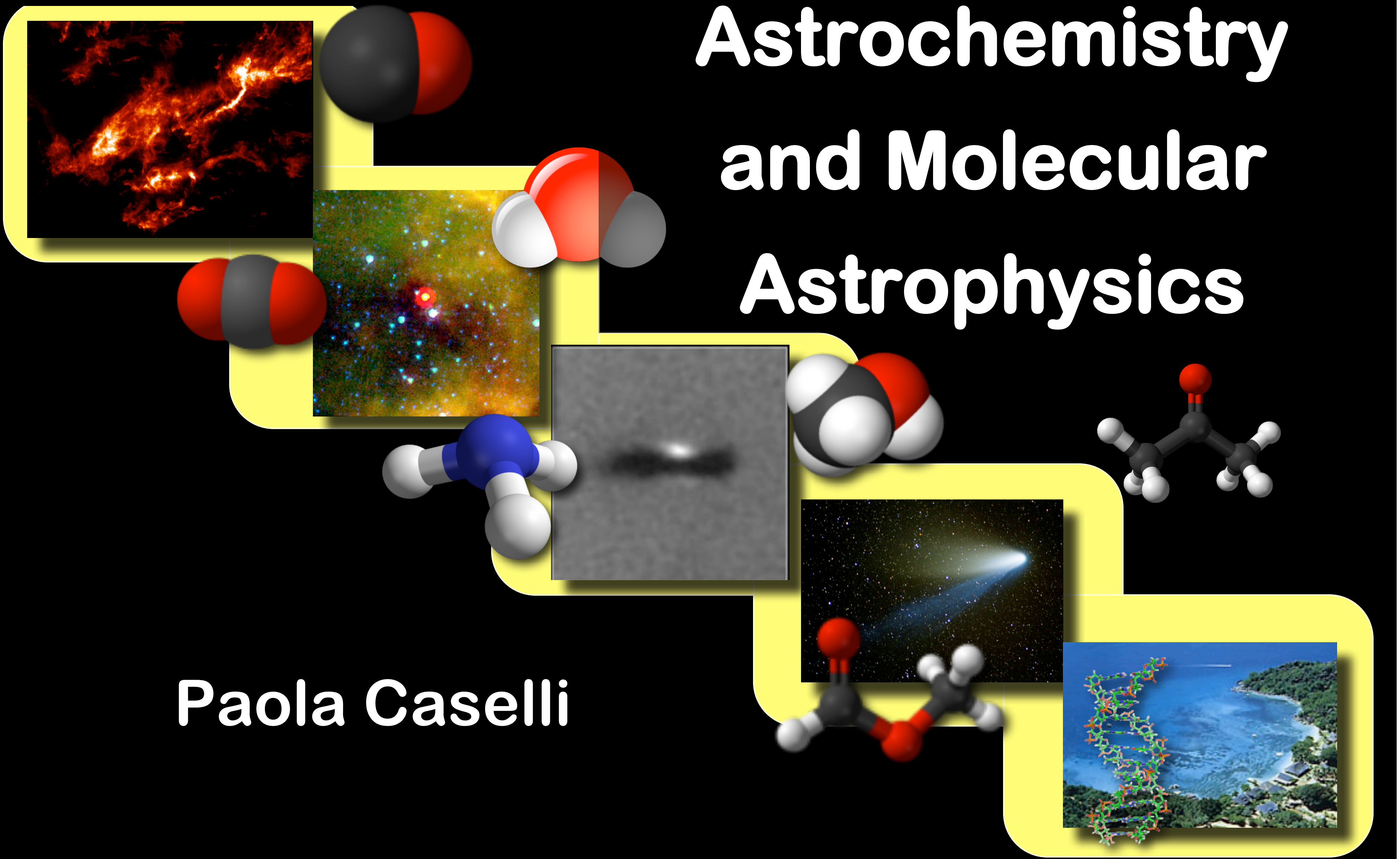
School of Physics and Astronomy
FACULTY OF MATHEMATICS & PHYSICAL SCIENCES

UNIVERSITY OF LEEDS

Astrochemistry and Molecular Astrophysics

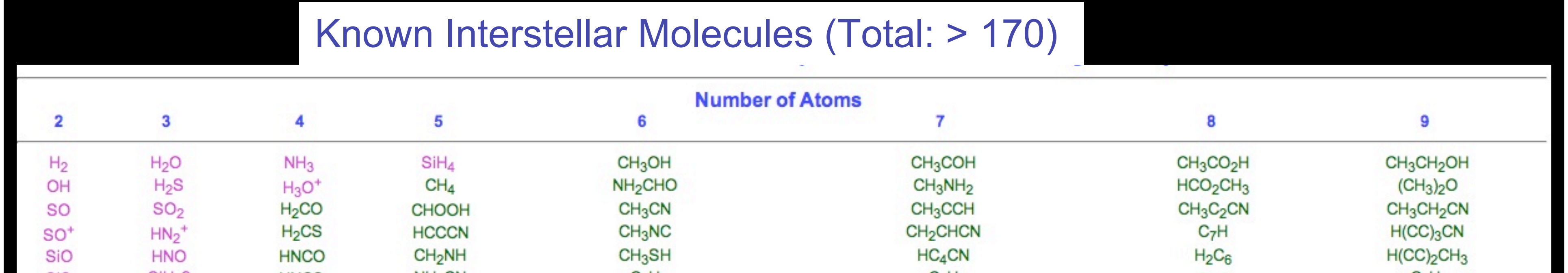


Paola Caselli

Outline

1. The formation of H_2
2. The formation of H_3^+
3. The chemistry initiated by H_3^+
4. Formation and destruction of CO
5. The two-level system
6. Transfer of radiation in spectral lines
7. The rotational temperature diagram
8. The escape probability method

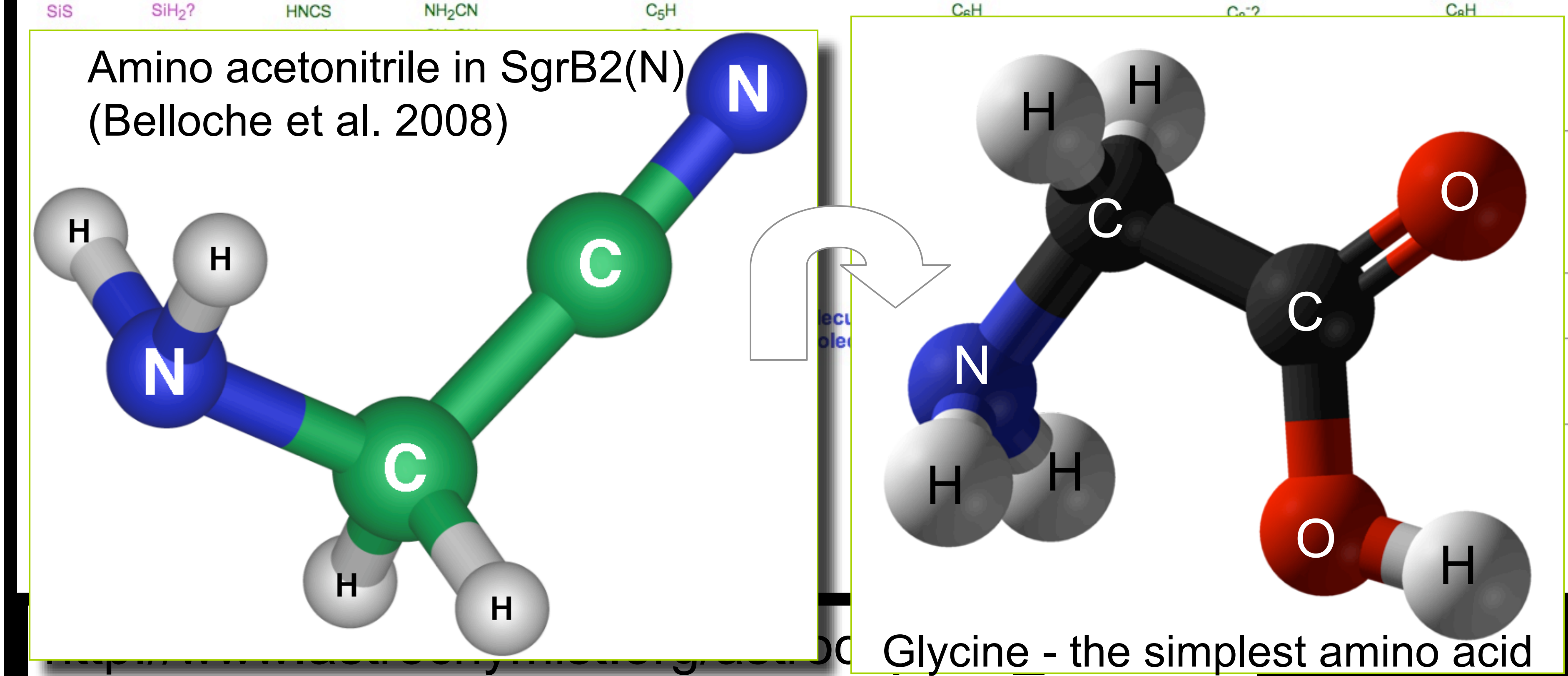
Interstellar Molecules



Known Interstellar Molecules (Total: > 170)

