Why do we do astronomical observations?

to know physical conditions up there.

what do you mean by "physical conditions"?

How much are they N_i

where in position?	morphology	$N_i(x)$
where in velocity?	kinematics	$N_i(\dot{x})$
relatively?	chemistry	N_i / N_j
relatively (in level)?	temperature	N_{i+1} / N_i

↔

model

ρ (density)

excitation mechanisms

shock, radiation

chemical compositions

t, history

story

How it comes to present state

How to measure N_i ?

1. what molecules do?
2. when to observe what?
3. convert E to N_i
4. calculate T_{ex} from N_{i+1} / N_i

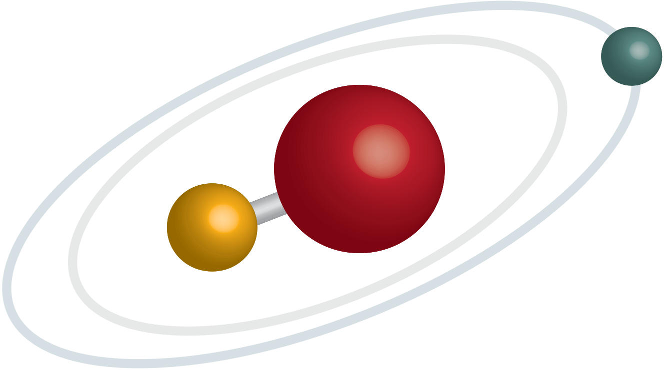
collisional excitation

in emission / absorption

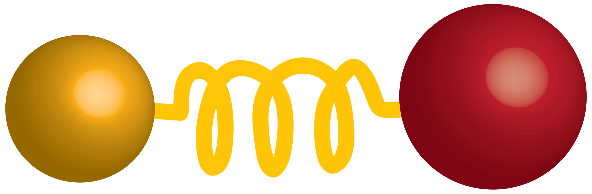
Boltzmann distribution

What do molecules do?

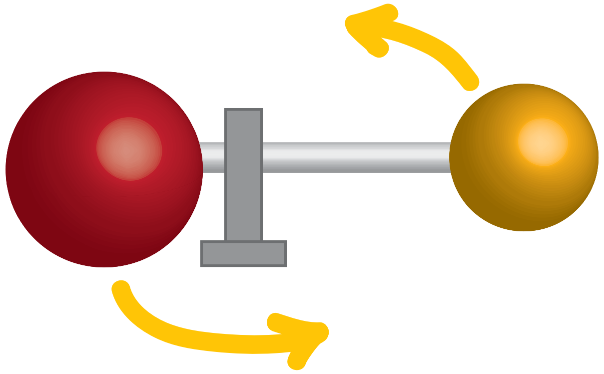
when they have >2 point mass



1. have electrons

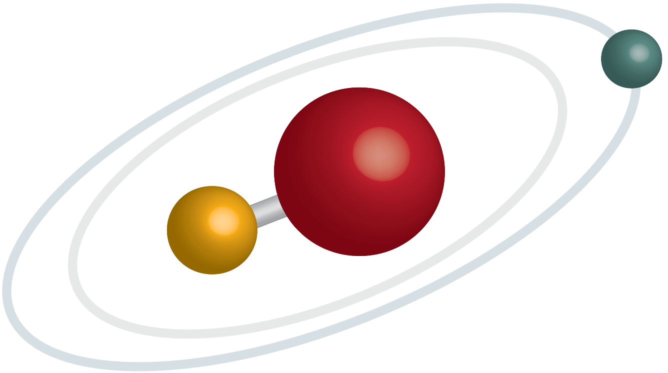


2. vibrate



3. rotate

What do molecules do?

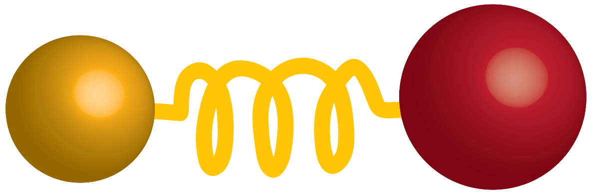


① have electrons

UV / optical

1000-10000 Å

1-10 eV



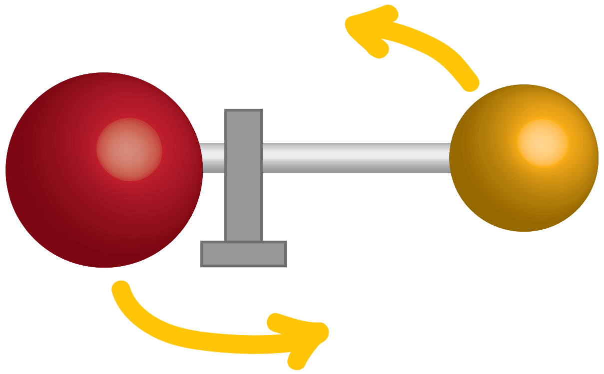
② vibrate

IR

1-100 μm

1-100 THz

100-10000 cm^{-1}



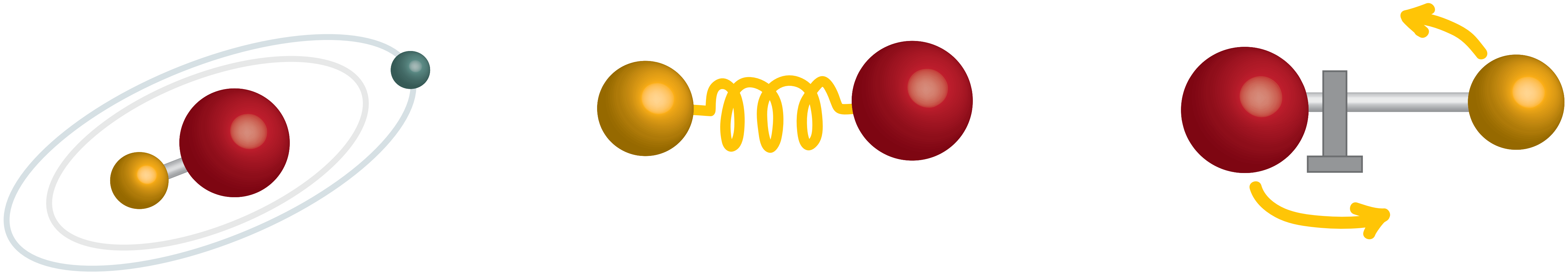
③ rotate

sub-mm - cm

0.1-10 mm

1-100 GHz

What do molecules do?

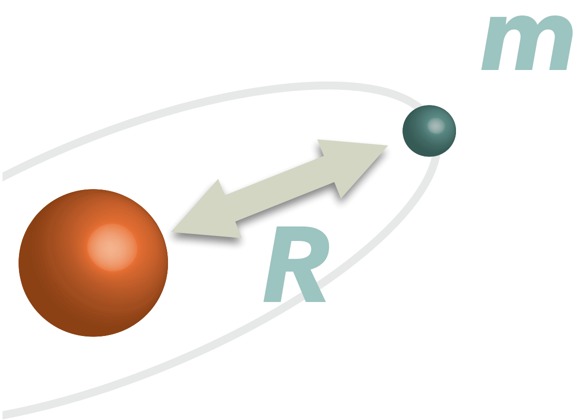


① have electrons	② vibrate	③ rotate
UV / optical	**IR**	**sub-mm - cm**
1000-10000 Å	1-100 μm	0.1-10 mm
1-10 eV	1-100 THz	1-100 GHz
	100-10000 cm^{-1}	
0.1 μm	10 μm	1000 μm

x 100

x 100

electron orbital



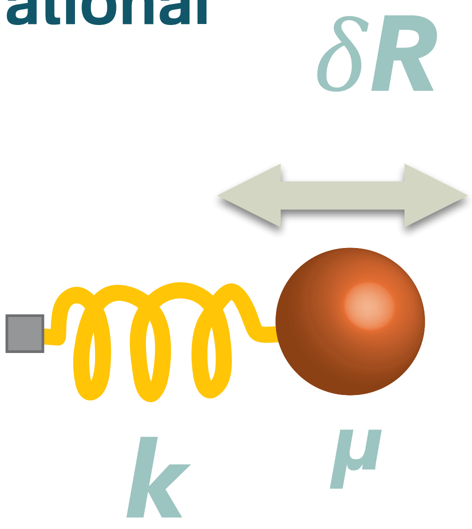
energy

$$E_{elec} = \frac{1}{2} mv^2$$

angular momentum

$$mRv = \hbar$$

vibrational



spring constant

energy

$$E_{vib} = \frac{1}{2}\mu V_b^2 = \frac{1}{2}k(\delta R)^2$$

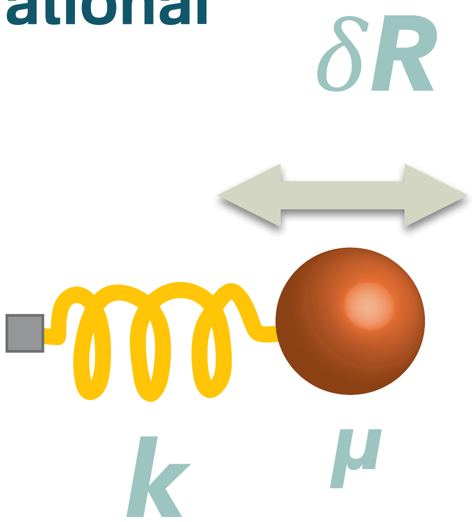
angular momentum

$$\mu(\delta R)V_b = \hbar$$

vibrational

energy

angular momentum



spring constant

$$E_{vib} = \frac{1}{2}\mu V_b^2 = \frac{1}{2}k(\delta R)^2$$

$$\mu(\delta R)V_b = \hbar$$

Reduced mass

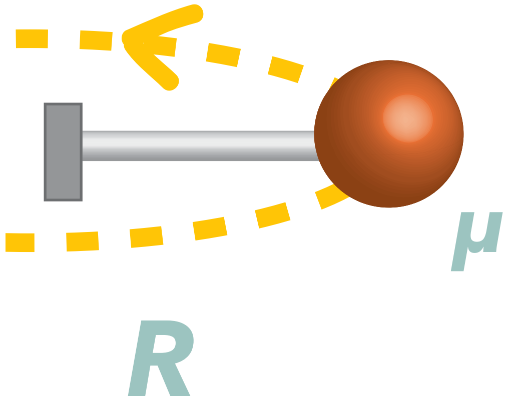
$$\frac{1}{\mu} = \frac{1}{M_1} + \frac{1}{M_2}$$

$$M_1 << M_2$$

$$\mu \sim M_1 \sim Mp$$

smallest one

rotational



energy

$$E_{rot} = \frac{1}{2}\mu V_r^2$$

angular momentum

$$\mu R V_r = \hbar$$

Reduced mass

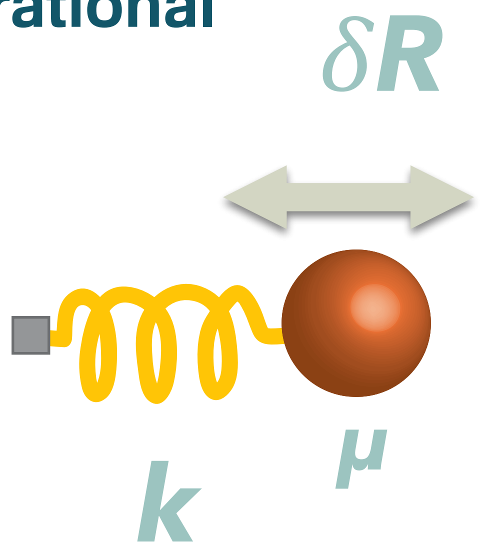
$$\frac{1}{\mu} = \frac{1}{M_1} + \frac{1}{M_2}$$

