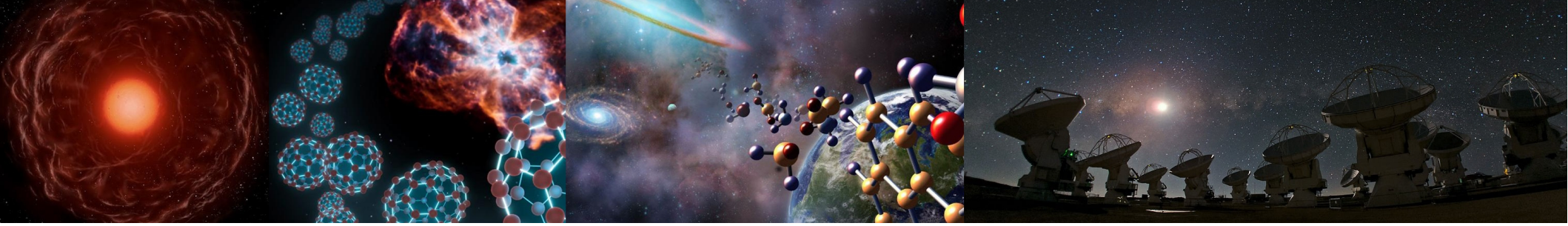


Lecture:

CIRCUMSTELLAR CHEMISTRY

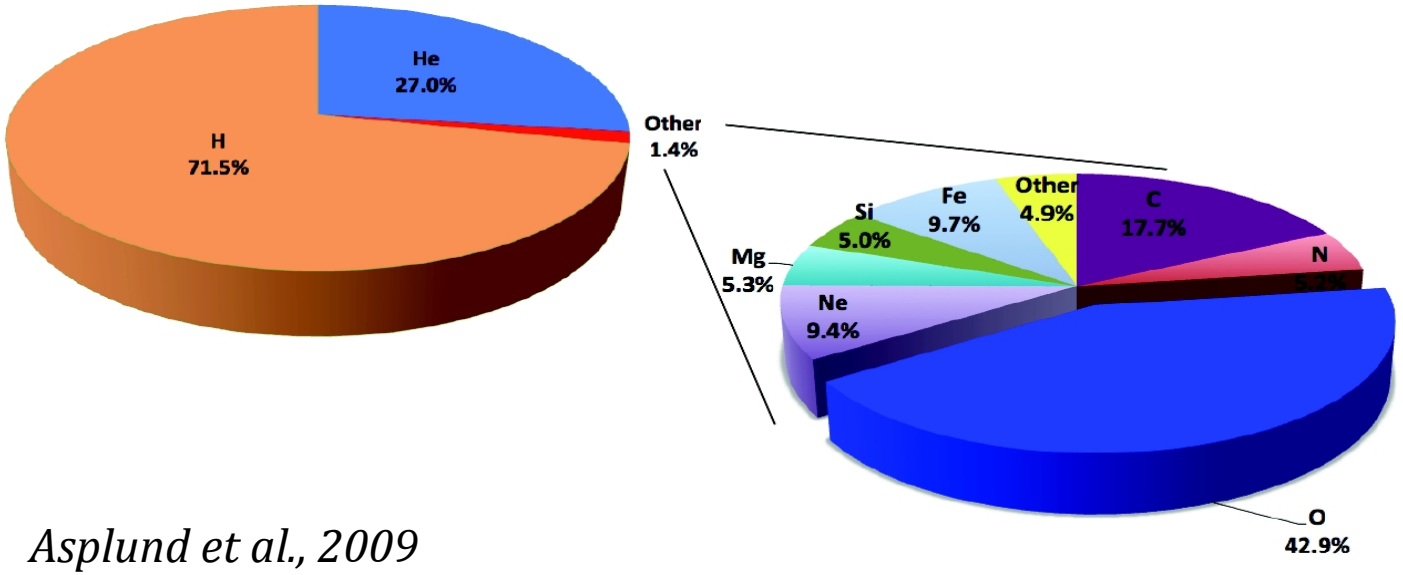
OUTLINE:

- *Chemical differentiation: carbon to oxygen ratio*
- *Thermodynamical equilibrium: formation of molecules*
- *Types of reactions*
- *Chemical kinetics*
- *Other chemical processes: dust grains and shocks*
- *Circumstellar chemistry*
- *Laboratory work*
- *Chemical databases*

The term "circumstellar chemistry" refers in this case to the chemical processes occurring in the ejecta of an evolved star. However, you could consider also the processes that transform e.g. the chemical nature of a cloud of gas and dust surrounding young stars.

Chemical differentiation: C/O ratio, types of CSEs

- *Circumstellar chemistry depends on the carbon-to-oxygen ratio:*



Asplund et al., 2009

Most stars are O-rich (C/O<1) like the Sun.

However, dredge-up processes may invert this ratio: C-rich (C/O>1).

There are also stars with C/O~1 (S-type stars)

$$\log(\epsilon_H) = 12.00$$

$$\log(\epsilon_x) = \log(N_x / N_H) + 12$$

Z	Element	Photosphere
1	H	12.00
2	He	[10.93 ± 0.01]
3	Li	1.05 ± 0.10
4	Be	1.38 ± 0.09
5	B	2.70 ± 0.20
6	C	8.43 ± 0.05
7	N	7.83 ± 0.05
8	O	8.69 ± 0.05
9	F	4.56 ± 0.30
10	Ne	[7.93 ± 0.10]
11	Na	6.24 ± 0.04
12	Mg	7.60 ± 0.04
13	Al	6.45 ± 0.03
14	Si	7.51 ± 0.03
15	P	5.41 ± 0.03
16	S	7.12 ± 0.03

Chemical differentiation: carbon monoxide and different species

- *After H_2, CO is the most abundant species formed (independent of the C/O ratio):*

It is a very stable molecule (Dissociation energy of the ground state: 89462 cm^{-1}=11.09 eV, λ<1118 Å)
Thus, all the possible CO is formed and then, depending on which element is in excess (C/O) C- or O-bearing molecules will be formed

	Tracing molecules	***Dust grains***
C-rich (e.g. IRC+10216)	*C_2H, SiC, HC_xN...*	*Carbonaceous*
O-rich (e.g. IK Tau)	*SO, SO_2, NO, OH ...*	*Silicates, Metal oxides*
S-type (e.g. χ Cyg)	*Mixed*	*Mixed*

However, O-bearing molecules are found in C-rich CSEs and vice versa

Thermodynamical equilibrium: molecular formation

- *Molecular formation under TE conditions in the atmosphere of the star:*

High densities ($n>10^{12}$ cm^{-3})

Temperatures (T_{kin} = 2000-3000)

→ *Favourable conditions*

- *Example: dissociation of H_2*

$$\mathrm{H_2} \rightleftharpoons \mathrm{H} + \mathrm{H}$$

$$p = p_{\mathrm{H_2}} + p_{\mathrm{H}} \quad \textit{(Partial pressures)}$$

$$K_{p,\mathrm{H_2}} = \frac{p_{\mathrm{H}} p_{\mathrm{H}}}{p_{\mathrm{H_2}}}$$

Dissociation constant can be calculated using thermodynamical properties (see bibliography and additional slides)

$$\frac{p_{\mathrm{H}}^2}{K_p} + p_{\mathrm{H}} - p = 0$$

$$\begin{cases} p_{\mathrm{H}} = \dfrac{-1+\sqrt{1+4p/K_p}}{2/K_p} \\ \\ p_{\mathrm{H_2}} = p - \left(\dfrac{-1+\sqrt{1+4p/K_p}}{2/K_p} \right) \end{cases}$$

Thermodynamical equilibrium: general case

- *For each molecule in our system, we can write:*

$$\underbrace{\mathrm{X}_x\mathrm{Y}_y\mathrm{Z}_z}_{i} \rightleftharpoons x\mathrm{X} + y\mathrm{Y} + z\mathrm{Z} \qquad K_{p,i} = \frac{(p_{\mathrm{X}})^x (p_{\mathrm{Y}})^y (p_{\mathrm{Z}})^z}{p_i}$$

- *For each element in our system, we can write these conservation equations:*

$$\begin{aligned}
n^0_{\mathrm{H}} &= n_{\mathrm{H}} + x\ n_{\mathrm{AH_x}} + y\ n_{\mathrm{BH_y}} + z\ n_{\mathrm{BH_z}} + \ldots \\
n^0_{\mathrm{C}} &= n_{\mathrm{C}} + x\ n_{\mathrm{AC_x}} + y\ n_{\mathrm{BC_y}} + z\ n_{\mathrm{BC_z}} + \ldots \\
n^0_{\mathrm{O}} &= n_{\mathrm{O}} + x\ n_{\mathrm{AO_x}} + y\ n_{\mathrm{BO_y}} + z\ n_{\mathrm{BO_z}} + \ldots \\
&\ldots
\end{aligned}$$

- *You can write this densities as a function of H density:* $n^0_{\mathrm{C}} = \epsilon_{\mathrm{C}} n^0_{\mathrm{H}}$

... and make use of the ideal gas law

Thermodynamical equilibrium: computational model

- *We have a system of equations as follows:*

$$\varepsilon_i kT = p_i + \sum_{n=1}^{N_i} \frac{(p_i)^{h_n} (p_j)^{c_n} (p_k)^{o_n} \dots}{K_{p,n}}$$

…

…

The system of non-linear algebraic equations can be solved by using a Newton-Raphson method, with a set of initial abundances, a temperature, and the dissociation constants.

Tsuji, 1973

1973A&A....23..411T

Astron. & Astrophys. 23, 411—431 (1973)

Molecular Abundances in Stellar Atmospheres. II.

T. Tsuji*

Observatoire de Paris-Meudon

Received March 31, revised September 22, 1972

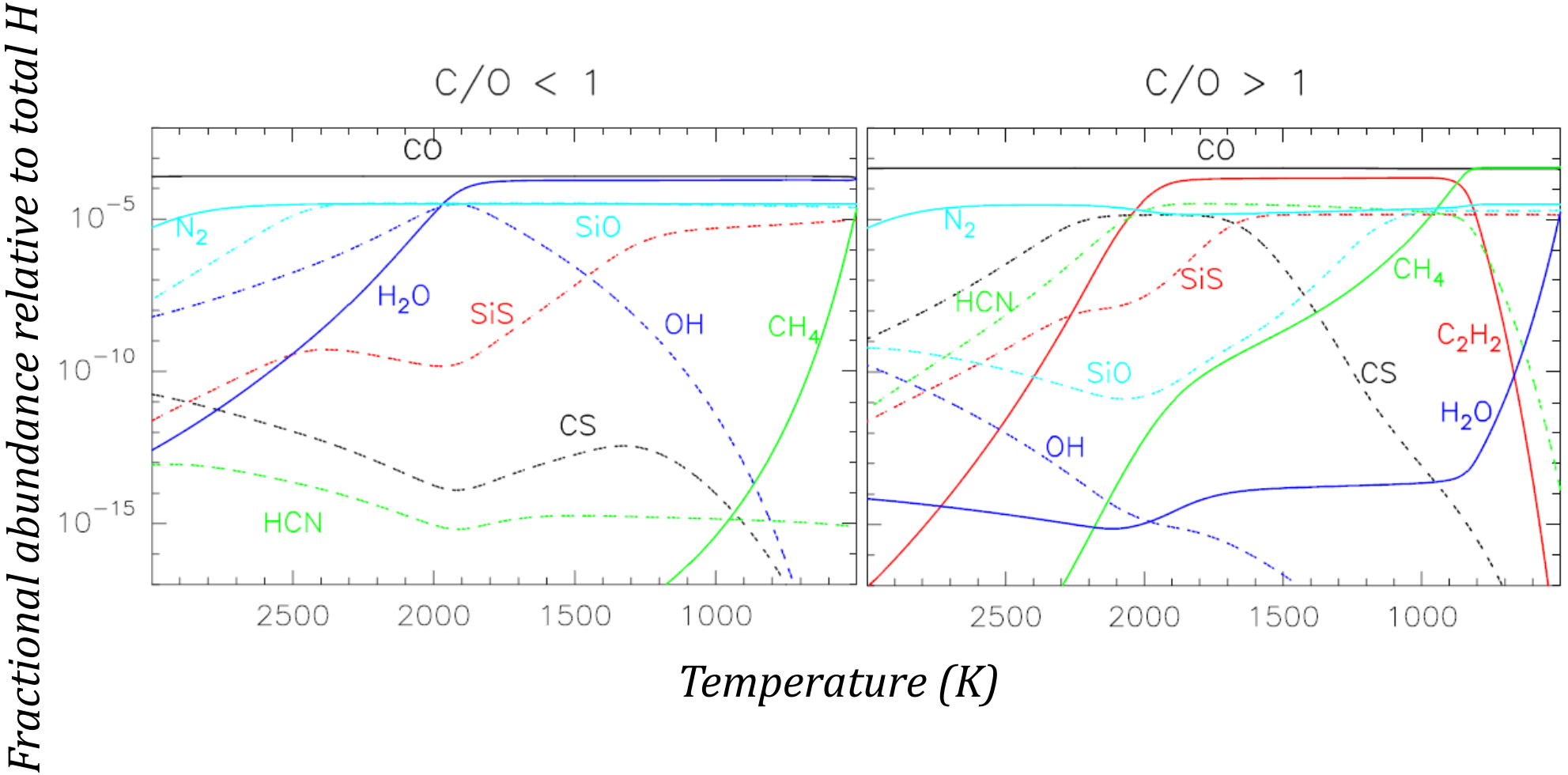
Summary. Chemical equilibria of 36 elements are solved for the physical conditions of cool stellar atmospheres. It is found that the molecular species formed (monoxide, dioxide, halide etc.) and the degree of molecular association, (i.e. the fraction of atoms locked in molecules) are well correlated with the position of each element (both Group and atomic weight) in the periodic table.

In the atmospheres of carbon-rich stars, molecular formation is generally less important than in oxygen-rich atmospheres except for some carbon compounds. The metal oxides in oxygen-rich atmospheres are generally replaced by metal carbides, especially by dicarbides, in carbon-rich atmospheres. The formation of carbides in carbon-rich atmospheres, however, is less effective than that of the corresponding metal oxides in oxygen-rich atmospheres. In carbon stars, it is shown that the Si/S ratio plays a critical role just like the C/O ratio.