Number of Atoms

2	3	4	5	6	7	8	9
H_2	H_2O	NH_3	SiH_4	CH_3OH	CH_3COH	CH_3CO_2H	CH_3CH_2OH
OH	H_2S	H_3O^+	CH_4	NH_2CHO	CH_3NH_2	HCO_2CH_3	$(CH_3)_2O$
SO	SO_2	H_2CO	CHOOH	CH_3CN	CH_3CCH	CH_3C_2CN	CH_3CH_2CN
SO^+	HN_2^+	H_2CS	HCCCN	CH_3NC	CH_2CHCN	C_7H	$H(CC)_3CN$
SiO	HNO	HNCO	CH_2NH	CH_3SH	HC_4CN	H_2C_6	$H(CC)_2CH_3$
SiS	SiH_2?	HNCS	NH_2CN	C_5H	C_6H	[illegible]	C_8H



Amino acetonitrile in SgrB2(N)
(Belloche et al. 2008)

Glycine - the simplest amino acid

How do molecules form in the interstellar medium ?

The most elementary chemical reaction is the association of A and B to form a molecule AB with internal energy:

$$A + B \rightarrow AB^*$$

The molecule AB^* must lose the internal energy. In the Earth atmosphere, where the number of particles per cubic centimeter (cc) is very large (~10^{19}), the molecule looses its energy via three-body reactions:

$$AB^* + M \rightarrow AB$$

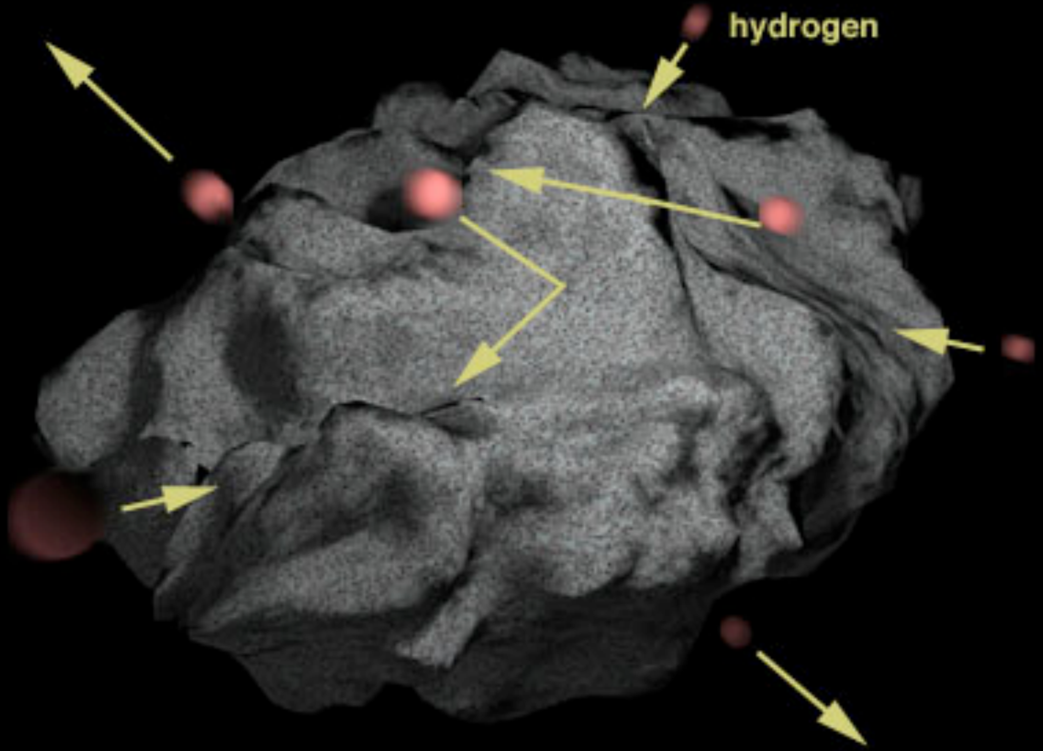
But this is not an efficient process in interstellar clouds, where the number of particles per cc ranges between a few hundred and ~10^8.

1. The formation of H_2

The reaction that starts the chemistry in the interstellar medium is the one between two hydrogen atoms to form molecular hydrogen:

$$H + H \rightarrow H_2$$

This reaction happens on the surface of dust grains.

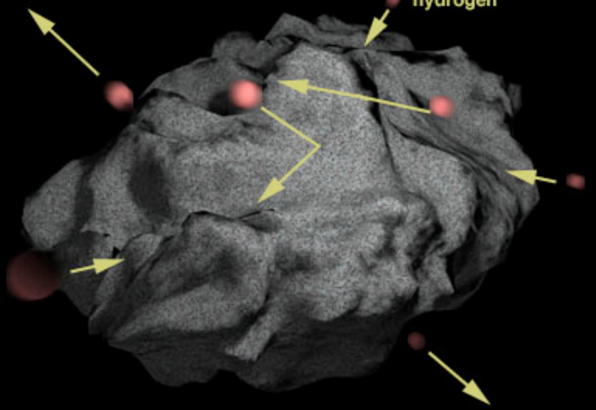


1. The formation of H_2

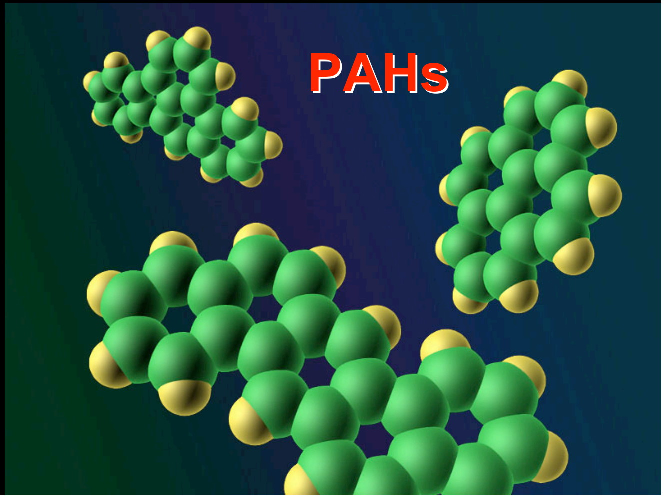
The H_2 formation rate ($cm^{-3}\ s^{-1}$) is given by (Gould & Salpeter 1963; Hollenbach & Salpeter 1970; Jura 1974; Pirronello et al. 1999; Cazaux & Tielens 2002; Bergin et al. 2004; Cuppen & Herbst 2005; Cazaux et al. 2008):

$$R_{H_2} = \frac{1}{2} n_H v_H A n_g S_H \gamma$$

$$\cong 10^{-17}\ -\ 10^{-16}\ \mathrm{cm^{-3}s^{-1}}$$



$n_H \equiv$ gas number density
$v_H \equiv$ H atoms speed in gas-phase
A ≡ grain cross sectional area
$n_g \equiv$ dust grain number density
$S_H \equiv$ sticking probability
$\gamma \equiv$ surface reaction probability



Once H2 is formed, the fun starts…

H_2 is the key to the whole of interstellar chemistry. Some important species that might react with H_2 are C, C+, O, N… To decide whether a certain reaction is chemically favored, we need to examine internal energy changes.

Molecule	Dissociation energy (eV)
H_2	4.48
CH	3.47
OH	4.39
CH^+	4.09
OH^+	5.10

Question: Can the following reactions proceed in the cold interstellar medium?

$C + H_2 \rightarrow CH + H$??
$C^+ + H_2 \rightarrow CH^+ + H$??

$O + H_2 \rightarrow OH + H$??
$O^+ + H_2 \rightarrow OH^+ + H$??