$$M_1 << M_2$$

$$\mu \sim M_1 \sim Mp$$

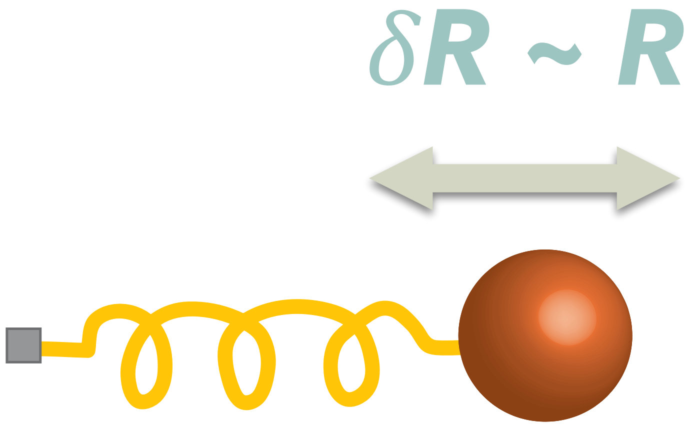
smallest one

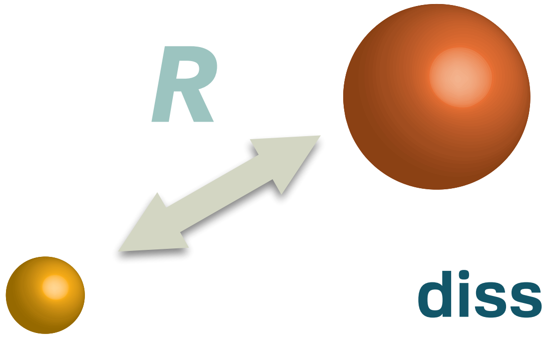
vibrational



$$E_{vib} = \frac{1}{2}\mu V_b{}^2 = \frac{1}{2}k(\delta R)^2$$

when vibration goes extreme





dissociation

$$\frac{1}{2}kR^2 \sim E_{elec}$$

Born-Oppenheimer constant

$$\kappa^4 = \frac{m}{Mp}$$

$$\frac{\text{electron mass}}{\text{proton mass}}$$

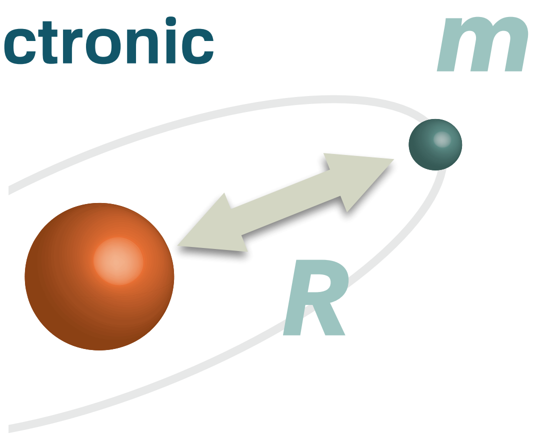
$$= \frac{m}{\mu}$$

$$\kappa = 0.1$$

energy

angular momentum

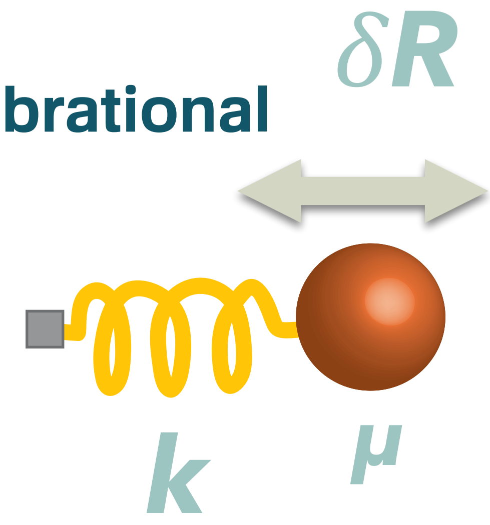
electronic



$$E_{elec} = \frac{1}{2} mv^2 = \frac{1}{2} kR^2 \quad \boxed{1}$$

$$mRv = \hbar \quad \boxed{3}$$

vibrational



$$E_{vib} = \frac{1}{2} \mu V_b^2 = \frac{1}{2} k(\delta R)^2 \quad \boxed{2}$$

$$\mu(\delta R)V_b = \hbar \quad \boxed{4}$$

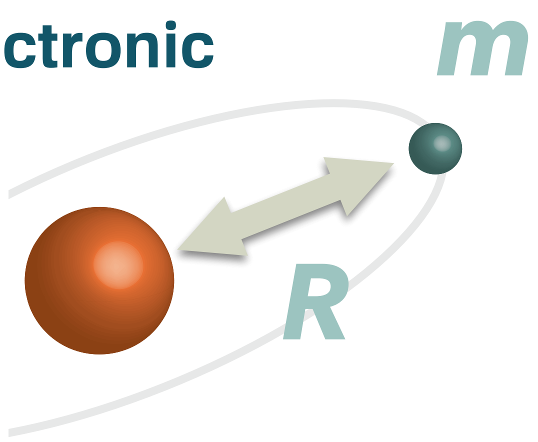
T. Oka, in Handbook of High-Resolution Spectroscopy,
“Orders of magnitude and Symmetry in Molecular Spectroscopy

$\kappa^4 = \frac{m}{\mu}$ $\quad \kappa \sim 0.1$

energy

angular momentum

electronic



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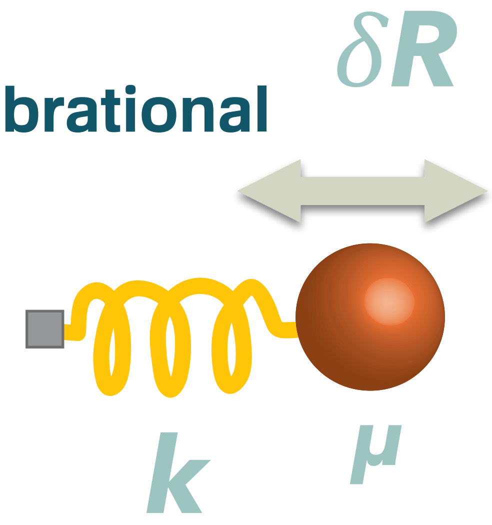
vibrational



$\boxed{1}\ \boxed{2}$

$$\frac{E_{elec}}{E_{vib}} = \frac{m v^2}{\mu V_b^2} = \frac{R^2}{(\delta R)^2}$$

$$\kappa^4 \frac{v^2}{V_b^2} = \frac{R^2}{(\delta R)^2}$$

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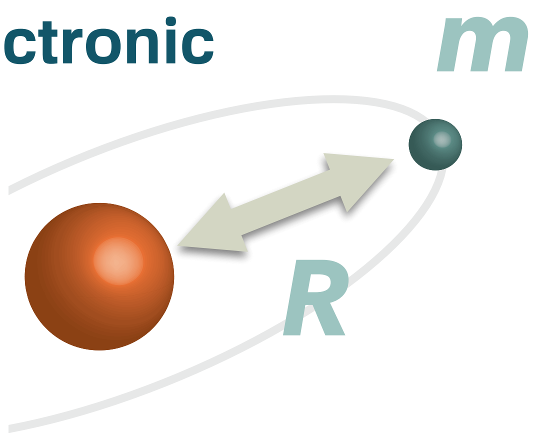
energy

angular momentum

electronic



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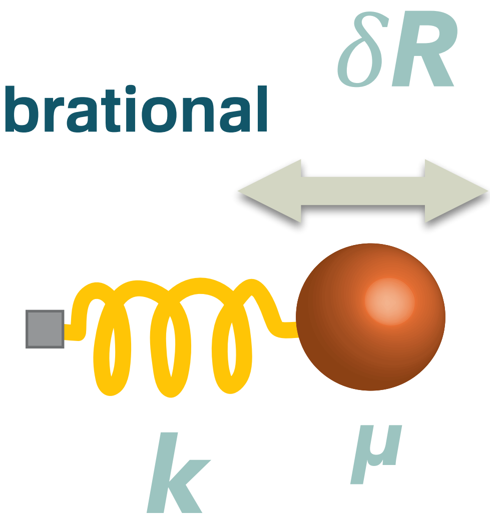
vibrational



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$\boxed{1}$ $\boxed{2}$

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$$\kappa^4 \frac{v^2}{V_b^2} = \frac{R^2}{(\delta R)^2}$$

$\boxed{3}$ $\boxed{4}$

$$\frac{m R v}{\mu (\delta R) V_b} = 1$$

$$\kappa^4 \frac{v}{V_b} = \frac{\delta R}{R}$$

$$\frac{v}{V_b} = \frac{\delta R}{R} \frac{1}{\kappa^4}$$

T. Oka, in Handbook of High-Resolution Spectroscopy,
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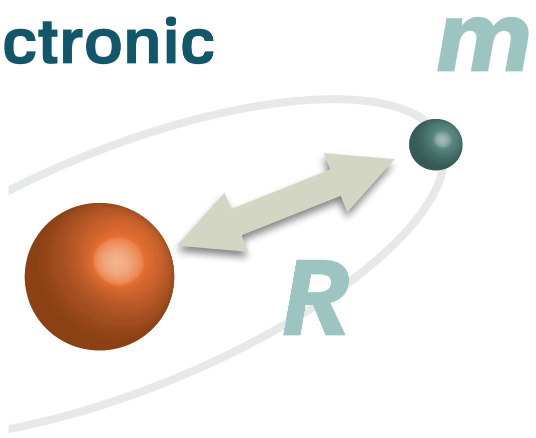
$\kappa^4 = \frac{m}{\mu}$ $\kappa \sim 0.1$

energy

angular momentum

electronic



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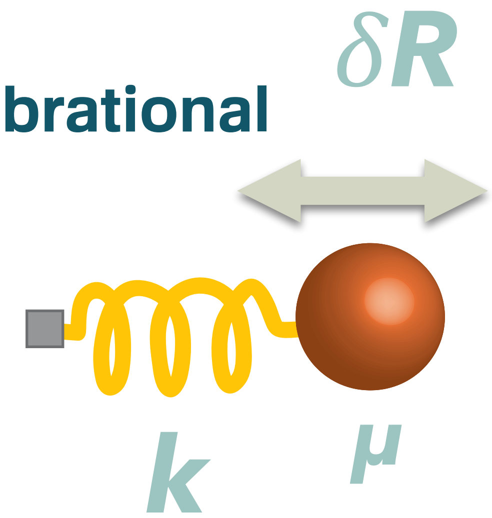
vibrational



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$\boxed{3}$ $\boxed{4}$

$$\frac{mRv}{\mu(\delta R)V_b} = 1$$

$$\kappa^4 \frac{v^2}{V_b^2} = \frac{R^2}{(\delta R)^2}$$

$$\kappa^4 \frac{v}{V_b} = \frac{\delta R}{R}$$

$$\frac{v}{V_b} = \frac{\delta R}{R} \frac{1}{\kappa^4}$$

$$\kappa^4 \left(\frac{\delta R}{R} \frac{1}{\kappa^4} \right)^2 = \frac{R^2}{(\delta R)^2}$$

electron orbital / vibration radius

$$\frac{R^4}{(\delta R)^4} = \frac{1}{\kappa^4} \qquad \frac{R}{\delta R} = \frac{1}{\kappa} \qquad \frac{E_{elec}}{E_{vib}} = \frac{1}{\kappa^2} = \sqrt{\frac{M}{m}}$$

0.1 μm

10 μm

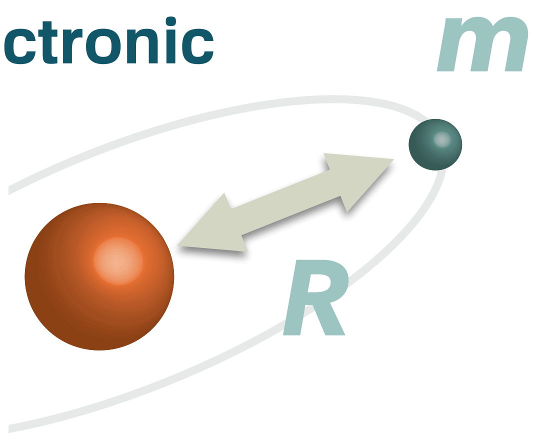
T. Oka, in Handbook of High-Resolution Spectroscopy,
"Orders of magnitude and Symmetry in Molecular Spectroscopy