Key words: equilibrium constants – chemical equilibrium – molecular abundance – atmospheres of cool stars

Thermodynamical equilibrium: results, C-rich vs O-rich

- *These are the results of chemical modelling for a C-rich and an O-rich CSE:*



Types of reactions

- *Chemical reactions occuring in a CSE are similar to those occuring in the ISM:*

Type	Example	Units of k
CR direct processes	$H_2 + \zeta \rightarrow H_2^+ + e^-$	s^{-1}
Neutral-neutral	$H_2 + OH \rightarrow H + H_2O$	$cm^3\ s^{-1}$
Ion-neutral	$CH^+ + H_2O \rightarrow HCO^+ + H_2$	$cm^3 s^{-1}$
Radiative association	$Si + O \rightarrow SiO + \gamma$	$cm^3\ s^{-1}$
Dissociative recombination	$HCO^+ + e^- \rightarrow CO + H$	$cm^3\ s^{-1}$
Mutual neutralisation	$H_2CO^+ + e^- \rightarrow H_2CO + \gamma$	$cm^3\ s^{-1}$
3-body reactions	$H + H + H_2 \rightarrow H_2 + H_2$	$cm^6\ s^{-1}$
Thermal dissociation	$CH + H \rightarrow C + H + H$	$cm^3\ s^{-1}$
γ-induced reactions	$HCN + \gamma \rightarrow CN + H$	s^{-1}

ζ: Cosmic ray. γ: Photon.

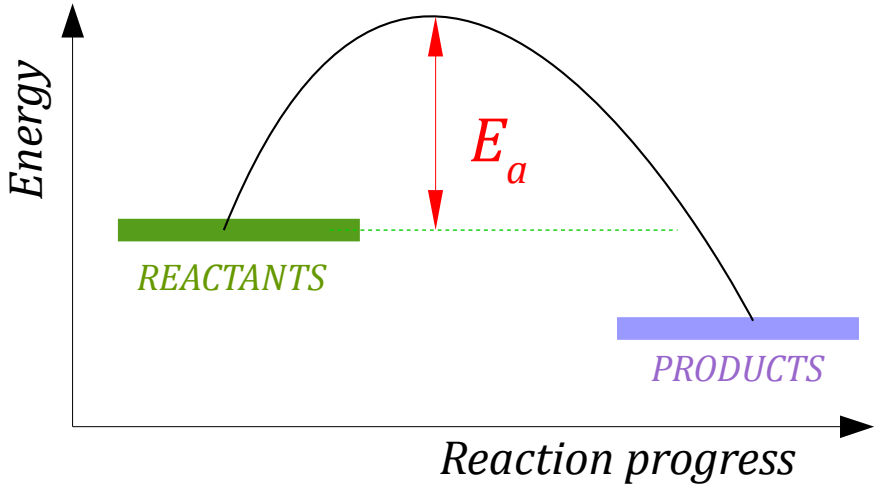
And also photoprocesses induced indirectly by cosmic rays

Chemical kinetics: description

- *A simple reaction:* $A + B \longrightarrow C + D$

$$v = \frac{-dn(A)}{dt} = \frac{-dn(B)}{dt} = \frac{dn(C)}{dt} = \frac{dn(D)}{dt} = k\,n(A)\,n(B)$$

Rate constant, f(T)



- *Arrhenius law:*

$$k = A\exp\left(-E_a/kT\right) \longrightarrow k(T) = \alpha(T/300)^{\beta}\exp\left(-\gamma/T\right)$$

E_a: activation energy = minimum energy of the reactants system to form the products

A: pre-exponential factor = fraction of collisions that have $E>E_a$

Chemical kinetics: generalisation and computational model

- *For a first order reaction:* $\frac{dn_i}{dt} = -k_i\, n_i \;\rightarrow\; n_i = n_{0,i} e^{-k_i t}$

- *We must consider all the species in our system, a chemical reactions network, an initial guess of the abundances, and a physical model (T(r), n(H_2), mass loss rate, A_v, cosmic-ray ionisation rate...):*

$$\frac{dn_i}{dt} = \underbrace{\sum_{j=1}^{N_f} k_j \prod_{l=1}^{N_{reac}^{j}} n_{j,l}}_{\text{Formation of } i} - \underbrace{\sum_{m=1}^{N_d} k_m n_i \prod_{s=1}^{N_{reac}^{m}} n_{m,s}}_{\text{Destruction of } i}$$

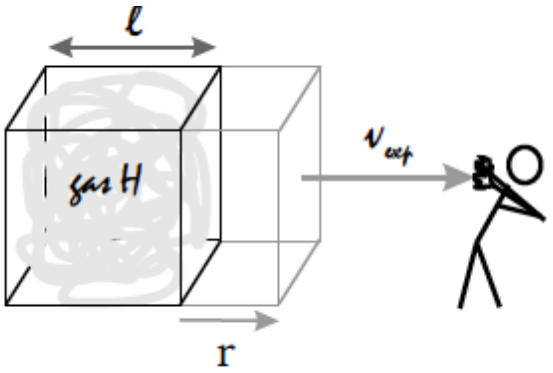
- *Using the physical model of the corresponding CSE, and as initial abundances, you can start using the output from a TE model or observational constraints*

The system of non-linear ODEs can be solved by using a Runge-Kutta method, with a set of initial abundances, a physical model (T(r), n(r)), and the reaction rates for the chemical network considered.

Chemical kinetics: an example

- *Consider pure hydrogen gas in expansion:* $\mathrm{H_2} \rightleftharpoons \mathrm{H} + \mathrm{H}$

$T = 2000$ K $\quad n = 10^{12}$ cm^{-3}



Initial state: Hydrogen gas at P_o and T_o, with n_H and n_{H2} at chemical eq.

Final state: adiabatic expansion (P and T decrease), abundances will evolve according to chemical kinetics

- *Chemical network and rates:*

$$\mathrm{H} + \mathrm{H} + \mathrm{H} \rightarrow \mathrm{H_2} + \mathrm{H} \qquad k_{\mathrm{M,H}} = 8.82 \times 10^{-33}\ \mathrm{cm^6 s^{-1}}$$
$$\mathrm{H} + \mathrm{H} + \mathrm{H_2} \rightarrow \mathrm{H_2} + \mathrm{H_2} \qquad k_{\mathrm{M,H_2}} = 2.65 \times 10^{-31} T^{-0.6}\ \mathrm{cm^6 s^{-1}}$$
$$\mathrm{H_2} + \mathrm{H} \rightarrow \mathrm{H} + \mathrm{H} + \mathrm{H} \qquad k_{\mathrm{d,H}} = 1.11 \times 10^{-9} T^{0.36} e^{-52043/T}\ \mathrm{cm^3 s^{-1}}$$
$$\mathrm{H_2} + \mathrm{H_2} \rightarrow \mathrm{H} + \mathrm{H} + \mathrm{H_2} \qquad k_{\mathrm{d,H_2}} = 3.32 \times 10^{-8} T^{-0.24} e^{-52043/T}\ \mathrm{cm^3 s^{-1}}$$

- *System of equations:*

$$\frac{dn_{\mathrm{H}}}{dt} = \left(2k_{\mathrm{d,H}} n_{\mathrm{H_2}} n_{\mathrm{H}} + 2k_{\mathrm{d,H_2}} n_{\mathrm{H_2}}^2\right) - \left(2k_{\mathrm{M,H}} n_{\mathrm{H}}^3 + 2k_{\mathrm{M,H_2}} n_{\mathrm{H}}^2 n_{\mathrm{H_2}}\right)$$

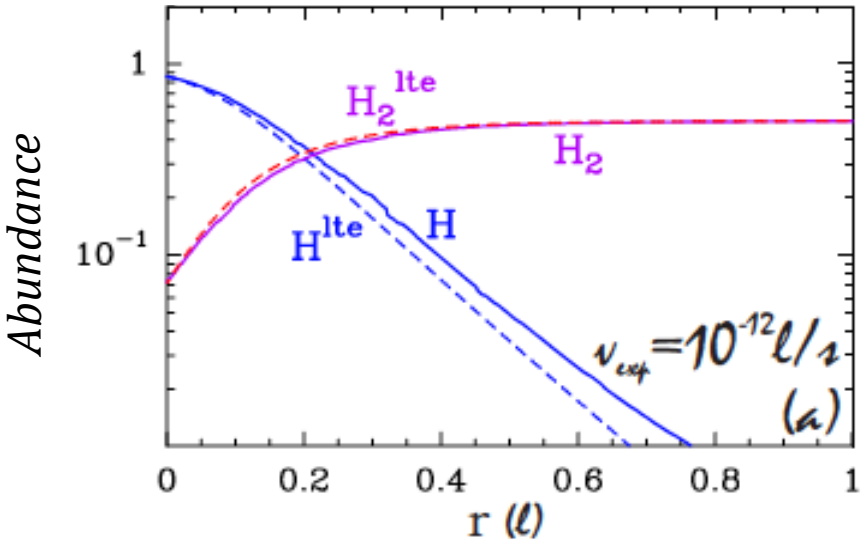
$$\frac{dn_{\mathrm{H_2}}}{dt} = \left(k_{\mathrm{M,H}} n_{\mathrm{H}}^3 + k_{\mathrm{M,H_2}} n_{\mathrm{H}}^2 n_{\mathrm{H_2}}\right) - \left(k_{\mathrm{d,H}} n_{\mathrm{H_2}} n_{\mathrm{H}} + k_{\mathrm{d,H_2}} n_{\mathrm{H_2}}^2\right)$$

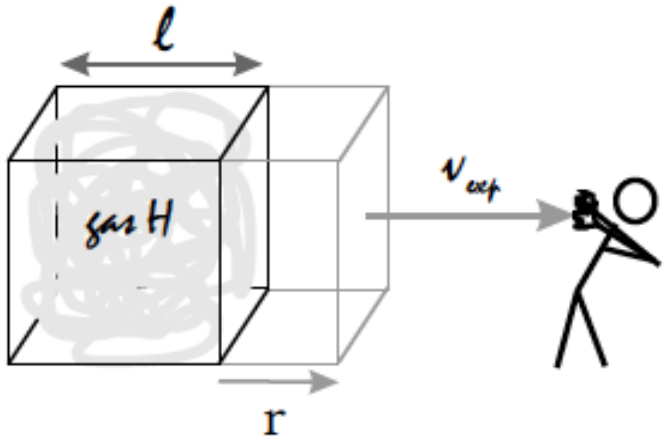
Chemical kinetics: example results

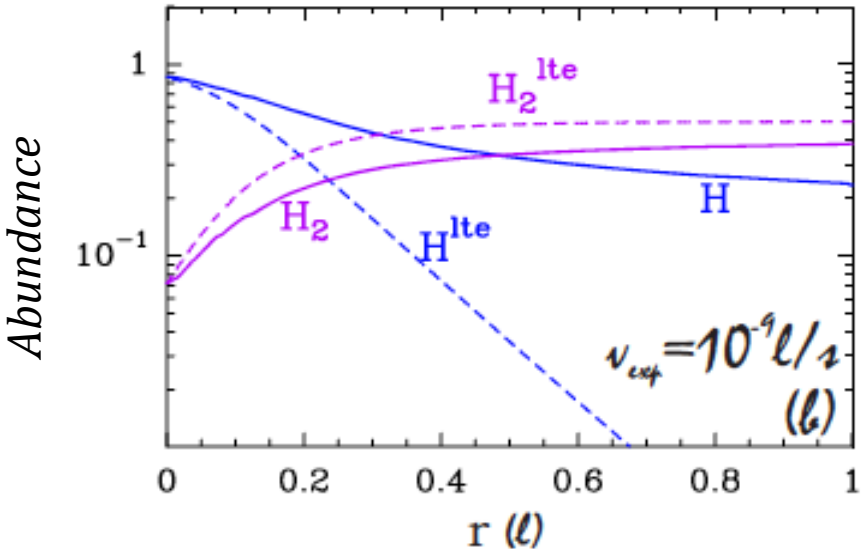
- *Consider pure hydrogen gas in expansion:*