Once H2 is formed, the fun starts…

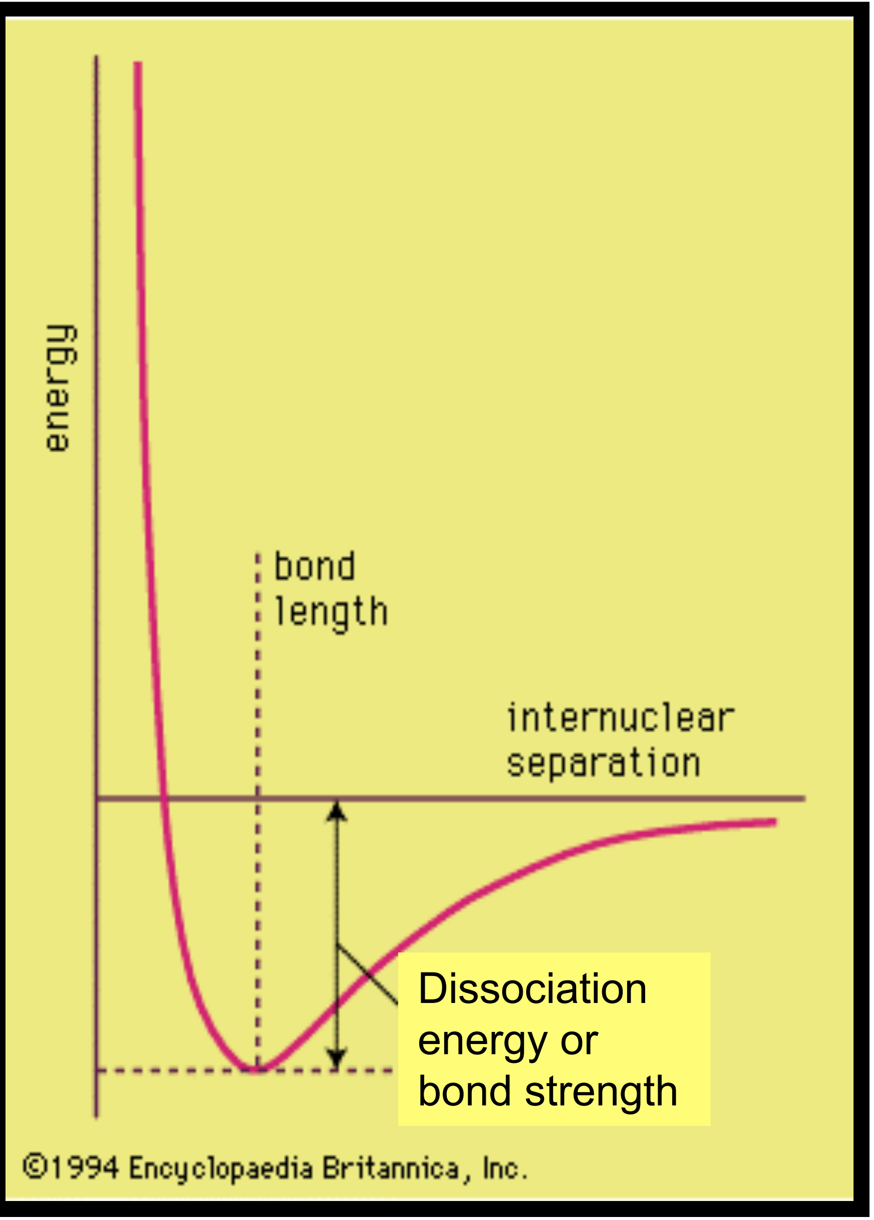
$C + H_2 \rightarrow CH + H$??

4.48 eV

3.47 eV

The bond strength of H_2 is larger than that of CH ➔the reaction is not energetically favorable.

The reaction is **endothermic** (by 4.48-3.47 = 1.01 eV) and cannot proceed in cold clouds, where $k_b T < 0.01$ eV !



Dissociation energy or bond strength

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Once H2 is formed, the fun starts…

Molecule	Dissociation energy (eV)
H_2	4.48
CH	3.47
OH	4.39
CH^+	4.09
OH^+	5.10

$\text{C} + \text{H}_2 \not\rightarrow \text{CH} + \text{H}$ (endothermic by 1.01 eV)

$\text{C}^+ + \text{H}_2 \not\rightarrow \text{CH}^+ + \text{H}$ (endothermic by 0.39 eV)

$\text{O} + \text{H}_2 \not\rightarrow \text{OH} + \text{H}$ (endothermic by 0.09 eV)

$\text{O}^+ + \text{H}_2 \xrightarrow{\checkmark} \text{OH}^+ + \text{H}$ (**exothermic** by 0.62 eV!)

Rate coefficients and activation energies

The rate coefficient *k* (cm^3 s^{-1}) of a generic reaction A + B -> C + D is given by:

$$\boxed{k = < \sigma \mathrm{v} >}$$

$\sigma \equiv$ total cross section of the reactants
v ≡ relative velocity
<The average is performed over the thermal distribution>

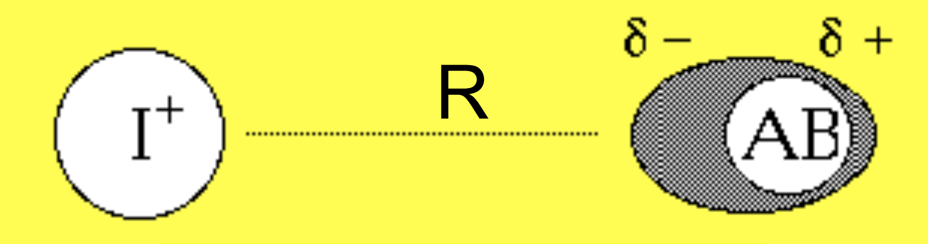
Most reactions possess activation energies E_a (~0.1-1 eV) even if exothermic and *k* is given by the Arrhenius formula (Herbst 1990):

$$\boxed{k = a(T)\exp(-E_a / k_B T)}$$

Ion-Neutral reactions

$$\mathbf{A^+ + B \rightarrow C^+ + D}$$

Exothermic ion-molecule reactions do not possess activation energy because of the strong long-range attractive force (Herbst & Klemperer 1973; Anicich & Huntress 1986):



$$V(R) = -\ \alpha\ e^2/2R^4$$

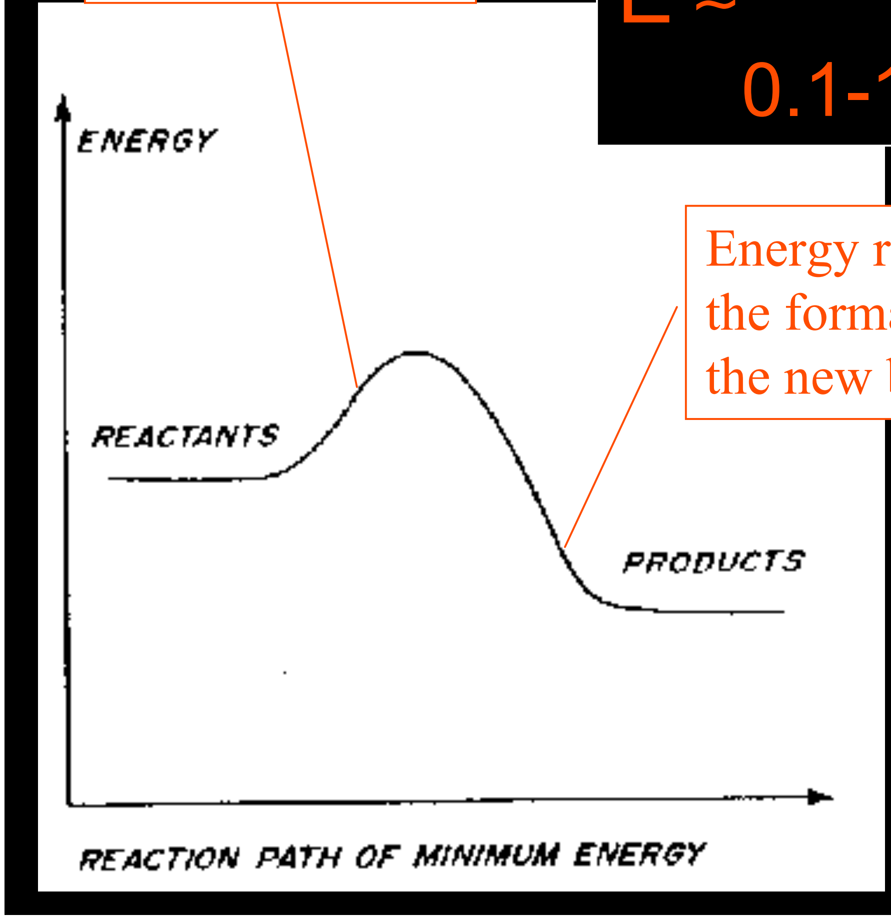
$$k_{LANGEVIN} = 2\ \pi e(\alpha/\mu)^{1/2}$$

$$\sim 10^{-9}\ cm^3\ s^{-1}$$

independent of T

Neutral-Neutral reactions

$A + BC \rightarrow AB + C$



Energy to break the bond of the reactant.

Energy released by the formation of the new bond.