$\kappa^4 = \frac{m}{\mu}$ $\quad$ $\kappa \sim 0.1$

energy

angular momentum

electronic



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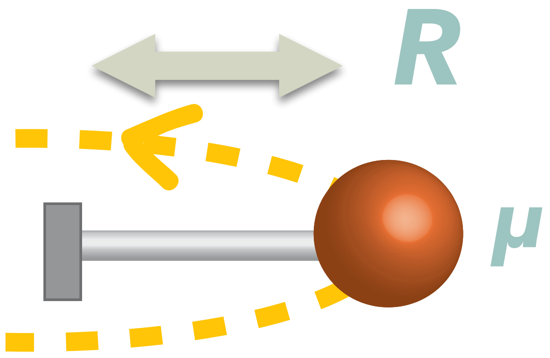
$$m R v = \hbar \quad \boxed{3}$$

$$E_{rot} = \frac{1}{2} \mu V_r^2 \quad \boxed{2}$$

$$\mu R V_r = \hbar \quad \boxed{4}$$

rotational



$\boxed{1}\ \boxed{2}$

$$\frac{E_{elec}}{E_{rot}} = \frac{m v^2}{\mu V_r^2} = \kappa^4 \frac{v^2}{V_r^2}$$

$\boxed{3}\ \boxed{4}$

$$\frac{m R v}{\mu R V_r} = 1$$

$$\kappa^4 \frac{v}{V_r} = 1$$

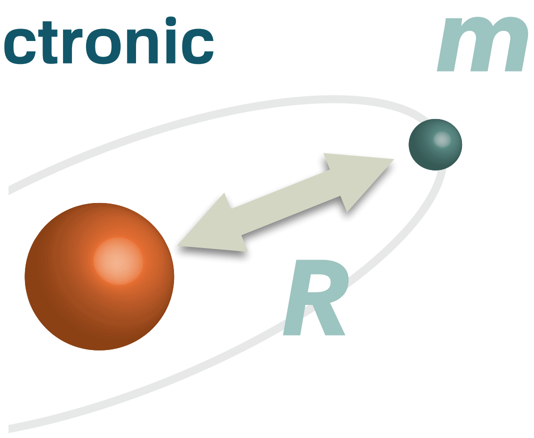
T. Oka, in Handbook of High-Resolution Spectroscopy,
"Orders of magnitude and Symmetry in Molecular Spectroscopy

$\kappa^4 = \frac{m}{\mu}$ $\kappa \sim 0.1$

energy

angular momentum

electronic



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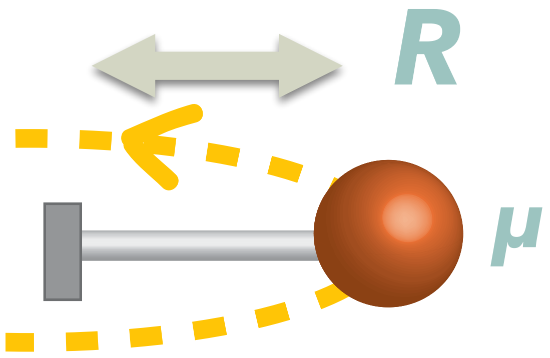
rotational



$\boxed{1}\ \boxed{2}$

$$\frac{E_{elec}}{E_{rot}} = \frac{m v^2}{\mu V_r^2} = \kappa^4 \frac{v^2}{V_r^2}$$

$$= \frac{1}{\kappa^4}$$

$$= \frac{\mu}{m}$$

0.1 μm

1 mm

$\boxed{3}\ \boxed{4}$

$$\frac{m R v}{\mu R V_r} = 1$$

$$\kappa^4 \frac{v}{V_r} = 1$$

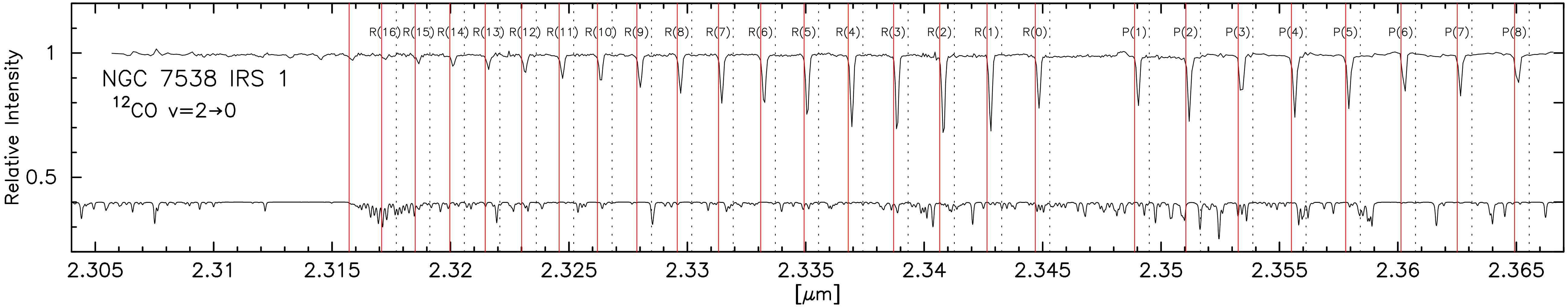
$$\frac{v}{V_r} = \frac{1}{\kappa^4}$$

T. Oka, in Handbook of High-Resolution Spectroscopy,
"Orders of magnitude and Symmetry in Molecular Spectroscopy

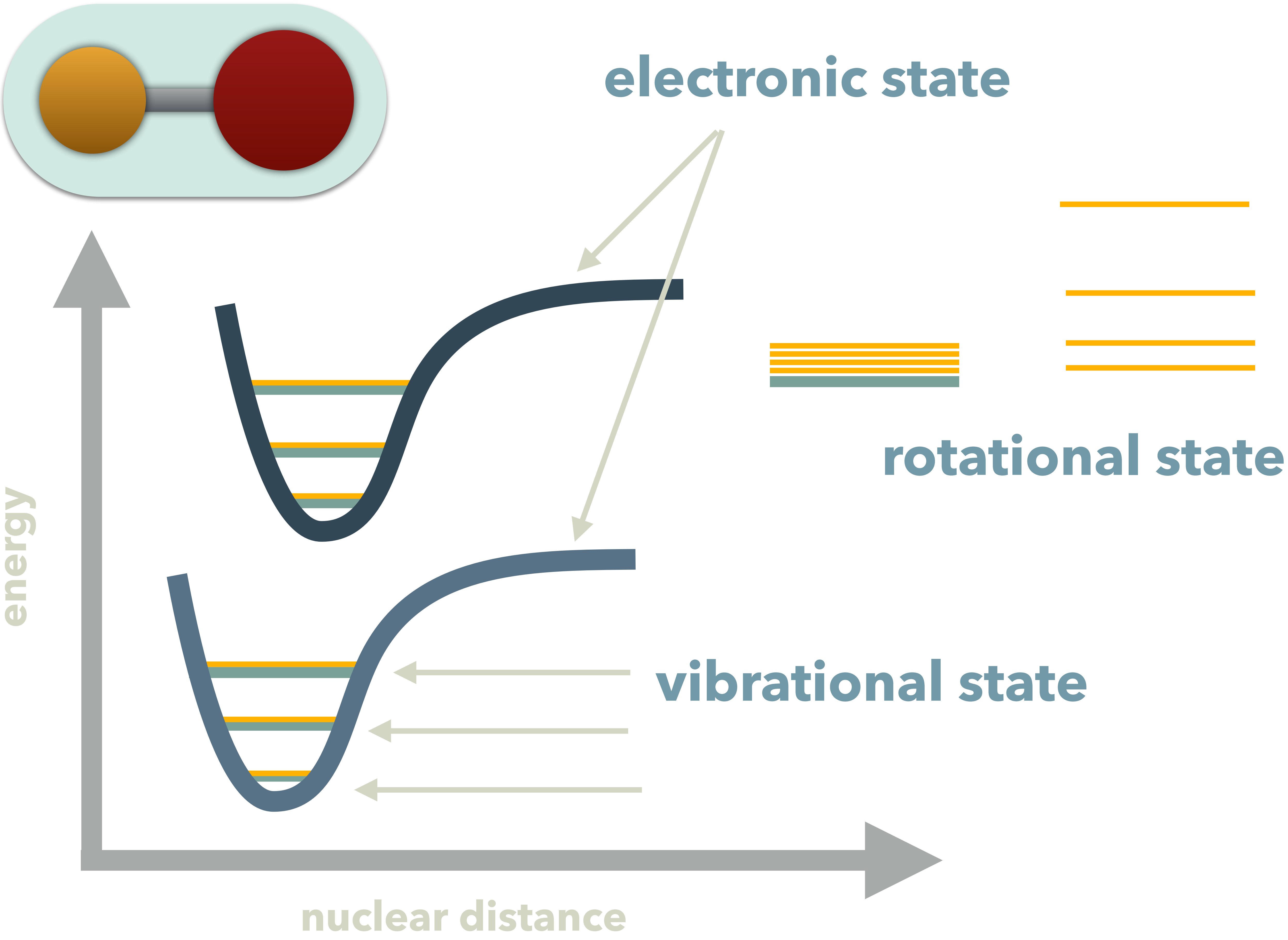
In the universe where $\frac{M_p}{m_e} \sim 10000$

		energy	
electronic transition	10 eV		UV - vis
		1/100	
vibrational transitions	1-10 μm		infrared spectroscopy
		1/100	
rotational transitions	1 mm		sub-mm spectroscopy

CO v=2-0



why do we see many lines?



