Information from fine structure lines: How to excite C$^+$, O and N$^+$?

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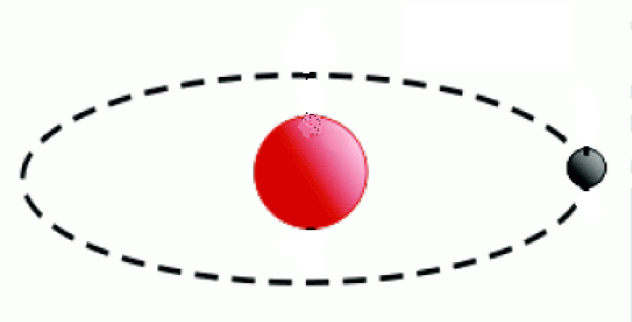
Overview

Table of contents

- **Line frequencies**
  - Basic atomic physics: The hydrogen atom
  - Fine structure
  - Hyperfine structure
  - Metals

- **Line intensities**
  - Excitation: n-level, 2-level, 3-level problems
  - LTE
  - Collision partners
  - Optically thin emission
  - Radiative trapping
  - Abundances

Basics of spectroscopy: The hydrogen atom



Repetition of basic atomic physics:

The H-atom

- Simple problem: p + e$^-$
  - Pure Coulomb problem: $$\hat{H} = \frac{\vec{p}^2}{2m_r} - \frac{(Z)e^2}{4\pi\epsilon_0|\vec{r}|}$$
    - With reduced mass $$m_r = \frac{m_e m_p}{m_e + m_p}$$
  - Solution has eigenvalues $$E = -R\frac{(Z^2)}{n^2}$$
    - With Rydberg constant $$R = \frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\frac{m_r}{\hbar^2} \approx 13.605\text{eV}$$

Z = charge for more general case of multiple protons

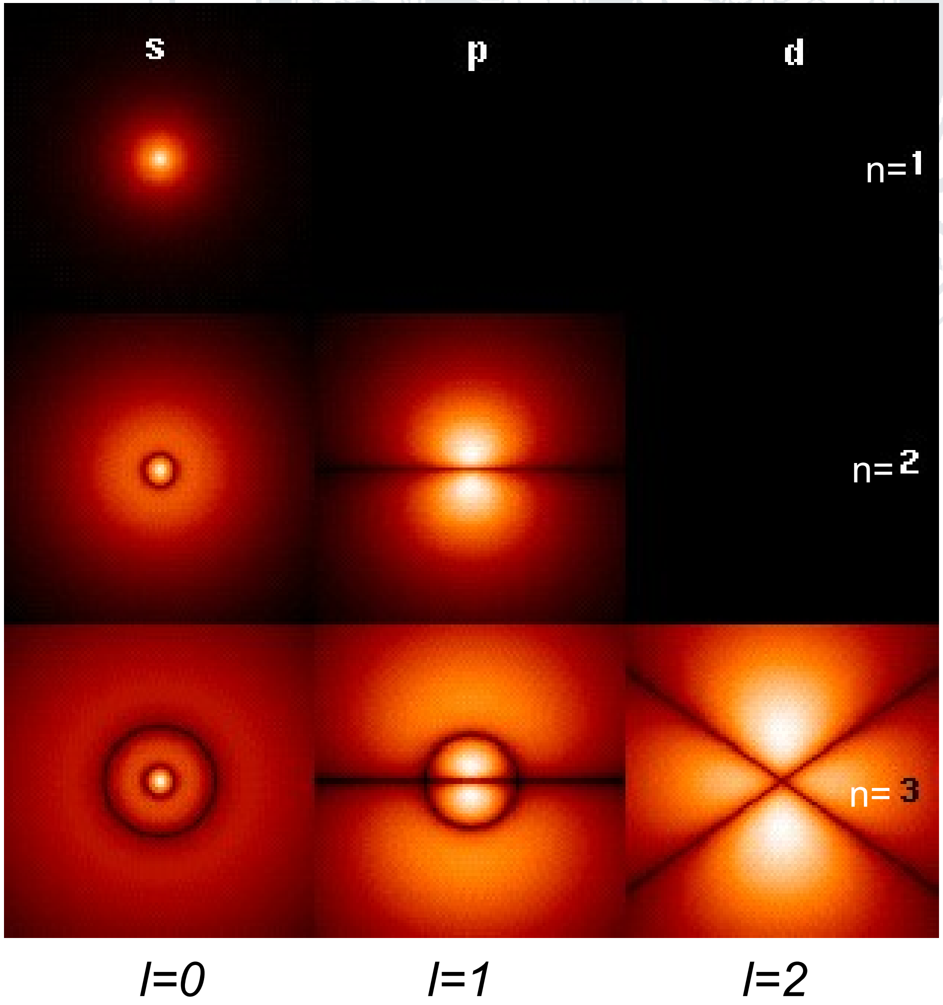
n = main quantum number

Basics of spectroscopy: The hydrogen atom

Repetition of basic atomic physics:

The H-atom

- Orbits: Solution of the full spatial problem
  - Provides in total 3 quantum numbers: n, l, m_l
    - l = orbital quantum number $l=0...n-1$
    - m_l = projection of l on z-axis: $m_l=-l...l$
    - Energy levels n are degenerate with respect to l and m_l
    - Corresponding eigenvector: $|n, l, m_l>$



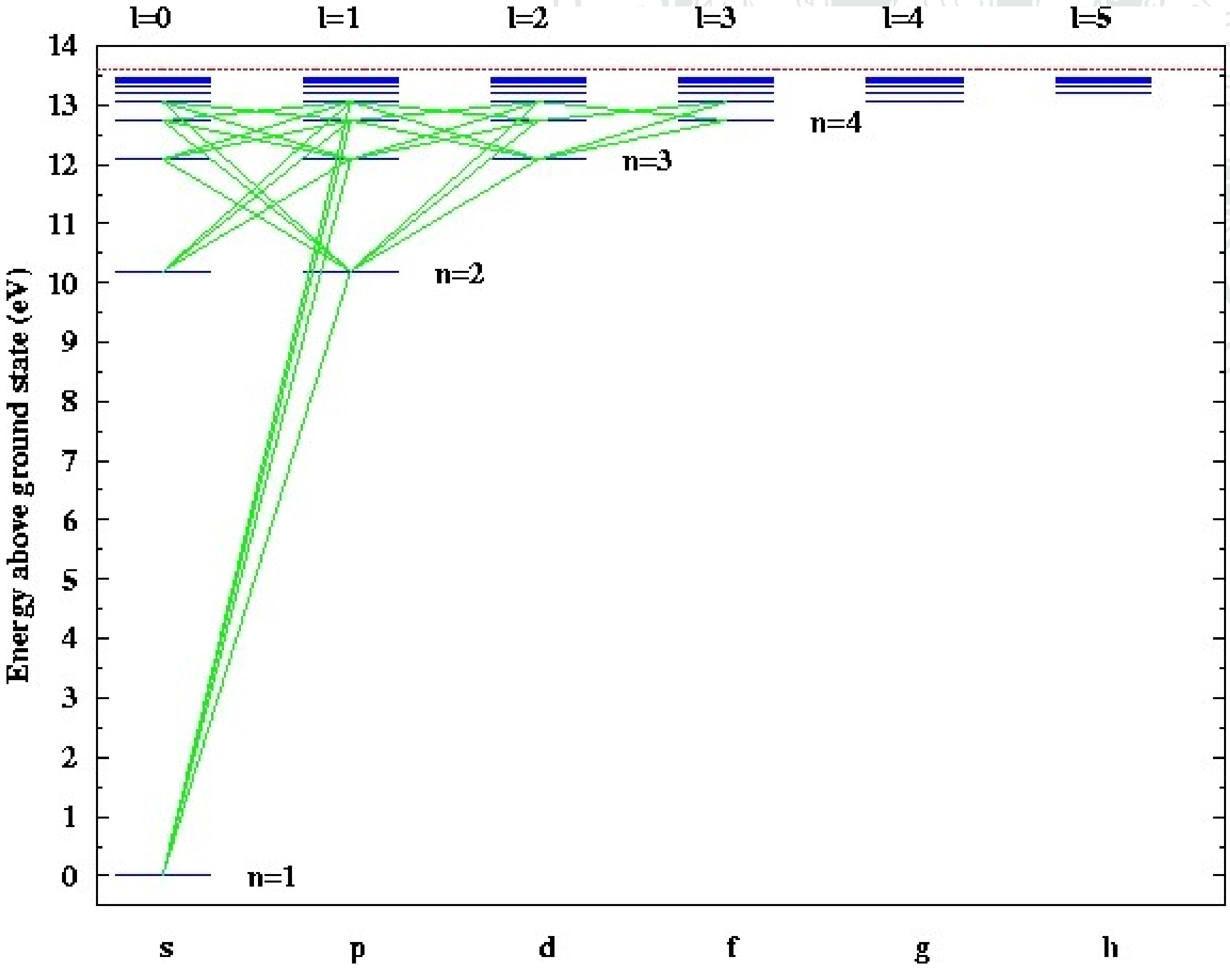
Basics of spectroscopy: The hydrogen atom

Repetition of basic atomic physics:

The H-atom

- Possible transitions
  - from level *n* to *n'*

$$E_n - E_{n'} = -(Z^2)R\left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$$



Basics of spectroscopy: The hydrogen atom

Repetition of basic atomic physics:

The H-atom

- Possible transitions
  - from level *n* to *n'*
- Gives series for different *n'*
    - *n'*=1 = Lyman
    - *n'*=2 – Balmer
    - *n'*=3 – Paschen
    - *n'*=4 – Bracket
    - *n'*=5 – Pfund

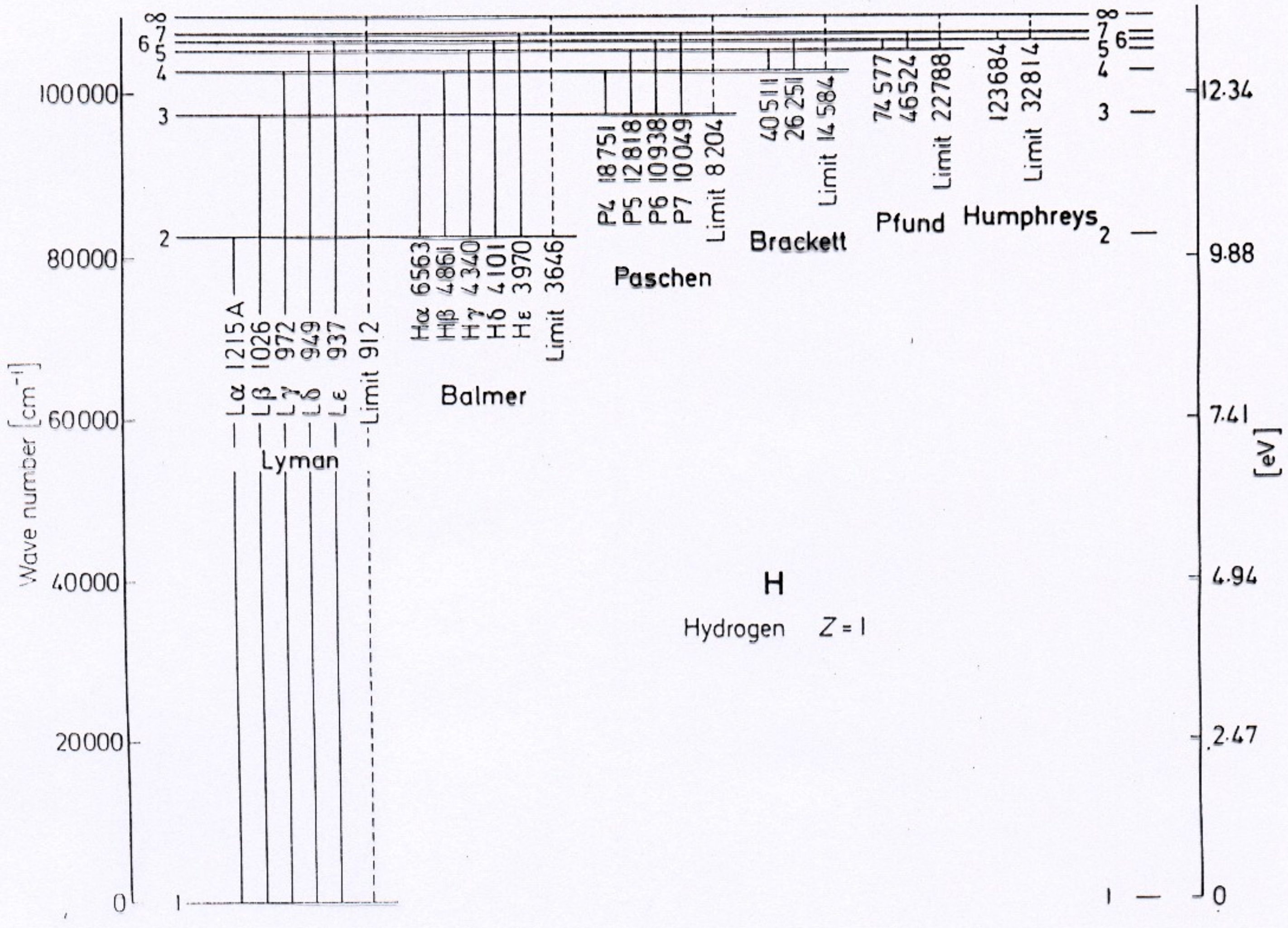


Fig. 13. Grotrian diagrams for H, He I, He II, C II, C III, C IV, O I, O II, O III, N II, Mg I, Mg II, Ca I, Ca II, Fe I, and Fe II. (After Moore and Merrill, 1968)

Basics of spectroscopy: Fine structure

The electron spin

- Adds spin system |s,m_s> with s=1/2
- Provides additional coupling term between orbital momentum and spin

$$\hat{H}_{fs} = \frac{e}{2m_e^2c^2}\left(-\frac{1}{r}\frac{\partial}{\partial r}\frac{(Z)e^2}{4\pi\epsilon_0|\vec{r}|}\right)\hat{\vec{s}}\,\hat{\vec{l}}$$

  - Solution has eigenvalues

$$E_{FS} = \alpha^2 R\frac{(Z^4)}{n^3}\frac{j(j+1)-l(l+1)-s(s+1)}{l(l+1)(2l+1)}$$

  - *j* = total angular momentum from $\vec{j} = \vec{l} + \vec{s}$ → *j=l-s...l+s*
  - $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$ Sommerfeld fine structure constant

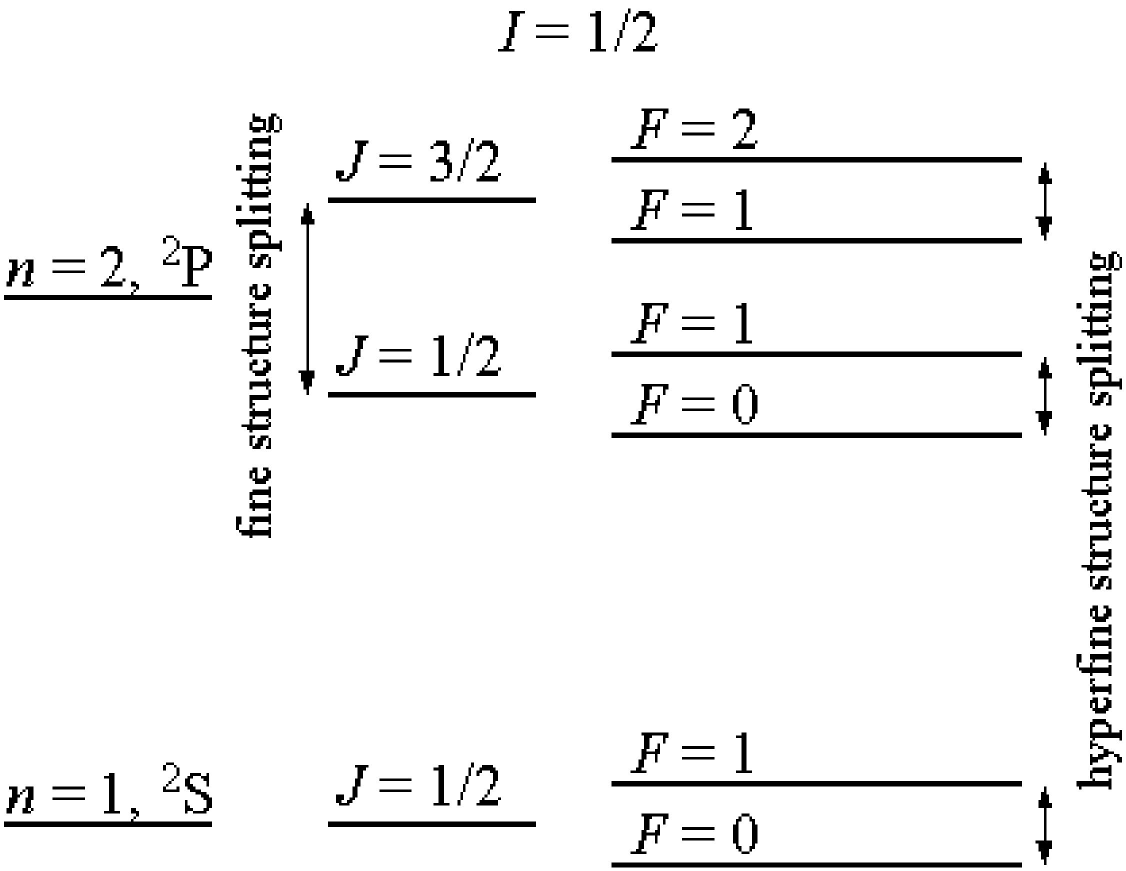
Basics of spectroscopy: Fine structure

The electron spin

- Fine structure energies are scaled by α^2 relative to main level energies
- H-atom
  - No split for *n=1, l=0* because *j=1/2* independent of m_s
  - First split for *n=2, l=1* → *j=1/2, 3/2*

$$\Delta E_{fs} = 4.53\,10^{-5}\mathrm{eV}$$
$$= 10.9\mathrm{GHz}$$

  - Requires *n=2* excitation: 10.2eV = 120000K
  - Not directly observable due to other splits



Basics of spectroscopy: Notation

Spectroscopy notation

$$^{2s+1}l_j^{(p)}$$

- *l* encrypted in letters
  - *0 = s, 1 = p, 2 = d, 3 = f, 4 = g, 5 = h, ...*
- p = parity
  - Blank for parity = even, o for parity = odd
  - Characterizes whether wave function changes sign under reflection of all electron positions through the origin.