$E \sim$ 1 eV for endothermic reactions

$E \sim$ 0.1-1 eV for exothermic reactions

$k_b T < 0.01$ eV in molecular clouds

Example: $O + H_2 \not\rightarrow OH + H$
(does not proceed in cold clouds)

Duley & Williams 1984, *Interstellar Chemistry;*
Bettens et al. 1995, ApJ

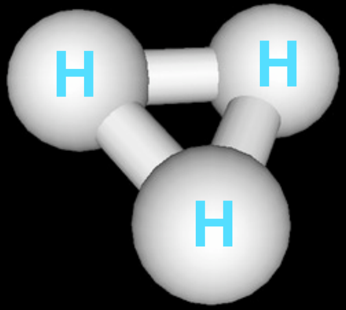
2. *The formation of H_3^+*

After the formation of molecular hydrogen, cosmic rays ionize H_2 initiating fast routes towards the formation of complex molecules in dark clouds:

$$H_2 + c.r. \rightarrow H_2^+ + e^- + c.r.$$

Once H_2^+ is formed (in small percentages), it very quickly reacts with the abundant H_2 molecules to form H_3^+, the most important molecular ion in interstellar chemistry:

$$H_2^+ + H_2 \rightarrow H_3^+ + H$$

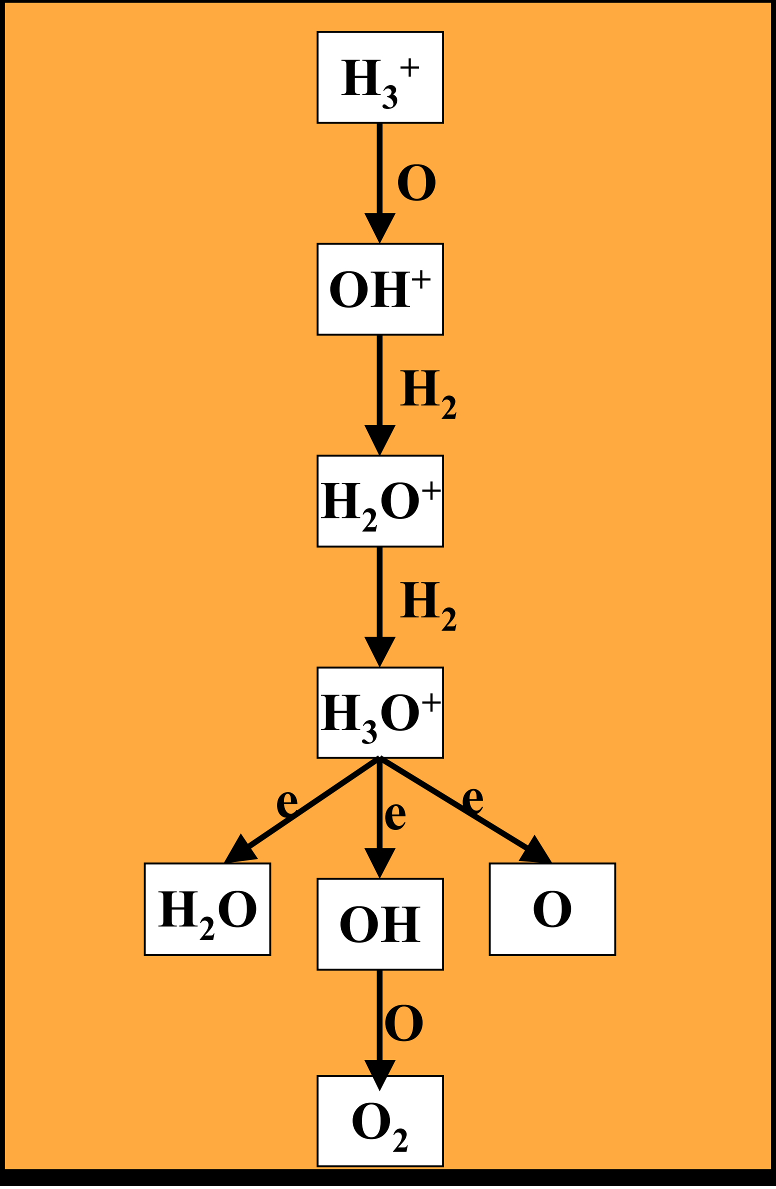


3. The chemistry initiated by H_3^+

Once H_3^+ is formed, a cascade of reactions greatly enhance the chemical complexity of the ISM.

In fact, H_3^+ can easily donate a proton and allow larger molecules to form.

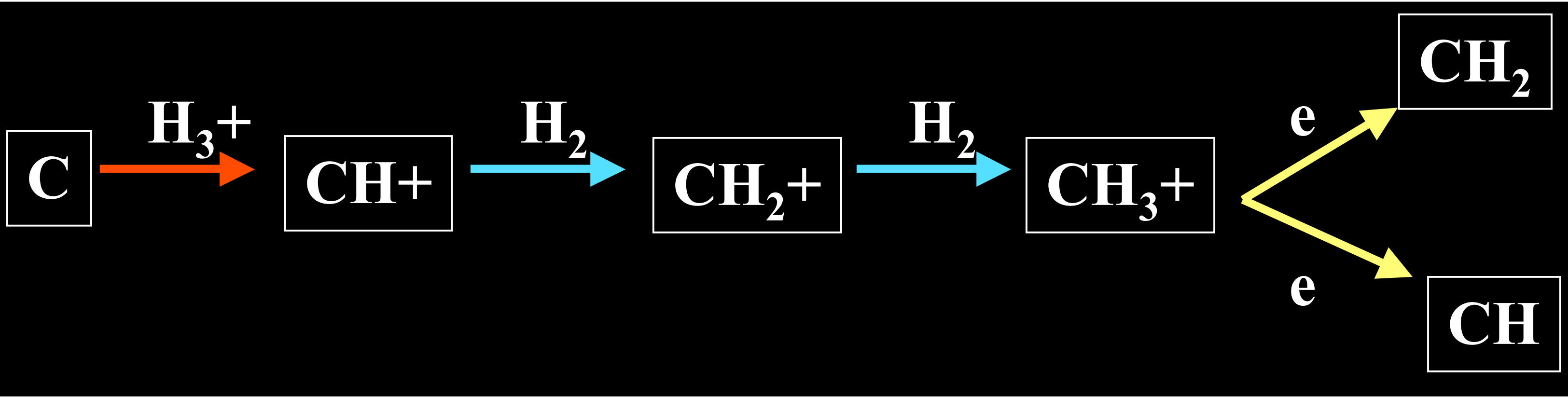
Example →
OXYGEN CHEMISTRY (the formation of water in dark clouds)



3. The chemistry initiated by H_3^+

CARBON CHEMISTRY (the formation of hydrocarbons)

The formation of more complicated species from neutral atomic carbon begins with a sequence very similar to that which starts the oxygen chemistry:



$$C \xrightarrow{H_3+} CH+ \xrightarrow{H_2} CH_2+ \xrightarrow{H_2} CH_3+$$

$$CH_3+ \xrightarrow{e} CH_2$$

$$CH_3+ \xrightarrow{e} CH$$

A. Proton transfer from H_3^+ to a neutral atom;
B. Hydrogen abstraction reactions terminating in a molecular ion that does not react with H_2;
C. Dissociative recombination with electrons.

4. Formation and destruction of CO

[a] $C + H_3O^+ \rightarrow HCO^+ + H_2$

[b] $O + CH_3^+ \rightarrow HCO^+ + H_2$

[c] $HCO^+ + e \rightarrow CO + H$ is the most important source of CO.

CO is very stable and difficult to remove. It reacts with H_3^+:

[d] $H_3^+ + CO \rightarrow HCO^+ + H_2$

but reaction (c) immediately reform CO.

The main mechanisms for removing CO are:

[e] $He^+ + CO \rightarrow He + C^+ + O$

[f] $h\nu + CO \rightarrow C + O$

Some of C^+ can react with OH and H_2O (but not with H_2):

[g] $C^+ + OH \rightarrow CO^+ + H$

[h] $CO^+ + H_2 \rightarrow HCO^+ + H$

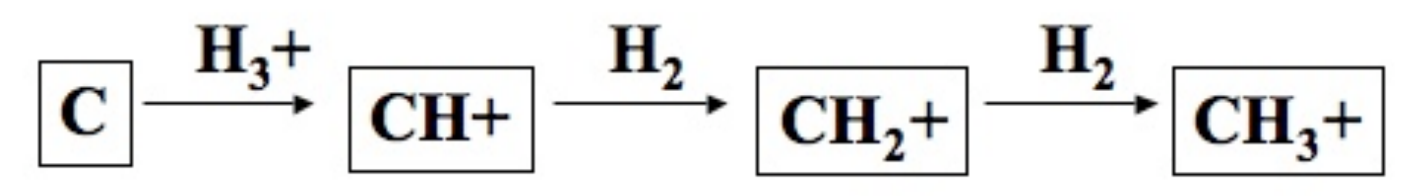
[i] $C^+ + H_2O \rightarrow HCO^+ + H$

The timescale to form CO

Assume: dark region where all H is in H_2 and all atoms more massive than He are in neutral atomic form.