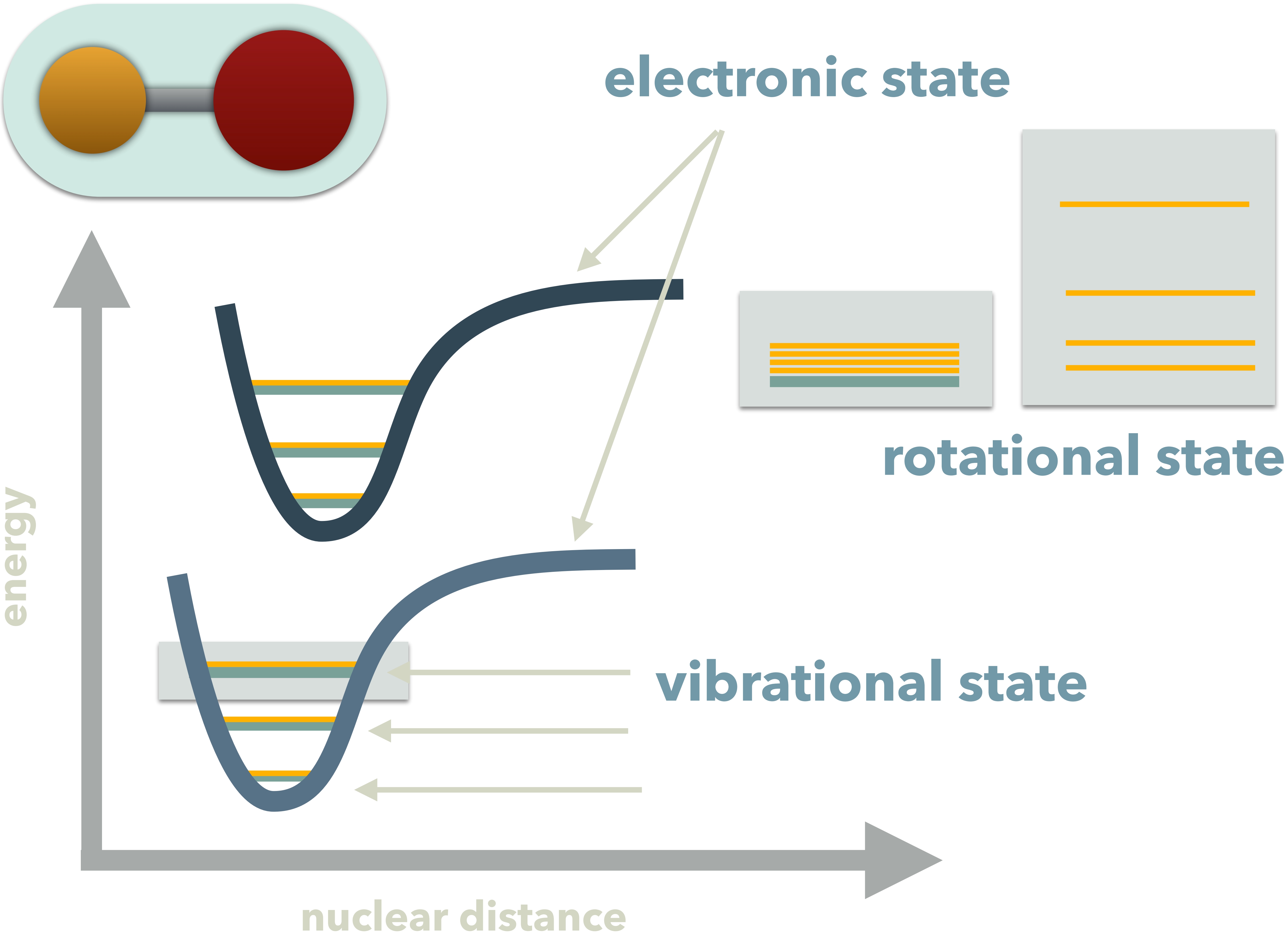
electronic state

rotational state

vibrational state

energy

nuclear distance



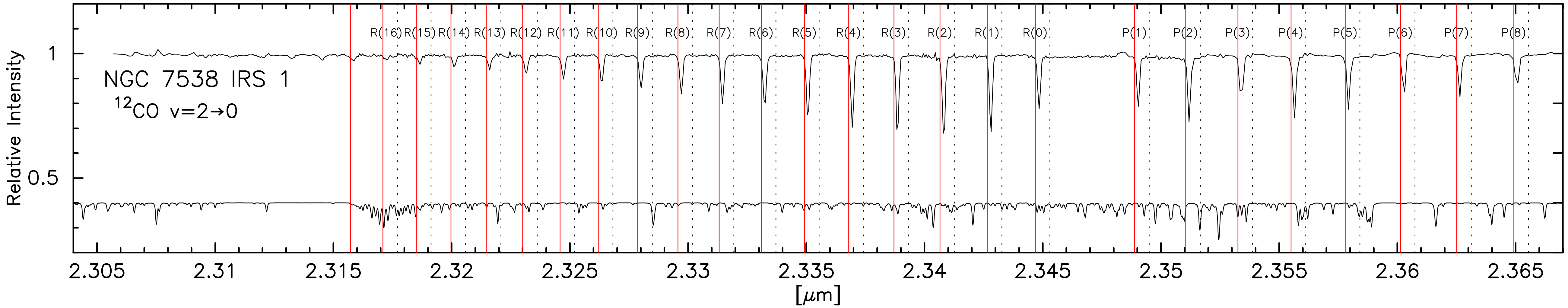
electronic state

rotational state

vibrational state

energy

nuclear distance



R-branch ΔJ = +1

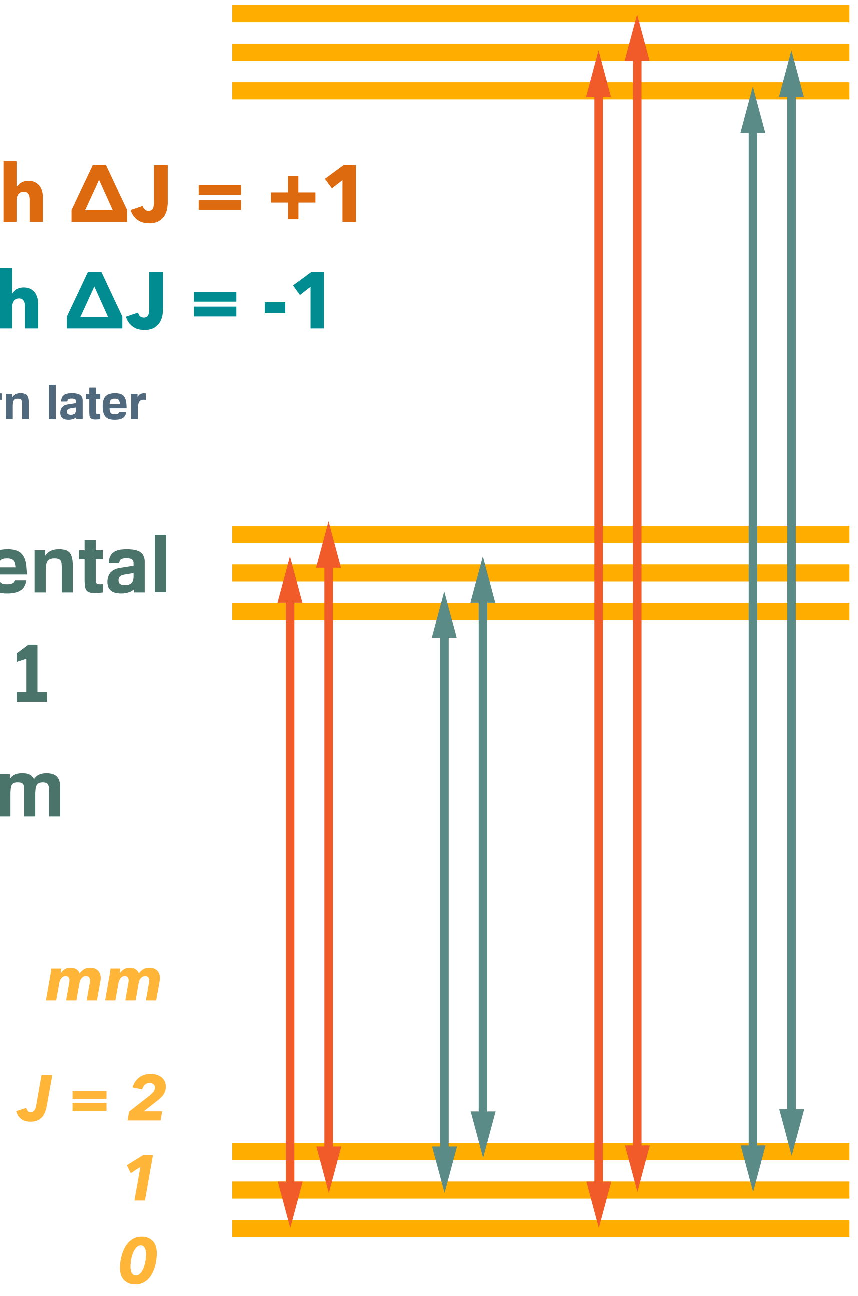
P-branch ΔJ = -1

★ will learn later

fundamental

Δv = 1

4.6 µm



***v* = 2**

overtone

2.3 µm

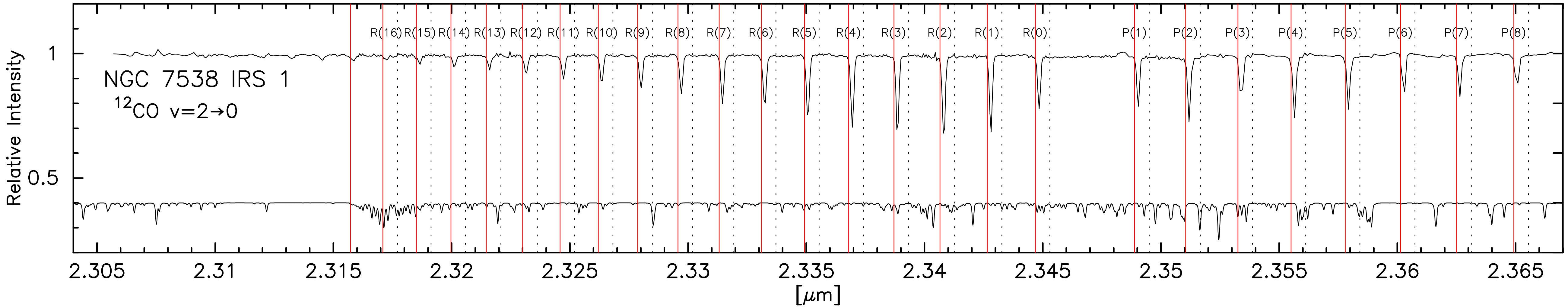
***Δv* = 2**

***v* = 1**

infrared spectroscopy covers many lines in one shot

➡ **population diagram**

***v* = 0**



rotational levels

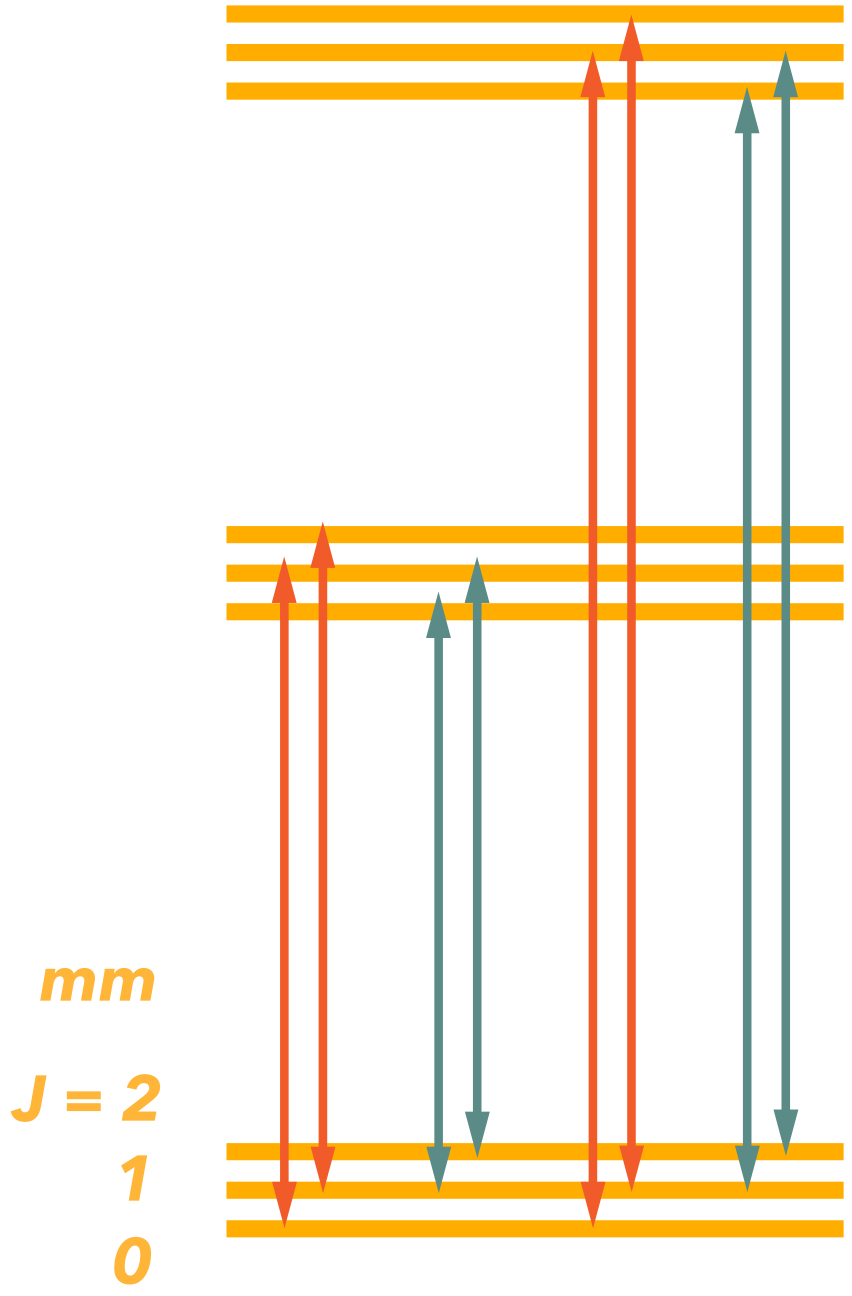
$E_J = BJ(J+1)$

★ will learn later

$J=1\text{–}0$ $E_1\text{-}E_0 = 2B$ 115 GHz

$J=2\text{–}1$ $E_2\text{-}E_1 = 4B$ 230 GHz

$J=3\text{–}2$ $E_3\text{-}E_2 = 6B$ 345 GHz



$E_3 = 12B$

$E_2 = 6B$

$E_1 = 2B$

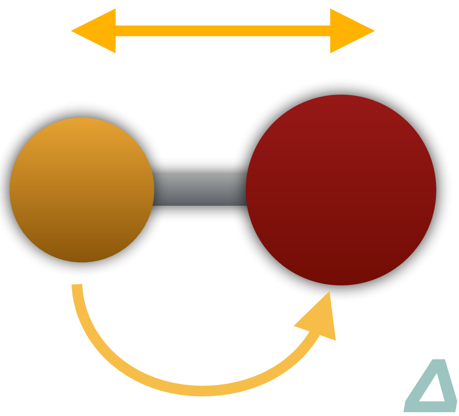
$E_0 = 0B$

have to observe one by one

type of vibration

$v = 1\text{-}0$	**fundamental**
$v = 2\text{-}0$	**first overtone**
$v = 3\text{-}0$	**second overtone**
$v = 2\text{-}1$	**hot band**