- Examples:
  - $^2s_{1/2}$ = ground state
  - $^2p_{1/2}$, $^2p_{3/2}$ = first excited state (Balmer level)

Basics of spectroscopy: Hyperfine splitting

The nuclear spin

- Adds nuclear spin system $|i,m_i>$ with $i=1/2$ for every nucleon
- Treatment equivalent to fine-structure splitting
- New quantum number $\vec{f} = \vec{j} + \vec{i}$
  - f = total angular momentum from → $f=j-i...j+i$
- Eigenvalues of hyperfine coupling

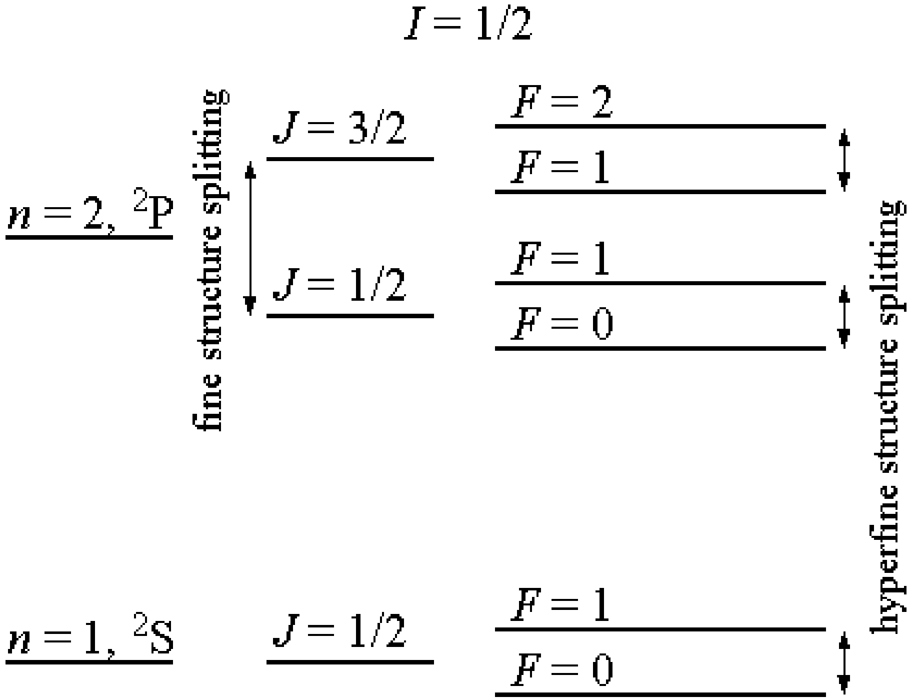
$$E_{HF} = g_N \frac{m_e}{m_p} \alpha^2 R \frac{(Z^4)}{n^3} \frac{f(f+1) - j(j+1) - i(i+1)}{j(j+1)(2j+1)}$$

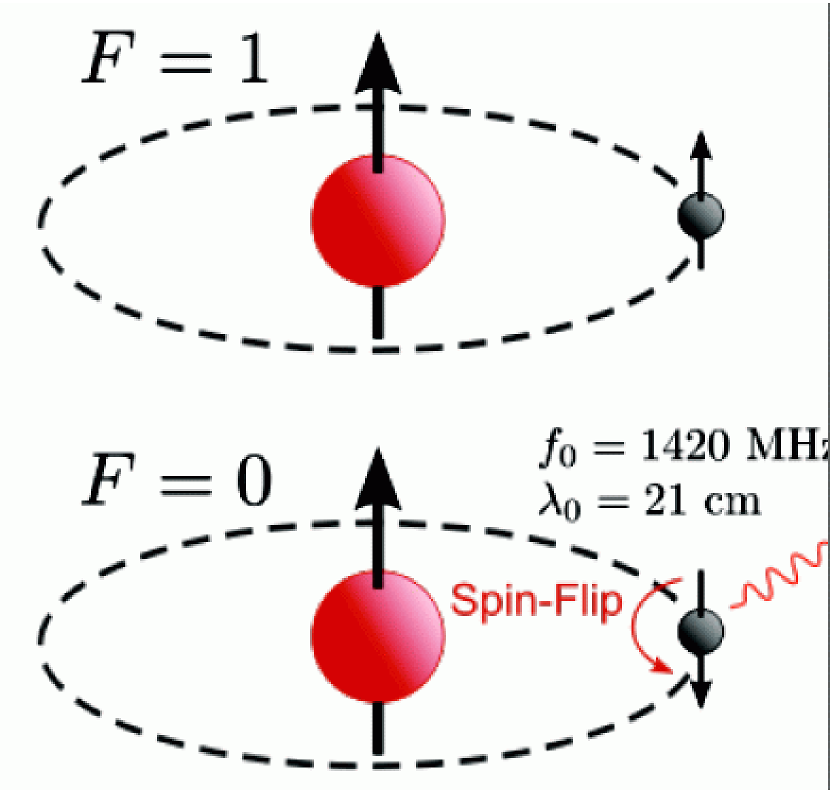
  - Hyperfine splitting typically lower than fine-structure splitting by factor $\frac{m_e}{m_p}$
  - g_N – Gaunt factor of the core
- Spectroscopic notation: explicite writing of f

Basics of spectroscopy: Hyperfine structure splitting

Hyperfine structure

- H-atom
  - for *n=1* (ground state, *l=0*): $^2s_{1/2}$: *f=1-0*
  - Can be observed for “cold hydrogen”



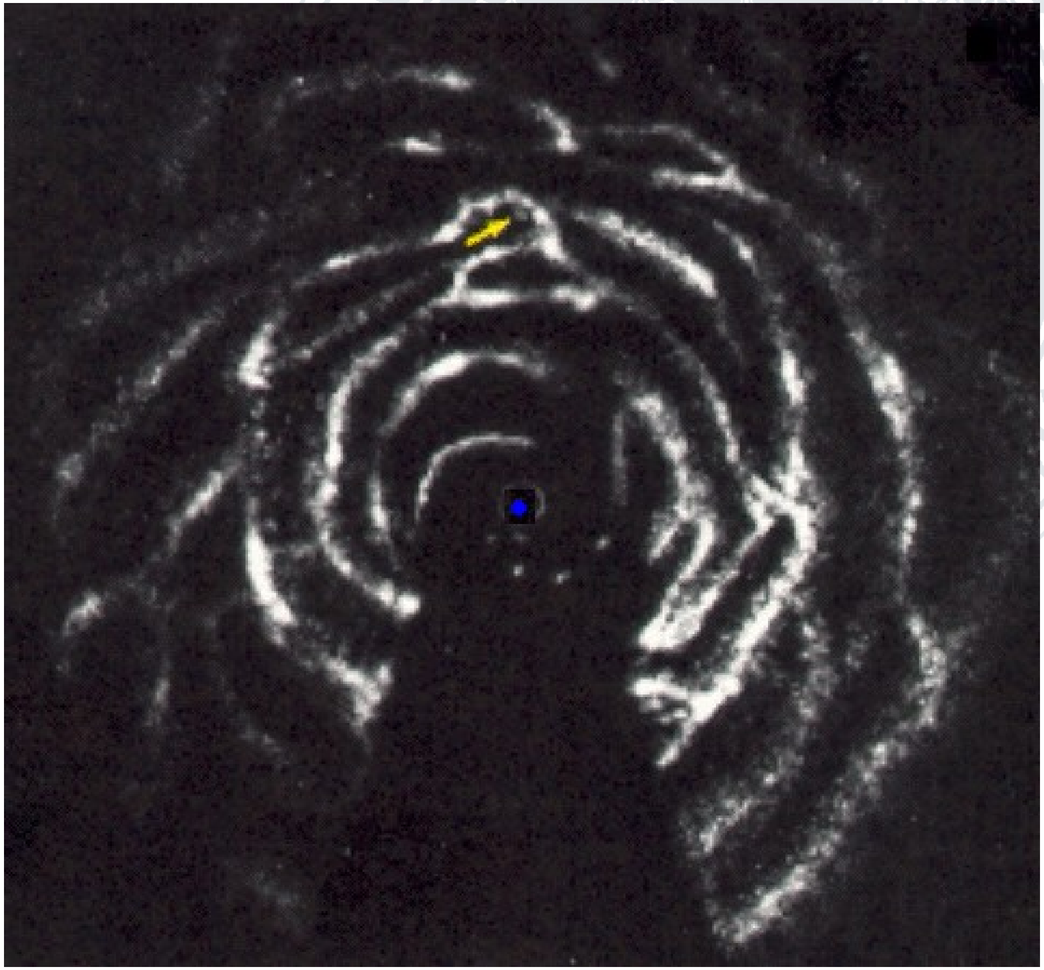


- famous 21cm line = 1.42GHz
- allows for mapping of the Milky Way
- magnetic dipole transition → forbidden
  - $A= 2.9\ 10^{-15}\ \mathrm{s}^{-1}$
  - $t=10^7$ a

Basics of spectroscopy: Hyperfine structure splitting

Hyperfine structure

- H-atom
  - for *n=1* (ground state, *l=0*): $^2s_{1/2}$: *f=1-0*
  - Can be observed for “cold hydrogen”
- allows for mapping of neutral interstellar gas



1951 Lyman Spitzer: Mapping of the Milky Way

Basics of spectroscopy: Atoms

Multiple electrons

- Arrangement in subshells with increasing energy level

  = increasing main and orbital quantum numbers *n, l*

  - Example: $C^+ = 1s^2\ 2s^2\ 2p^1$
    - 3 subshells occupied
    - Closed shells: Sum of orbital momenta and spins always = 0
      - No contribution to radiative interaction
      - Can be ignored
    - 3rd subshell is open:
      - can take 6 electrons: $m_l = -1, 0, 1$, $m_s = -½, ½$
      - dominates radiative interaction as
      - Only electrons in open shell need to be considered

Basics of spectroscopy: Atoms

Multiple electrons

- Coupling between different electrons
  - Provides additional term to Hamiltonian
  - No analytic solution
  - Approximation through Russell-Sounders coupling
    - Inter-electron coupling stronger than spin-orbit coupling
    - Individual orbital momentums and spins add up $\sum \vec{l} = \vec{L} \text{ and } \sum \vec{s} = \vec{S}$

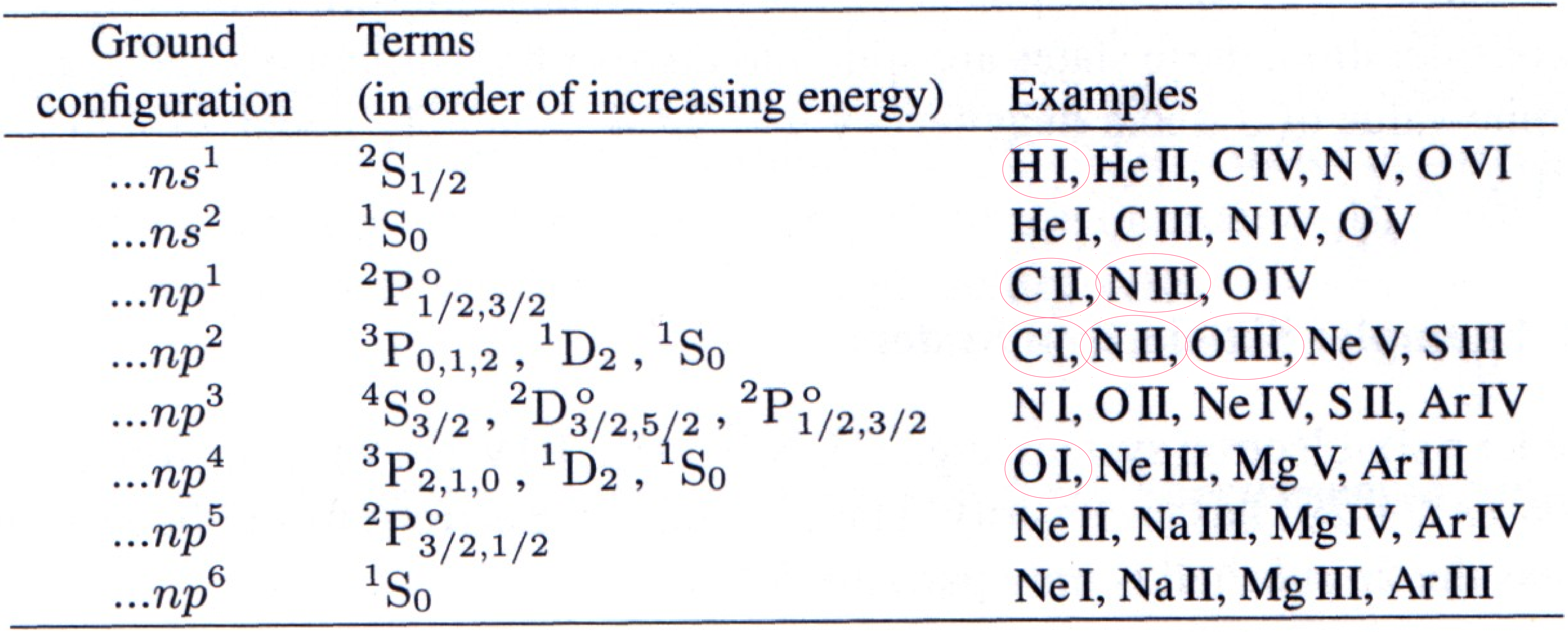
$$\vec{J} = \vec{L} + \vec{S}$$

    - Remember: approximation only → *L*,*S*, *J* are no “good” quantum numbers
    - Different approximation for heavy elements
- Spectroscopic notation:
  - capital letters for sum over multiple electrons in open shell
  - explicite writing of *F* for sum of total angular momentum including nuclear spin

Basics of spectroscopy: Multiple electrons

Astrophysically relevant subterms

- Remember H-atom: $^{2s+1}l_j^{(p)}$
- Equivalently for multi-electron atoms $^{2S+1}L_J^{(P)}$



Ground configuration	Terms (in order of increasing energy)	Examples
$...ns^1$	$^2\mathrm{S}_{1/2}$	H I, He II, C IV, N V, O VI
$...ns^2$	$^1\mathrm{S}_0$	He I, C III, N IV, O V
$...np^1$	$^2\mathrm{P}^{\mathrm{o}}_{1/2,3/2}$	C II, N III, O IV
$...np^2$	$^3\mathrm{P}_{0,1,2}$, $^1\mathrm{D}_2$, $^1\mathrm{S}_0$	C I, N II, O III, Ne V, S III
$...np^3$	$^4\mathrm{S}^{\mathrm{o}}_{3/2}$, $^2\mathrm{D}^{\mathrm{o}}_{3/2,5/2}$, $^2\mathrm{P}^{\mathrm{o}}_{1/2,3/2}$	N I, O II, Ne IV, S II, Ar IV
$...np^4$	$^3\mathrm{P}_{2,1,0}$, $^1\mathrm{D}_2$, $^1\mathrm{S}_0$	O I, Ne III, Mg V, Ar III
$...np^5$	$^2\mathrm{P}^{\mathrm{o}}_{3/2,1/2}$	Ne II, Na III, Mg IV, Ar IV
$...np^6$	$^1\mathrm{S}_0$	Ne I, Na II, Mg III, Ar III

Basics of spectroscopy: Multiple electrons

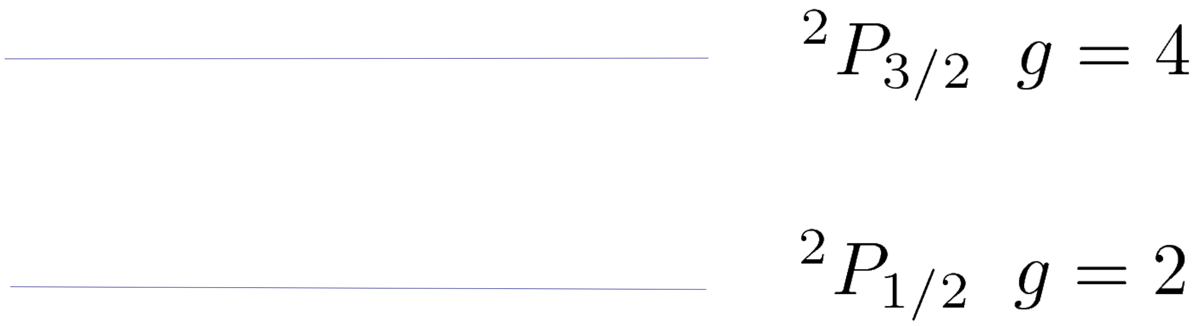
Russel-Sounders coupling

- Solution
  - “Hund rules”:
    1) higher S → lower energies
    2) higher L → lower energies
    3) lower J and shell ≤ half-full → lower energies
    shell > half-full → higher energies
  - Example: $C^+ = 1s^2\ 2s^2\ 2p^1$
    - 2p electron has $S = ½$, $L = 1$