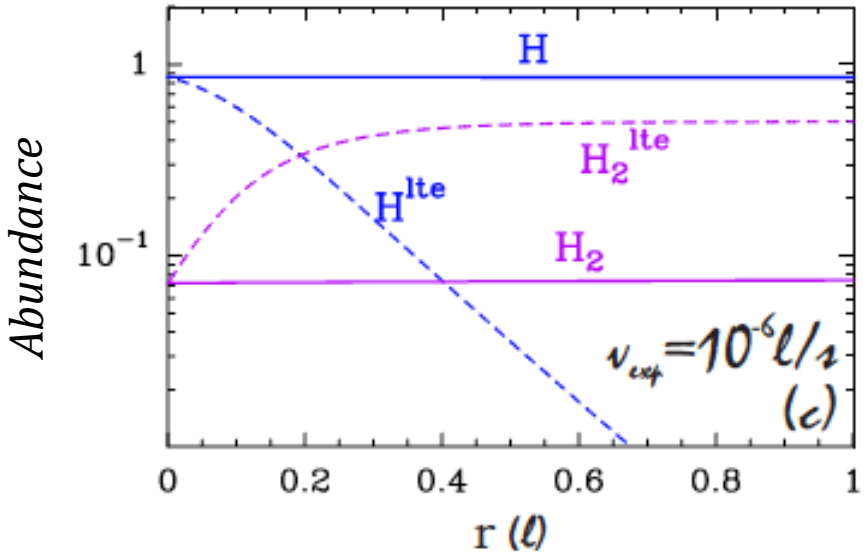
$$H_2 \rightleftharpoons H + H$$

Initial state *Final state*





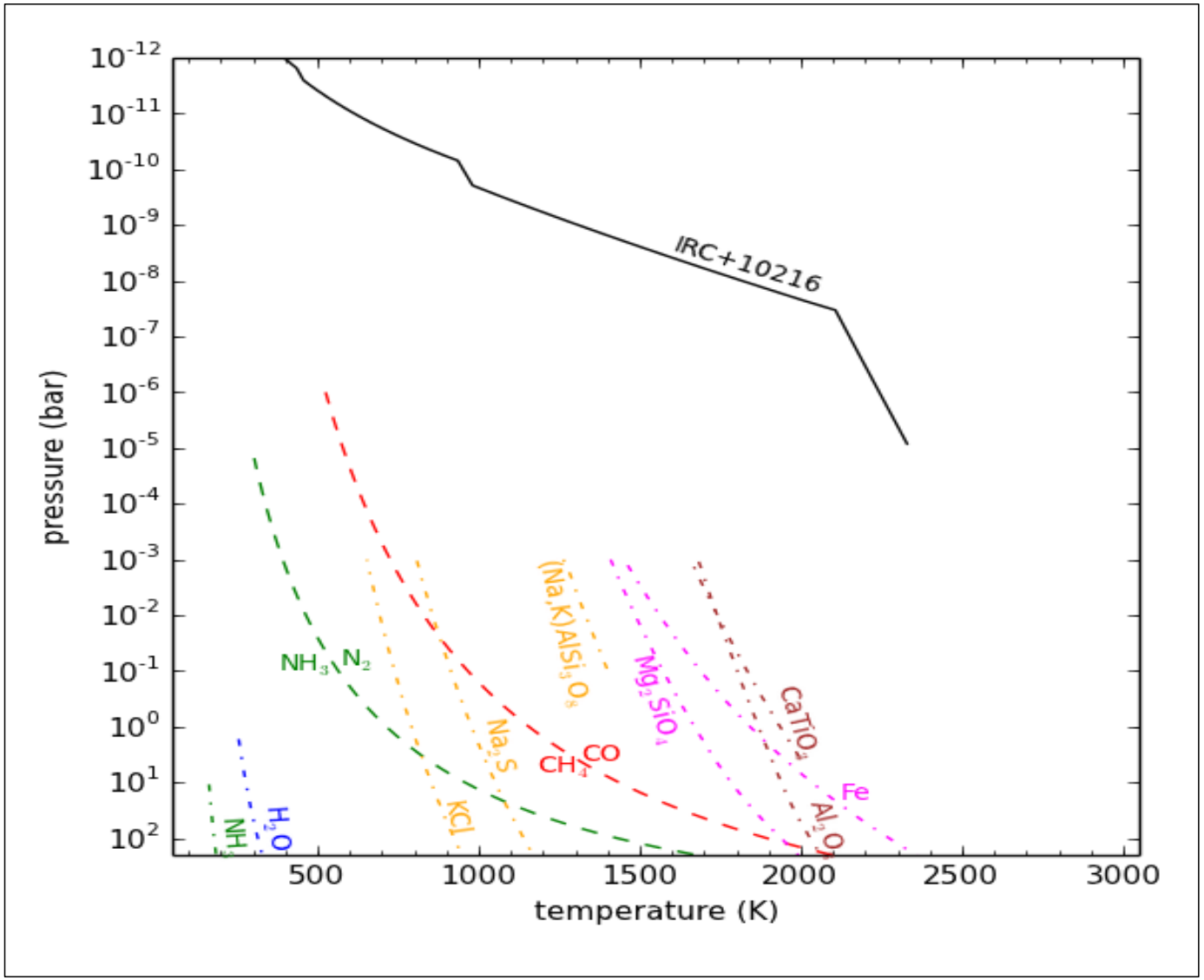




Dust formation

- *Dust formation:*

A species will condense if its partial pressure is larger than its vapor pressure



Grain growth through condensation and aggregation of species

Water ice mantles observed in some OH/IR sources (Justtanont et al. 2006)

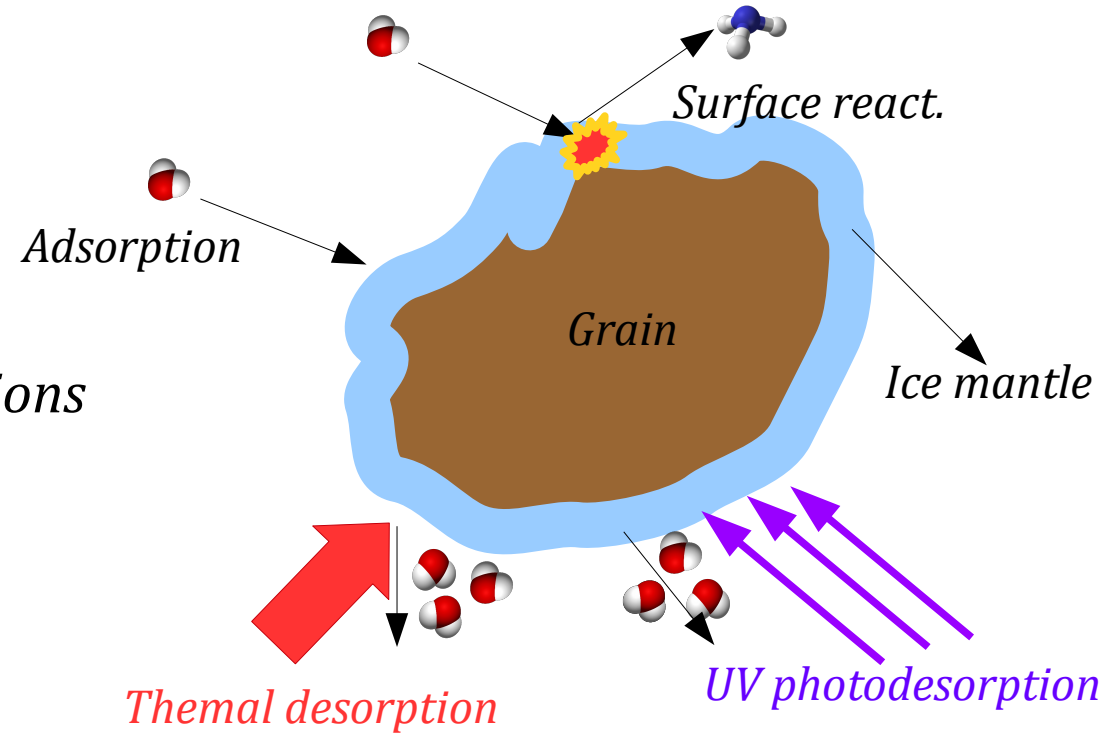
Other chemical processes: dust grains and shocks

- *Dust grains chemistry:*

  Adsorption

  Desorption

  Grain-surface (catalytic) reactions



- *Shock-induced chemistry:*

  - Gas compression and heating

Shocks can produce different effects on the chemistry, which are difficult to characterise:

- *Dissociating or not?*
- *UV radiation*
- *molecular reformation after shock passage*

Circumstellar chemistry: general ideas

- *Studied because physical conditions are well-constrained*
- *Importance of chemical and dynamical times:*

Chemical kinetics depends on time. As the gas of the CSE expands, molecules have to re-adapt their abundances to the new physical conditions (n, T) encountered during the expansion. If the dynamical time ($t_d = r/v_{exp}$) is shorter than the chemical time (i.e. the characteristic time of a given reaction), the abundances will remain constant during the expansion. This is called frozen chemistry.

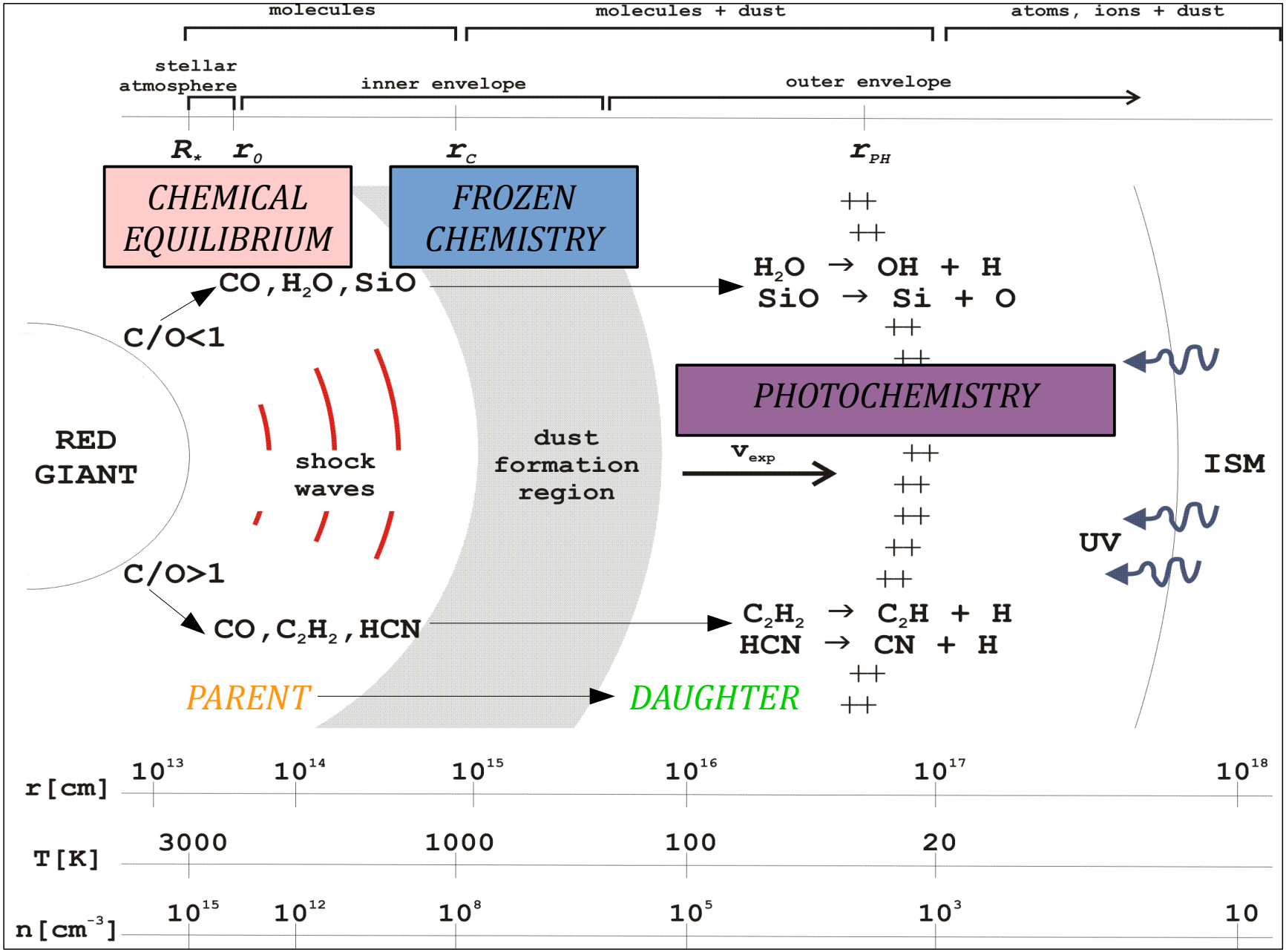
- *Parent and daughter species:*

Parent molecules: *abundant species that have been formed in the innermost parts of a CSE and are injected into the intermediate envelope in gas phase.*

Daughter molecules: *molecules that are formed in the outermost parts of a CSE, as a result of chemical reactions involving parent species. Daughter species are usually distributed in a hollow shell.*

