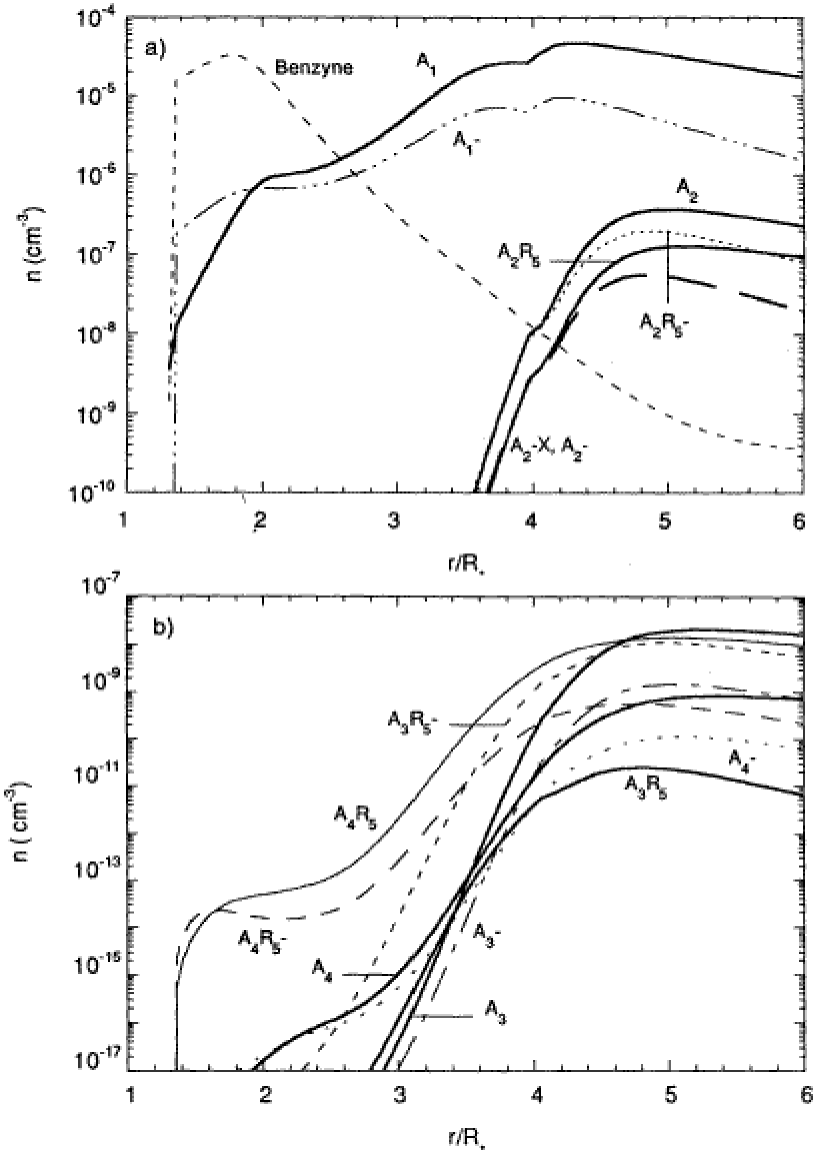
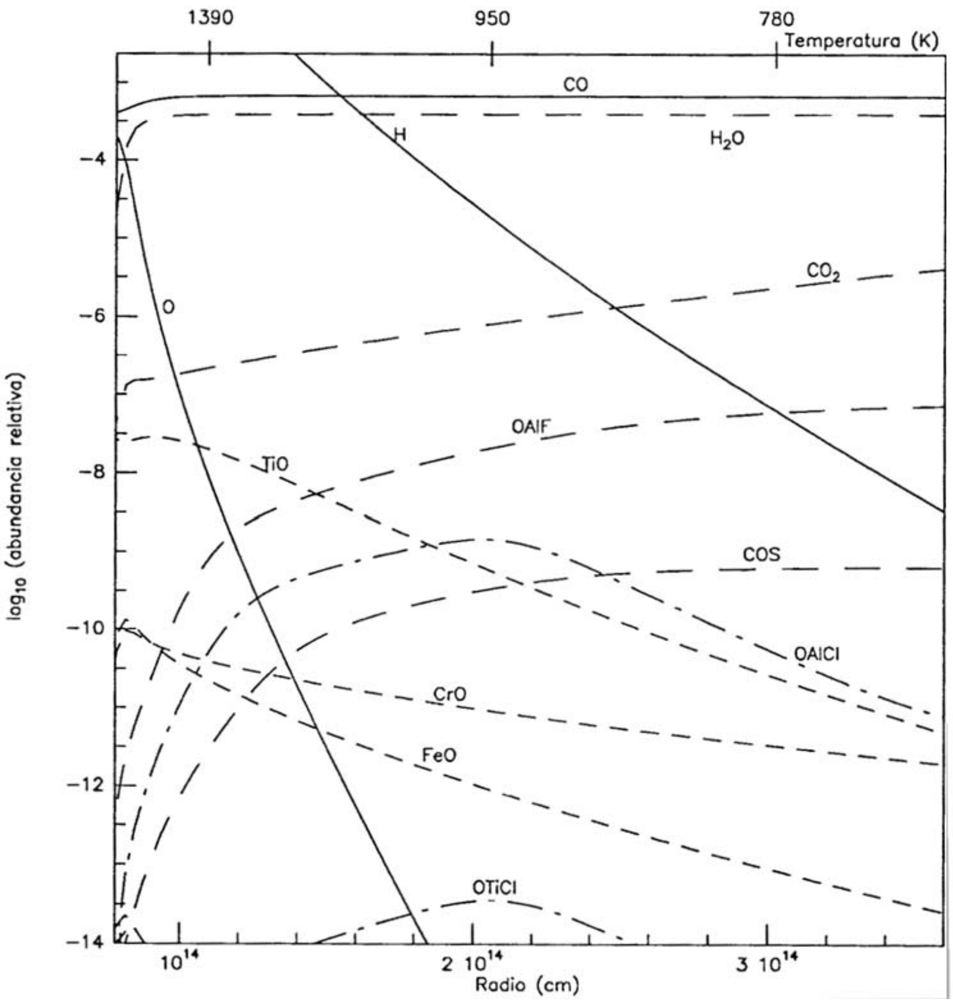