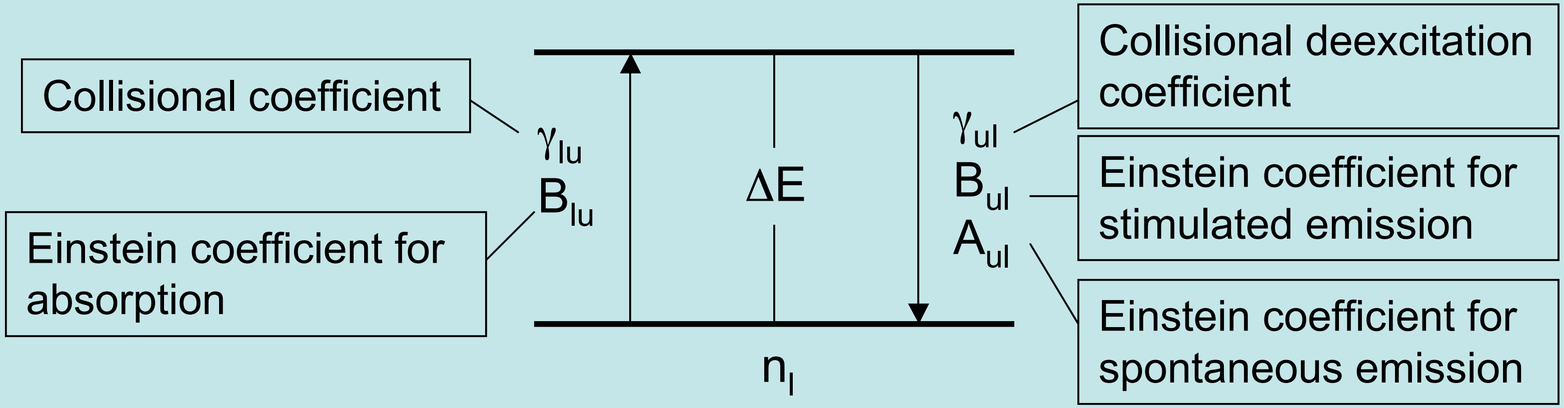
The timescale on which almost all carbon becomes contained in CO ($n_O > n_C$) is at least equal to the timescale for one H_2 to be ionized for every C: $n_C/[\zeta\, n(H_2)] = 2\, n_C/[\zeta\, n_H]$

For $\zeta = 3\times10^{-17}$ s^{-1} and $n_C/n_H = 10^{-4}$, the above expression gives a value of about 2×10^5 yr.



$\xrightarrow{O} HCO^+ \xrightarrow{e^-} CO$

5. The two-level system



Collisional coefficient

Einstein coefficient for absorption

Collisional deexcitation coefficient

Einstein coefficient for stimulated emission

Einstein coefficient for spontaneous emission

Problem: find the level populations n_u and n_l as a function of the ambient kinetic temperature T_{kin} and density n_{tot}.

In order for the populations of both levels to remain constant in time, we need:

$$\gamma_{lu} n_{tot} n_l + B_{lu} \bar{J} n_l = \gamma_{ul} n_{tot} n_u + B_{ul} \bar{J} n_u + A_{ul} n_u$$

Total rate of collisional excitations per unit time and per unit volume

Probability per unit time of being excited radiatively

$$\bar{J} \equiv \int_0^\infty J_\nu \phi(\nu) d\nu$$

In Local Thermodinamic Equilibrium (i.e. when radiative transitions are negligible):

$$\frac{\gamma_{lu}}{\gamma_{ul}} = \frac{n_u}{n_l} = \frac{g_u}{g_l}\exp\left(-\frac{\Delta E}{k_B T_{kin}}\right) \quad (T_{ex} = T_{kin}, \text{ in LTE})$$

When n_{tot} is so low that that radiative transitions dominate:

$$\bar{J} = \frac{A_{ul} n_u}{B_{lu} n_l \quad B_{ul} n_u} = \frac{A_{ul} / B_{ul}}{(g_l B_{lu} / g_u B_{ul}) \exp(\# E / k_B T_{rad}) \quad 1}$$

Under the assumption of thermodynamic equilibrium ($J_\nu = B_\nu$):

$$\bar{J} \approx B_{\nu 0} = \frac{2h\nu_0^3 / c^2}{\exp(\Delta E / k_B T_{rad}) - 1}$$

↓

$$A_{ul} = \frac{2h\nu_0^3}{c^2} B_{ul} \qquad g_l B_{lu} = g_u B_{ul}$$

$$\boxed{\gamma_{lu} n_{tot} n_l + B_{lu} \bar{J} n_l = \gamma_{ul} n_{tot} n_u + B_{ul} \bar{J} n_u + A_{ul} n_u}$$

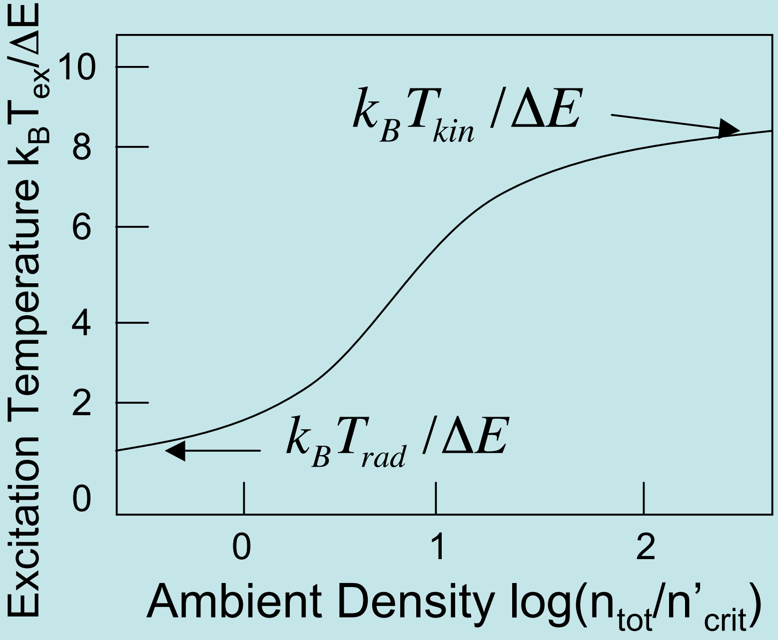
$$\Downarrow$$

$$\exp\left(-\frac{\Delta E}{k_B T_{ex}}\right) = f_{coll} \exp\left(-\frac{\Delta E}{k_B T_{kin}}\right) + (1 - f_{coll}) \exp\left(-\frac{\Delta E}{k_B T_{rad}}\right)$$

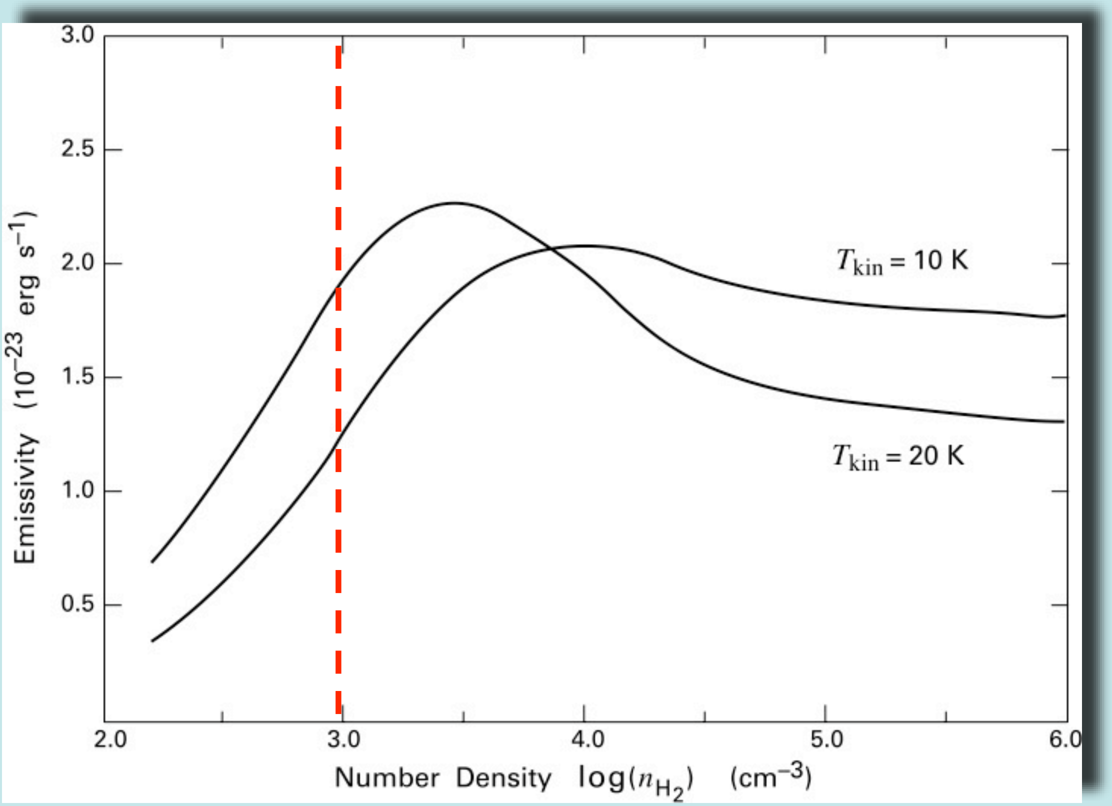
$$f_{coll} \equiv \frac{n_{tot}}{n_{tot} + n_{crit}(1 + c^2 \bar{J} / 2h\nu_0^3)}$$