Circumstellar chemistry: chemical regions of a CSE

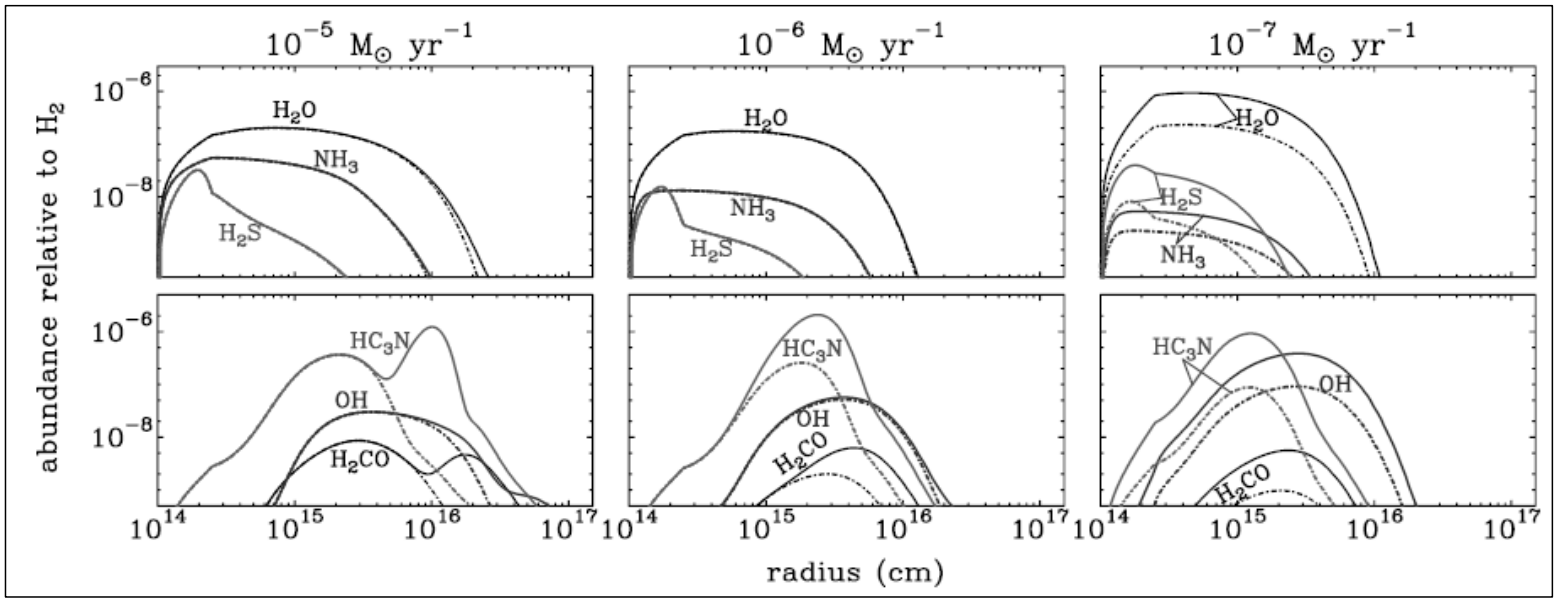
- *Standard scenario:*

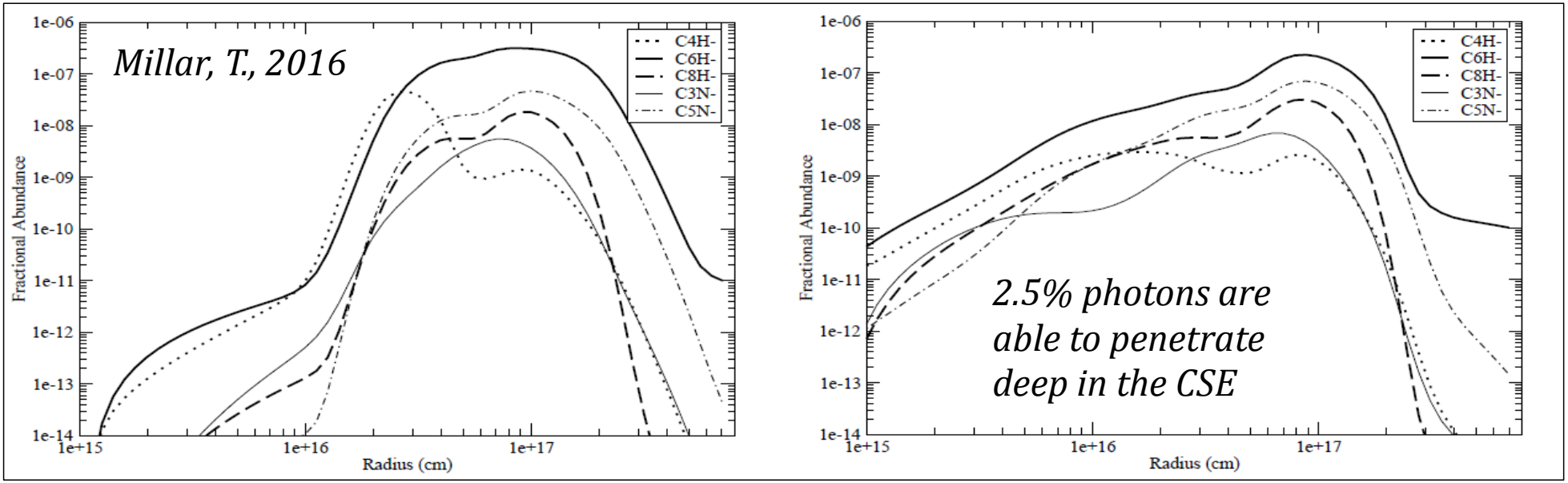


Circumstellar chemistry: C-rich CSE

- *Chemical models:*

Agúndez et al., 2010





Circumstellar chemistry: C-rich CSE

- *The case of IRC+10216:*

10^{-3}	CO	1(−3)											
				Up-to-date as of 2009									
10^{-4}													
			C_2H_2	8(−5)									
					HCN	2(−5)							
10^{-5}													
			CH_4	3.5(−6)									
			C_2H	3(−6)	NH_3	2(−6)							
			C_4H	2.5(−6)	CN	1.7(−6)							
			C_2	1(−6)	HC_3N	1.4(−6)			SiC_2	1.2(−6)			
10^{-6}			C_3	1(−6)					SiS	1(−6)			
					C_3N	4(−7)	CS	5(−7)					
									SiH_4	2.2(−7)			
					HC_5N	2(−7)			SiO	1.2(−7)			
10^{-7}	H_2O	1(−7)	C_5	1(−7)	HNC	1(−7)							
			l-C_3H	5(−8)									
	OH	4(−8)	C_6H	4(−8)					SiC	4(−8)			
			C_5H	3(−8)	CH_3CN	3(−8)	C_2S	3(−8)				AlCl	3.5(−8)
			c-C_3H_2	3(−8)									
			CH_3C_2H	3(−8)									
			c-C_3H	2(−8)	HC_7N	2(−8)					HCP	2.5(−8)	
			C_2H_4	2(−8)								NaCN	*
	H_2CO	1.3(−8)	H_2C_4	1.4(−8)			C_3S	1.2(−8)					
10^{-8}											CP	1(−8)	
			C_8H	8(−9)	HC_9N	8(−9)	H_2CS	7(−9)	SiN	8(−9)	PH_3	8(−9)	MgNC 8(−9)
					CH_2CN	7(−9)						AlF	7.5(−9)
					HC_2N	6(−9)							
					C_5N	4(−9)							
			C_7H	3(−9)	HCCNC	4(−9)							
			H_2C_6	3(−9)	C_2H_3CN	4(−9)	H_2S	4(−9)	c-SiC_3	4(−9)			
			C_6H^-	3(−9)	C_5N^-	2.3(−9)			SiC_4	3(−9)			
	C_3O	2(−9)	C_8H^-	1.5(−9)	HC_4N	2(−9)			SiCN	2(−9)			
			H_2C_3	1.5(−9)	C_3N^-	1.1(−9)	C_5S	1.2(−9)	SiNC	1.1(−9)	PN	1(−9)	NaCl 1(−9)
10^{-9}											C_2P	1(−9)	AlNC 1(−9)
	HCO^+	7(−10)			HNCCC	5(−10)							MgCN 5(−10)
			C_4H^-	3(−10)									KCl 2.5(−10)
10^{-10}													

More molecules found:

Si_2C

CCN

$SiHC_3N$

NCCP

MgCCH

C_5S

HMgNC

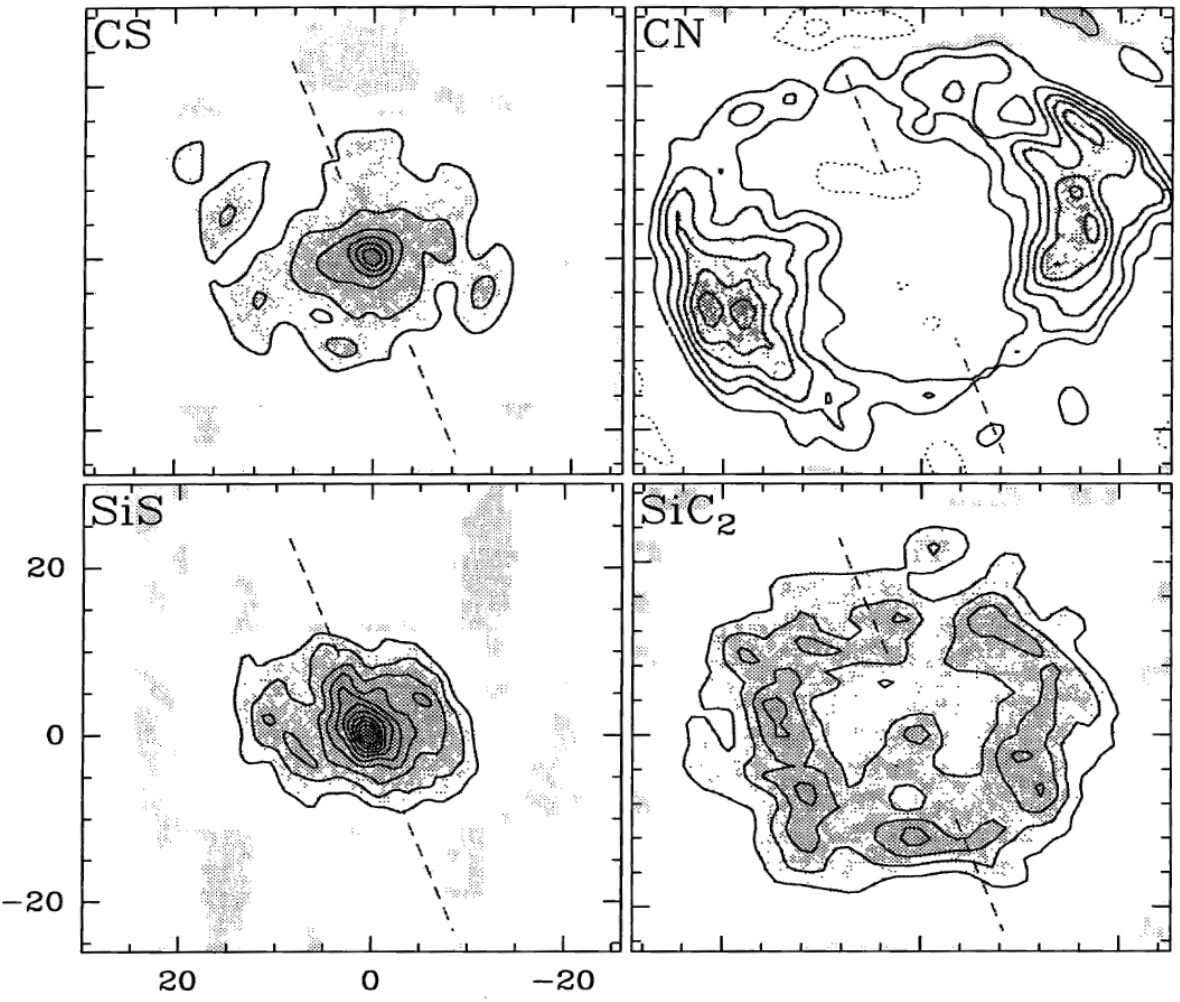
FeCN

KCN

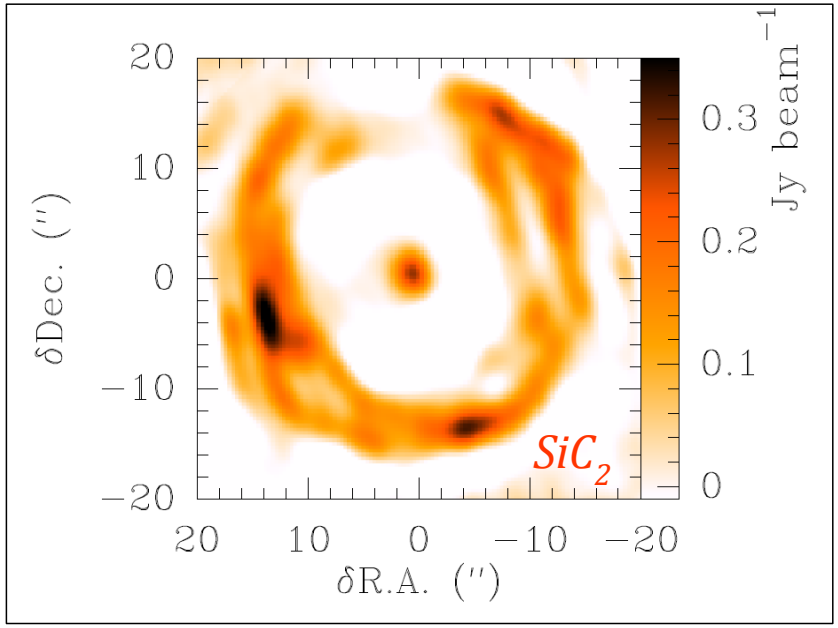
CN^-

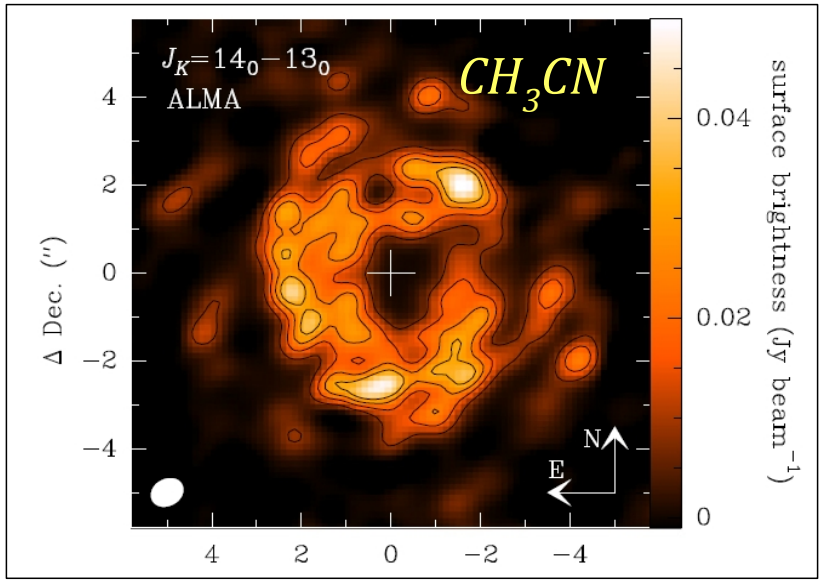
Circumstellar chemistry: C-rich CSE

- *The case of IRC+10216:*



Lucas et al., 1995



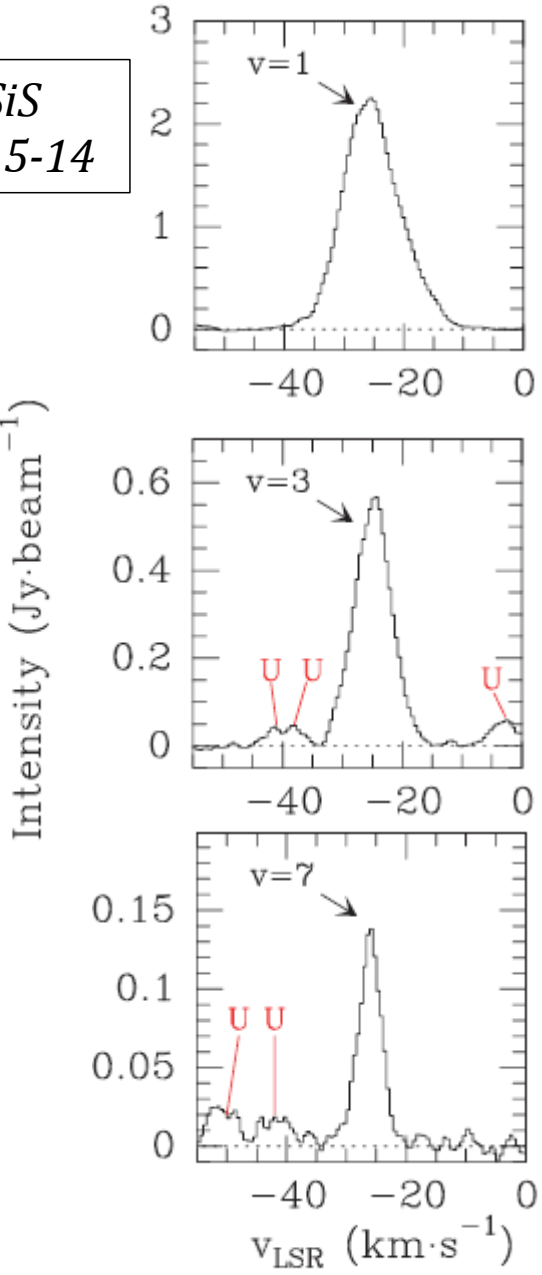


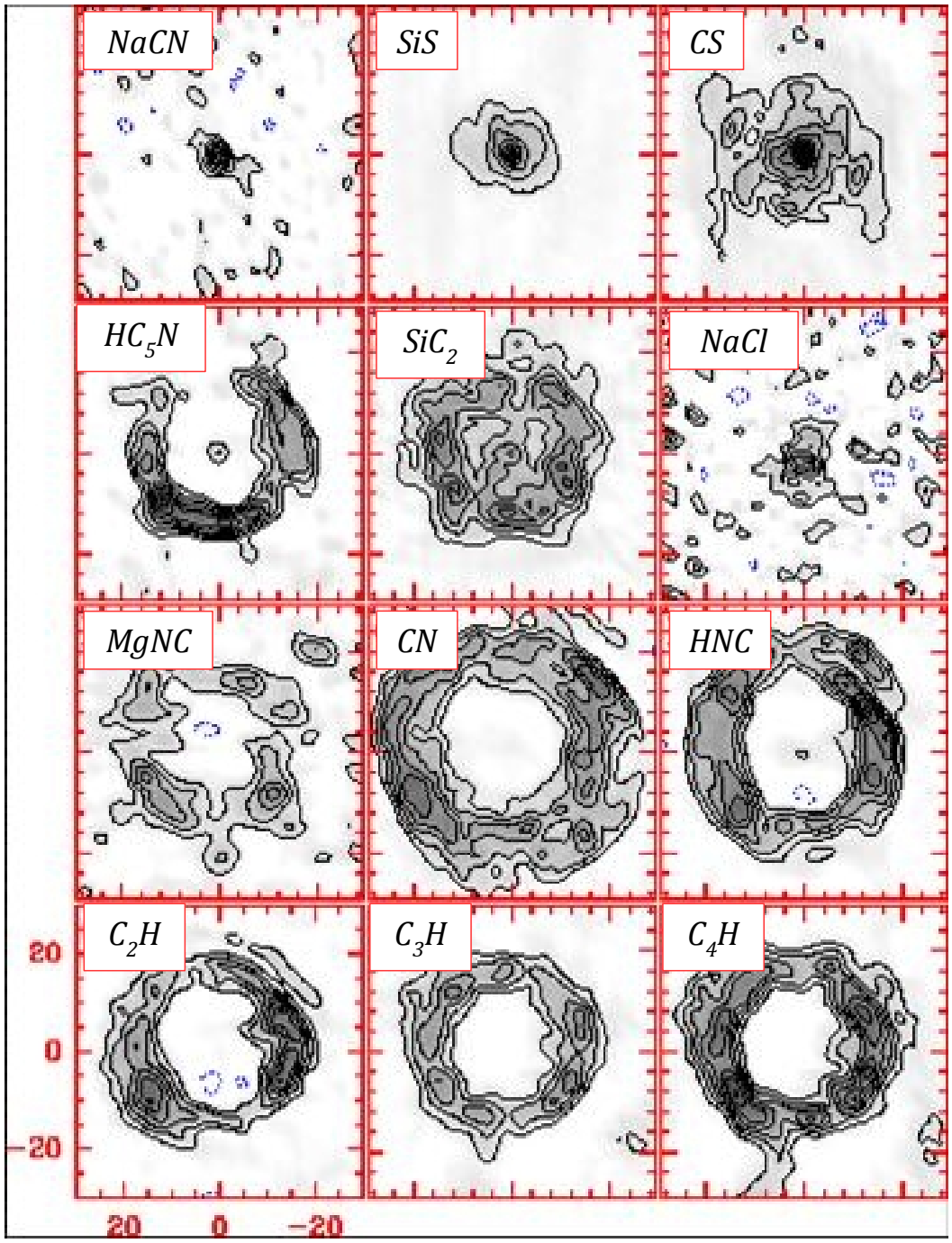
Agúndez et al., 2015

Circumstellar chemistry: C-rich CSE

- *The case of IRC+10216:*

SiS
J=15-14



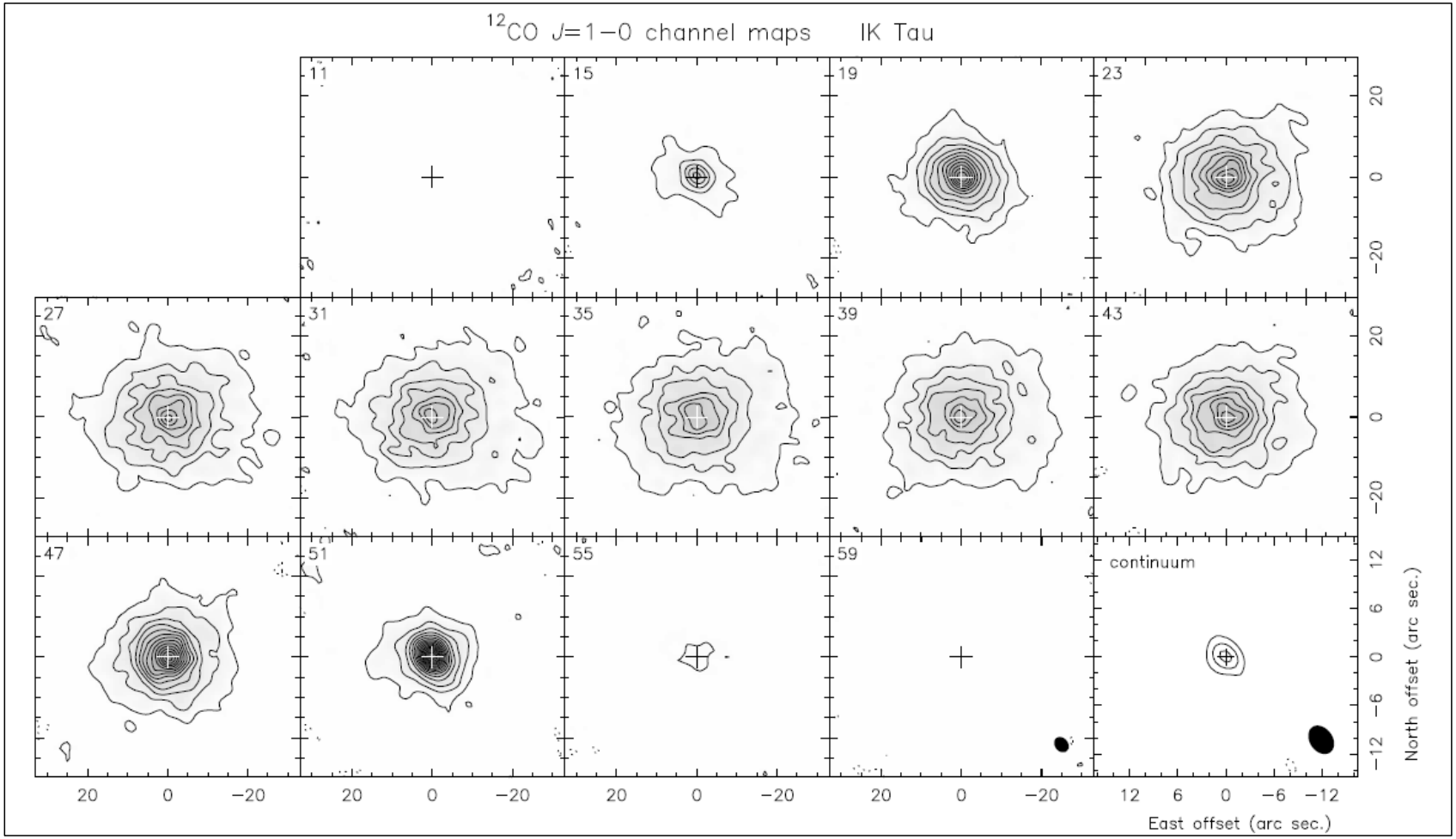


Velilla Prieto et al., 2015

Circumstellar chemistry: O-rich CSE

- *Observational studies of O-rich CSEs:*

O-rich CSEs are not so well studied.
Most observational works are limited to CO and maser emission (SiO, H_2O, and OH), and single-dish observations of other species (e.g. SiO or HCN).

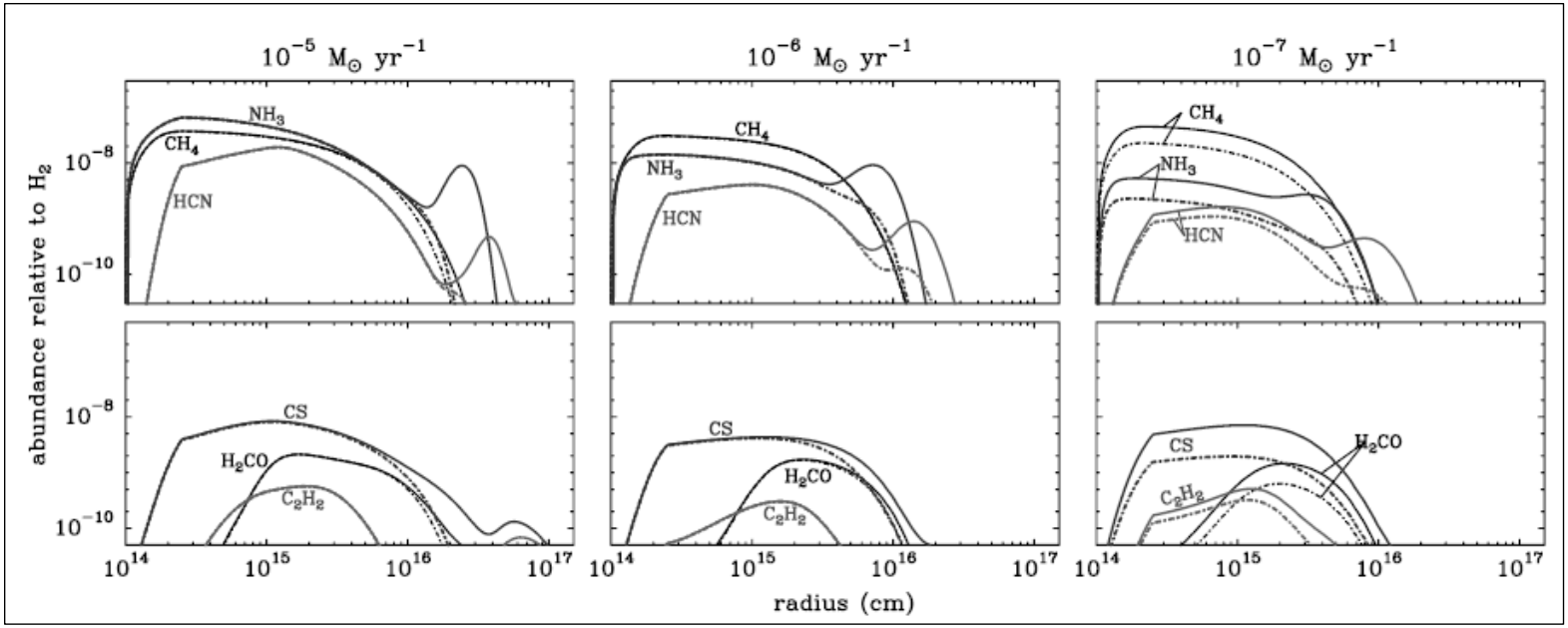


Castro-Carrizo et al., 2010

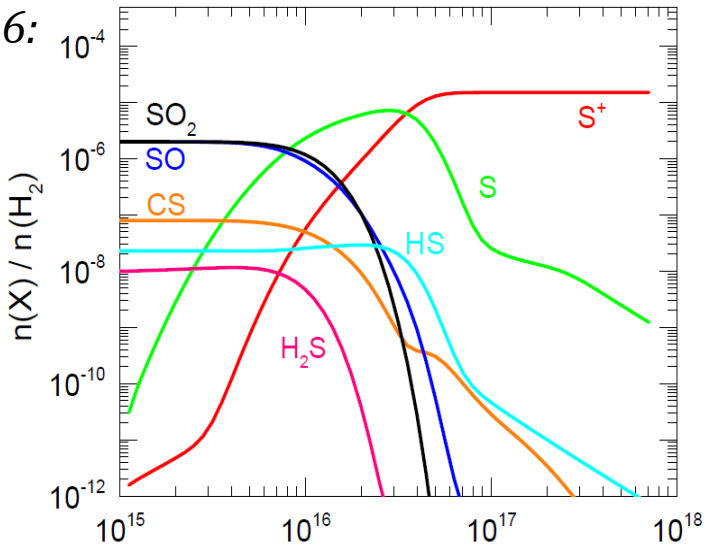
Circumstellar chemistry: O-rich CSE

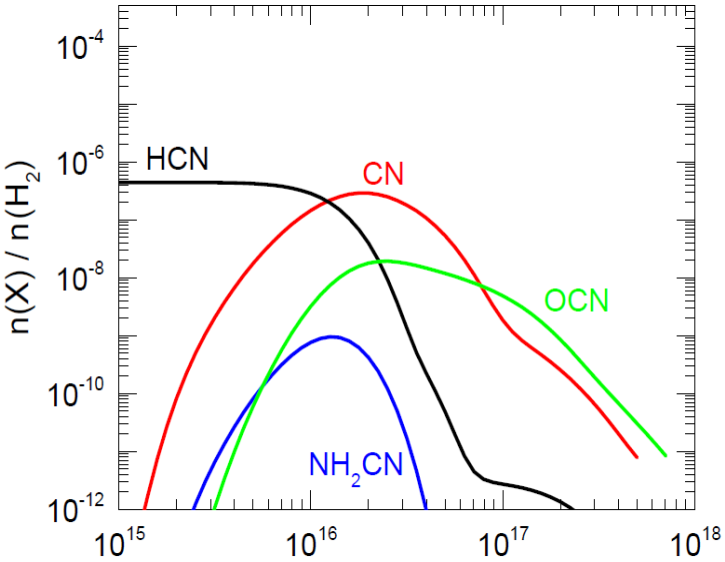
- *Chemical models:*

Agúndez et al., 2010



Li et al., 2016:

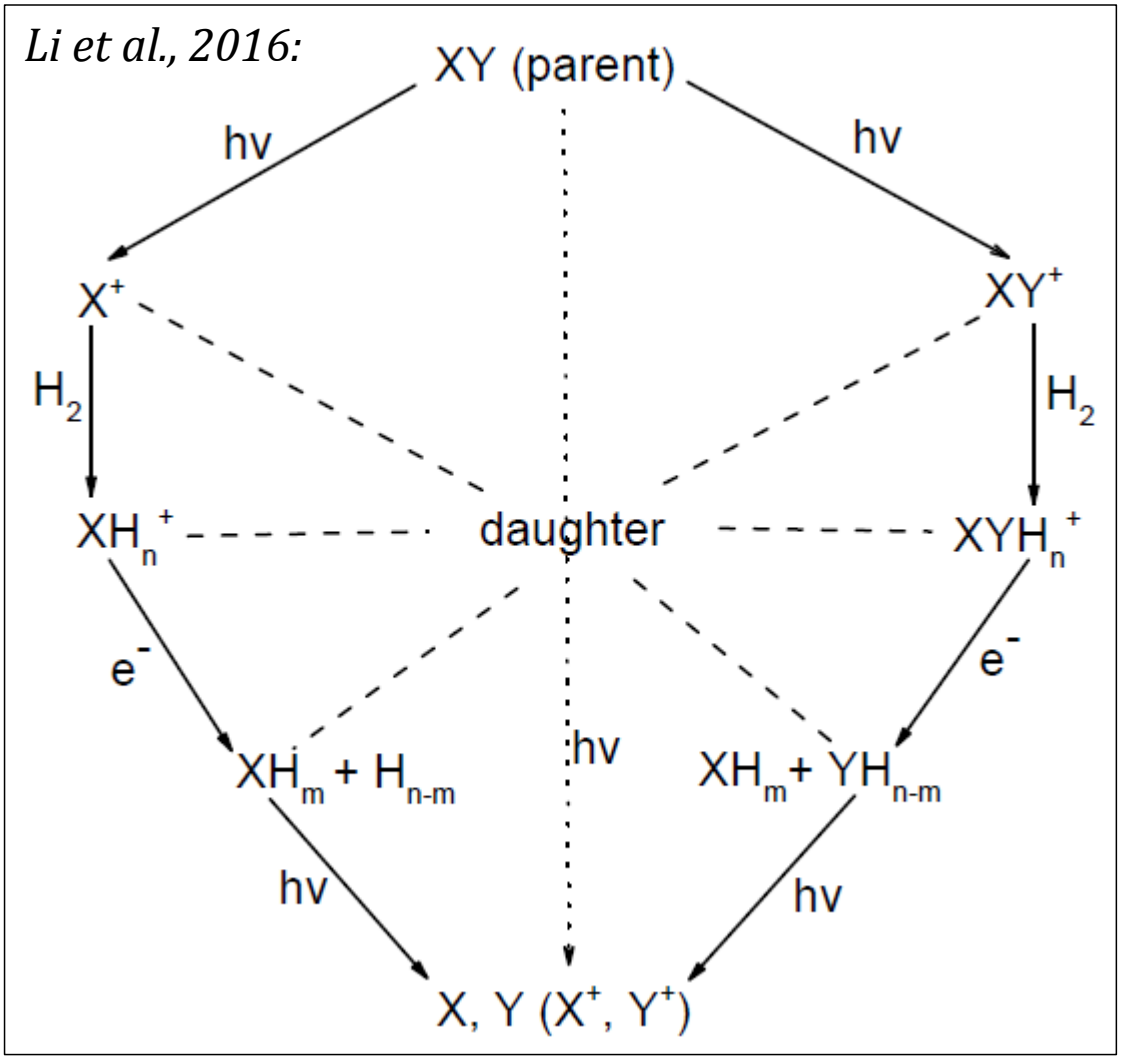




Circumstellar chemistry: chemical routes

- *Chemical models:*

Li et al., 2016:



Inner e^- source: (both C- and O-rich):

$$H_2 + crp \rightarrow H_2^+ + e^-$$

H_3^+ its very important:

$$H_3^+ + O \rightarrow H_2O^+ + H$$

$$H_2O^+ + H_2 \rightarrow H_3O^+ + H$$

Example of neutrals reaction;

$$N + OH \longrightarrow NO + H$$

Example: formation of HNCO:

$$CN + OH \longrightarrow NCO + H$$

$$H_3^+ + NCO \longrightarrow HNCO^+ + H_2$$

$$HNCO^+ + H_2 \longrightarrow HNCOH^+ + H$$

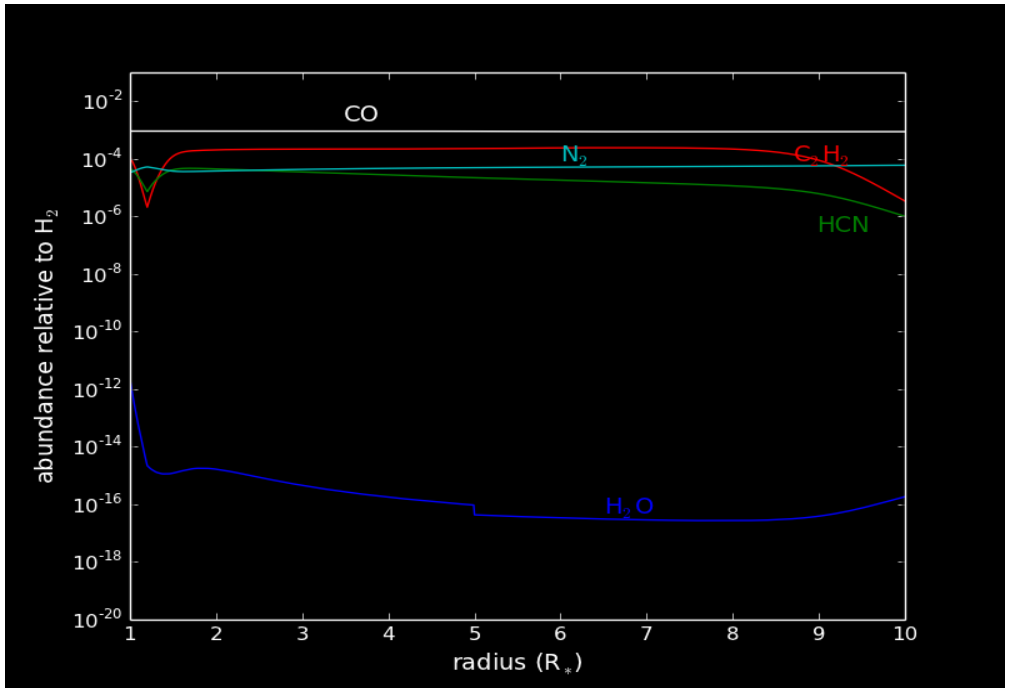
$$HNCOH^+ + e^- \longrightarrow HNCO + H$$

Circumstellar chemistry: unsolved mysteries I

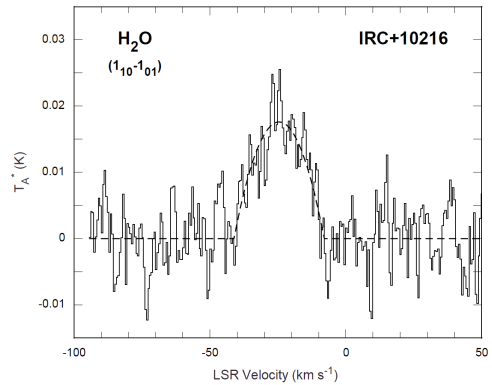
Water in C-rich CSEs

- *Presence of O-bearing molecules in C-rich CSEs and vice versa:*

TE models do not predict high abundances of water vapor in C-rich CSEs:



Melnick et al. 2001, detected the o-H_2O $1_{1,0}$-$1_{0,1}$ line (556.9 GHz) toward IRC+10216:

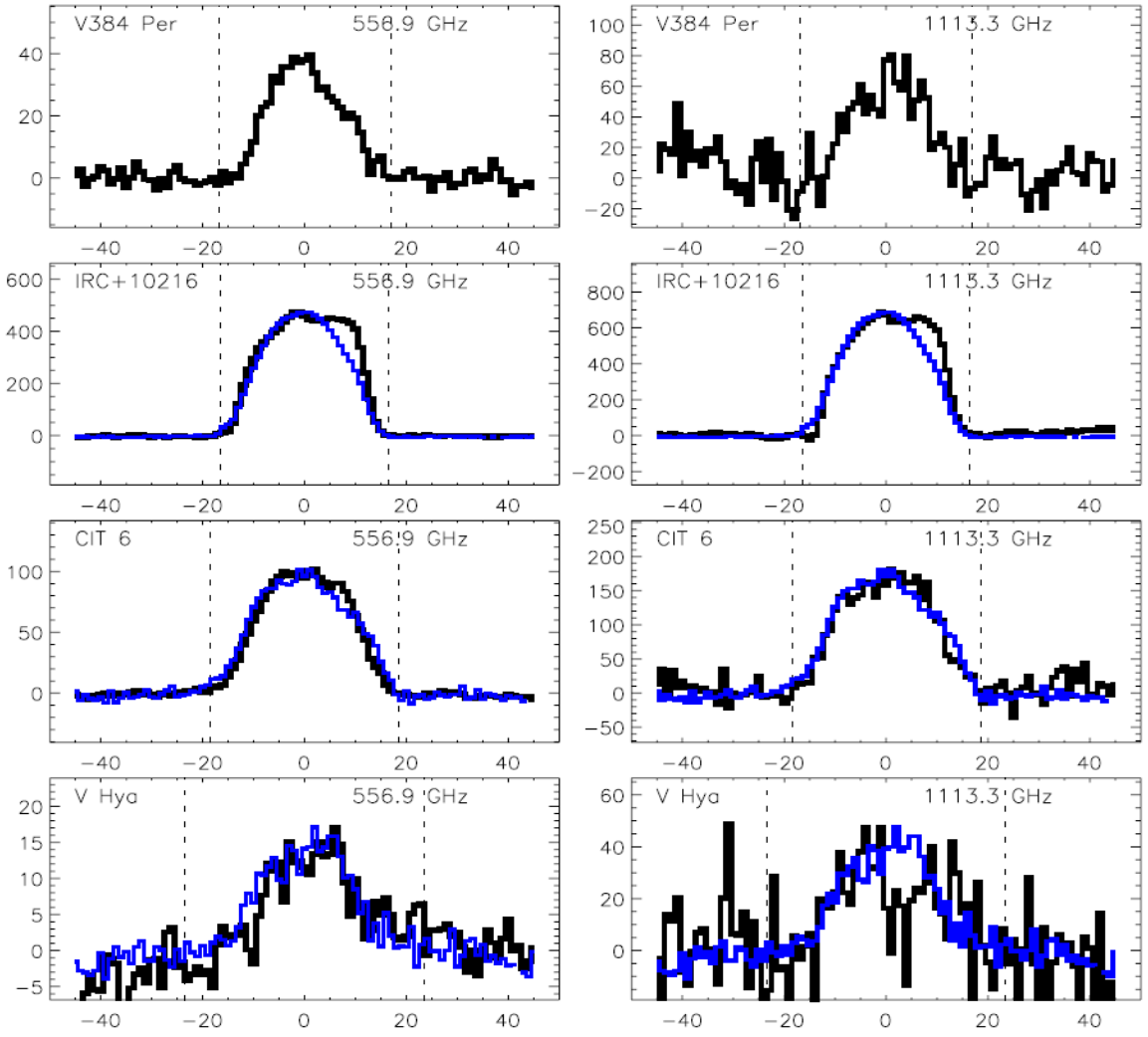


Circumstellar chemistry: unsolved mysteries I

Water in C-rich CSEs

- *Presence of O-bearing molecules in C-rich CSEs and vice versa:*

Water vapor lines were detected toward different C-rich CSEs with HIFI-HSO (Neufeld et al. 2011):



Black spectra represent the o-H2O $1_{1,0}$-$1_{0,1}$ and p-H2O $1_{1,1}$-$0_{0,0}$ lines at 556.9 and 1113.3 GHz, respectively. The blue spectra represent the scaled CO J=10-9 line (when available). Units are in antenna temperature (K) and veloctiy ($km \cdot s^{-1}$).

There should be a kind of universal mechanism to form H_2O in the CSEs of C-rich AGB stars.

Circumstellar chemistry: unsolved mysteries II

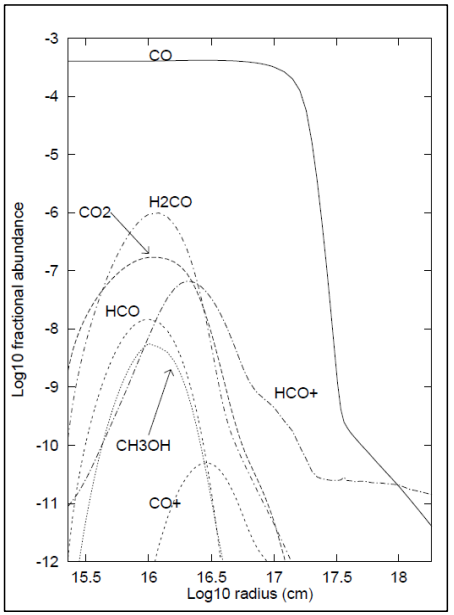
- *C-bearing molecules in O-rich CSEs:*

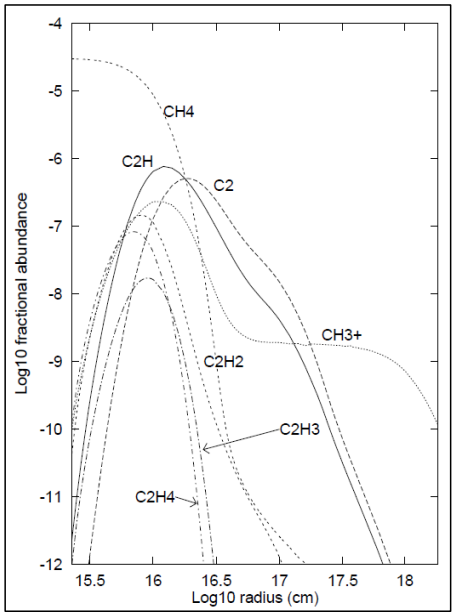
Willacy & Millar (1997) proposed CH_4 as a parent molecule in O-rich CSEs. Their model predict the formation of CH_3OH and C_2H.