CO



1 vibration

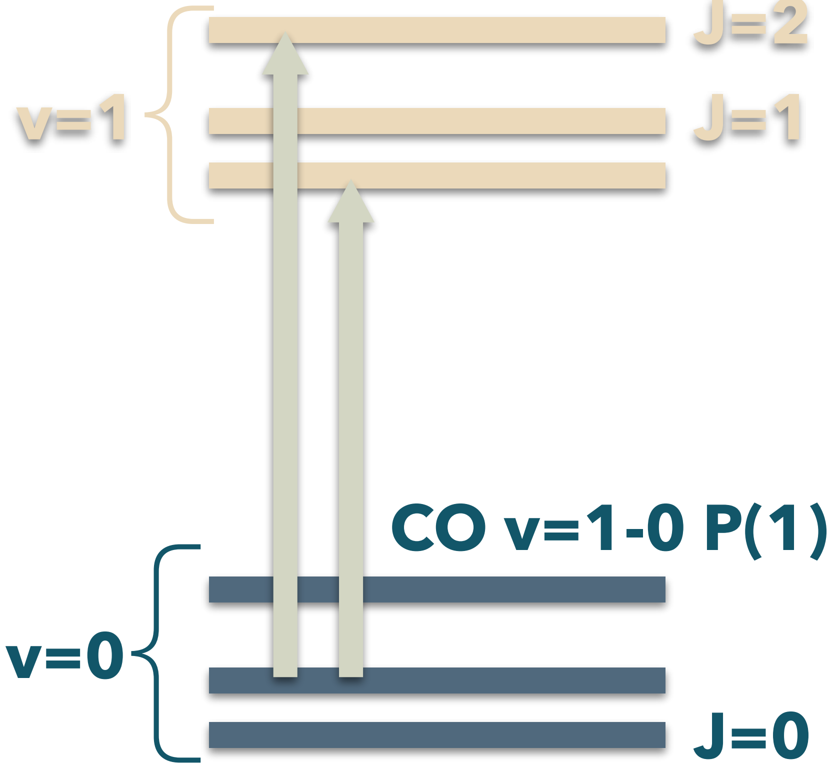
1 rotation

$\Delta J = +-1$

$R: \quad \Delta J = +1$

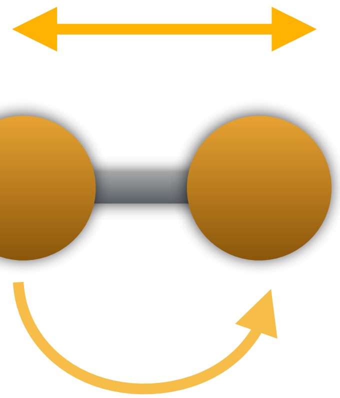
$P: \quad \Delta J = -1$ **only**

CO v=1-0 R(1)



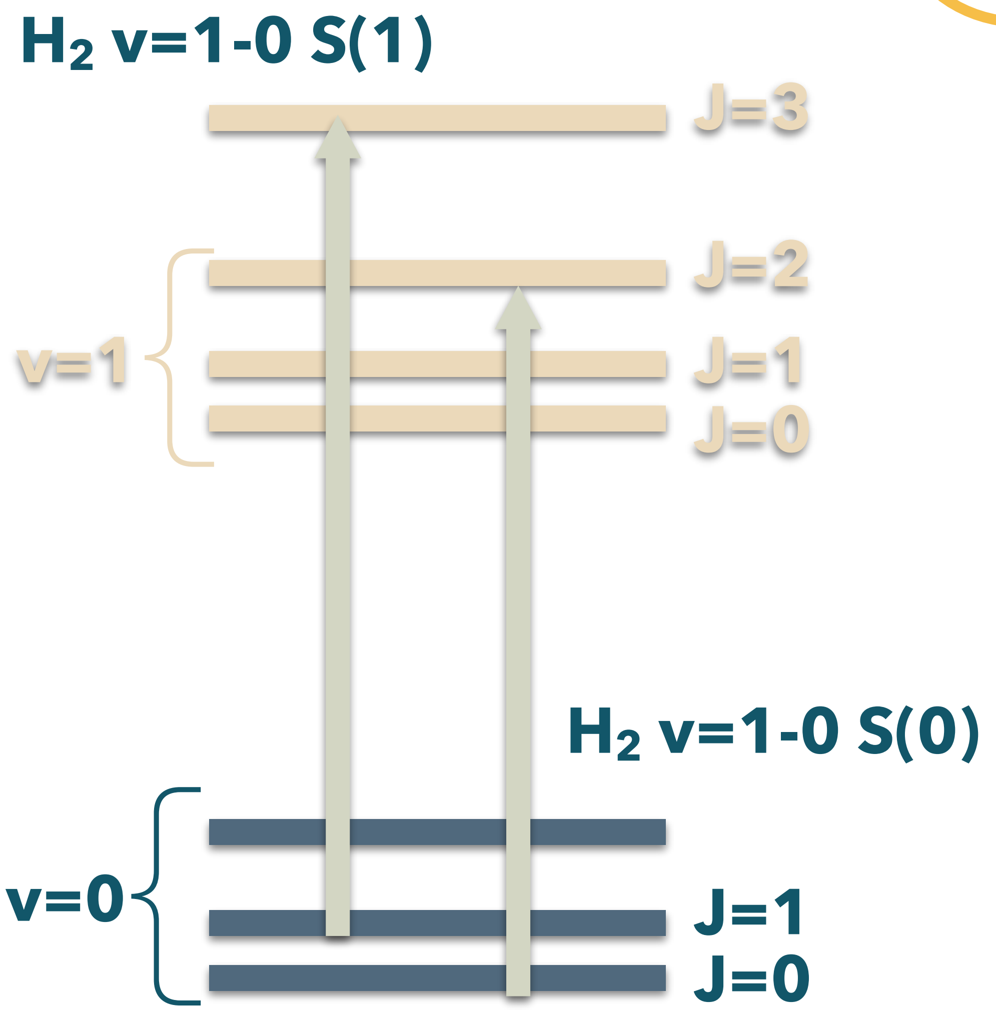
"CO 1-0" usually means CO J=1-0 but confusing

H_2



1 vibration $v = 1\text{-}0$

1 rotation $\Delta J = 0, +\text{-}2, \ldots$



H_2 v=1-0 S(1)

v=1

J=3

J=2

J=1

J=0

H_2 v=1-0 S(0)