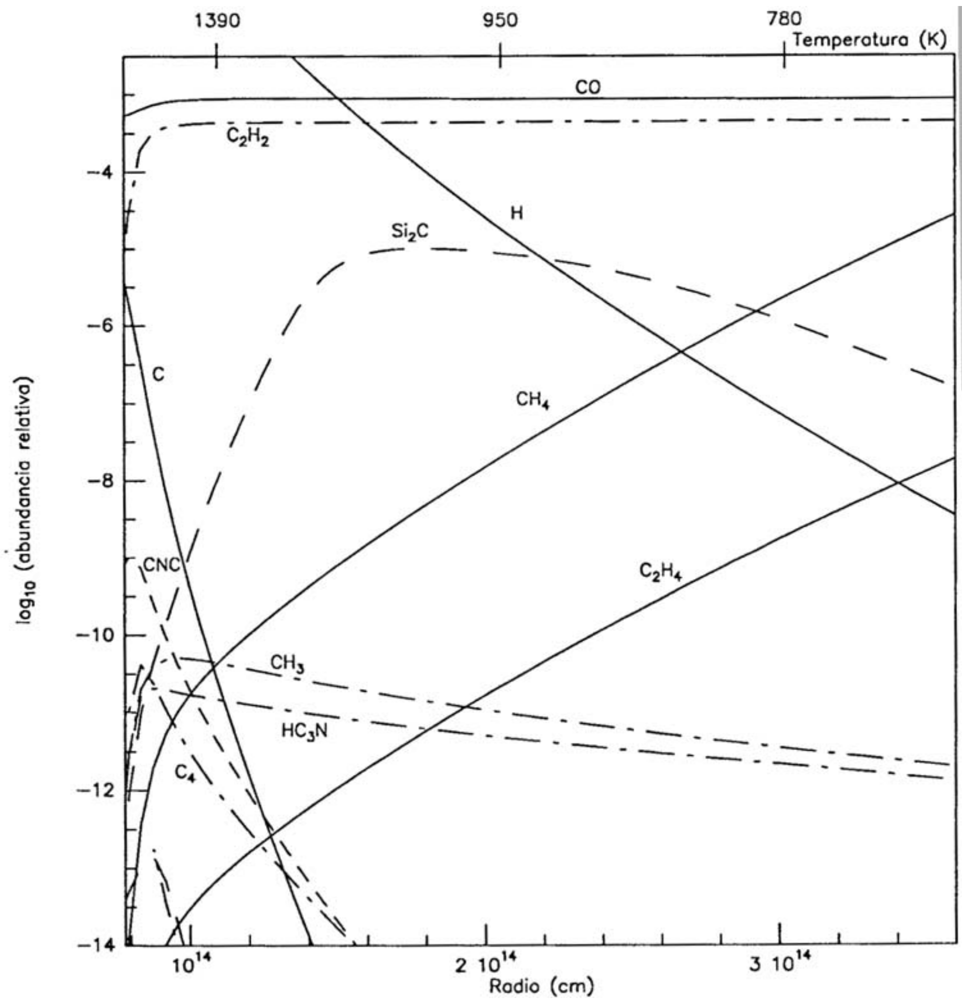