      → gives $J = ½$ ($m_J = -½, ½$)

      or $J = 3/2$ ($m_J = -3/2, -1/2, 1/2, 3/2$) = *2-level system*
    - Only 3rd Hund rule applies:

$$\Delta E = 7.86\mathrm{meV} \\ = 1900.536\mathrm{GHz} \\ = 157.7\mu\mathrm{m}$$



$$^2P_{3/2} \quad g = 4$$

$$^2P_{1/2} \quad g = 2$$

- Equivalent for N^{++}: ΔE=57μm

Basics of spectroscopy: Hyperfine structure in atoms

Hyperfine structure

- Superimposed if nuclear spin does not sum up to 0

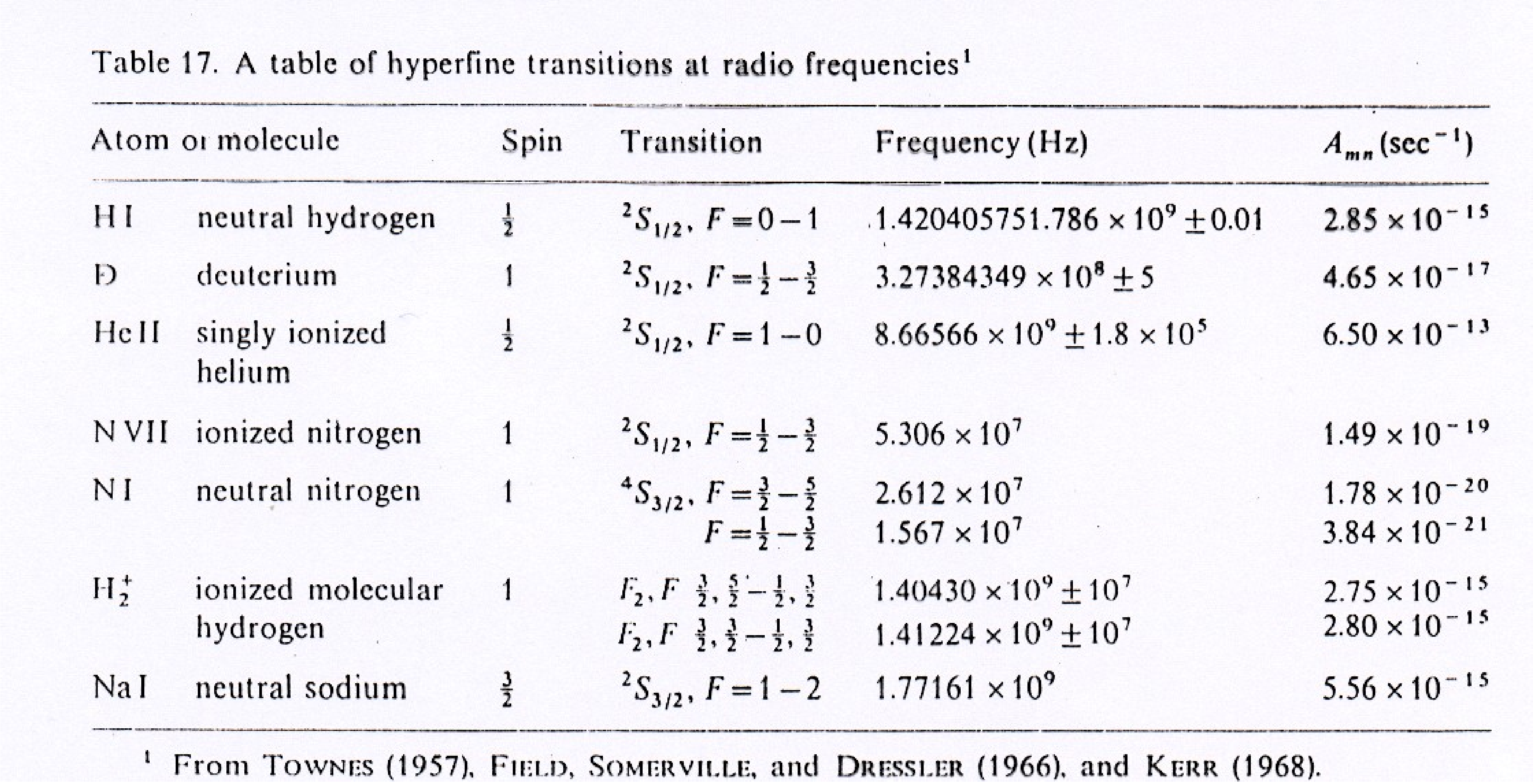


Table 17. A table of hyperfine transitions at radio frequencies[1]

Atom or molecule		Spin	Transition	Frequency (Hz)	A_{mn} (sec^{-1})
H I	neutral hydrogen	$\frac{1}{2}$	$^2S_{1/2}$, $F = 0 - 1$	$1.420405751.786 \times 10^9 \pm 0.01$	2.85×10^{-15}
D	deuterium	1	$^2S_{1/2}$, $F = \frac{1}{2} - \frac{3}{2}$	$3.27384349 \times 10^8 \pm 5$	4.65×10^{-17}
He II	singly ionized helium	$\frac{1}{2}$	$^2S_{1/2}$, $F = 1 - 0$	$8.66566 \times 10^9 \pm 1.8 \times 10^5$	6.50×10^{-13}
N VII	ionized nitrogen	1	$^2S_{1/2}$, $F = \frac{1}{2} - \frac{3}{2}$	5.306×10^7	1.49×10^{-19}
N I	neutral nitrogen	1	$^4S_{3/2}$, $F = \frac{3}{2} - \frac{5}{2}$ $F = \frac{1}{2} - \frac{3}{2}$	2.612×10^7 1.567×10^7	1.78×10^{-20} 3.84×10^{-21}
H_2^+	ionized molecular hydrogen	1	F_2, F $\frac{3}{2}, \frac{5}{2} - \frac{1}{2}, \frac{3}{2}$ F_2, F $\frac{3}{2}, \frac{3}{2} - \frac{1}{2}, \frac{3}{2}$	$1.40430 \times 10^9 \pm 10^7$ $1.41224 \times 10^9 \pm 10^7$	2.75×10^{-15} 2.80×10^{-15}
Na I	neutral sodium	$\frac{3}{2}$	$^2S_{3/2}$, $F = 1 - 2$	1.77161×10^9	5.56×10^{-15}

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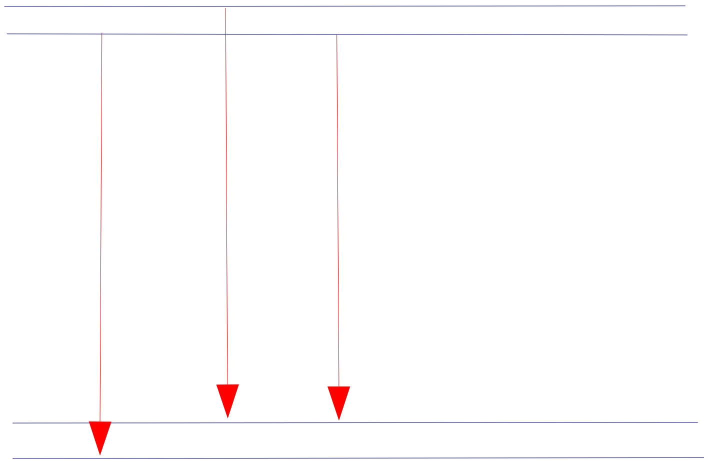
[1] From TOWNES (1957), FIELD, SOMERVILLE, and DRESSLER (1966), and KERR (1968).

Basics of spectroscopy: Hyperfine structure in atoms

Hyperfine structure

- Example: $^{13}\mathrm{C}^+$
  - *I* = ½ combines with *J* = ½ to *F=0* (m_F= *0*) *or F=1* (m_F= *-1, 0, 1*)

    with *J* = *3/2* to *F=1* (m_F= *-1, 0, 1*) *or F=2* (m_F= *-2,-1, 0, 1, 2*)
  - C^+ levels split up



$$^2P_{3/2}\ F=2\ \ g=5$$

$$^2P_{3/2}\ F=1\ \ g=3$$

$$^2P_{1/2}\ F=1\ \ g=3$$

$$^2P_{1/2}\ F=0\ \ g=1$$

  - 3 possible transitions, *F* = *2* → *0* is forbidden

Basics of spectroscopy: Multiple electrons in one subshell

Combination of states

- Example: $N^+ = 1s^2\ 2s^2\ 2p^2$
  - Combination of two electrons with $s = \frac{1}{2}$ ($m_s=-\frac{1}{2}, \frac{1}{2}$), $l = 1$ ($m_l=-1,0,1$)
    → gives 6x6=36 possible combinations
    - Pauli exclusion principle:
      - 2 electrons never in same state
      - Electrons indistiguishable, i.e. wave functions antisymmetric with respect of exchange of 2 electrons
  - 15 allowed combinations remaining
    - $l_1 \uparrow\uparrow l_2$, $s_1 \uparrow\downarrow s_2$: $L=2, S=0$ → $J=2$ ($m_J=-2,-1,0,1,2$) → ${}^1D_2$, $g=5$
    - $l_1 \uparrow\downarrow l_2$, $s_1 \uparrow\downarrow s_2$: $L=0, S=0$ → $J=0$ ($m_J=0$) → ${}^1S_0$, $g=1$
    - $l_1 \perp l_2$, $s_1 \uparrow\uparrow s_2$: $L=1, S=1$ → $J=0$ ($m_J=0$) → ${}^3P_0$, $g=1$

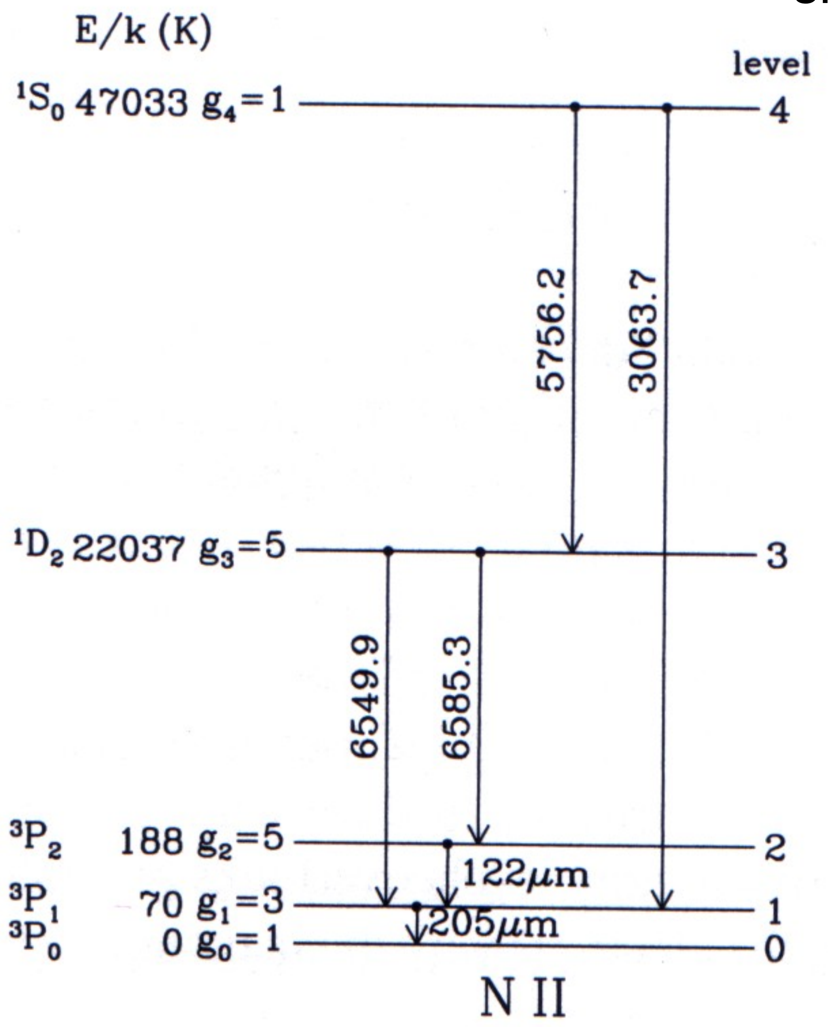
      → $J=1$ ($m_J=-1,0,1$) → ${}^3P_1$, $g=3$

      → $J=2$ ($m_J=-2,-1,0,1,2$) → ${}^3P_2$, $g=5$

Basics of spectroscopy: Combination of states

$N^+ = 1s^2\, 2s^2\, 2p^2$

- "Hund rules": 1) higher *S* → lower energies
  2) higher *L* → lower energies
  3) lower *J* and shell ≤ half-full → lower energies
  shell > half-full → higher energies