v=0

J=1

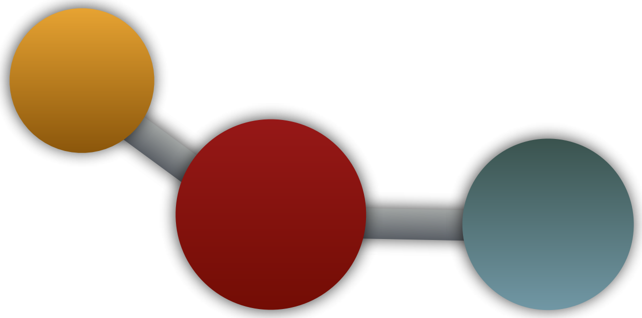
J=0

O, P, Q, R, S, …

$\Delta J =$ **-2, -1, 0, +1, +2**

★ will learn later

non-linear molecule



vibration

change of shape of molecule

bonds distance

bonds angle

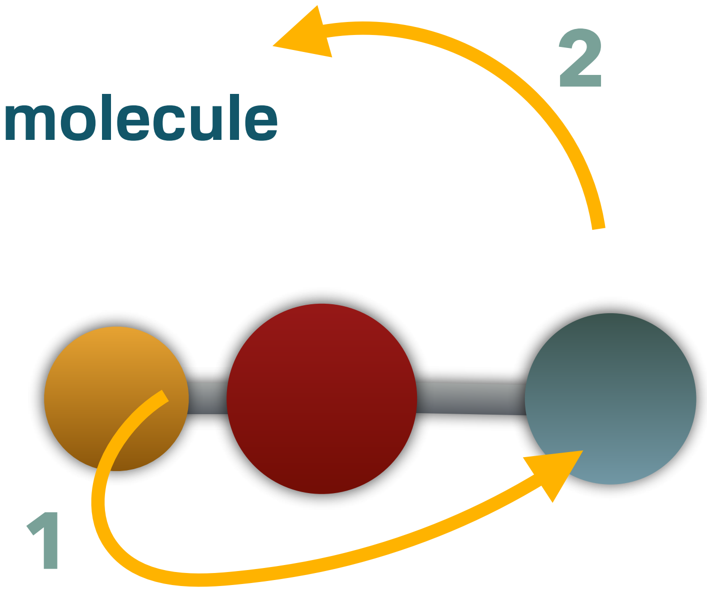
degree of freedom : 3N

translational : -3 does not change molecular shape

rotation : -3 does not change molecular shape

number of vibrational modes : 3N - 6

linear molecule



vibration

change of shape of molecule

bonds distance

bonds angle

degree of freedom : 3N

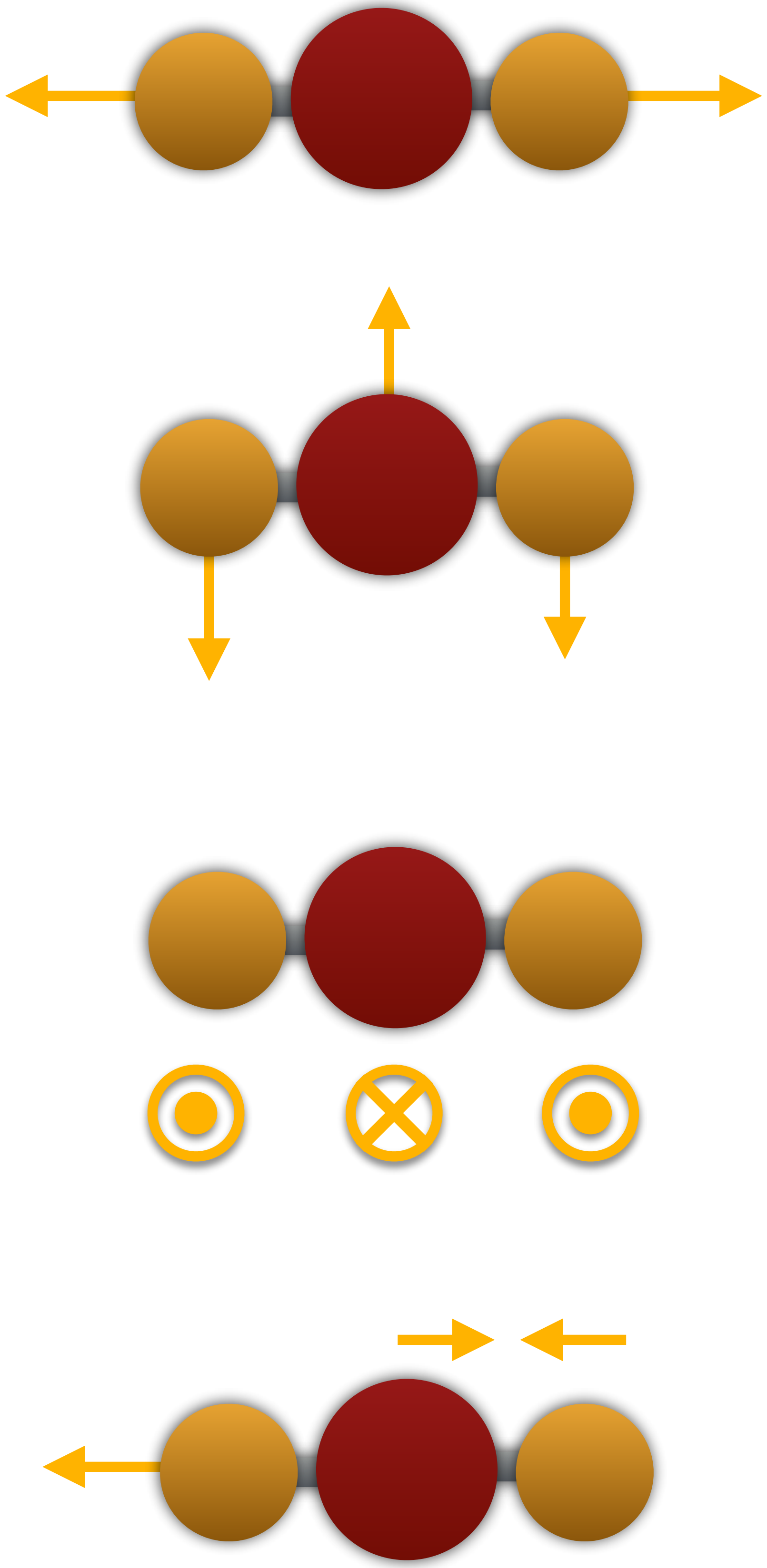
translational : -3 does not change molecular shape