FIG. 6.—Concentration profiles for case 1: (*a*) small PAH molecules; (*b*) large PAH molecules.

Molecular abundances in O-rich stars

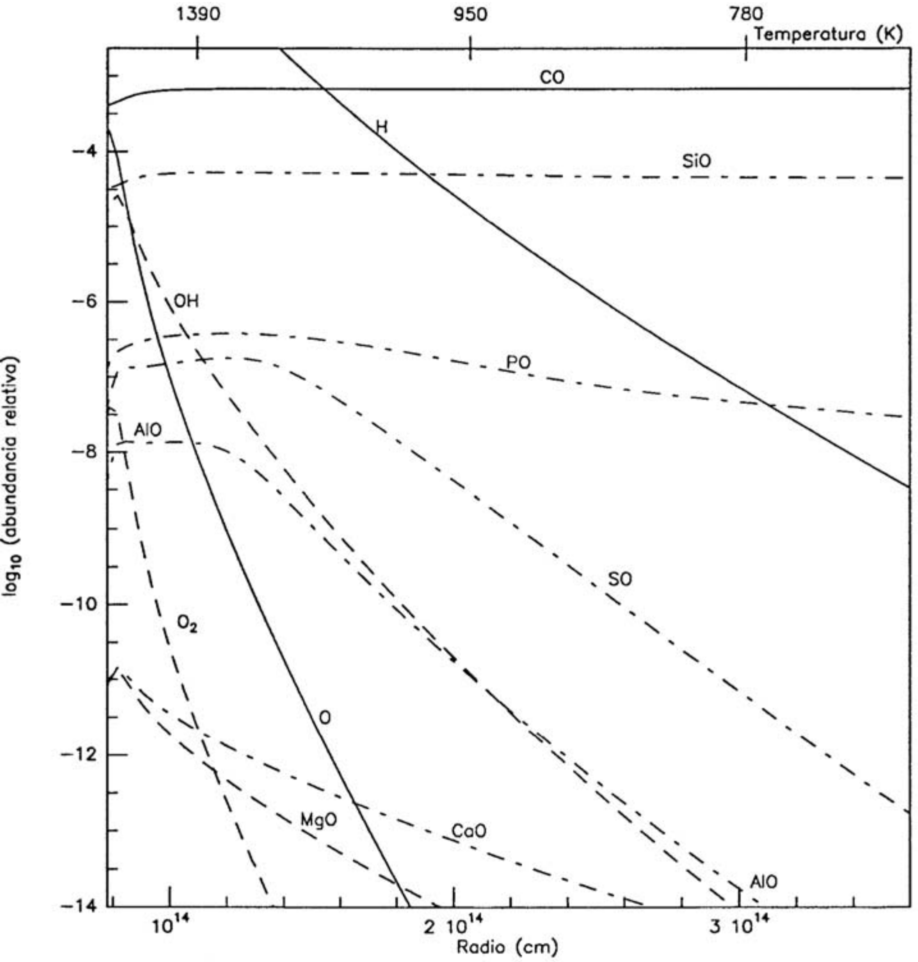


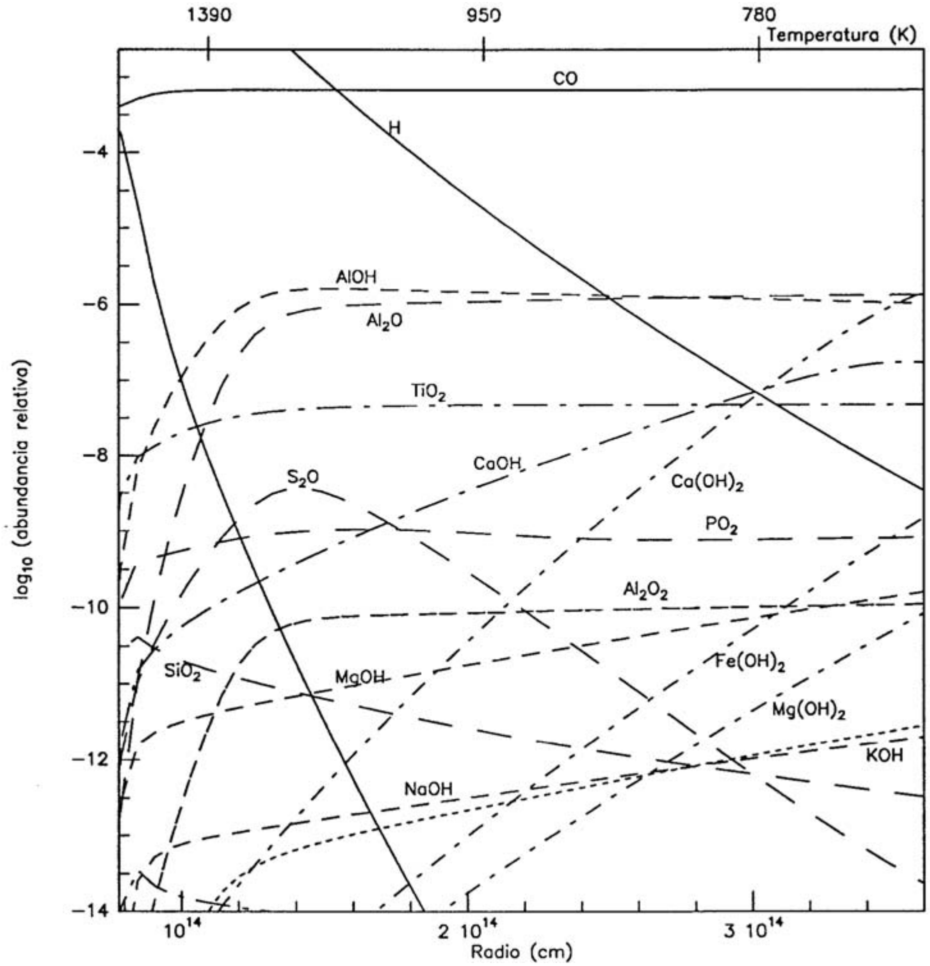
O-rich



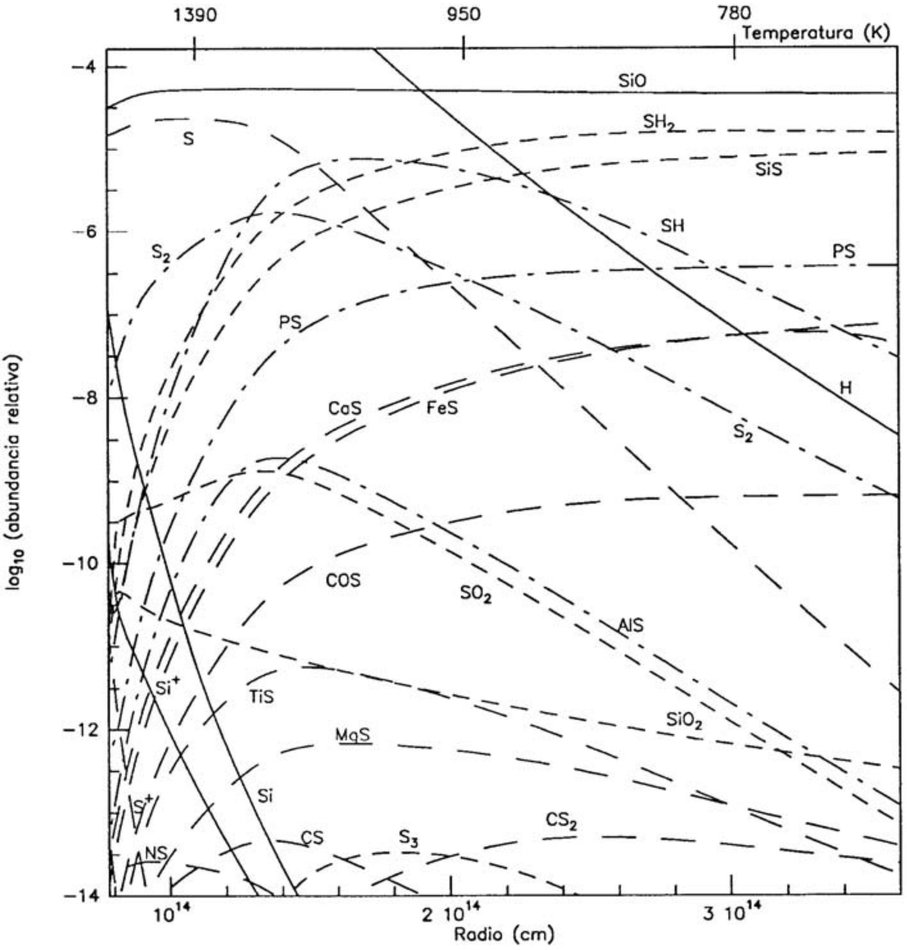
C-rich

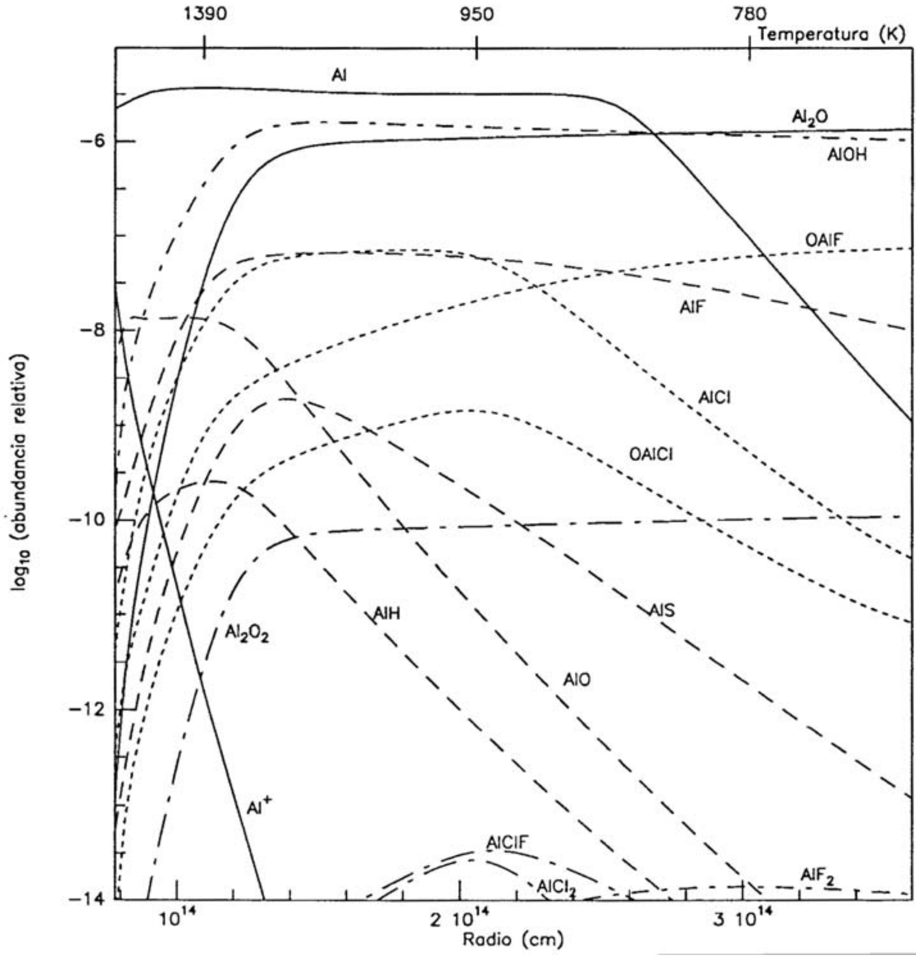
O-rich


1390
950
780
Temperatura (K)
CO
H
SiO
OH