The *S=0* states need very high excitation energy

→ usually not relevant for ISM physics

→ treat N^+ as 3-level system

Only 2 radiative transitions. *J = 2 → 0* forbidden

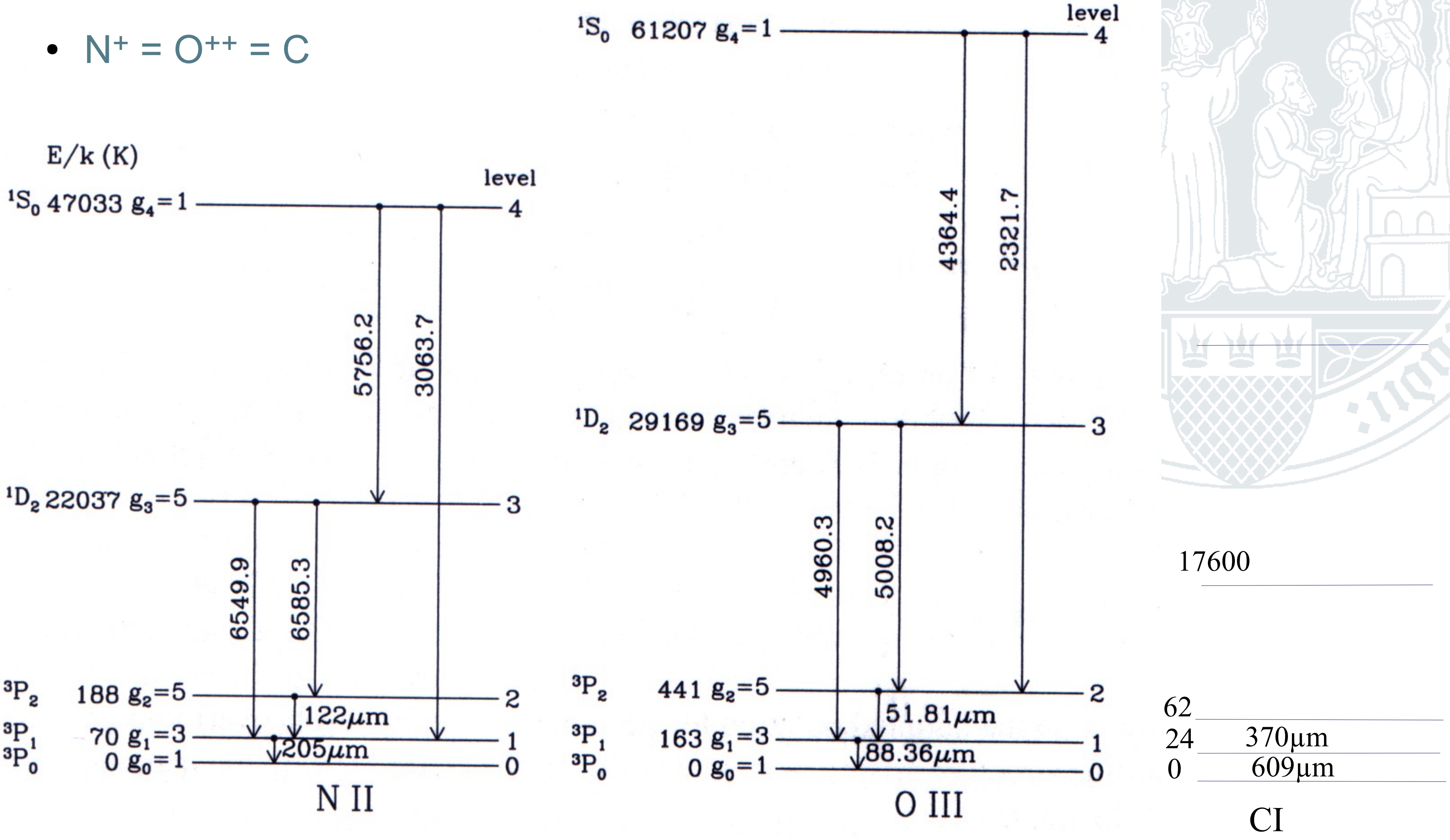
122μm = 2457 GHz

205μm = 1458 GHz

Basics of spectroscopy: Combination of states

Other atoms with same configuration: $^3P_{0,1,2}$

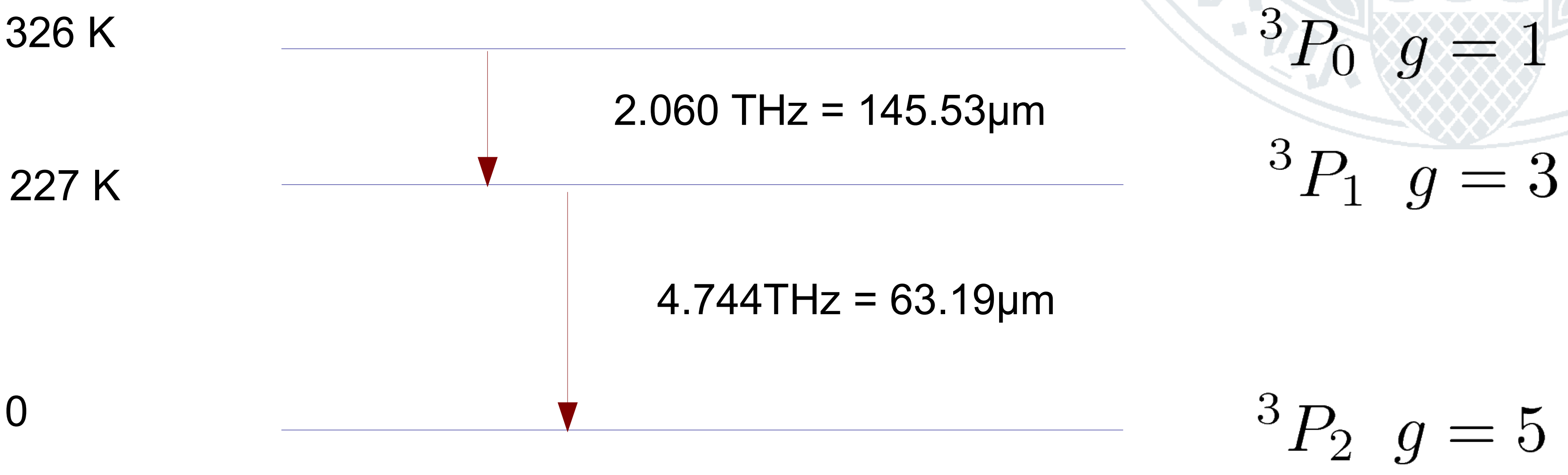
- $N^+ = O^{++} = C$



Basics of spectroscopy: Combination of states

O = $1s^2\ 2s^2\ 2p^4$

- Similar addition of configurations for all 4 electrons
- Now third Hund rule with “shell > half-full” applies → reverse order: $^3P_{2,1,0}$
- Only *S=1* states excited at moderate temperatures (below 20000K)
    - Effectively 3-level system as well
    - Radiative transitions only J = 2 → 1 and J = 1 → 0



326 K

$^3P_0 \quad g = 1$

2.060 THz = 145.53µm

227 K

$^3P_1 \quad g = 3$

4.744THz = 63.19µm

0

$^3P_2 \quad g = 5$

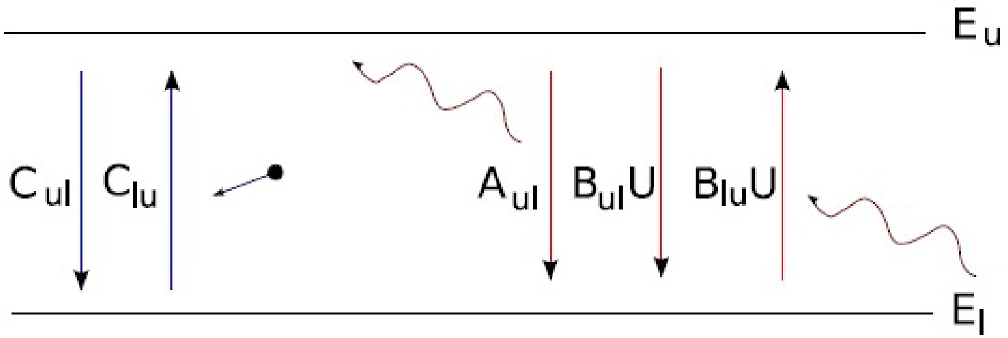
Basics of spectroscopy: Summary

Few cases to distinguish:

- 2-level systems: HI, C^+, N^{++}
- 3-level systems: C, N^+, O^{++}, O
  - $^2P_{0,1,2}$ (C, N^+, O^{++}): ground-state transition has lower frequency
  - $^2P_{2,1,0}$ (O): ground-state transition has higher frequency
- 4-level systems: $^{13}C^+$

- $2p^3$ systems: N, O^+ → “Darkness”
  - no fine-structure transitions excited at temperatures << 20000K

Excitation analysis: Introduction of quantities



- Consider transitions between 2 levels:
  - Spontaneous emission: A_{ul}
  - Stimulated emission: $B_{ul}U$
  - Absorption: $B_{lu}U$
  - Collisional transitions: C_{ul}, C_{lu}

$$U = \iint \frac{I_\nu \phi(\nu)}{c} d\nu d\Omega = \frac{4\pi}{c} \langle I_{\rm line} \rangle$$

- Rate coefficients are mutually dependent:

$$C_{lu} = C_{ul} \frac{g_u}{g_l} \exp\left(-\frac{h\nu}{kT_{\rm kin}}\right)$$

  - Number conservation:

$$B_{lu} = B_{ul} \frac{g_u}{g_l}$$

  - Quantum mechanics:

$$B_{ul} = A_{ul} \frac{c^3}{8\pi h \nu^3}$$

Excitation analysis: Balance equation

General case: transitions between multiple levels

- To determine the excitation of the system the matrix of balance equations had to be solved

$$n_i \left(\sum_{j<i} A_{ij} + \sum_{j\neq i} B_{ij} u_{ij} + \sum_{j\neq i} C_{ij} \right) = \sum_{j>i} A_{ji} n_j + \sum_{j\neq i} B_{ji} u_{ij} n_j + \sum_{j\neq i} C_{ij} n_j$$

- n_i - level population of level *i*
- A_{ij}, B_{ij} - spontaneous, induced radiative rate coefficients

  u_{ij} - radiative energy density at transition frequency
- $C_{ij} = \sum_{i_{coll}}^{n_{coll}} n_{i_{coll}} \gamma_{ij,i_{coll}}$ - collisional rate coefficients for different collision partners i_{coll} :

  H_2, H, H^+, He, electrons, ...

Excitation analysis: n-level systems

Description of level populations by excitation temperature T_{ex}

$$\frac{n_j}{n_i} = \frac{g_j}{g_i} \exp\left(-\frac{h\nu_{ij}}{kT_{ex,ij}}\right)$$

- Usually different for every pair of levels i,j
- Can be obtained exploiting properties of Einstein coefficients

- Radiation: $B_{ij} g_i = B_{ji} g_j$

- Collisions: $C_{ij} = C_{ji} \frac{g_j}{g_i} \exp\left(-\frac{h\nu_{ij}}{kT_{kin}}\right)$
  - for *j* > *I*

→ 3 limiting cases

Excitation analysis: Excitation temperature

Limiting cases

- Collision-dominated ($n_{i_{coll}}$ large): $C_{ij} \gg A_{ij}, B_{ij}u_{ij}$ for all i,j

→ Balance equation: $$\frac{n_i}{g_i}\sum_{j\neq i} C_{ij} = \sum_{j\neq i}\frac{n_j}{g_j} C_{ij} \exp\left(\frac{h\nu_{ij}}{kT_{kin}}\right)$$

  - Solution:
    - $T_{ex,ij} = T_{kin}$ for all i,j

= LTE (local thermodynamical equilibrium)

Excitation analysis: Excitation temperature

Limiting cases

- Radiation dominated (u_{ij} large): $B_{ij}u_{ij} \gg A_{ij}, C_{ij}$ for all i,j

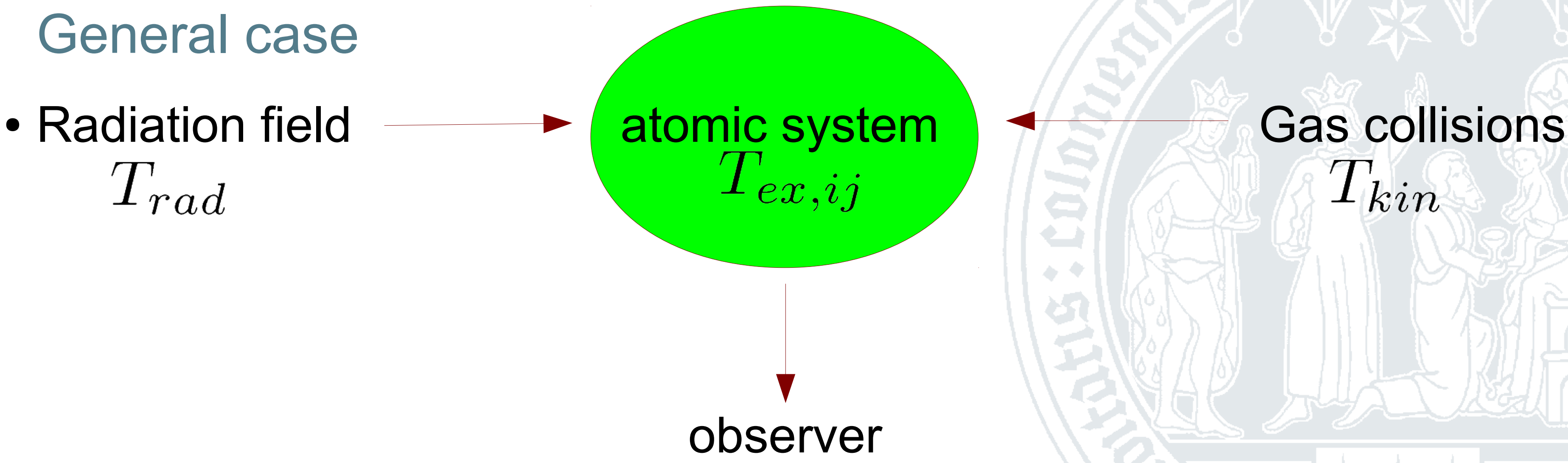
→ Balance equation: $\frac{n_i}{g_i}\sum_{j\neq i} B_{ij}u_{ij} = \sum_{j\neq i}\frac{n_j}{g_j}B_{ij}u_{ij}$

  - Solution:
    - $n_i/g_i = \text{const.}$
    - $T_{ex,ij} = \infty$

- Vacuum ($n_{i_{coll}}, u_{ij}$ small): $A_{ij} \gg B_{ij}u_{ij}, C_{ij}$ for all i,j
  - Solution:
    - $n_i \ll 1 \;\; \forall i > 0$
    - $T_{ex,ij} = T_{bg}$

Excitation analysis: Excitation temperature

General case



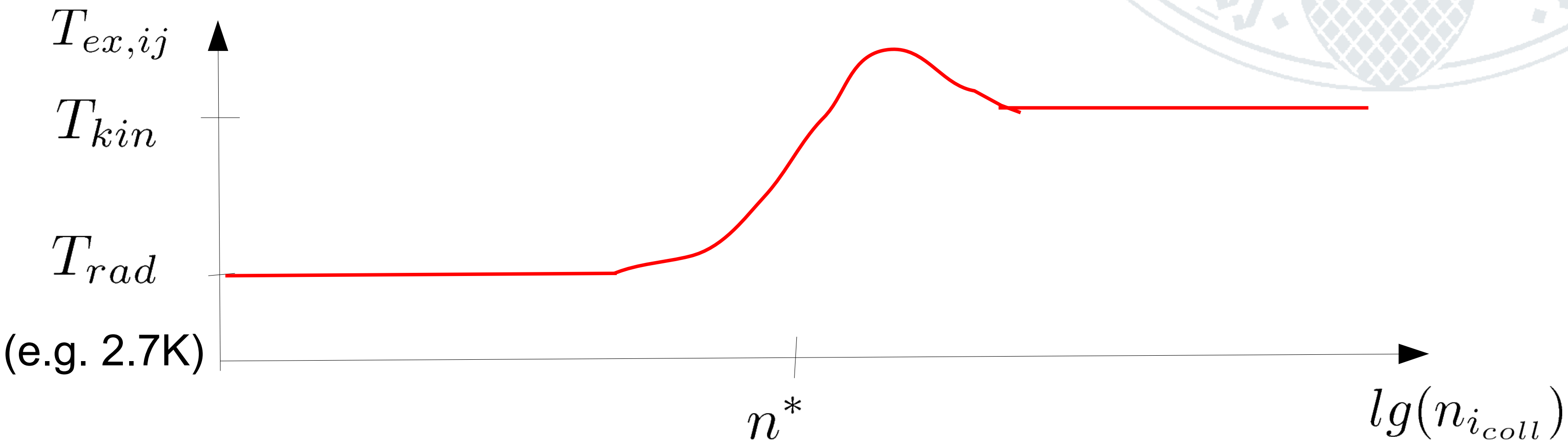
- Radiation field T_{rad}

atomic system $T_{ex,ij}$

Gas collisions T_{kin}

observer

- Observable excitation temperature:



- Transition roughly around critical density: $n^*_{i_{coll}} = A_{ij}/\gamma_{ij,i_{coll}}$

Collision partners: Environmental conditions

Gas-phase conditions

Element	number abundance	1st ionization potential	2nd ionization potential
H	100	13.6 eV	
He	9	24.6 eV	54.4 eV
O	0.026	13.6 eV	35.1 eV
C	0.012	11.3 eV	24.4 eV
N	0.008	14.5 eV	29.6 eV

Wakelam & Herbst (2008)

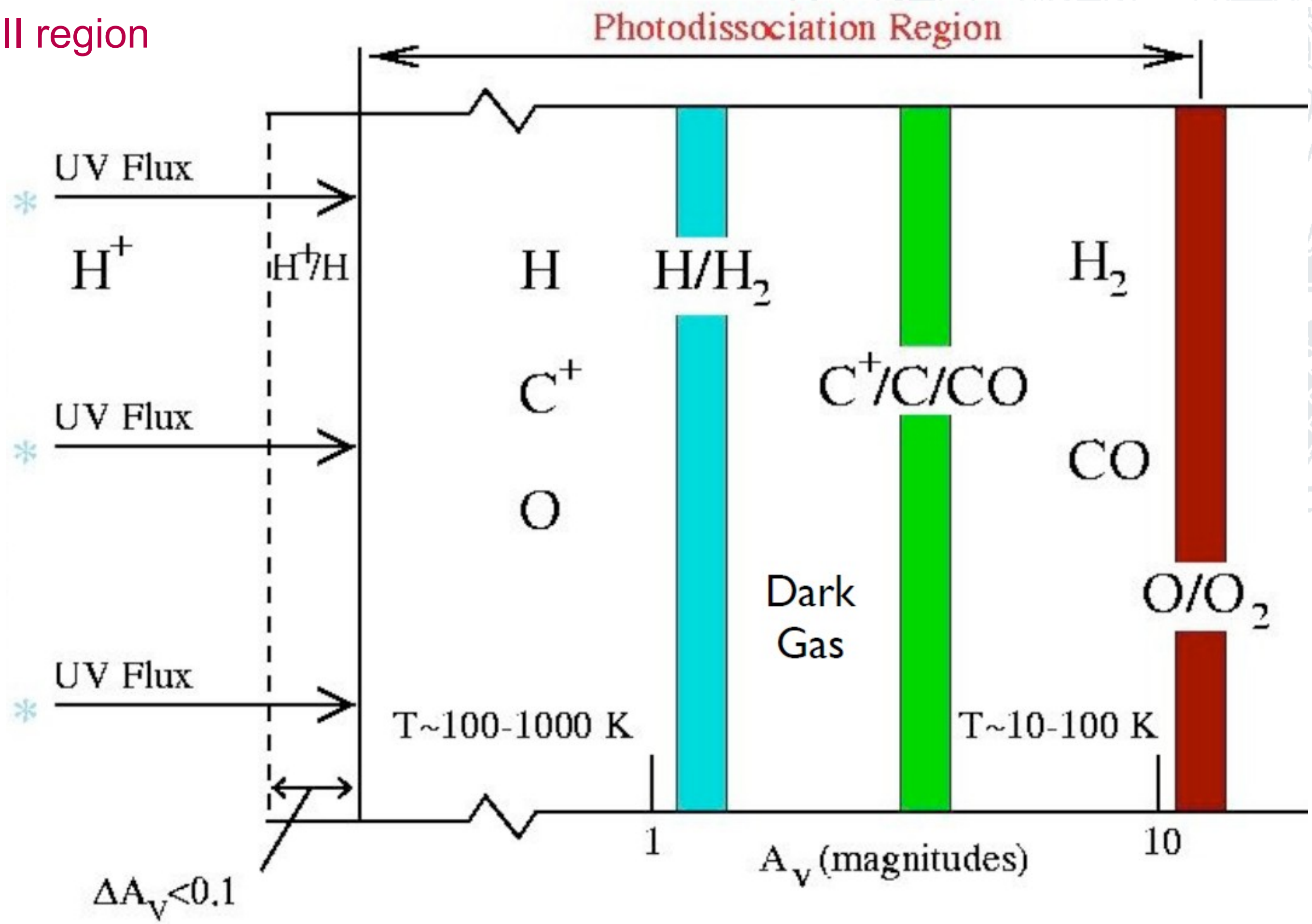
- O is neutral whenever H is neutral
- Only C can be (singly) ionized in regions where H is neutral
- OIII traces very energetic UV fields