rotation : -2 does not change molecular shape

number of vibrational modes : 3N - 5

CO_2

3N - 5 = 4



higher symmetry
counted first

ν_1

inactive

complicated motion
count later

ν_{2a}

15 µm

ν_1 : symmetric stretch

ν_{2b}

15 µm

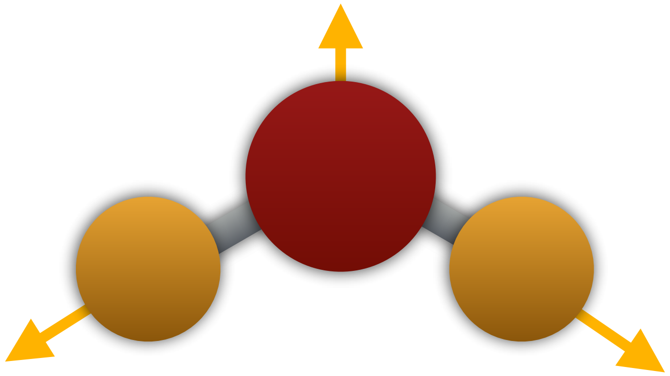
ν_3

4.3 µm

ν_3 : asymmetric stretch

H_2O

$3N - 6 = 3$

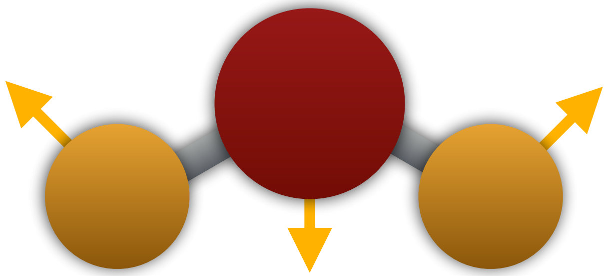


ν_1

3.0 µm

higher symmetry
counted first

complicated motion
count later

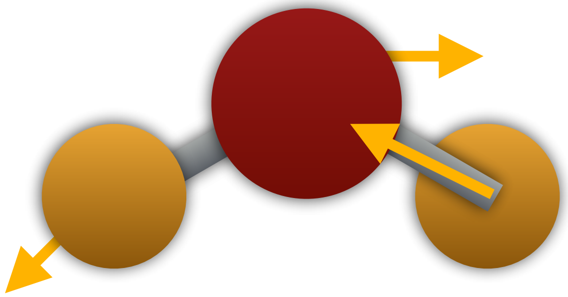


ν_2

6.0 µm

ν_1 : symmetric stretch

ν_2 : bending mode



ν_3

3.0 µm

ν_3 : asymmetric stretch

check with textbooks when doubt

Critical density

you have to be careful to whom to ask

① **optical spectroscopist**

AGN

extragalactic

② **sub-mm, rotational lines**

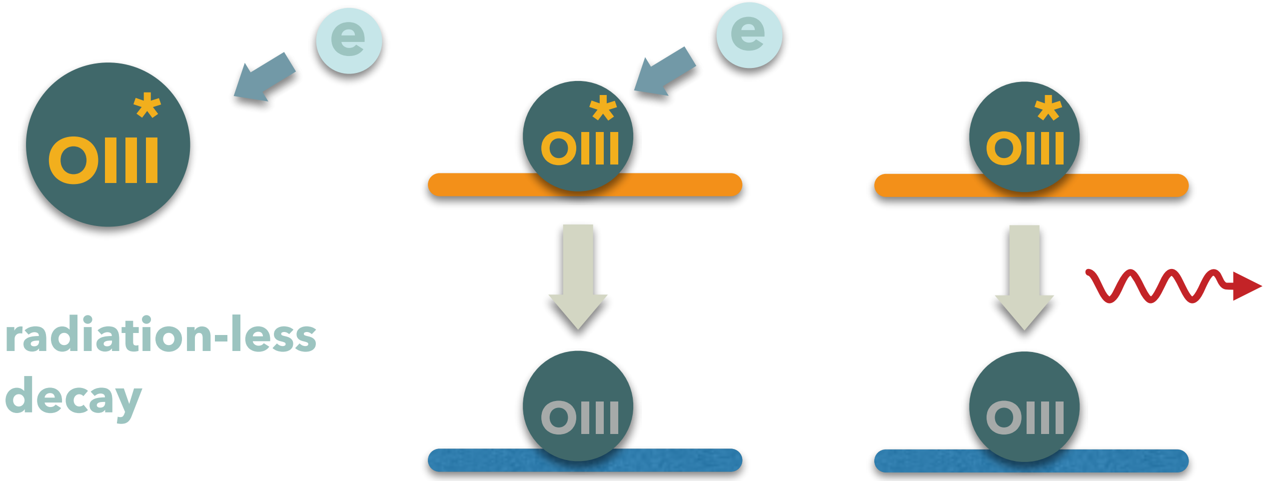
molecular cloud

[OIII] forbidden line

5007 A

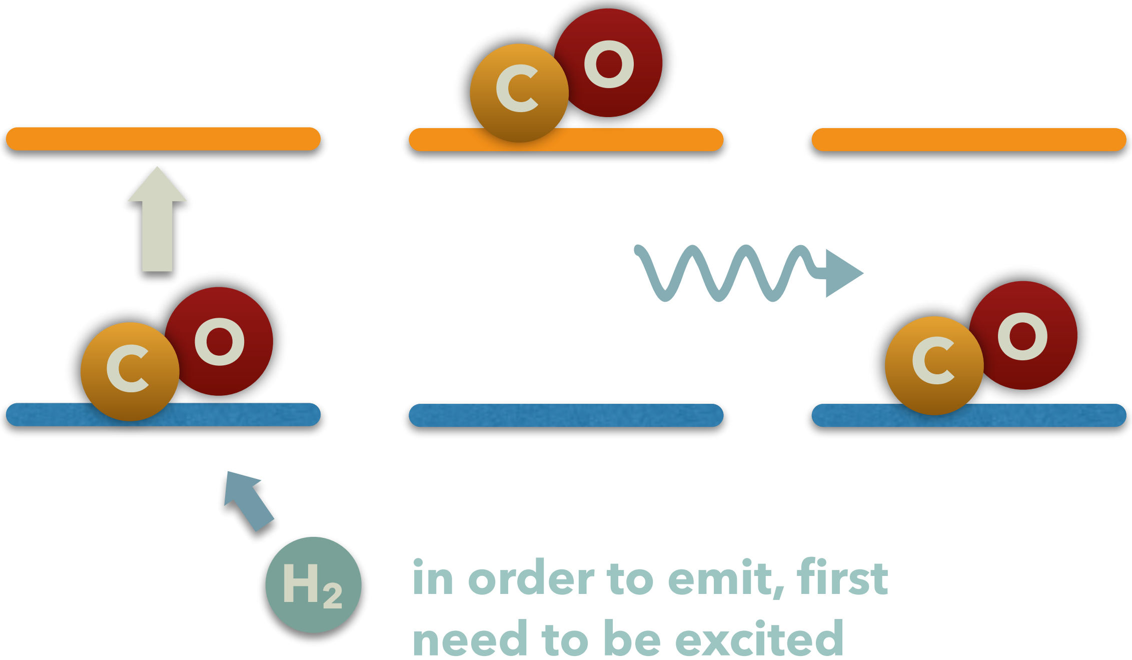
CO J=1-0 permitted

2.6 mm



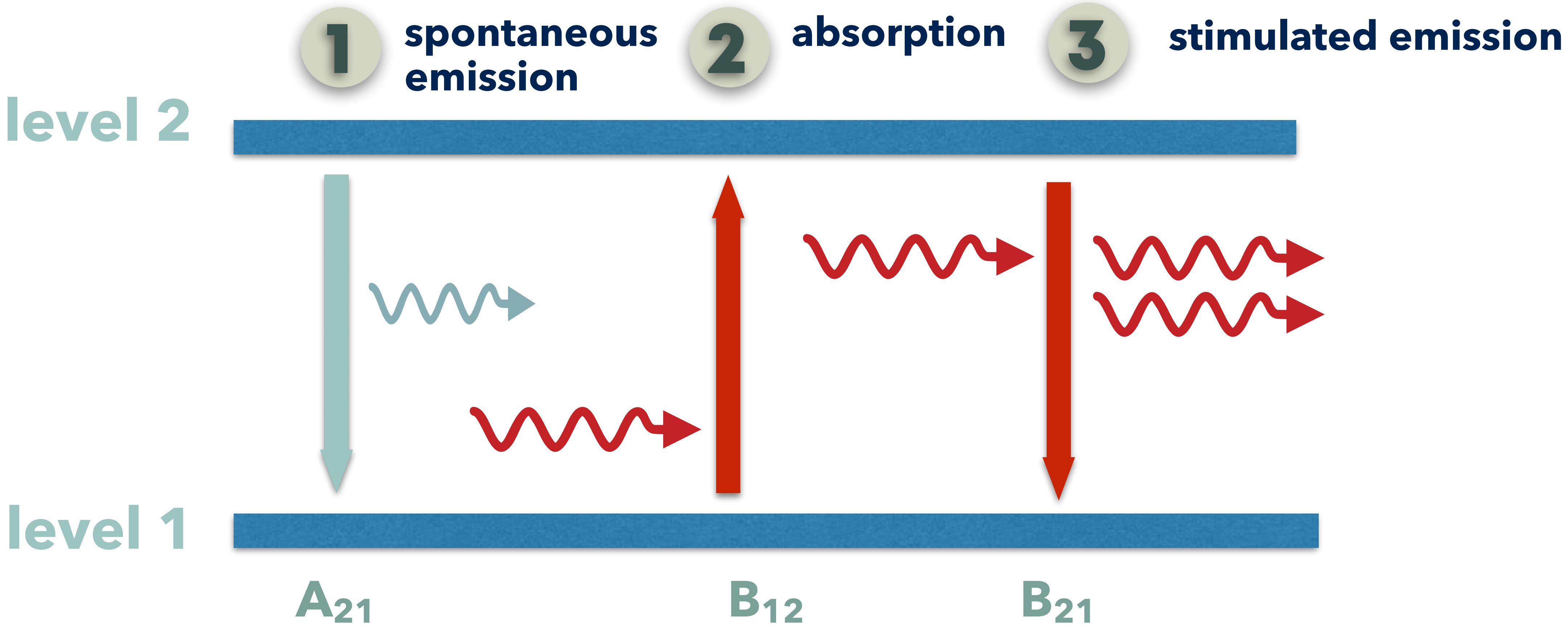
radiation-less decay

need enough time to radiate



in order to emit, first need to be excited

Einstein coefficient



① spontaneous emission

② absorption

③ stimulated emission

level 2

level 1

A_{21}

B_{12}

B_{21}

$$J = \frac{1}{4\pi}\int I \ \ d\Omega$$

system we were talking about

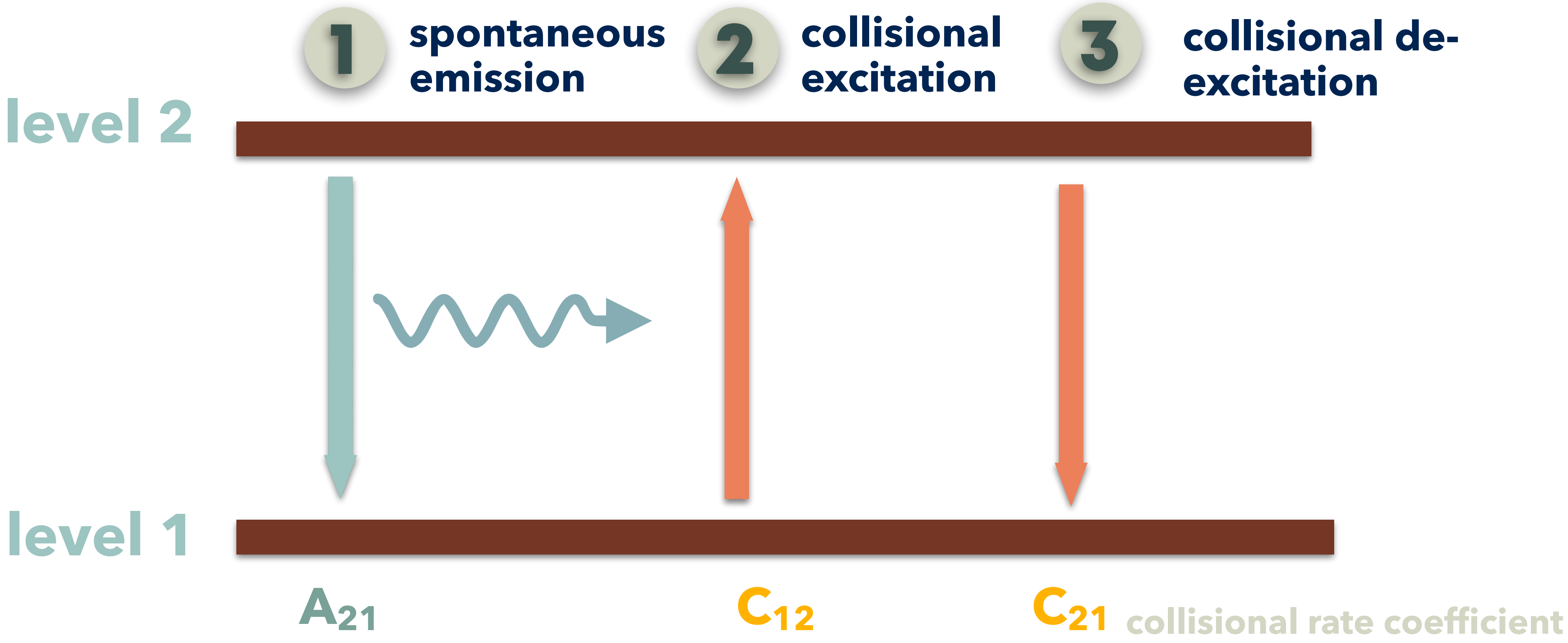
no collision

radiation only

two levels

thermal equilibrium

Collision dominated



① spontaneous emission

② collisional excitation

③ collisional de-excitation

level 2

level 1

A_{21}

C_{12}

C_{21} collisional rate coefficient

$$J = \frac{1}{4\pi}\int I \;\; d\Omega$$

↓

n_e

n_{H2}

density

system we were talking about

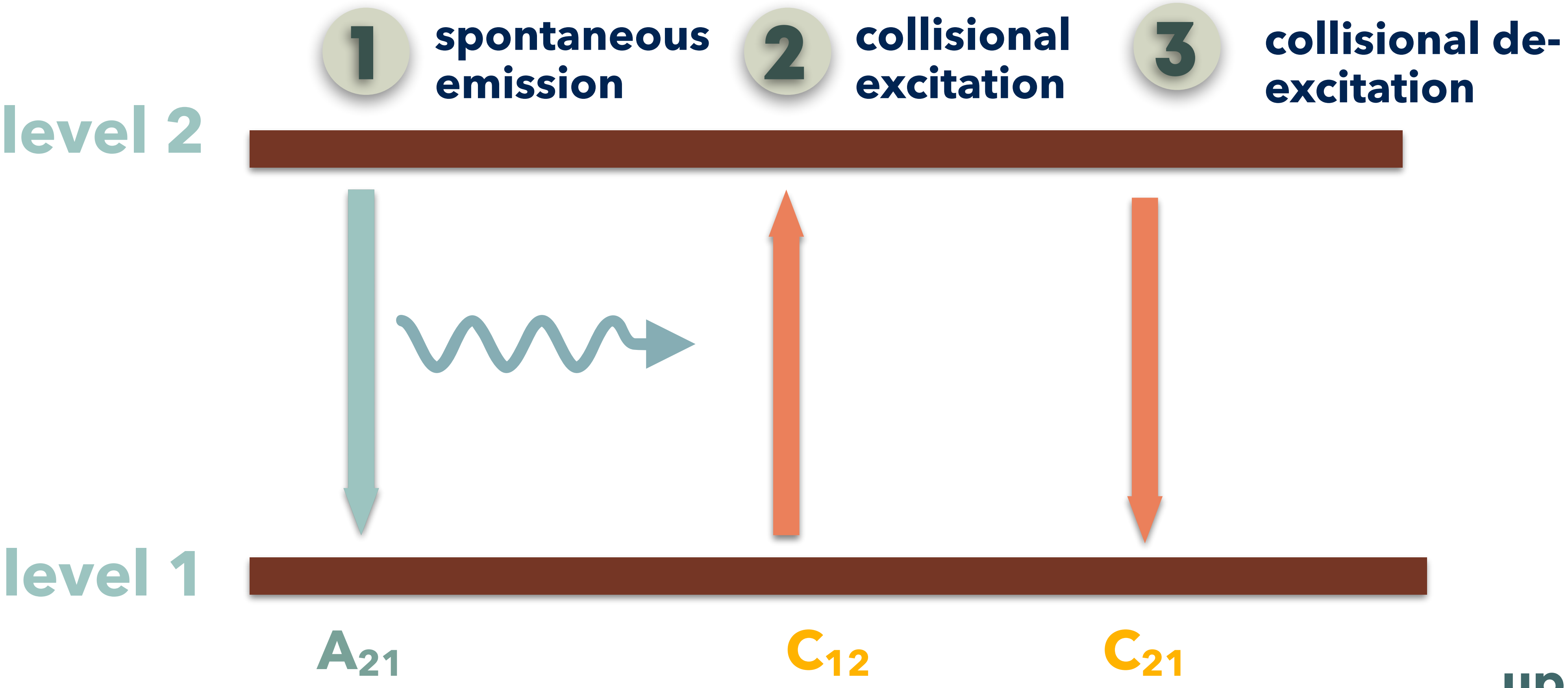
no collision → collision only

radiation only → no radiation

two levels

thermal equilibrium

Collision dominated



① **spontaneous emission**

② **collisional excitation**

③ **collisional de-excitation**

level 2

level 1

A_{21}

C_{12}

C_{21}

$$J = \frac{1}{4\pi}\int I \, d\Omega$$

n_e

n_{H2}

density

system we are talking about

collision only

no radiation

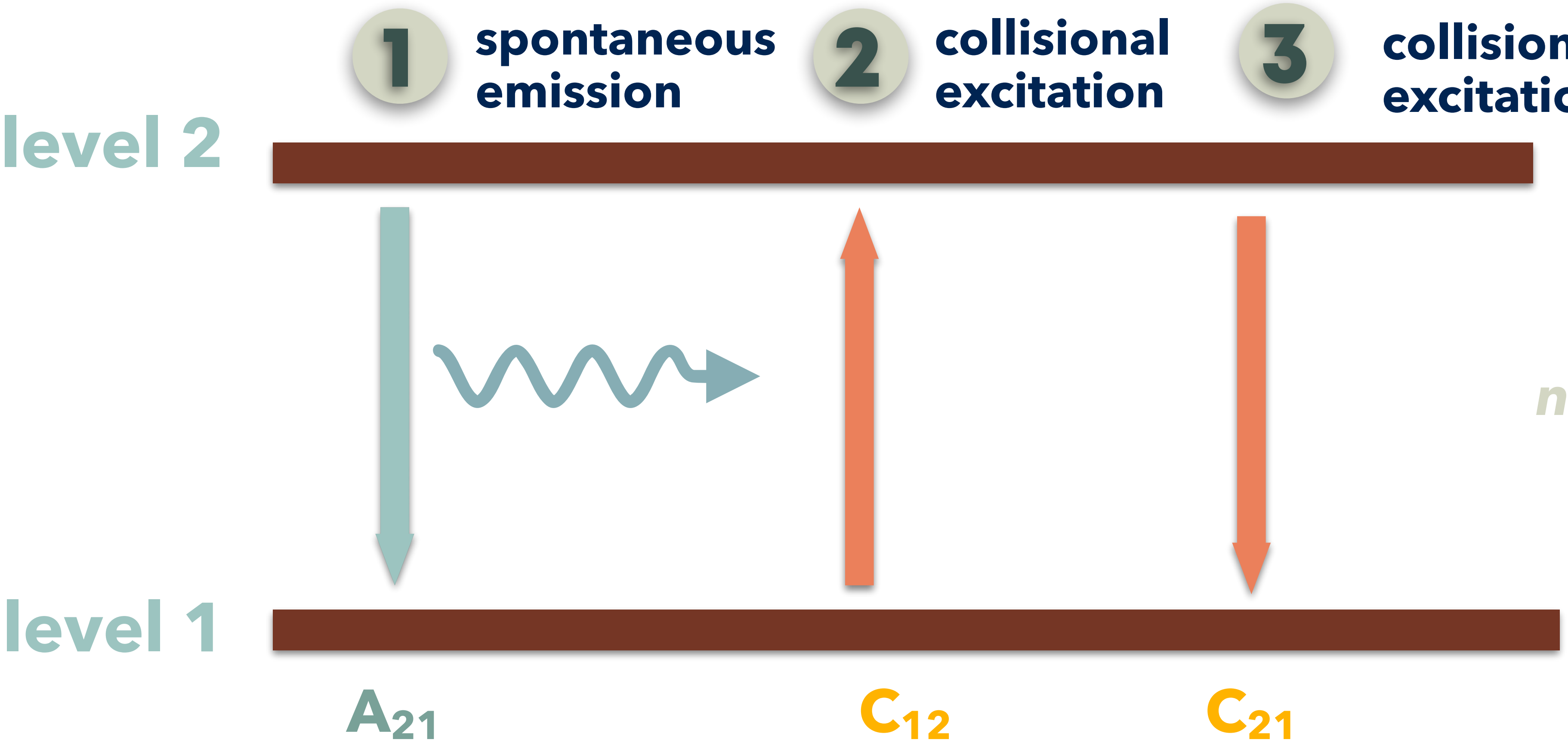
two levels

thermal equilibrium

$$\overbrace{Jn_1B_{12}}^{\text{up}} = \overbrace{n_2A_{21} + Jn_2B_{21}}^{\text{down}}$$