fraction of all downward transitions due to collisions

$$n_{crit} \equiv A_{ul} / \gamma_{ul}$$



Emission in the J=1→0 line of $^{12}C^{16}O$



Increasing the density in a cloud can enhance the J=1-0 emission, but only for subcritical values of n_{tot}.

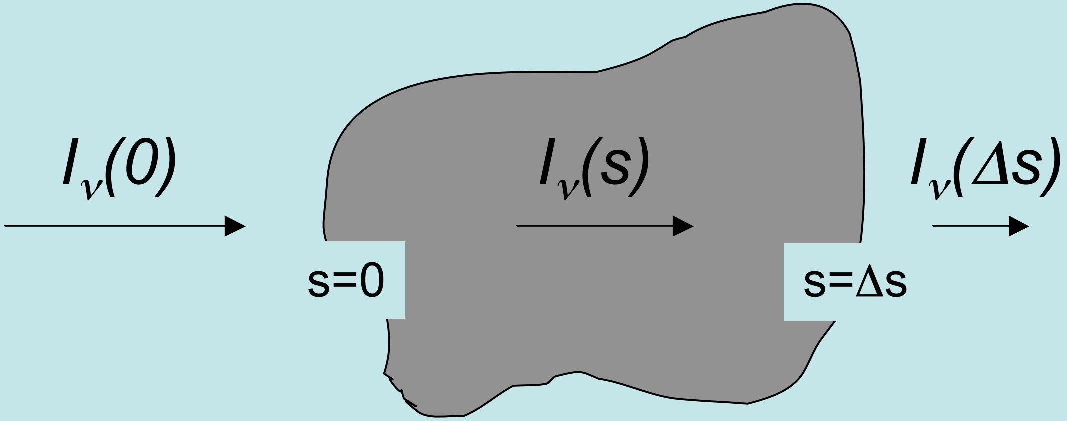
↓

Observations in a given transition are most sensitive to gas with densities near the corresponding n_{crit}.

Transfer of radiation in spectral lines

The propagation of the specific intensity I_ν is governed by the radiative transfer equation:

$$\boxed{\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu}$$



$$I_\nu(\Delta s) = I_\nu(0)\exp(-\alpha_\nu \Delta s) + \frac{j_\nu}{\alpha_\nu}[1 - \exp(-\alpha_\nu \Delta s)]$$

Stahler & Palla (2004)

We consider the case in which both absorption and emission are due to transitions between two discrete levels in an atom or molecule. The **macroscopic** emission and absorption coefficients can be written in terms of the **microscopic** Einstein coefficients:

$$j_\nu = \frac{h\nu_0}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\boxed{\phi(\nu) = \frac{2\sqrt{\ln 2}}{\sqrt{\pi}\,\Delta\nu}}$$

$$\alpha_\nu = \frac{h\nu_0}{4\pi}(n_l B_{lu} - n_u B_{ul})\phi(\nu)$$

$$\boxed{\frac{n_u}{n_l} = \frac{g_u}{g_l}\exp\left(-\Delta E / k\, T_{ex}\right)}$$

$$\Downarrow$$

$$\frac{j_\nu}{\alpha_\nu} = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} = \frac{2h\nu_0^3/c^2}{\exp(h\nu_0/k_B T_{ex}) - 1}$$

$$\Downarrow$$

$$I_{\nu_0}(\Delta\tau_0) = I_{\nu_0}(0)e^{-\Delta\tau_0} + \frac{2h\nu_0^3/c^2}{\exp(h\nu_0/k_B T_{ex}) - 1}\left(1 - e^{-\Delta\tau_0}\right)$$

The quantity of interest to the observer is not I_ν itself, but rather the **difference** between I_ν and the background intensity. Accordingly, we define a **brightness temperature T_B** by:

$$T_B \equiv \frac{c^2}{2\nu^2 k_B}[I_\nu(\Delta\tau_\nu) - I_\nu(0)]$$

If we make the final assumption that the background radiation field is Planckian with an associated temperature T_{bg}:

$$\boxed{T_{B_0} = T_0[f(T_{ex}) - f(T_{bg})]\left[1 - e^{-\Delta\tau_0}\right]}$$

$$T_{B_0} \equiv T_B(\nu = \nu_0), T_0 \equiv h\nu_0 / k_B$$

$$f(T) \equiv [\exp(T_0/T) - 1]^{-1}$$

T_{Bo} is what we measure if we are observing the source with a perfect telescope above the atmosphere, and with an angular resolution much smaller than the source size.

Antenna and Brightness Temperature

$$T_A \equiv \eta \frac{\Omega_S}{\Omega_A} T_B$$

Brightness temperature

Beam efficiency

Ratio of solid angles subtended by the source and the antenna beams ≡ *beam dilution factor*

The **brightness temperature** is the temperature which would result in the given brightness if inserted into the Rayleigh-Jeans law (T_0 / T<< 1 or *hν<<KT* , valid in radioastronomy)

$$\boxed{T_B = \frac{c^2}{2k}\frac{1}{\nu^2}B_\nu}$$

Column Density

$$\boxed{\alpha_\nu = \frac{h\nu_0}{4\pi}(n_l B_{lu} - n_u B_{ul})\phi(\nu)}$$

↓

$$\Delta\tau_0 = \frac{2\sqrt{\ln 2}\, c^3 A_{ul}(g_u/g_l)}{8\pi^{3/2}\nu_0^3 \Delta \mathrm{v}}\left[1-\exp\left(-\frac{\Delta E}{k_B T_{ex}}\right)\right] n_l \Delta s$$

For the two-level system, $n_l \sim n$ and $n_l \Delta s \sim N$, the **column density**. Such an approximation is however not adequate for a system in which the two levels are closely spaced rungs in the ladder (e.g. CO). In these cases:

$$n = n_l Q$$

Rotational partition function ←

$$Q = \sum_{j=0}^{\infty}(2J+1)\exp\left[-\frac{BhJ(J+1)}{k_B T_{ex}}\right]$$

The Rotational Temperature Diagram (RTD)

The RTD is a customary technique to analyze the data of an individual molecule with many transitions. This method assumes LTE conditions so that a single excitation temperature (T_{rot}) characterizes all transitions.

If the transitions are all optically thin, the RTD provides a good estimate of the column density of the molecule towards the source.