Marvel (2005) did not detect emission of these molecules, estimating upper limits to their abundances lower than the predicted values by Willacy & Millar (1997).

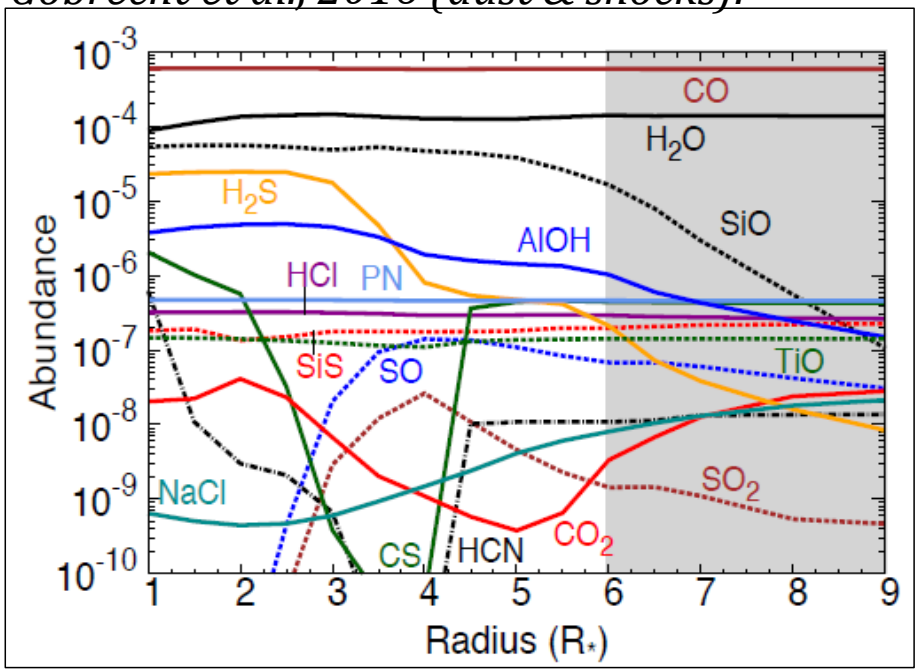
Species	Model
HCN	1.4 (-7)
HNC	2.0 (-8)
SiS	3.5 (-6)
CS	2.9 (-7)
SiO	3.2 (-5)
SO	9.1 (-7)
SO_2	2.2 (-7)
H_2S	1.3 (-5)
HCO^+	3.9 (-8)
CH_3OH	4.5 (-8)
C_2H	2.3 (-7)

Willacy & Millar, 1997:





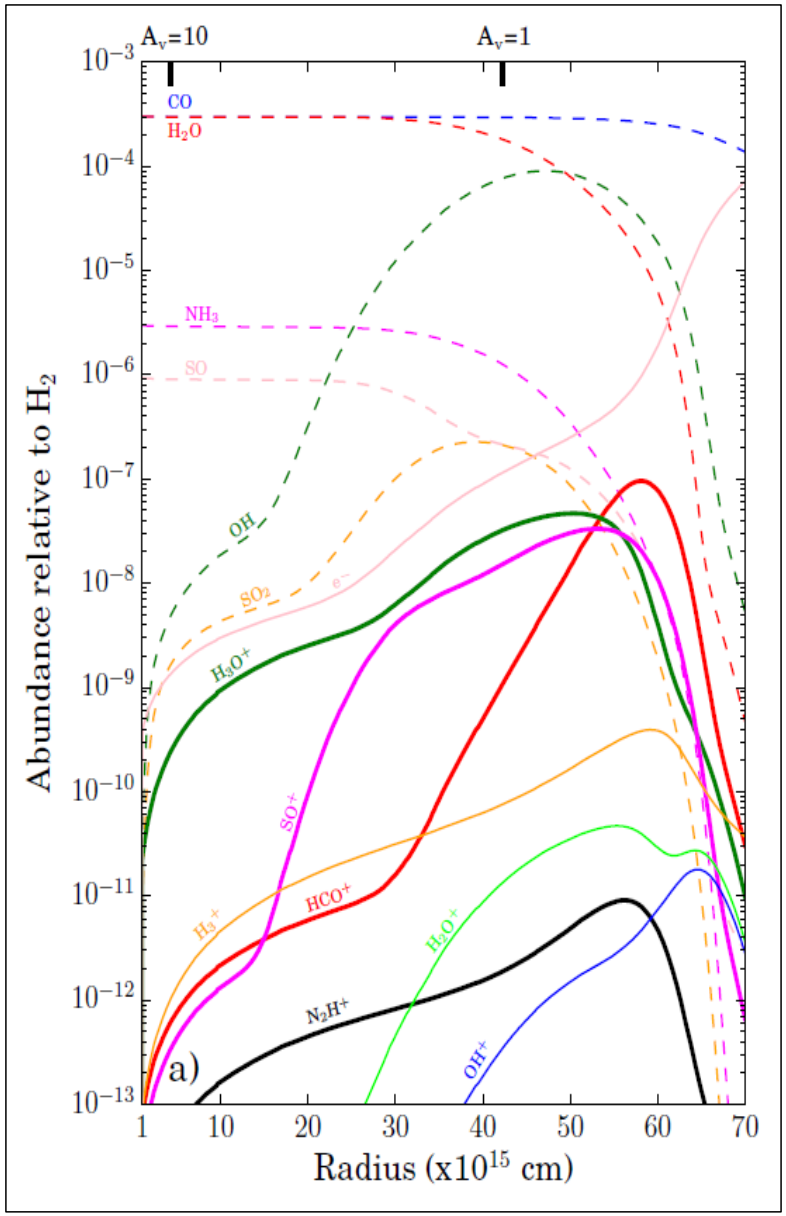
Gobrecht et al., 2016 (dust & shocks):

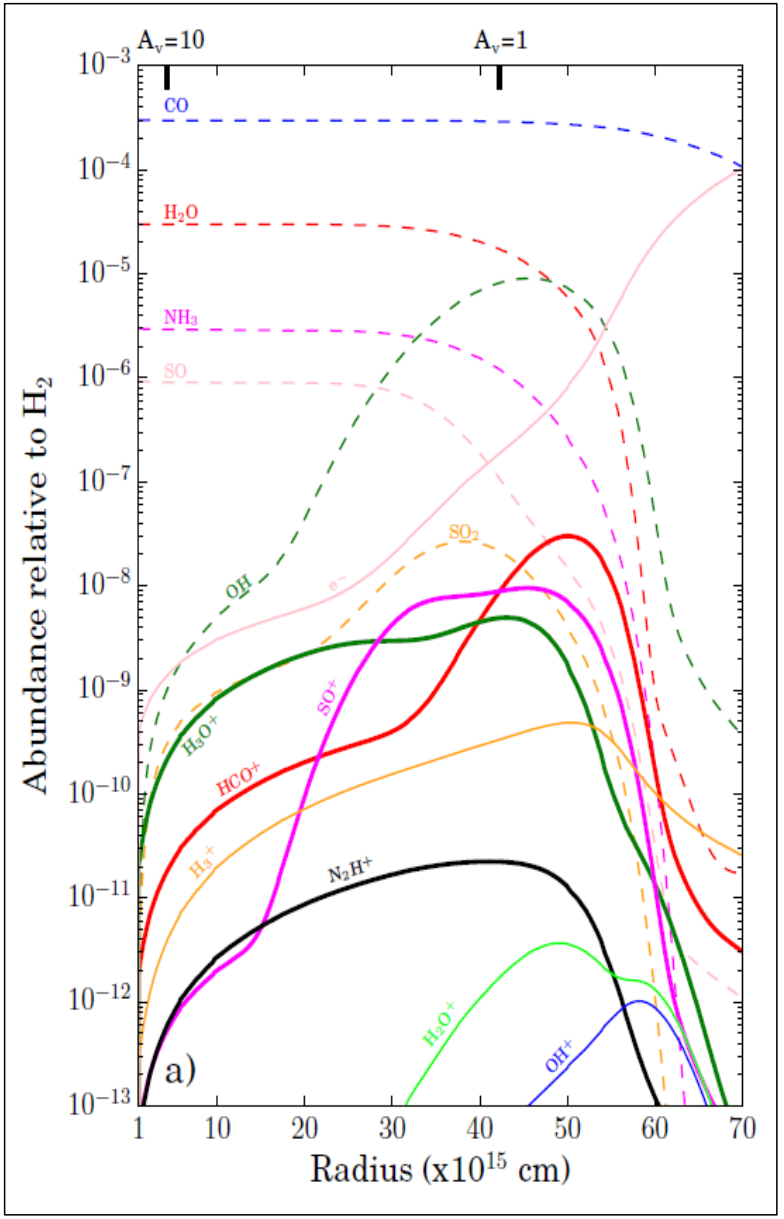


Recent observation of the O-rich CSE IKTau evidenced the presence of C-bearing molecules with abundances that are not compatible with predictions by chemical models. (Velilla Prieto et al. 2016).

Circumstellar chemistry: evolving toward the post-AGB phase

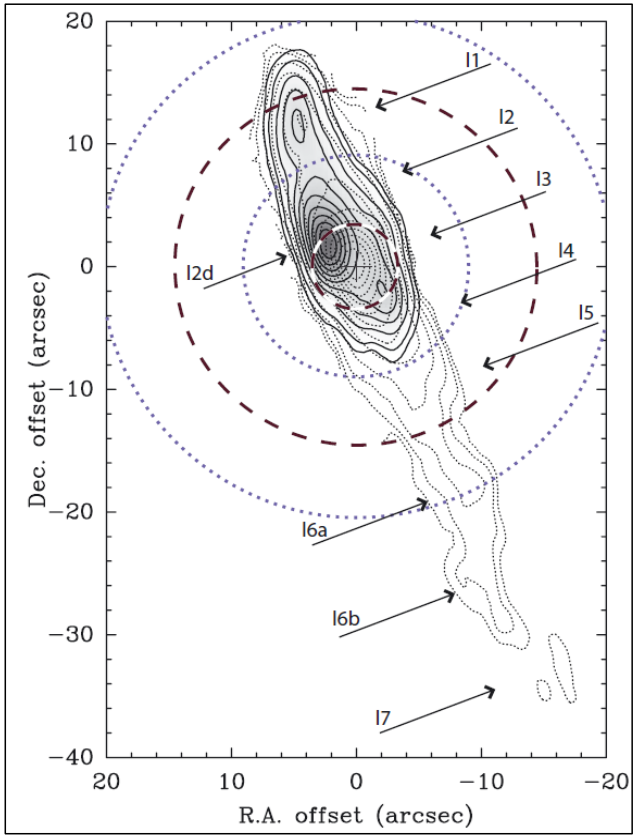
- *Shock-induced chemistry: The peculiar object OH231.8+4.2*





Circumstellar chemistry: evolving toward the post-AGB phase

- *Shock-induced chemistry: The peculiar object OH231.8+4.2*



HCO+ (1-0): *gray scale and solid contours*
CO (1-0): *dotted contours*

Formation of ions:

$$HOC^+ + H_2 \rightarrow HCO^+ + H_2$$
$$CO^+ + H_2 \rightarrow HCO^+ + H$$
$$C^+ + H_2O \rightarrow HCO^+ + H,$$

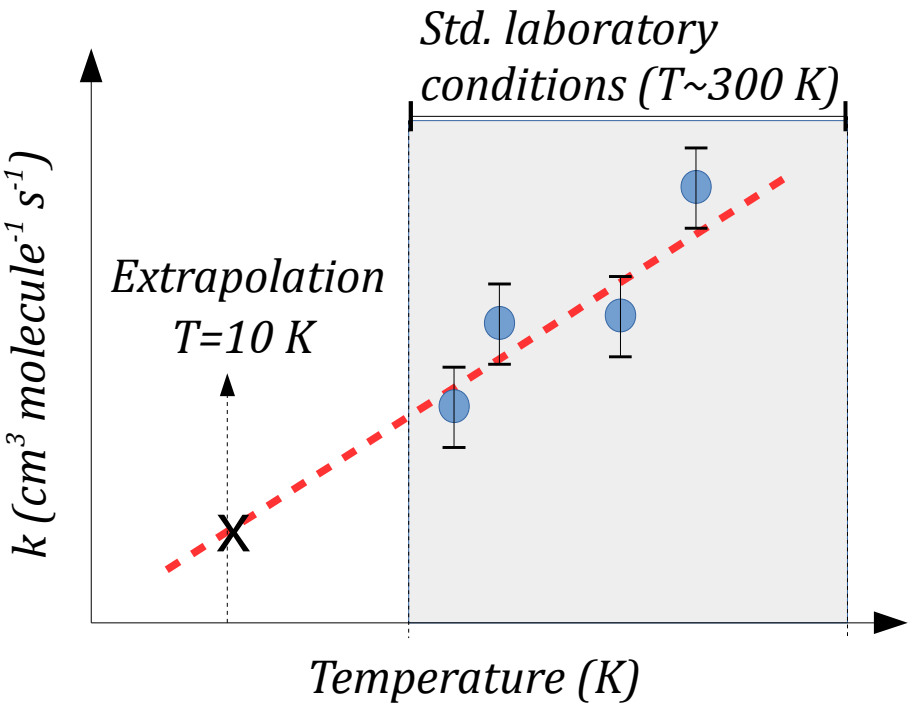
$$S^+ + OH \rightarrow SO^+ + H$$
$$SO + h\nu \rightarrow SO^+ + e^-$$
$$C^+ + SO_2 \rightarrow SO^+ + CO$$