Environmental conditions: abundances and collision partners

Spatial distribution

HII/OIII HII/NII/CII H/O/CII H_2/O/CII H_2/O/C

HII region



- Determines the main collision partners

Environmental conditions: abundances and collision partners

Layering:

HII/OIII HII/NII/CII H/O/CII H_2/O/CII H_2/O/C

determines the main collision partners:

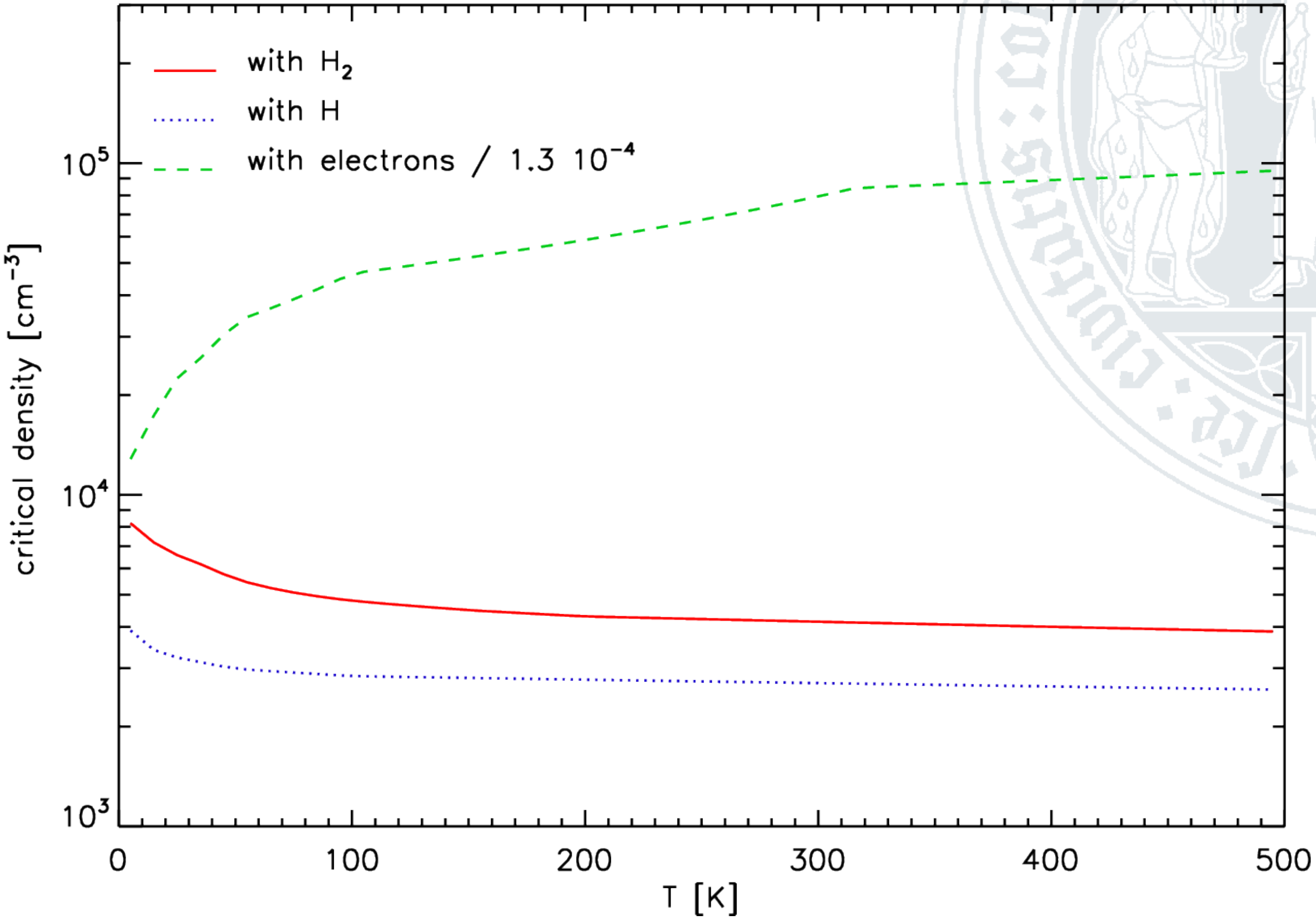
- **OIII**
  - Electrons: density given by number of H atoms
- **NII**
  - Electrons: density given by number of H atoms
- **CII**
  - Electrons: density given by H atoms or C atoms
  - H-atoms
  - H_2 molecules
- **CI**
  - H_2 molecules

(all have additional minor contribution from He)

Excitation analysis: Collisions

[CII] excitation:

- Critical densities for different relevant collision partners

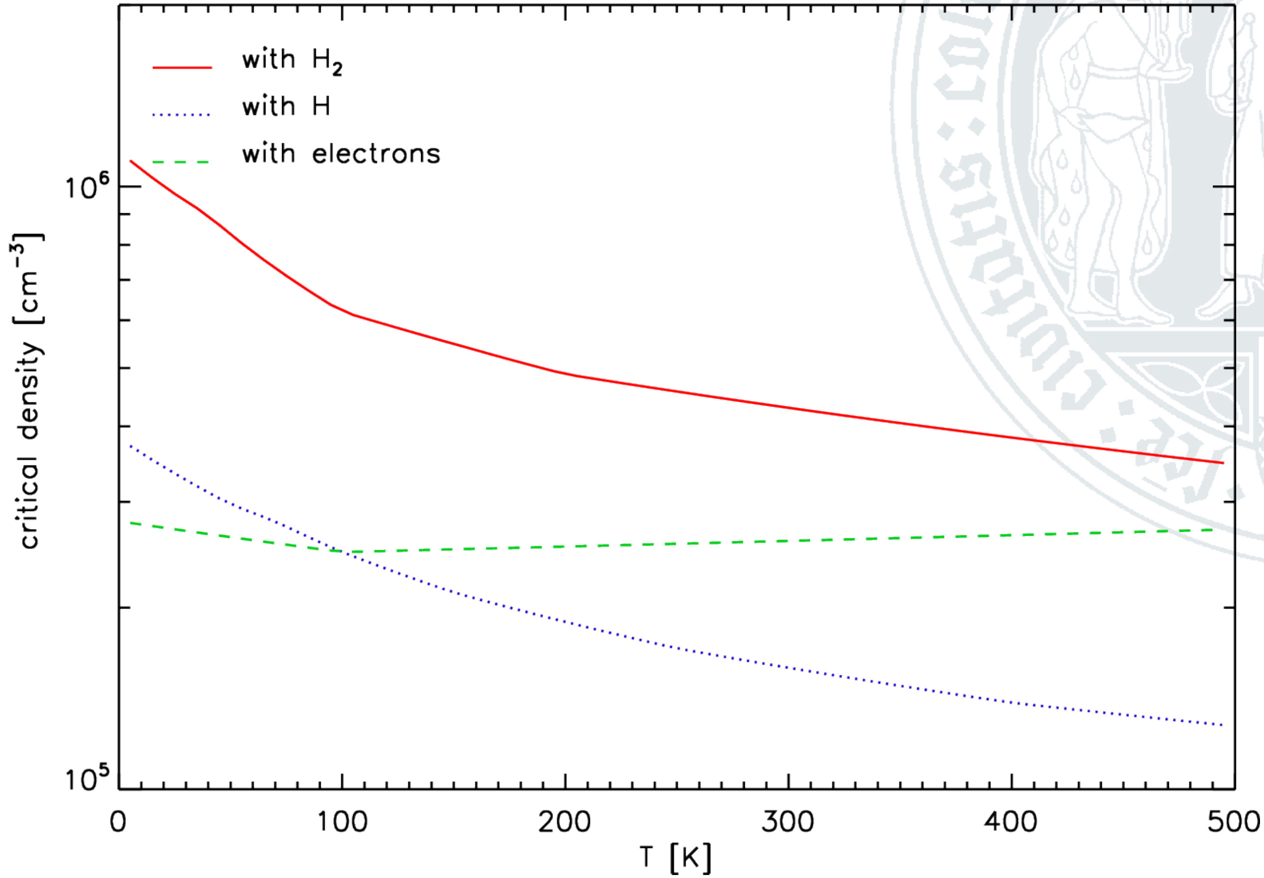


- Electrons only play a role if more than the carbon is ionized (X[C/H]=1.3 10^{-4}), i.e. in HII regions

Excitation analysis: Collisions

[OI] excitation:

- 63µm ground-state transition

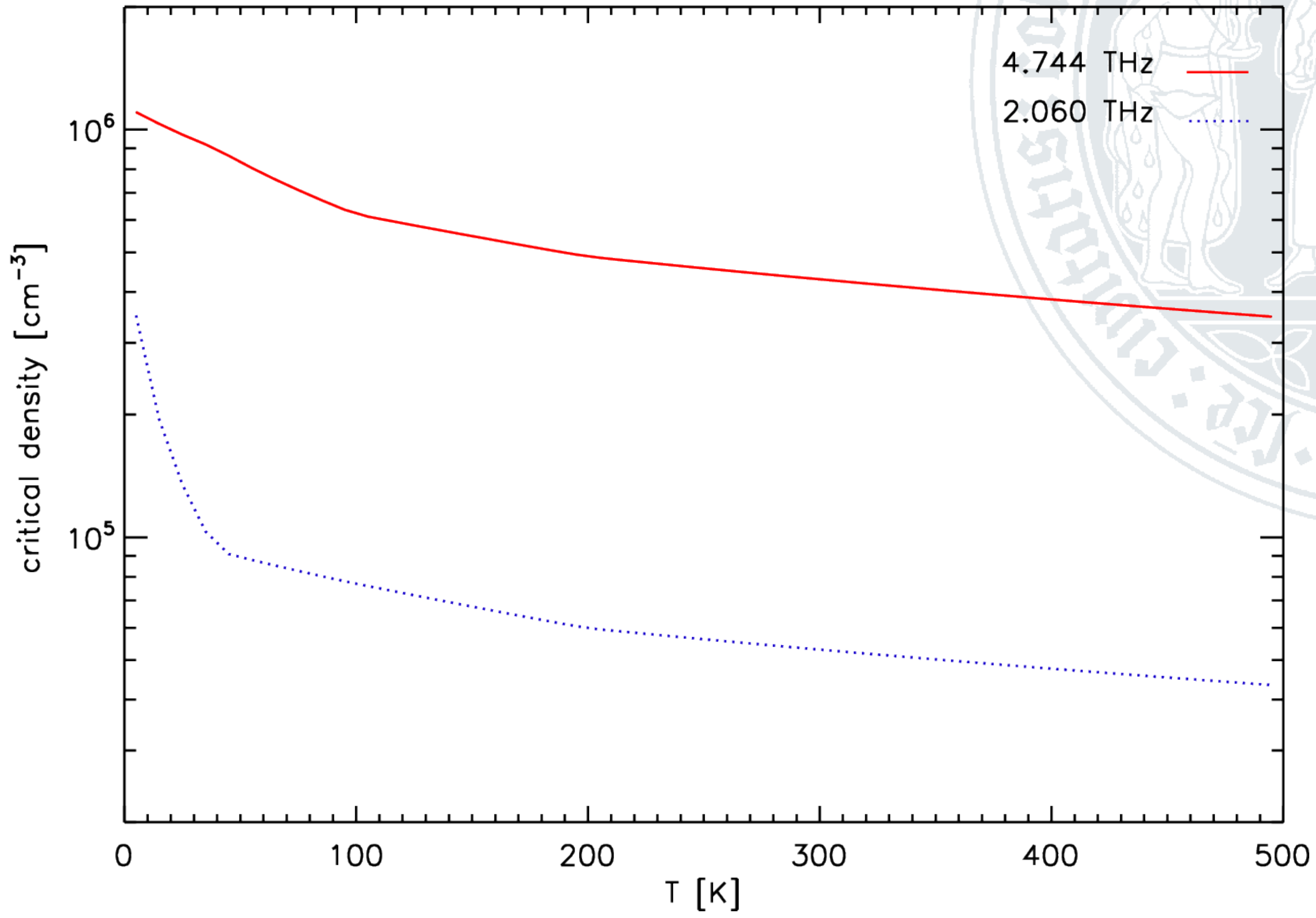


- H-excitation is most efficient, but regions with high fraction of atomic H always have low densities (or volumes) so that there O^+ is never in LTE
- High densities associated with H_2 – factor 3 less efficient

Excitation analysis: Collisions

[OI] excitation:

- Full 3-level system - critical densities for two transitions:



- Critical densities are temperature-dependent!
- Non-trivial behavior for n-level systems (n > 2)!

Line emission: Emission and absorption coefficients

n_i from balance equations

- Emission coefficient: $\epsilon_\nu(\vec{n}) = h\nu_{ij} n_i A_{ij} \frac{\phi_\nu(\vec{n})}{4\pi}$

  (spontaneous emission)

- Absorption coefficient: $\kappa_\nu(\vec{n}) = h\nu_{ij} \left(n_j B_{ji} - n_i B_{ij}\right) \frac{\phi_\nu(\vec{n})}{c}$

  (absorption and induced emission)

- With line profile

$$\phi_\nu(\vec{n}) = \int \delta\left(\nu - \nu_{ij}\left[1 + \frac{\vec{v}\vec{n}}{c}\right]\right) p(\vec{v})\, d^3\vec{v}$$

$$\approx \frac{1}{\sqrt{2\pi}\sigma} \frac{c}{\nu_{ij}} \exp\left(-\frac{c^2}{2\sigma^2}\left[\frac{\nu - \nu_{ij}}{\nu_{ij}}\right]^2\right)$$

  for Maxwellian velocity distribution

  - normalized so that omission of $\phi_\nu(\vec{n})$ gives line-integrated quantities

Line emission: Emission and absorption coefficients

Alternative expression

- $\epsilon_\nu(\vec{n}) = \kappa_\nu(\vec{n}) \times B_{\nu_{ij}}(T_{ex,ij})$
  - $B_{\nu_{ij}}(T_{ex,ij})$ - Planck function (blackbody emissivity)

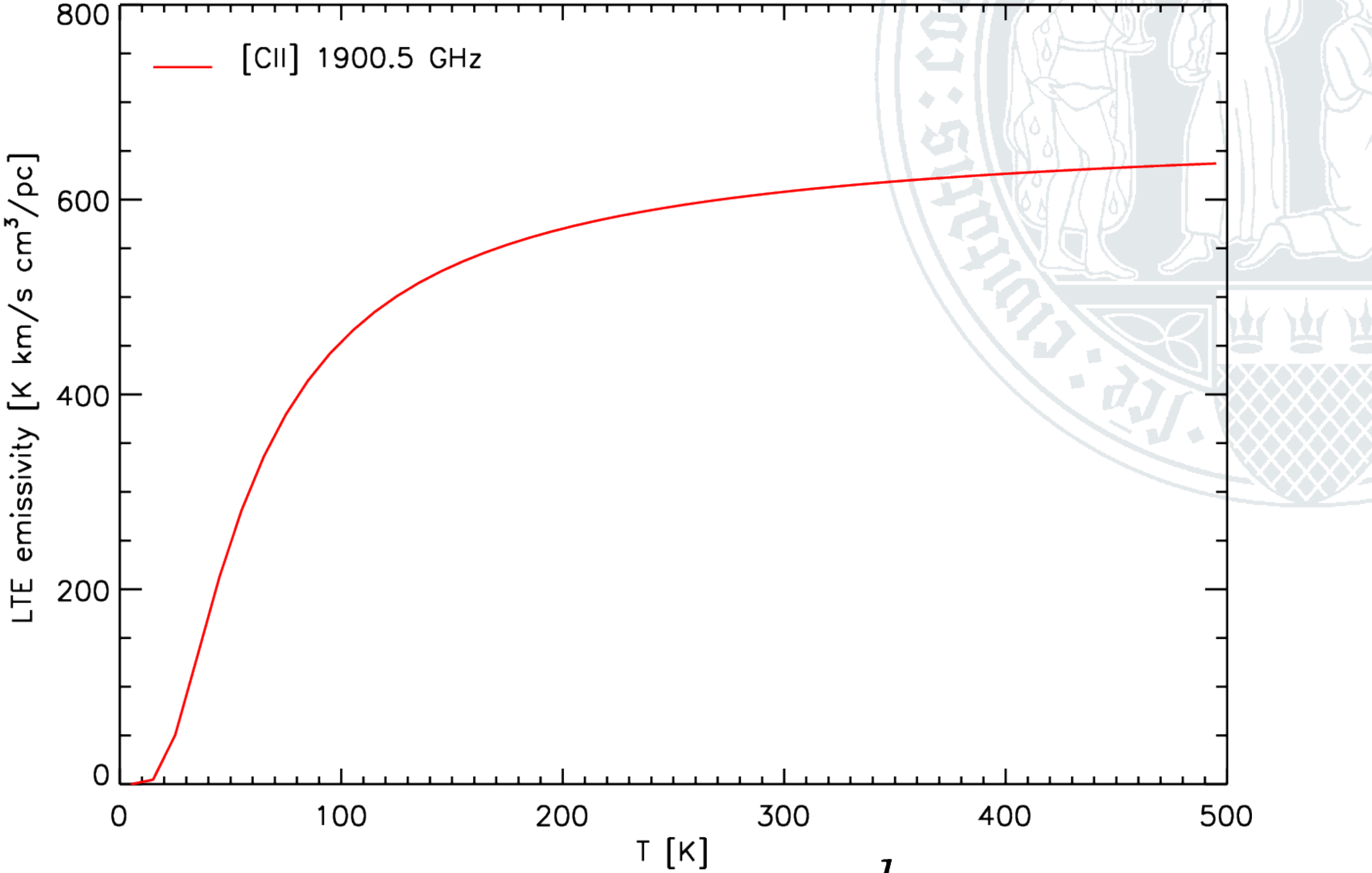
Practical computation:

- LTE
  - Boltzmann distribution of level populations *n*$_i$: $n_i \propto g_i \times \exp\left(-\frac{E_i}{kT_{kin}}\right)$
  - $T_{ex,ij} = T_{kin}$ i.e. $B_{\nu_{ij}}(T_{ex,ij}) = B_{\nu_{ij}}(T_{kin})$

Excitation analysis: LTE

LTE emissivity:

- Most simple: [CII] as two-level system $^2P_{1/2,3/2}$



- Constant emissivity at temperatures above $\frac{h\nu_{ij}}{k} = 91.2\mathrm{K}$

Excitation analysis: LTE

[CII] 1.9THz:

- Analytic description for emissivity

$$\int \epsilon \, dv = \frac{hc^3 A}{8\pi k \nu^2} \times N_{\mathrm{C+}} \frac{g_u \exp(-\Delta E/kT_{\mathrm{ex}})}{g_l + g_u \exp(-\Delta E/kT_{\mathrm{ex}})}$$

$$\approx 1011 \frac{\mathrm{K\,kms}^{-1}}{\mathrm{cm}^{-3}\,\mathrm{pc}} \times N_{\mathrm{C+}} \frac{2\exp(-91.2\mathrm{K}/T_{\mathrm{ex}})}{1+2\exp(-91.2\mathrm{K}/T_{\mathrm{ex}})}$$

and absorption/optical depth

$$\int \tau dv = 7.15\times10^{-18} \frac{\mathrm{kms}^{-1}}{\mathrm{cm}^{-2}} \times N_{\mathrm{C^+}} \frac{1-\exp(-91.2\,\mathrm{K}/T_{\mathrm{ex}})}{1+2\exp(-91.2\,\mathrm{K}/T_{\mathrm{ex}})}$$

$$\approx 7.15\times10^{-18} \frac{\mathrm{kms}^{-1}}{\mathrm{cm}^{-2}} \times N_{\mathrm{C^+}} \frac{32.9\,\mathrm{K}}{T_{\mathrm{ex}}}.$$

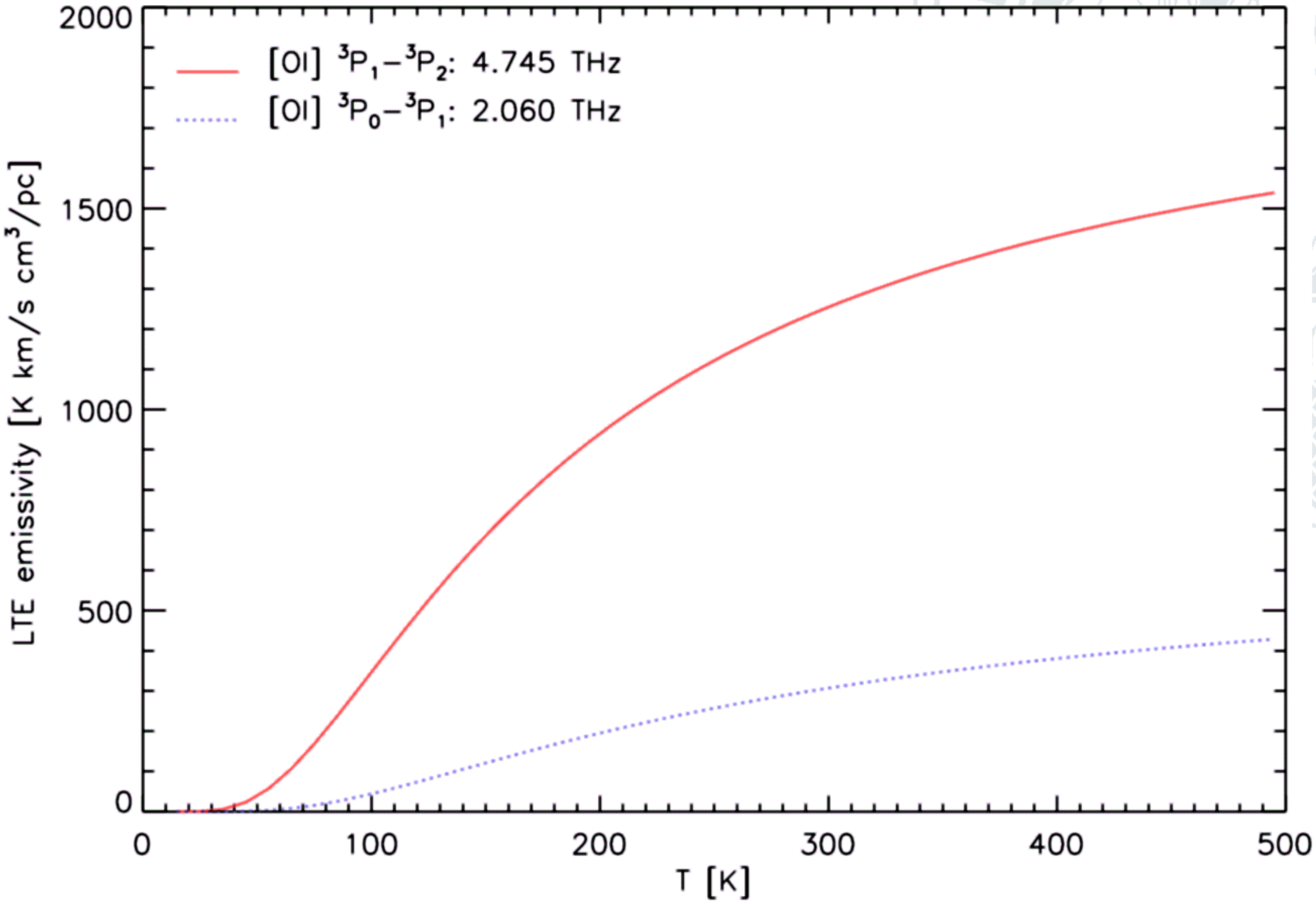
→ With X(C$^+$/H) =1.3 10^{-4}, [CII] turns optically thick for N_H ~ 2 10^{21} cm^{-2}, i.e. A_V ~ 1

Excitation analysis: LTE

LTE emissivity:

- [OI] as three-level system

$^3P_{2,1,0}$



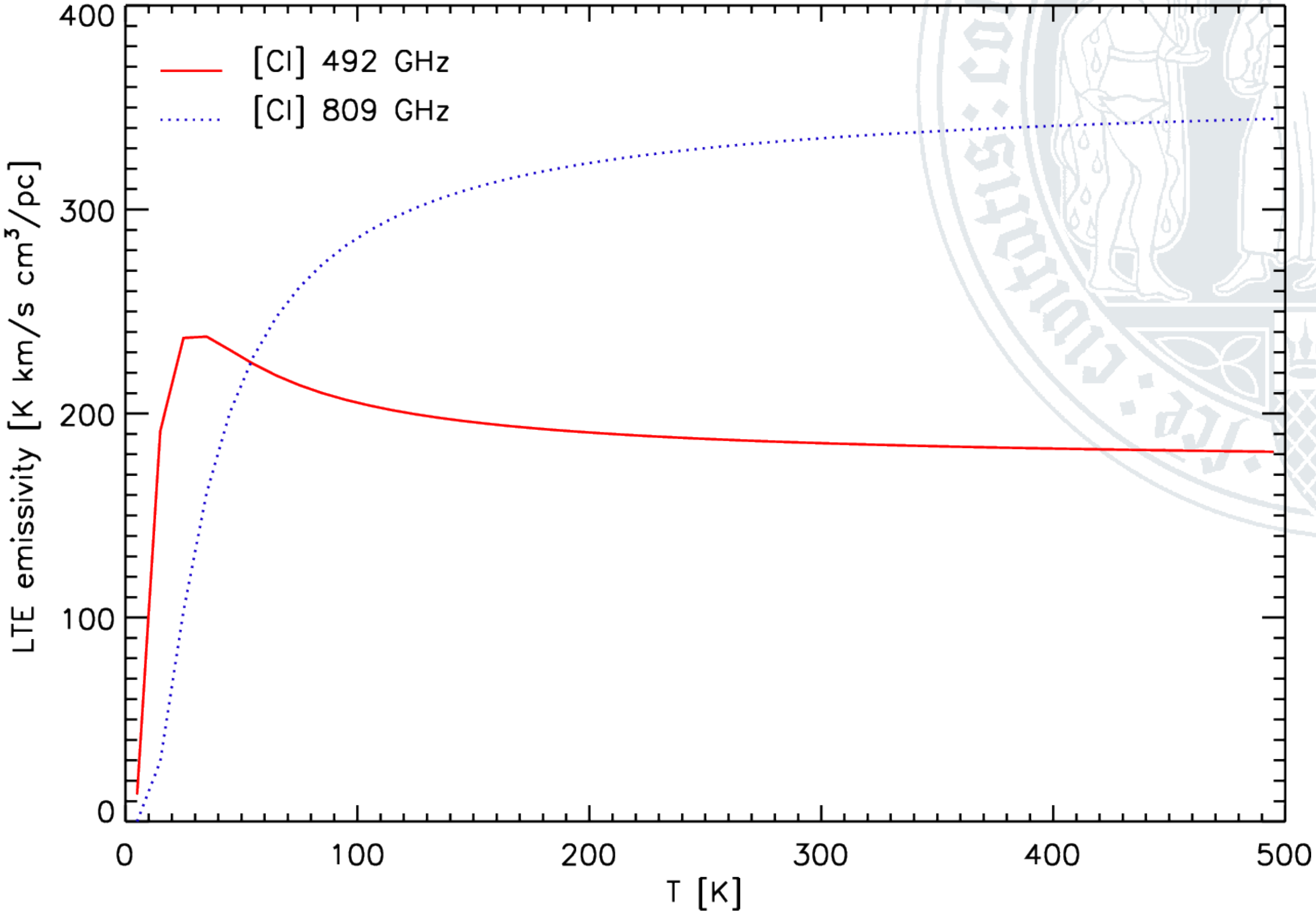
- Transition to constant emissivity shifted by factor 2 due to higher level energies

Excitation analysis: LTE

LTE emissivity:

- [CI] as three-level system

$^3P_{0,1,2}$



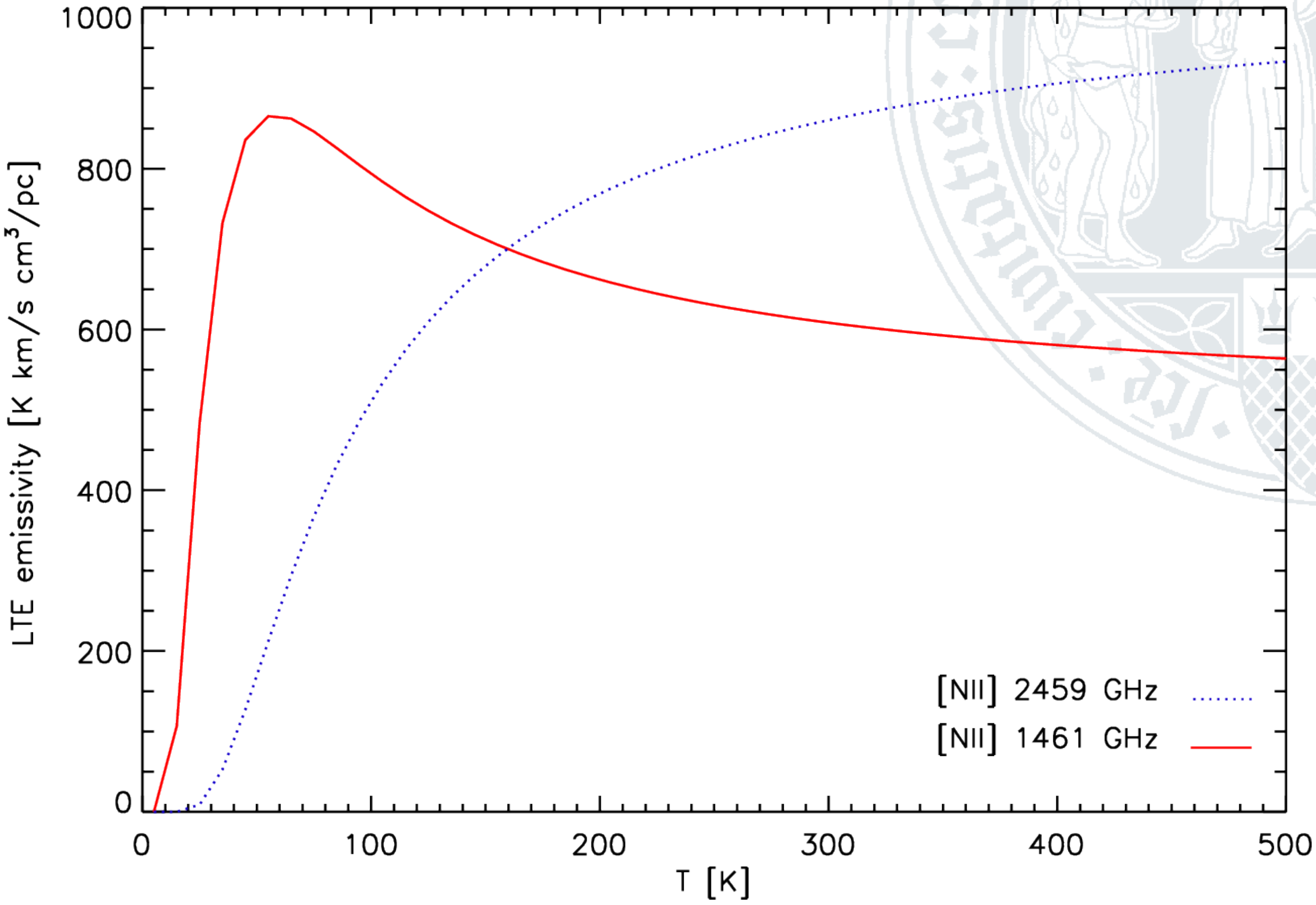
- “Overshooting” in ground-state line for all $^3P_{0,1,2}$ systems

Excitation analysis: LTE

LTE emissivity:

- [NII] as equivalent system

$^3P_{0,1,2}$



- [OIII] fully equivalent (not shown here)

Line emission: Non-LTE

Next-step approximation:

- Negligible radiative excitation: $B_{ij} u_{ij} \ll A_{ij}, C_{ij}$
  - Implies optically thin geometry
  - Analytic solutions for 2-level system:

$$n_u = \frac{g_u n_l}{g_l} \exp\left(-\frac{h\nu_{ul}}{kT_{kin}}\right) \frac{C_{ul} + A_{ul}}{C_{ul}}$$

  - and 3-level system:

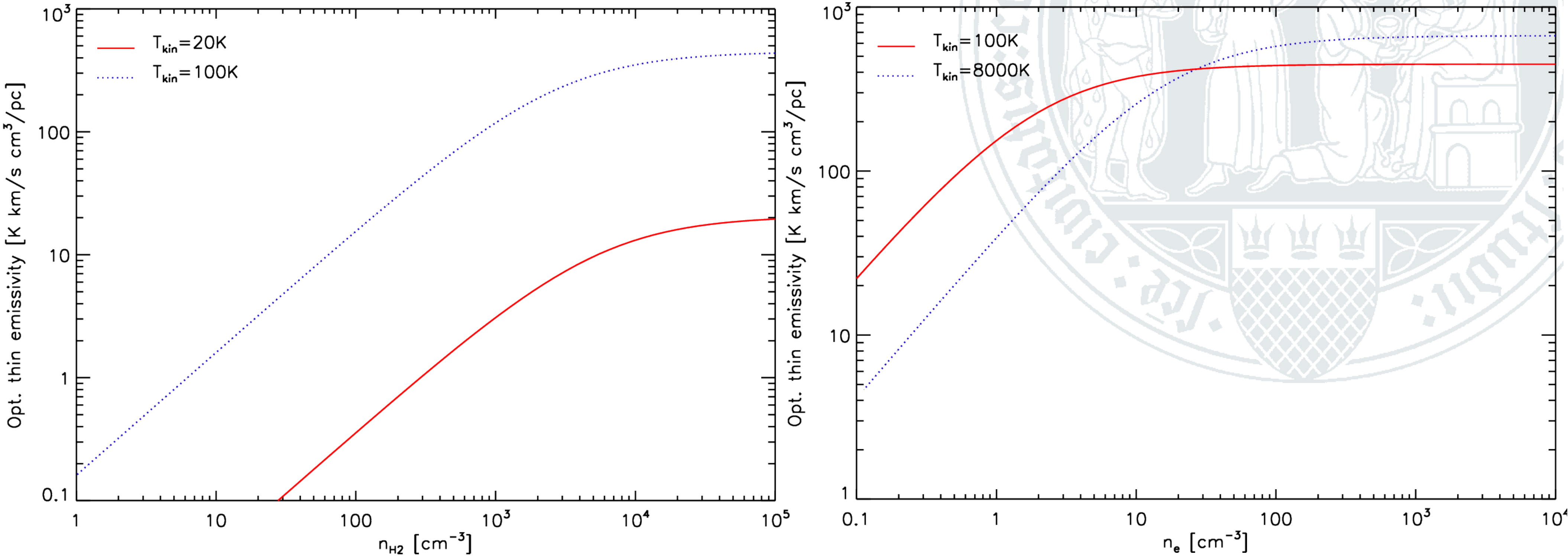
$$n_2 = \frac{g_2 n_0}{g_0} \frac{C_{12}C_{01} + C_{12}C_{10} + C_{02}C_{12}}{C_{21}C_{10} + C_{20}C_{10} + C_{21}C_{12}}$$

$$+ \frac{C_{20}A_{20}}{A_{10}(C_{21} + C_{20}) + A_{21}C_{10} + A_{10}A_{21}}$$

Line emissivity: Optically thin approximation

[CII] emissivity:

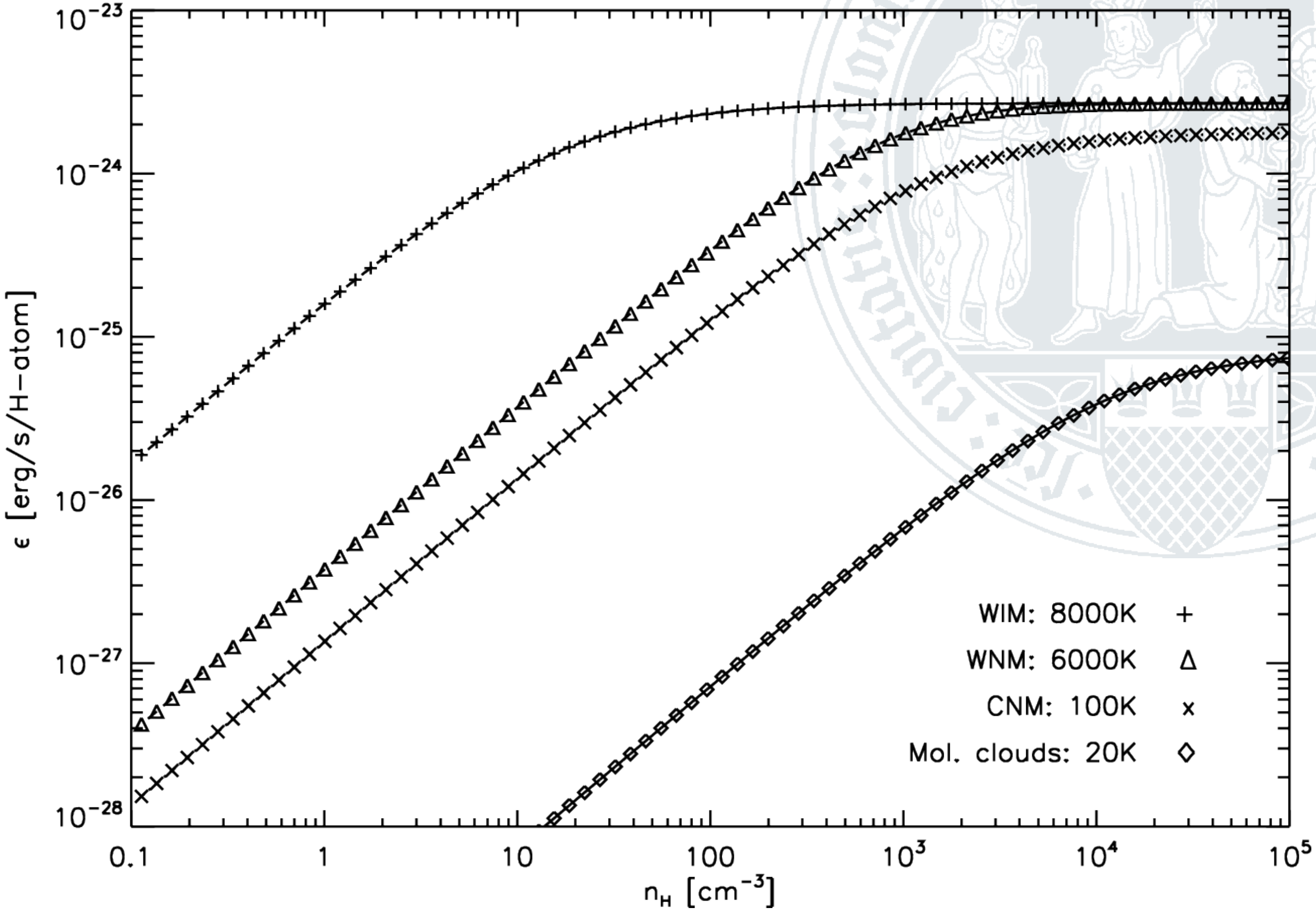
- For collisions with H_2 (left) and e^- (right)



- Transition from subthermal excitation at low densities to LTE at high densities
- At high densities only T_{kin} counts
- Critical density for electron-collisions lower by factor 1000

Line emissivity: Optically thin approximation

[CII] emissivity:

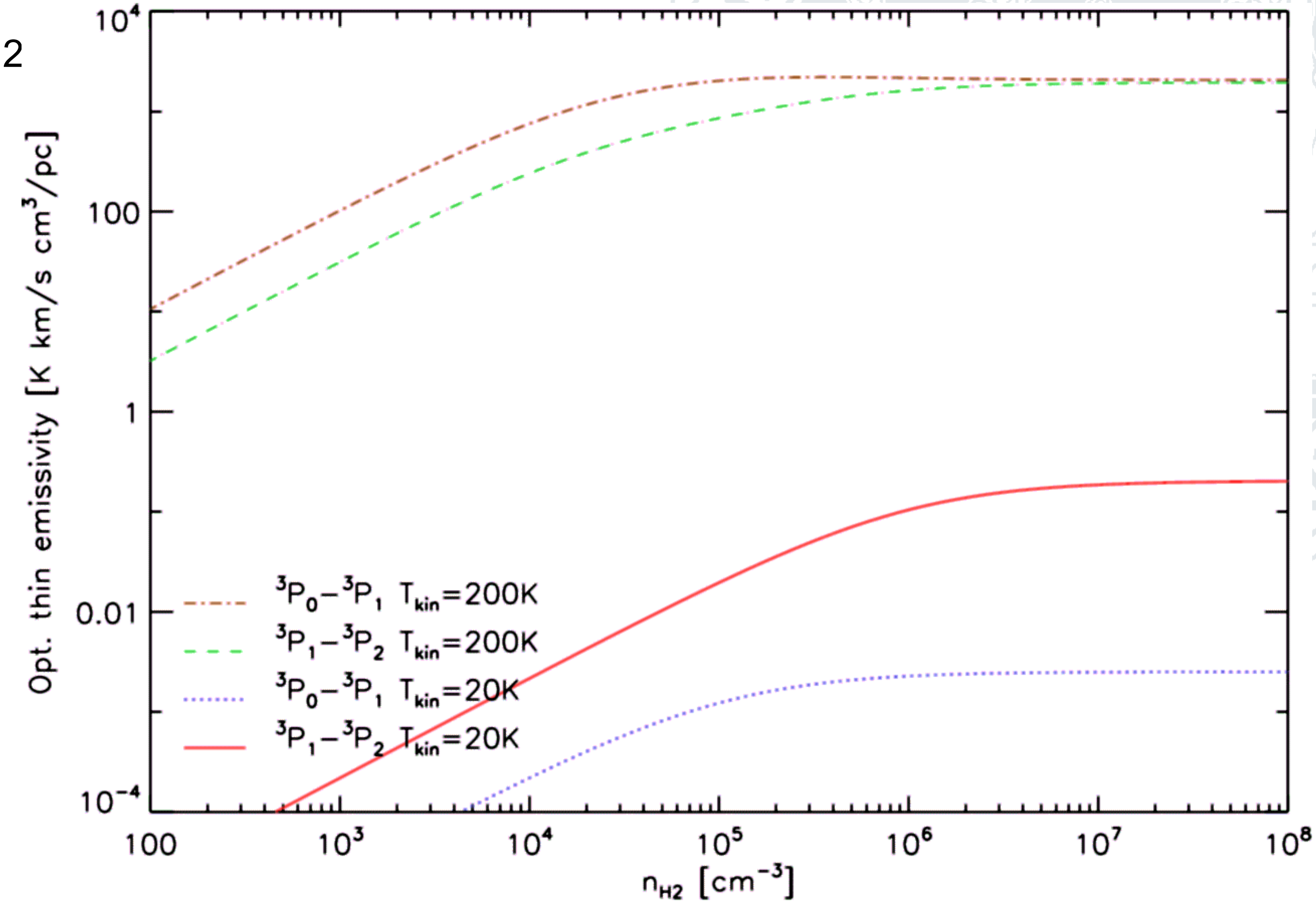


- Combination of higher emissivity above 91.2K and lower critical density for excitation through electron-collisions

Line emissivity: Optically thin approximation

[OI] emissivity:

- Excitation through H_2

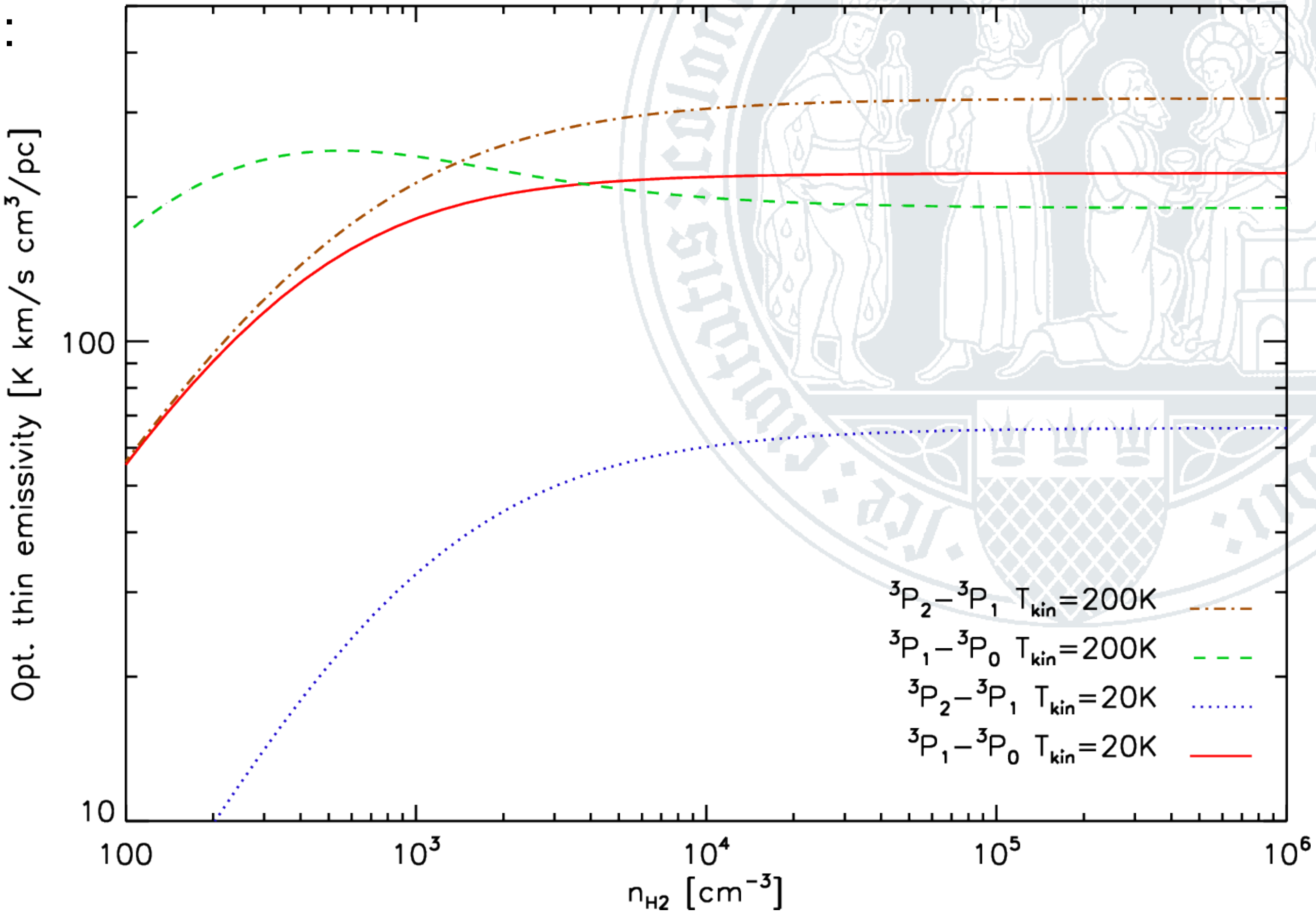


- Very simple: $\epsilon_\nu \propto n_{H_2}$ for subthermal excitation, monotonic transition to LTE
- High densities needed for thermal excitation
- Significant emission only for temperatures above 150K

Line emissivity: Optically thin approximation

[CI] emissivity:

- Excitation through H_2:

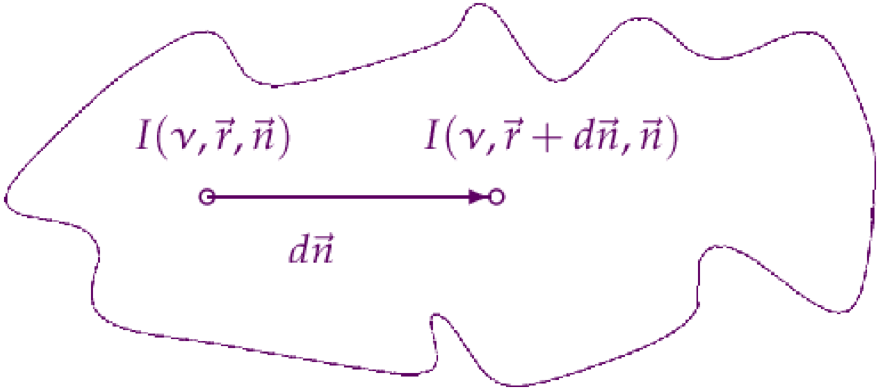


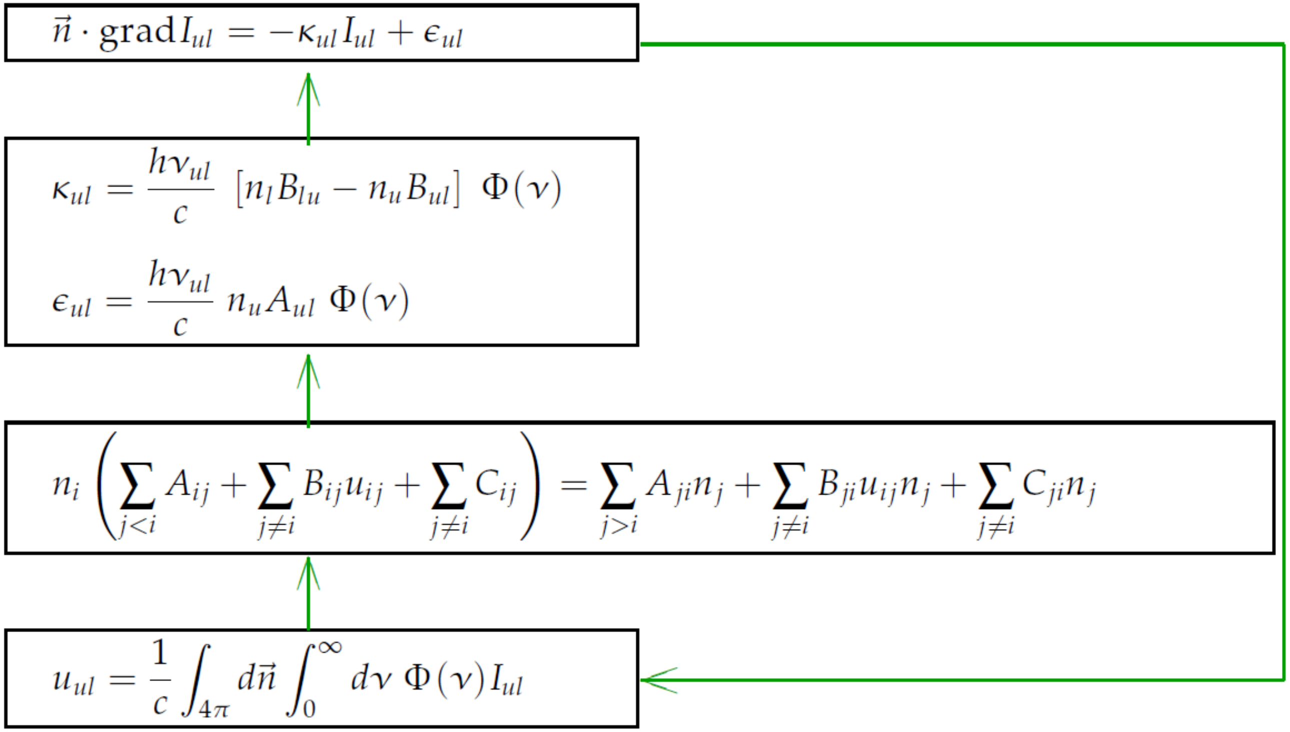
- Partially non-monotonic behaviour for ground-state transition
- Much lower densities and temperatures needed for excitation
- Qualitatively same for [NII]