PO
AlO
SO
O_2
O
MgO
CaO
AlO
-4
-6
-8
-10
-12
-14
10^{14}
$2\ 10^{14}$
$3\ 10^{14}$
Radio (cm)
$\log_{10}$ (abundancia relativa)


1390
950
780
Temperatura (K)
CO
H
AlOH
Al_2O
TiO_2
S_2O
CaOH
$Ca(OH)_2$
PO_2
Al_2O_2
SiO_2
MgOH
$Fe(OH)_2$
$Mg(OH)_2$
KOH
NaOH
-4
-6
-8
-10
-12
-14
10^{14}
$2\ 10^{14}$
$3\ 10^{14}$
Radio (cm)
$\log_{10}$ (abundancia relativa)

O-rich


1390
950
780
Temperatura (K)
-4
-6
-8
-10
-12
-14
log₁₀ (abundancia relativa)
SiO
S
SH₂
SiS
SH
PS
S₂
PS
H
CaS
FeS
S₂
COS
SO₂
AlS
Si⁺
TiS
SiO₂
MgS
Si
S⁺
NS
CS
S₃
CS₂
10¹⁴
2 10¹⁴
3 10¹⁴
Radio (cm)


1390
950
780
Temperatura (K)
-6
-8
-10
-12
-14
log₁₀ (abundancia relativa)
Al
Al₂O
AlOH
OAlF
AlF
AlCl
OAlCl
Al₂O₂
AlH
AlS
AlO
Al⁺
AlClF
AlCl₂
AlF₂
10¹⁴
2 10¹⁴
3 10¹⁴
Radio (cm)