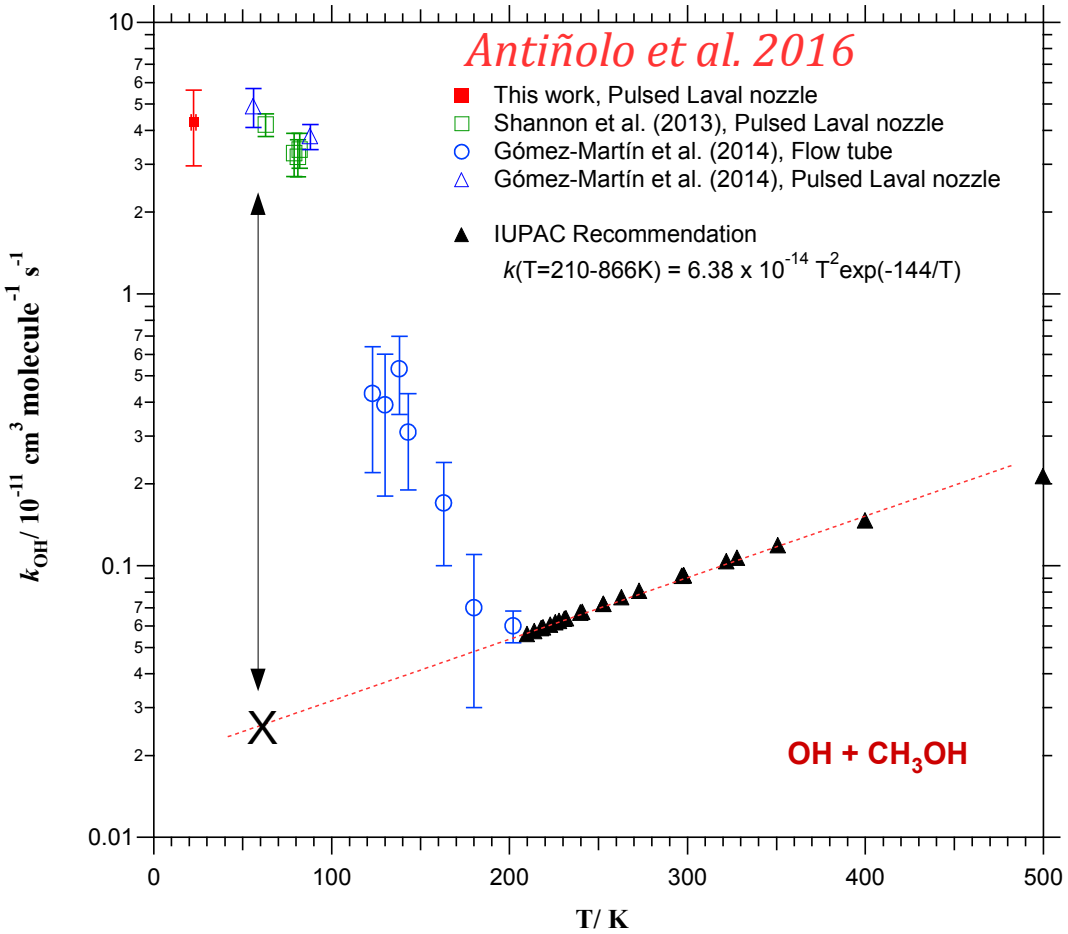
$$H_3^+ + N_2 \rightarrow N_2H^+ + H_2$$
$$N_2^+ + H_2 \rightarrow N_2H^+ + H$$
$$HCO^+ + N_2 \rightarrow N_2H^+ + CO$$

Its molecular content its similar to L1157

Laboratory work: reaction rates

- *The problem:*

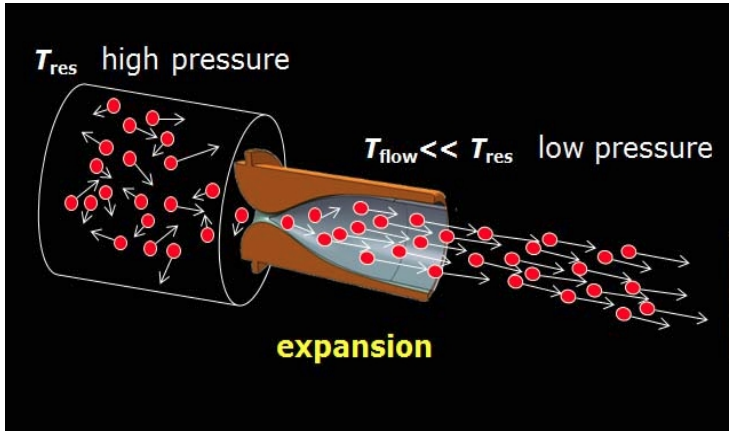




- *Cryogenic cooling: if $P>P_{sv}$ the gas will eventually condense on the walls of the vessel*

Laboratory work: reaction rates

- *The solution: CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme)*



Density of gas in the jet: 10^{16}-10^{17} cm^{-3}

↓

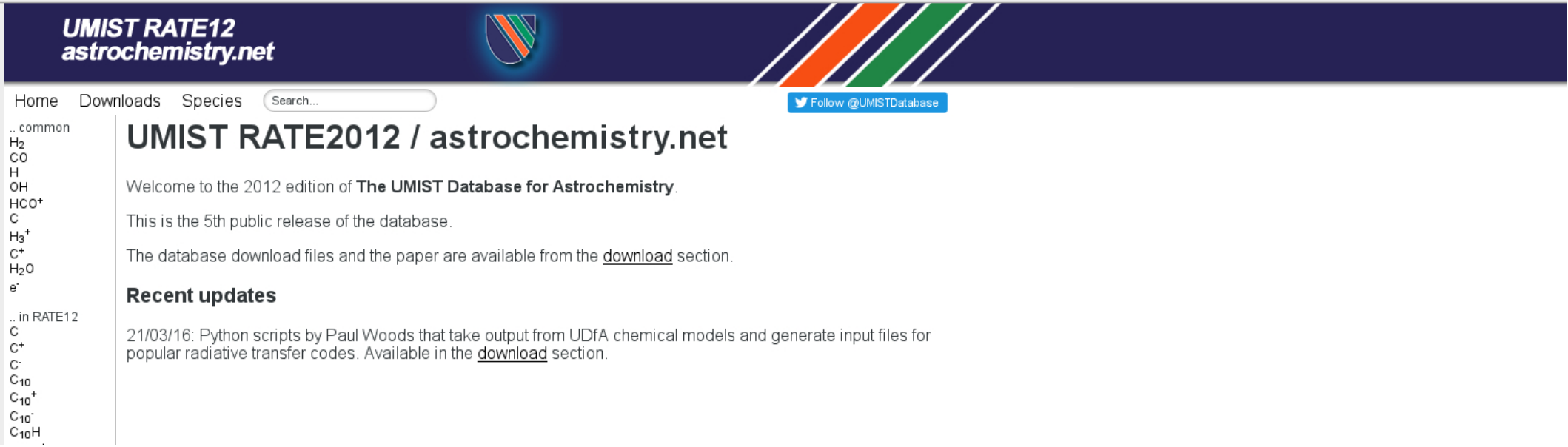
Thermal equilibrium

This technique allows to estimate reaction rates at temperatures as low as a ~20 K.

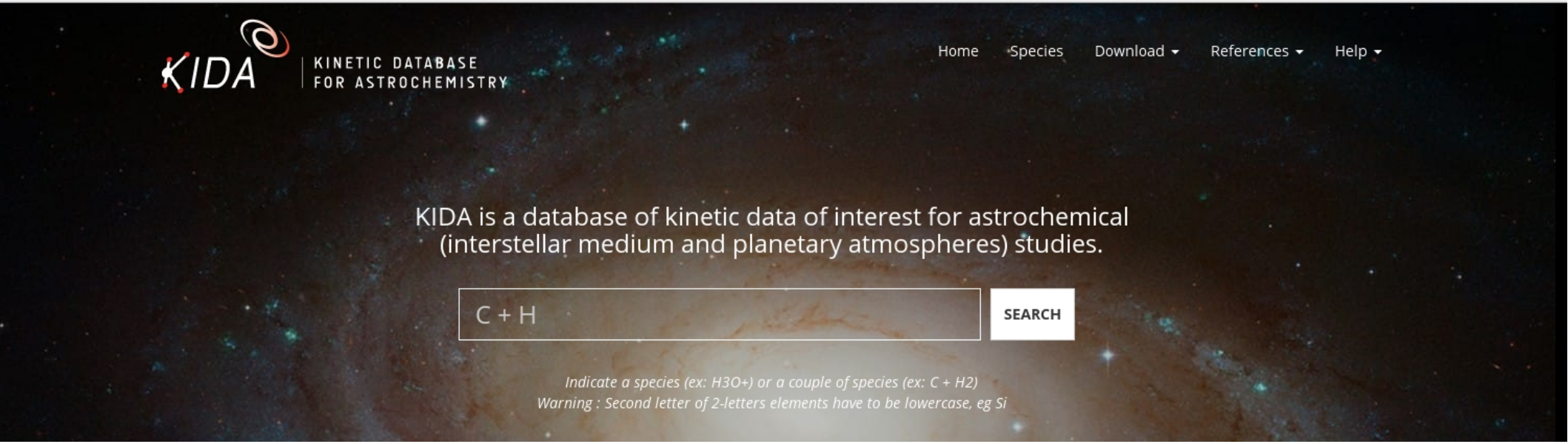
Such low temperatures are representative of ISM environments (like CSM).

Chemical databases: where to...

- *UMIST: http://udfa.ajmarkwick.net/*

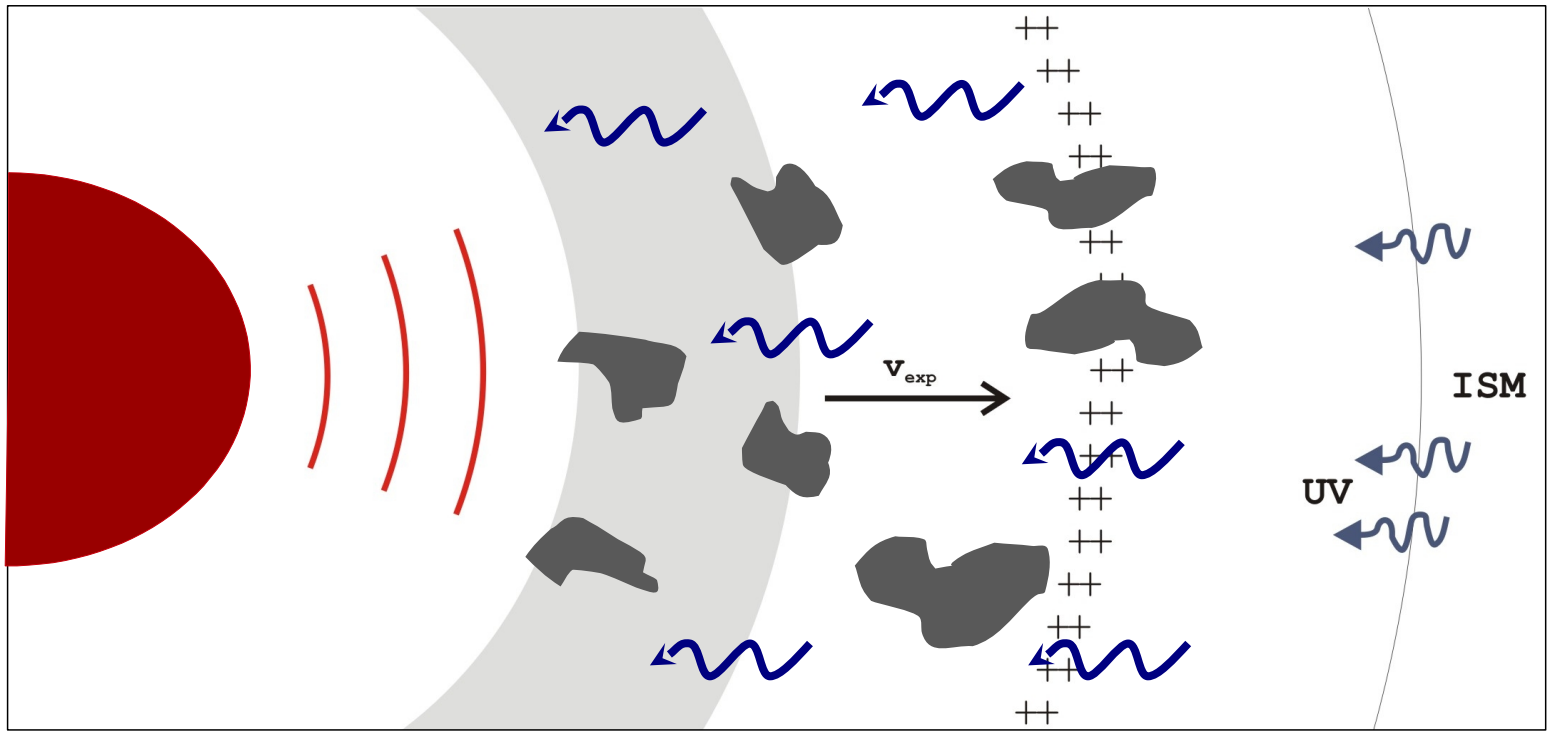


- *KIDA: http://kida.obs.u-bordeaux1.fr/*



Circumstellar chemistry: open questions

- *Clumpy envelope? Binarity?*
- *Shock-induced and dust grains chemistry?*



$$CO + h\nu \longrightarrow C + O$$
$$O + H_2 \longrightarrow OH + H$$
$$OH + H_2 \longrightarrow H_2O + H$$

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- *Marvel, K.B. 2005, AJ, 130, 261*
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- *Willacy, K., & Millar, T.J. 1997, A&A, 324, 237*

Additional slide: some formulas

- *Chemical thermodynamical equilibrium:*

$$K_p(T) = (p^0)^{\Delta\nu} \exp\{-\Delta G_r^0(T)/RT\}$$

$$\Delta G_r^0(T) = \Delta H_r^0(T) - T\Delta S_r^0(T)$$

$$\Delta H_r^0(T) = \sum_{i=1}^{N_{\text{prod}}} \Delta H_{f,i}^0(T) - \sum_{j=1}^{N_{\text{reac}}} \Delta H_{f,j}^0(T)$$

$$\Delta S_r^0(T) = \sum_{i=1}^{N_{\text{prod}}} S_i^0(T) - \sum_{j=1}^{N_{\text{reac}}} S_j^0(T)$$

G. Haro School on Molecular Astrophysics, 11-20 October 2016

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