Goldsmith & Langer (1999)

The Rotational Temperature Diagram (RTD)

$$T_A \equiv \eta \frac{\Omega_S}{\Omega_A} T_B \qquad T_B = \frac{c^2}{2k_B} \frac{1}{\nu^2} B_\nu$$

$$T_{B_0} = h\nu_0 / k_B [f(T_{rot}) - f(T_{bg})] \left[1 - e^{-\Delta\tau_0}\right]$$

$$T_{B_0} \equiv T_B(\nu = \nu_0)$$

$$f(T) \equiv [\exp(h\nu_0 / k_B T) - 1]^{-1}$$

Now we assume that $f(T_{rot}) >> f(T_{bg})$. We can then write B_{ν_0} as:

The Rotational Temperature Diagram (RTD)

$$B_{\nu_0} = T_0 f(T_{rot}) \frac{1-e^{-\tau}}{\tau}\tau \quad (\Delta\tau_0 \equiv \tau)$$

The optical depth of the transition can be written as:

Column density in the upper state

$$\tau \cong \frac{h}{\Delta v} N_u B_{ul} (e^{h\nu/kT_{rot}} - 1)$$

Half-maximum line width in units of velocity

Substituting these two expressions in: $T_B = \frac{c^2}{2k_B}\frac{1}{\nu^2}B_\nu$ ➔

The Rotational Temperature Diagram (RTD)

$$T_B = \frac{hc^3 N_u A_{ul}}{8\pi k_B \nu^2 \Delta \mathrm{v}} \left(\frac{1 - e^{-\tau}}{\tau} \right)$$

We can now invert the above equation to yield an expression for *N*$_u$. Considering the integrated line intensity, $W = \int T_B d\mathrm{v}$ ($\cong \mathrm{T_B \Delta v}$) we obtain:

$$N_u = \frac{8\pi k_B \nu^2 W}{hc^3 A_{ul}} \left(\frac{\tau}{1 - e^{-\tau}} \right)$$

The Rotational Temperature Diagram (RTD)

If the molecule is in LTE:

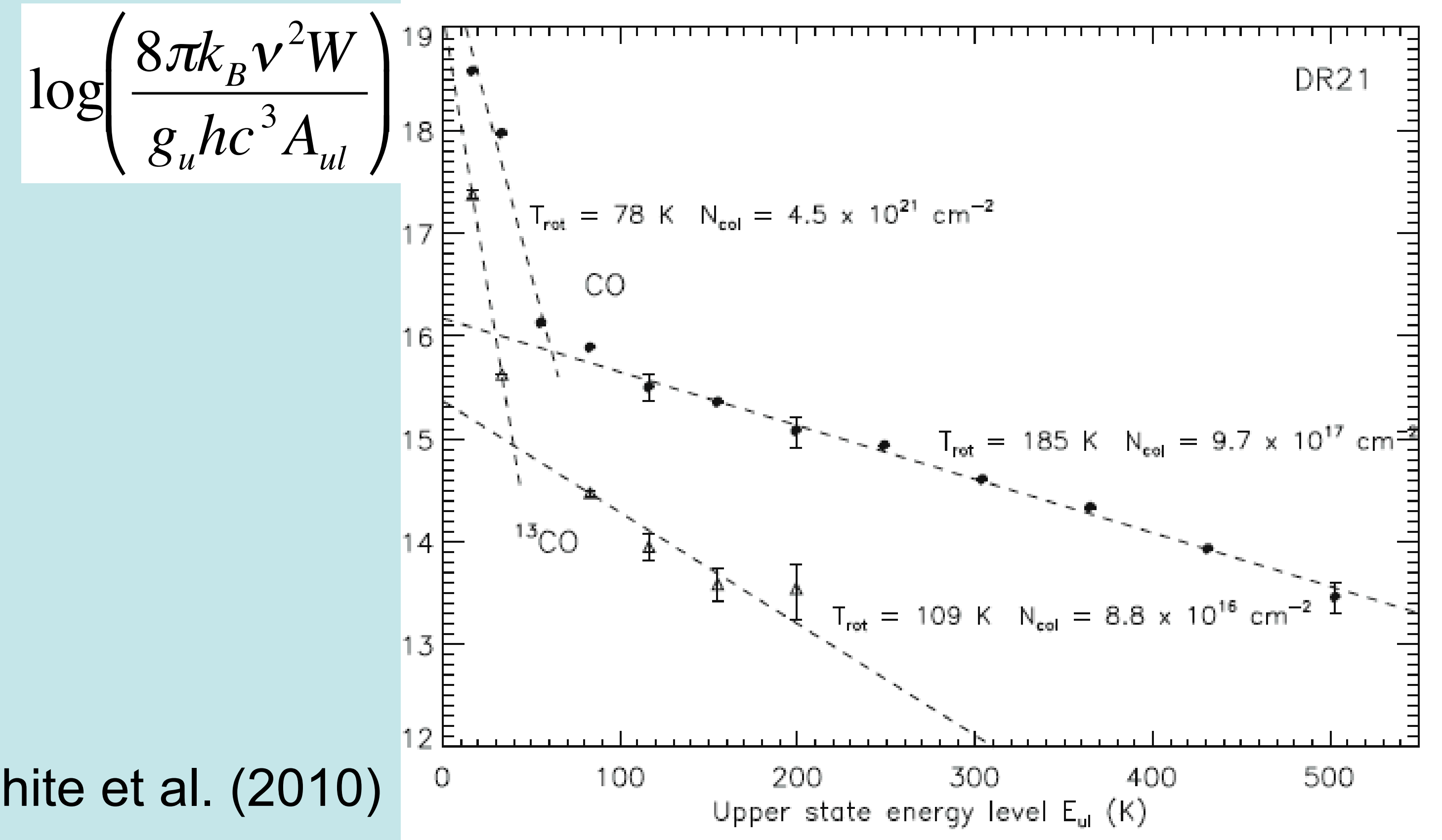
$$N_u = \frac{N}{Q} g_u e^{-E_u / kT}$$

Combining this with the previous expression of N_u, assuming optically thin conditions, and taking the *log* ➔

$$\log\left(\frac{8\pi k_B \nu^2 W}{g_u h c^3 A_{ul}}\right) = \log\left(\frac{N}{Q(T_{rot})}\right) - \frac{E_u \log e}{k_B T_{rot}}$$

The Rotational Temperature Diagram (RTD)

The previous expression shows that $\log\left(\dfrac{8\pi k_B \nu^2 W}{g_u h c^3 A_{ul}}\right)$ is a linear function of E_u/k_B, with slope $-(\log e)/T_{rot}$ and intercept $\log[N/Q(T_{rot})]$ at $E_u = 0$:



$$\log\left(\frac{8\pi k_B \nu^2 W}{g_u h c^3 A_{ul}}\right)$$

White et al. (2010)

Solving radiative transfer problems

For the two level system, the statistical equilibrium equations are:

$$\frac{dn_l}{dt} = -n_l(B_{lu}\bar{J} + \gamma_{lu}) + n_u(A_{ul} + B_{ul}\bar{J} + \gamma_{ul})$$

$$\frac{dn_u}{dt} = n_l(B_{lu}\bar{J} + \gamma_{lu}) - n_u(A_{ul} + B_{ul}\bar{J} + \gamma_{ul})$$

To solve this, we need to know the radiation field which was what we were after in the first place. This problem can be solved with some simplifying assumptions.

van der Tak et al. (2007)

Solving radiative transfer problems: escape probability

The problem is how to decouple the radiative transfer calculations from the calculations of the level populations.

The escape probability β is a factor which allows us to determine the chance that a photon at some position in the cloud can escape the system (based on Sobolev 1960).

We need to estimate $\bar{J}$ to calculate the level population. $\bar{J}$ is the amount of radiation "inside" the source. For a completely opaque source, $\bar{J}$ = S, the source function.

If β is the chance that a newly created photon can escape from the cloud, then

$$\bar{J} = S(1 - \beta)$$

Solving radiative transfer problems: escape probability

Now the statistical equilibrium equations can be simplified:

$$\frac{dn_l}{dt} = -n_l \gamma_{lu} + n_u \gamma_{ul} + \beta n_u A_{ul}$$

$$\frac{dn_u}{dt} = n_l \gamma_{lu} - n_u \gamma_{ul} - \beta n_u A_{ul}$$

And we can solve the level populations and the radiation field separately; they are decoupled. The contribution from background radiation can easily be added:

- take the background intensity. The average chance that it penetrates into the source is (1 - β).

Solving radiative transfer problems: escape probability

How to estimate β? Several forms have been proposed that depend on geometry (we have to find a form that estimates the average local escape probability over all directions).

A very crude form of β in a one-dimensional case can be estimated as:

$$\beta = < e^{-\tau} > = \frac{1}{\tau}\int_0^{\tau} e^{-\tau'}\,d\tau' = \frac{1 - e^{-\tau}}{\tau}$$

The form of β for a radially expanding sphere is equal to the above result. This is called the **Sobolev** or **large velocity gradient** (LVG) approximation (see also Elitzur 1992).