Line emission: Non-LTE

General case

- To derive physical parameters, the full radiative transfer problem needs to be solved





$$\vec{n}\cdot\mathrm{grad}\,I_{ul} = -\kappa_{ul} I_{ul} + \epsilon_{ul}$$

$$\kappa_{ul} = \frac{h\nu_{ul}}{c}\left[n_l B_{lu} - n_u B_{ul}\right]\,\Phi(\nu)$$

$$\epsilon_{ul} = \frac{h\nu_{ul}}{c}\,n_u A_{ul}\,\Phi(\nu)$$

$$n_i\left(\sum_{j<i} A_{ij} + \sum_{j\neq i} B_{ij}u_{ij} + \sum_{j\neq i} C_{ij}\right) = \sum_{j>i} A_{ji}n_j + \sum_{j\neq i} B_{ji}u_{ij}n_j + \sum_{j\neq i} C_{ji}n_j$$

$$u_{ul} = \frac{1}{c}\int_{4\pi} d\vec{n}\int_0^\infty d\nu\,\Phi(\nu) I_{ul}$$

- Practical way out: Local approximation – escape probability

Line emission: Escape probability

Probability that a line-photon escapes from the cloud β:

- Same probability that a background photon enters the cloud
- Consequence:
  - Radiation field given by “trapped” radiation field and external field:

$$u = (1-\beta) B_\nu(T_{ex}) + \beta B_\nu(T_{bg})$$

  - “Cooling of the system” not through all spontaneously emitted photons, but only through those photons also escaping from the cloud
    - Modified Einstein-A coefficient: $A_{ul} \times \beta$
  - Analytic solution for 2-level system:

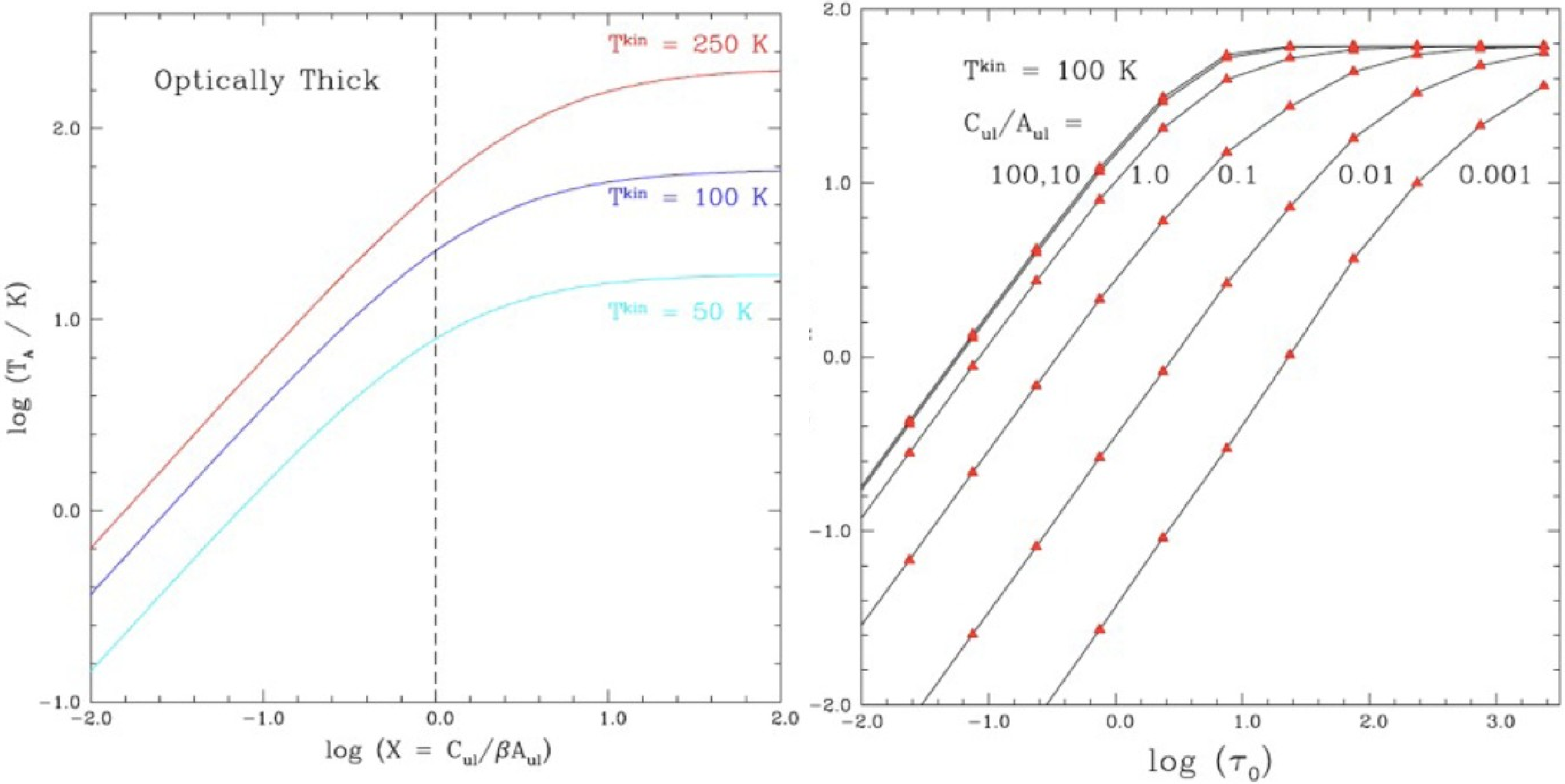
$$n_u = \frac{n_l g_u}{g_l} \frac{\beta A_{ul} G + C_{ul} \exp\left(-\frac{h\nu_{ul}}{kT_{kin}}\right)}{\beta A_{ul} (1+G) + C_{ul}}$$

    - with $G = \dfrac{1}{\exp\left(\frac{h\nu_{ul}}{kT_{bg}}\right) - 1}$

Goldsmith et al. (2013)

Line emissivity: Escape probability

Result



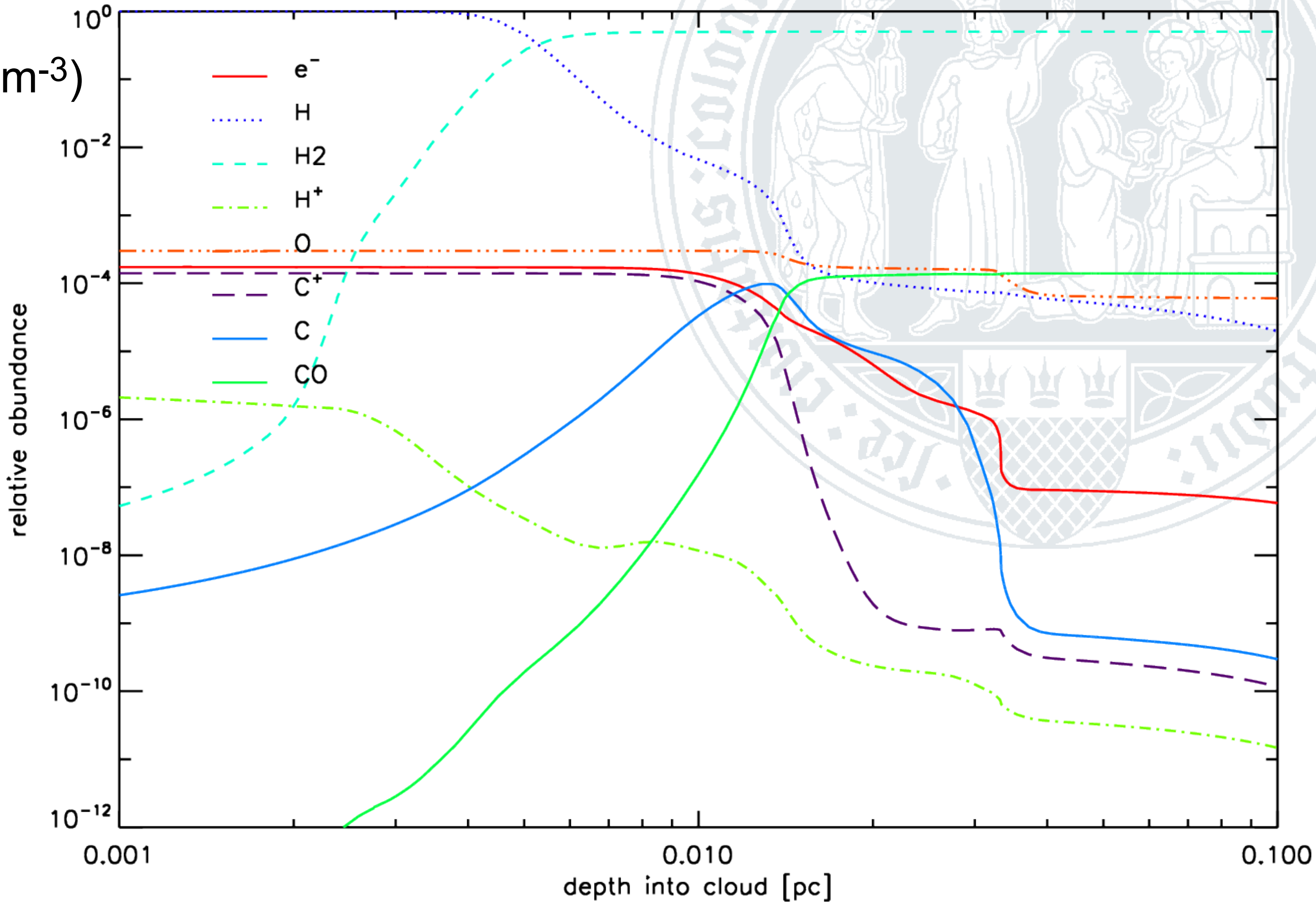
Goldsmith et al. (2013)

- Transition to LTE shifted to lower densities
- Emissivity remains proportional to column density in subthermal range

Line emissivity: Final step

Combination with model for chemical abundance

- e.g. PDR model ($\chi=10^4$, $n=10^5$ cm^{-3})

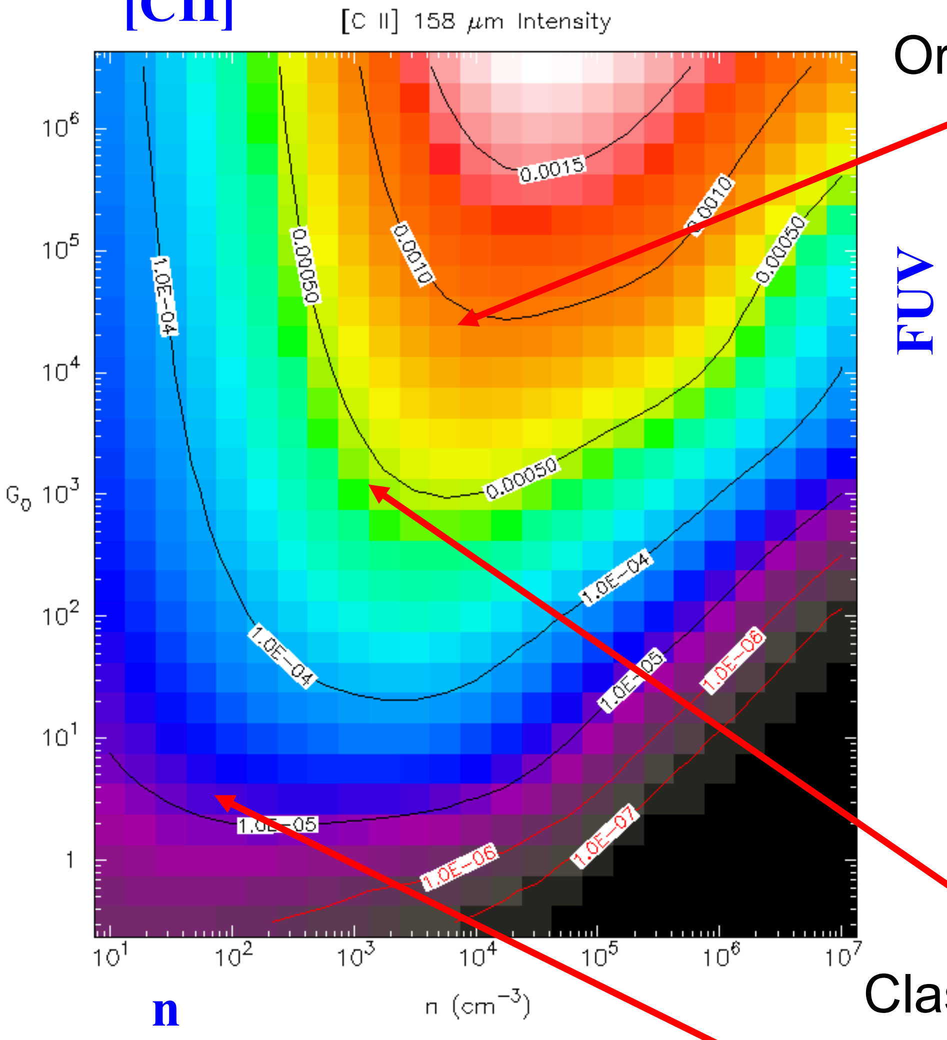


- Convolution of abundance profile with density and temperature for given chemical model needed.

Line emissivity: Final step

PDR emission:

[CII]

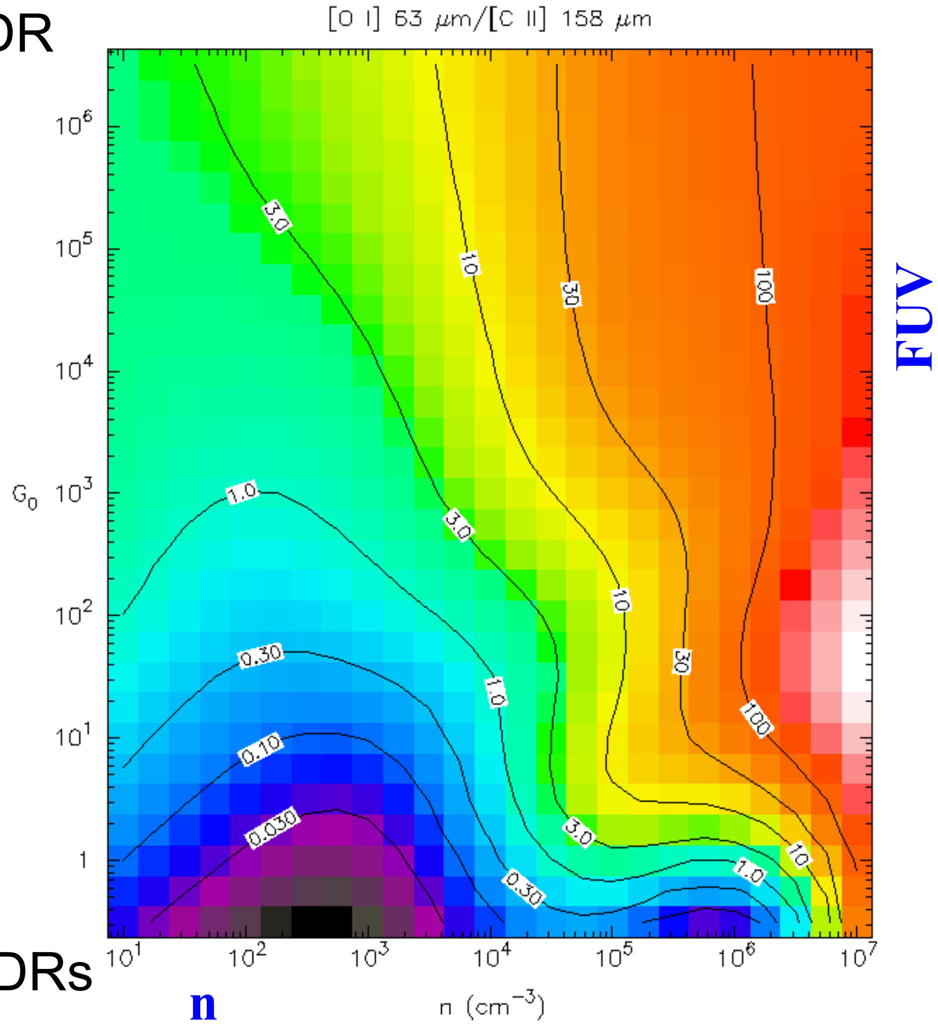


Orion PDR

Classic PDRs

Diffuse Gas

[OI]/[CII]



→ see talk by M. Röllig

Kaufman et al. 1999

Summary

Fine structure transitions are simple!

- Just a few numbers to describe them

- But always think of the dominant collision partners

	OIII	NII	CII	OI	CI
Line frequencies [GHz]	3393.0 5785.9	1461.3 2459.4	1900.5	4745.8 2060.0	492.2 809.3
Formation energy [eV]	35.1eV (IP)	14.5eV (IP)	11.2eV (IP)	11.1eV (CO diss.)	11.1eV (CO diss.)
Main collision partners	e^-	e^-	e^- H H_2	H_2	H_2
Typical critical densities [cm^{-3}]	500 4000	200 100	10 3000 5000	$5\ 10^5$ $8\ 10^4$	1000 1500
High-temperature LTE emissivities [K km/s cm^3 pc^{-1}]		550 940	699	1990 670	182 345