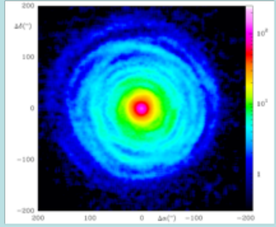
METHODS

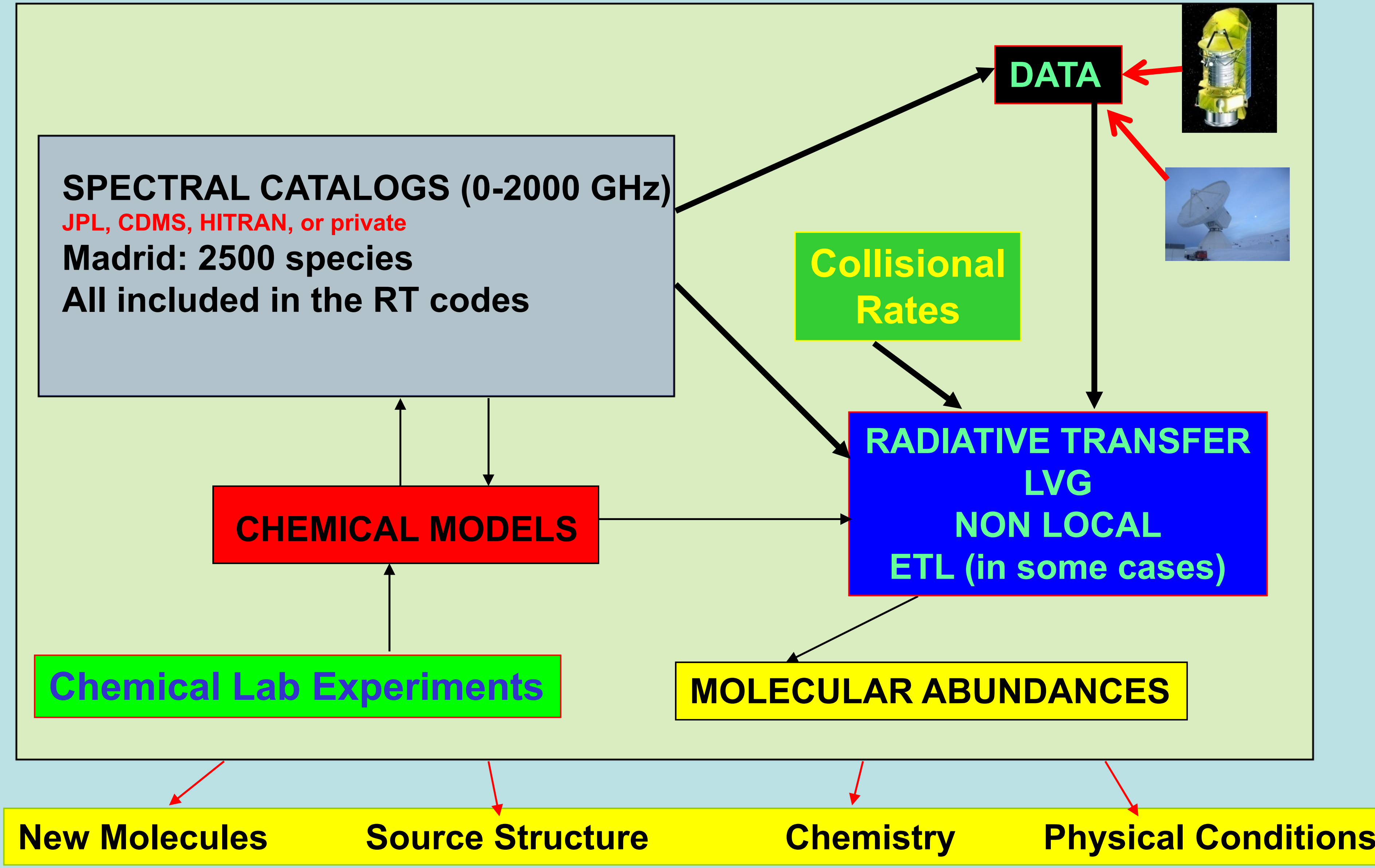
Astronomical Observations at all frequencies
optical, infrared and radio telescopes

Radiative transfer modeling

Chemical modeling

How we proceed to interpret astrophysical data?
In most cases the gas is out of equilibrium !!!!





DATA

SPECTRAL CATALOGS (0-2000 GHz)

JPL, CDMS, HITRAN, or private

Madrid: 2500 species

All included in the RT codes

Collisional Rates

RADIATIVE TRANSFER
LVG
NON LOCAL
ETL (in some cases)

CHEMICAL MODELS

Chemical Lab Experiments

MOLECULAR ABUNDANCES

New Molecules **Source Structure** **Chemistry** **Physical Conditions**

Three different approaches (single dish or interferometric observations):

I) Systematic observation of selected molecular lines in a large sample of objects:

- Physical conditions derived from each molecule
- Statistical studies
- Good estimation of mass loss rates

II) Systematic frequency coverage of a few prototypical objets:

- Full census of molecular lines. Spectroscopy in space
- Physical and chemical conditions
- New molecules. Chemical complexity

IRC+10216, CRL618, VyCMa, IK Tau, OH231 (see poster by Sanchez-Contreras et al.)

III) Identical to II but with spatial information:

- In most cases interferometric observations are needed
- But for a few cases (nearby objects) single dish observations can be used to get a complete line survey at different positions => Physical structure of the envelope.

IRC+10216