Solving radiative transfer problems: escape probability

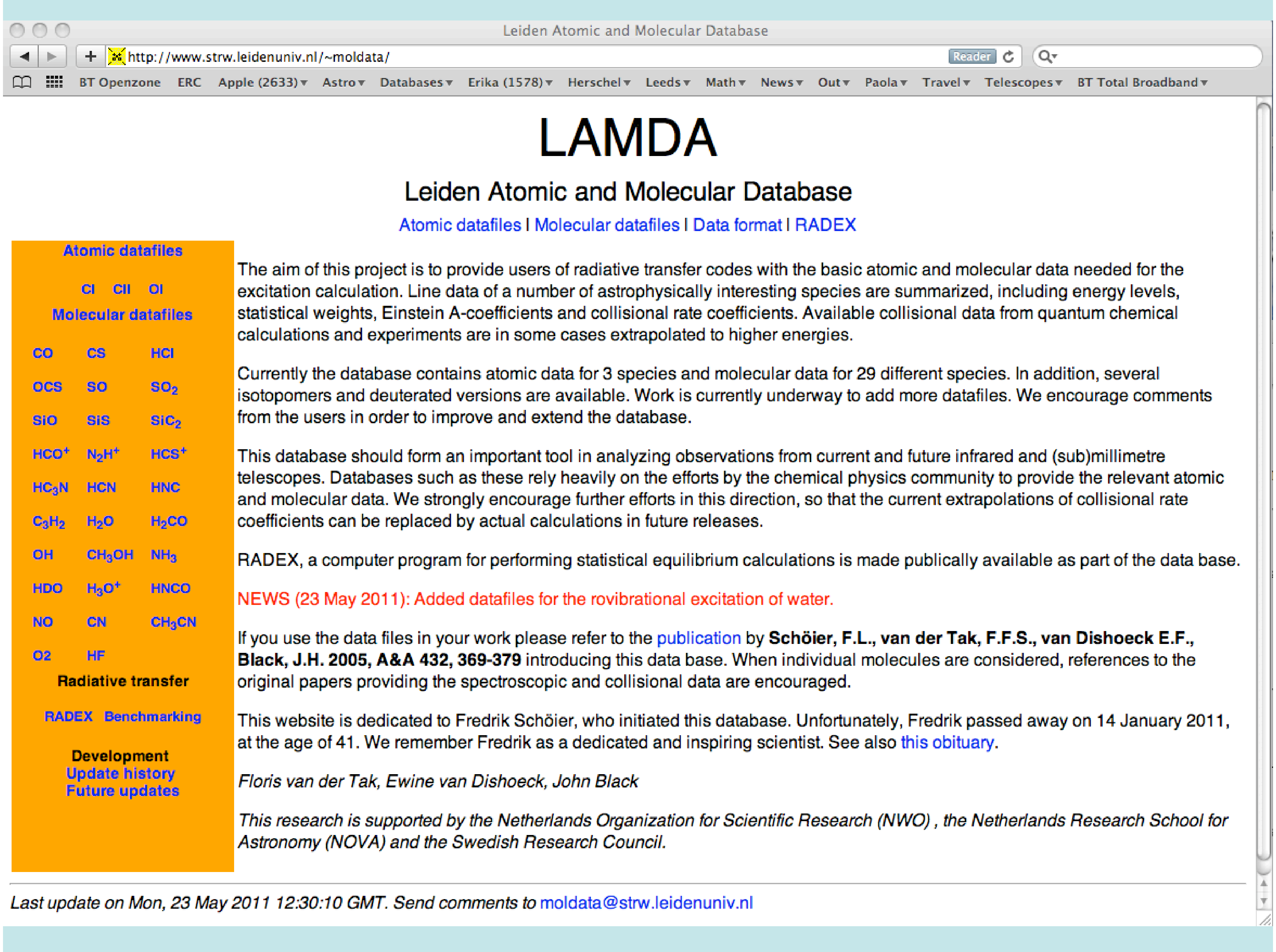
For a homogeneous slab:

$$\beta = \frac{(1 - e^{-3\tau})}{3\tau}$$

For a uniform sphere (Osterbrock 1974):

$$\beta = \frac{1.5}{\tau}\left[1 - \frac{2}{\tau^2} + \left(\frac{2}{\tau} + \frac{2}{\tau^2}\right)e^{-\tau}\right]$$

This last formula is used in RADEX (on-line code):
http://www.sron.rug.nl/~vdtak/radex/radex.php



LAMDA

Leiden Atomic and Molecular Database

Atomic datafiles | Molecular datafiles | Data format | RADEX

Atomic datafiles

CI CII OI

Molecular datafiles

CO CS HCl

OCS SO SO_2

SiO SiS SiC_2

HCO^+ N_2H^+ HCS^+

HC_3N HCN HNC

C_3H_2 H_2O H_2CO

OH CH_3OH NH_3

HDO H_3O^+ HNCO

NO CN CH_3CN

O2 HF

Radiative transfer

RADEX Benchmarking

Development
Update history
Future updates

The aim of this project is to provide users of radiative transfer codes with the basic atomic and molecular data needed for the excitation calculation. Line data of a number of astrophysically interesting species are summarized, including energy levels, statistical weights, Einstein A-coefficients and collisional rate coefficients. Available collisional data from quantum chemical calculations and experiments are in some cases extrapolated to higher energies.

Currently the database contains atomic data for 3 species and molecular data for 29 different species. In addition, several isotopomers and deuterated versions are available. Work is currently underway to add more datafiles. We encourage comments from the users in order to improve and extend the database.

This database should form an important tool in analyzing observations from current and future infrared and (sub)millimetre telescopes. Databases such as these rely heavily on the efforts by the chemical physics community to provide the relevant atomic and molecular data. We strongly encourage further efforts in this direction, so that the current extrapolations of collisional rate coefficients can be replaced by actual calculations in future releases.

RADEX, a computer program for performing statistical equilibrium calculations is made publically available as part of the data base.

NEWS (23 May 2011): Added datafiles for the rovibrational excitation of water.

If you use the data files in your work please refer to the publication by **Schöier, F.L., van der Tak, F.F.S., van Dishoeck E.F., Black, J.H. 2005, A&A 432, 369-379** introducing this data base. When individual molecules are considered, references to the original papers providing the spectroscopic and collisional data are encouraged.

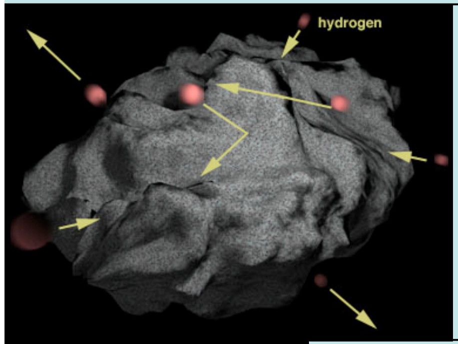
This website is dedicated to Fredrik Schöier, who initiated this database. Unfortunately, Fredrik passed away on 14 January 2011, at the age of 41. We remember Fredrik as a dedicated and inspiring scientist. See also this obituary.

Floris van der Tak, Ewine van Dishoeck, John Black

This research is supported by the Netherlands Organization for Scientific Research (NWO) , the Netherlands Research School for Astronomy (NOVA) and the Swedish Research Council.

Last update on Mon, 23 May 2011 12:30:10 GMT. Send comments to moldata@strw.leidenuniv.nl

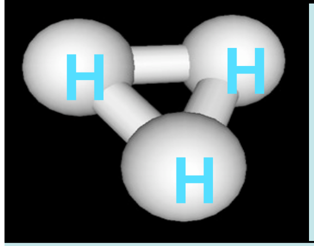
SUMMARY



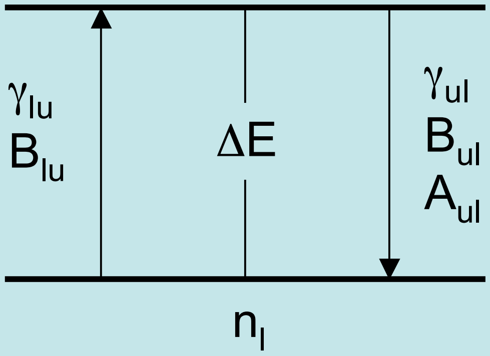
H_2 molecules are formed on the surface of dust grains with a rate

$$R_{H_2} = \frac{1}{2} n_H v_H A n_g S_H \gamma$$

$$\cong 10^{-17} \text{ - } 10^{-16} \text{ cm}^{-3}\text{s}^{-1}$$

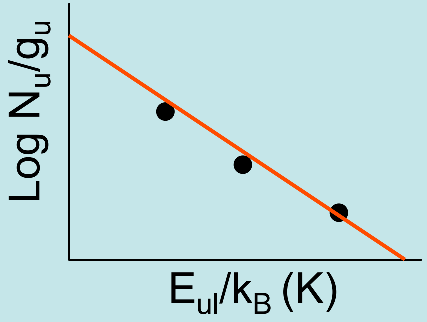


H_3^+ is formed from cosmic-ray ionization of H_2, followed by $H_2^+ + H_2$. This starts interstellar chemistry.



The two level system and the brightness temperature of a molecular line at frequency $\nu = \nu_0$.

$$T_{B_0} = T_0[f(T_{ex}) - f(T_{bg})]\left[1 - e^{-\Delta\tau_0}\right]$$



The rotational temperature diagram allows to derive the column density and gas temperature when multiple transitions of the same molecules are observed (assuming LTE and optically thin conditions).