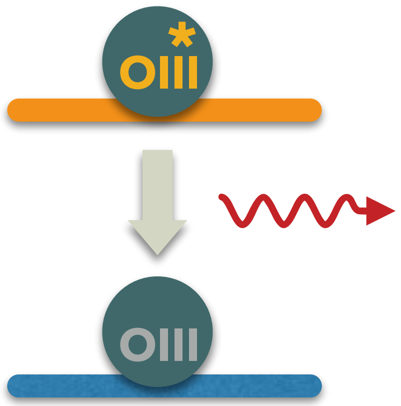
$$n_H n_1 C_{12} = n_2 A_{21} + n_H n_2 C_{21}$$

Collision dominated



$$n_H n_1 C_{12} = n_2 A_{21} + n_H n_2 C_{21}$$

1 need enough time to radiate

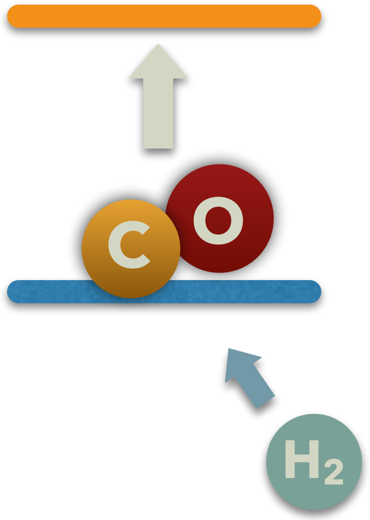


$$n_2 A_{21} > n_H n_2 C_{21}$$

$$n_H = \frac{A_{21}}{C_{21}}$$

critical density

2 in order to emit, first need to be excited

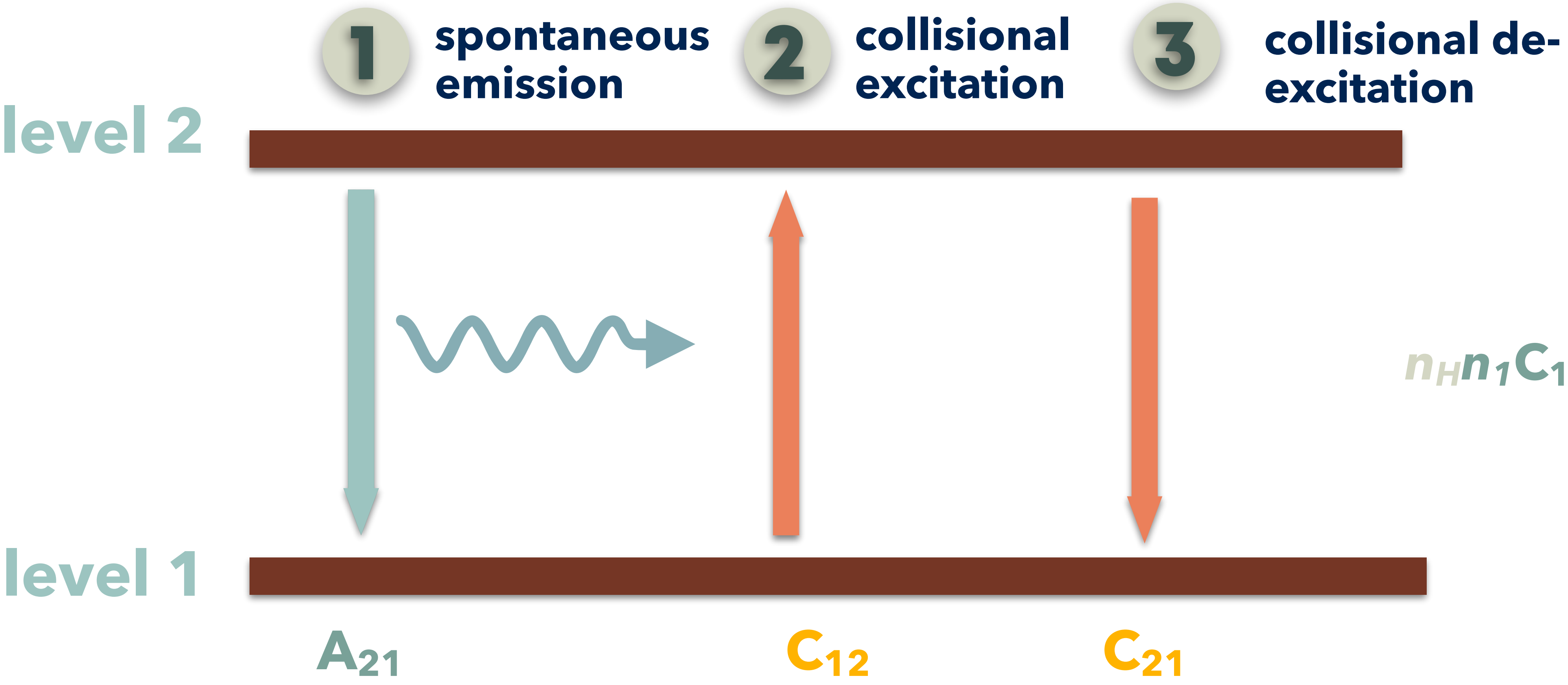


$$n_H n_1 C_{12} > n_2 A_{21}$$

$$n_H = \frac{n_2 A_{21}}{n_1 C_{12}}$$

critical density

Collision dominated



① spontaneous emission ② collisional excitation ③ collisional de-excitation

level 2

level 1

A_{21} C_{12} C_{21}

$$n_H n_1 C_{12} = n_2 A_{21} + n_H n_2 C_{21}$$

now a trick

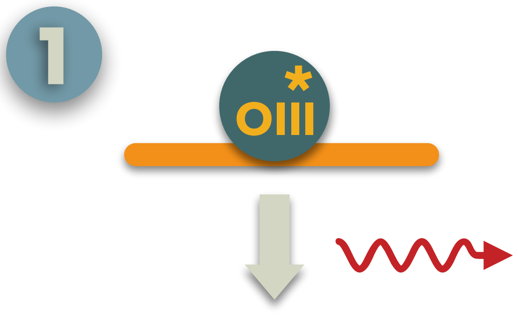
C_{12}, C_{21} are parameters you can calculate from molecular cross section and T_k

independent from n_H

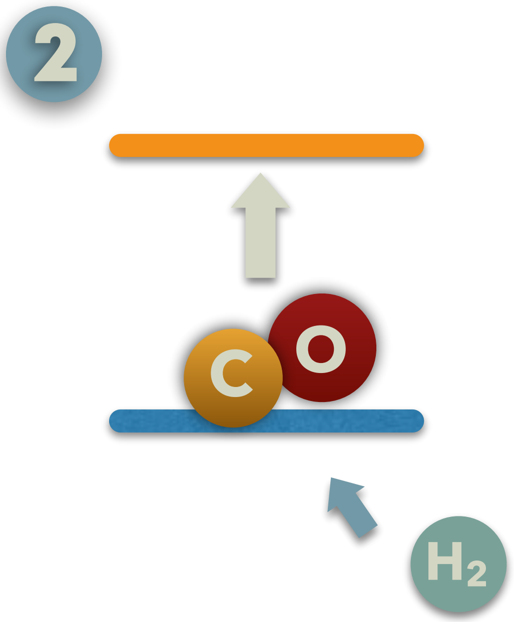
let's increase $n_H \gg 1$

level population is controlled collision only

$$n_1 C_{12} = n_2 C_{21}$$



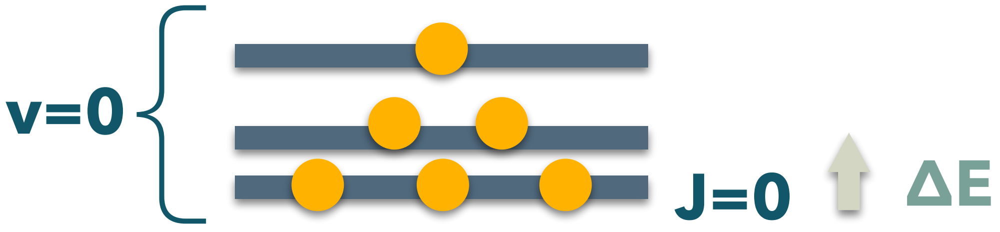
$$n_H = \frac{A_{21}}{C_{21}}$$



$$n_H = \frac{n_2 A_{21}}{n_1 C_{12}}$$

When to observe what?

sub-mm rotational emission lines



$$n_{cr} = \frac{A_{21}}{C_{21}} \quad \frac{[s^{-1}]}{[cm^3\ s^{-1}]} \quad [cm^{-3}]$$

① molecules has to exist

$n_X > 10^{-10} \times n_{H2}$

② a molecular line prove medium that is about

$n_{H2} \sim n_{cr}$

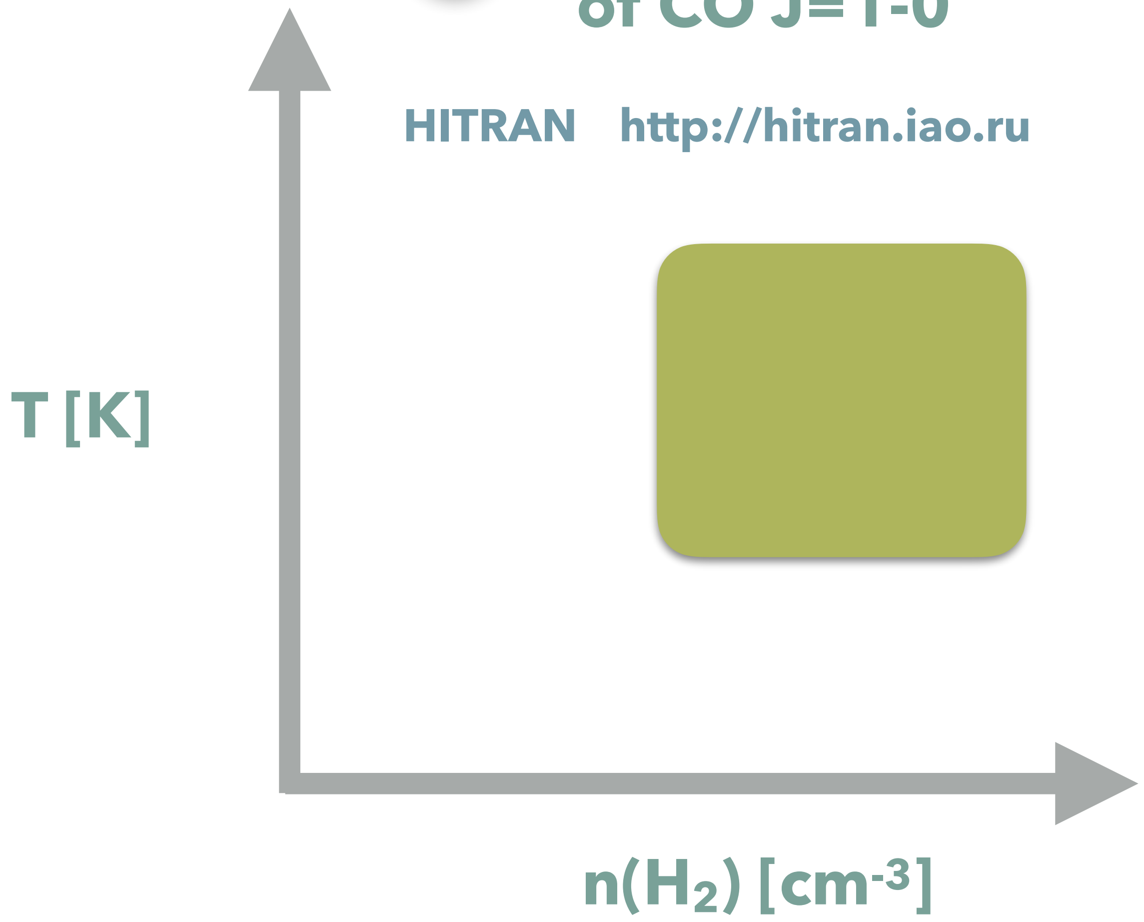
③ medium has to be warm about

$kT \sim \Delta E$

④ desirably not optically thick

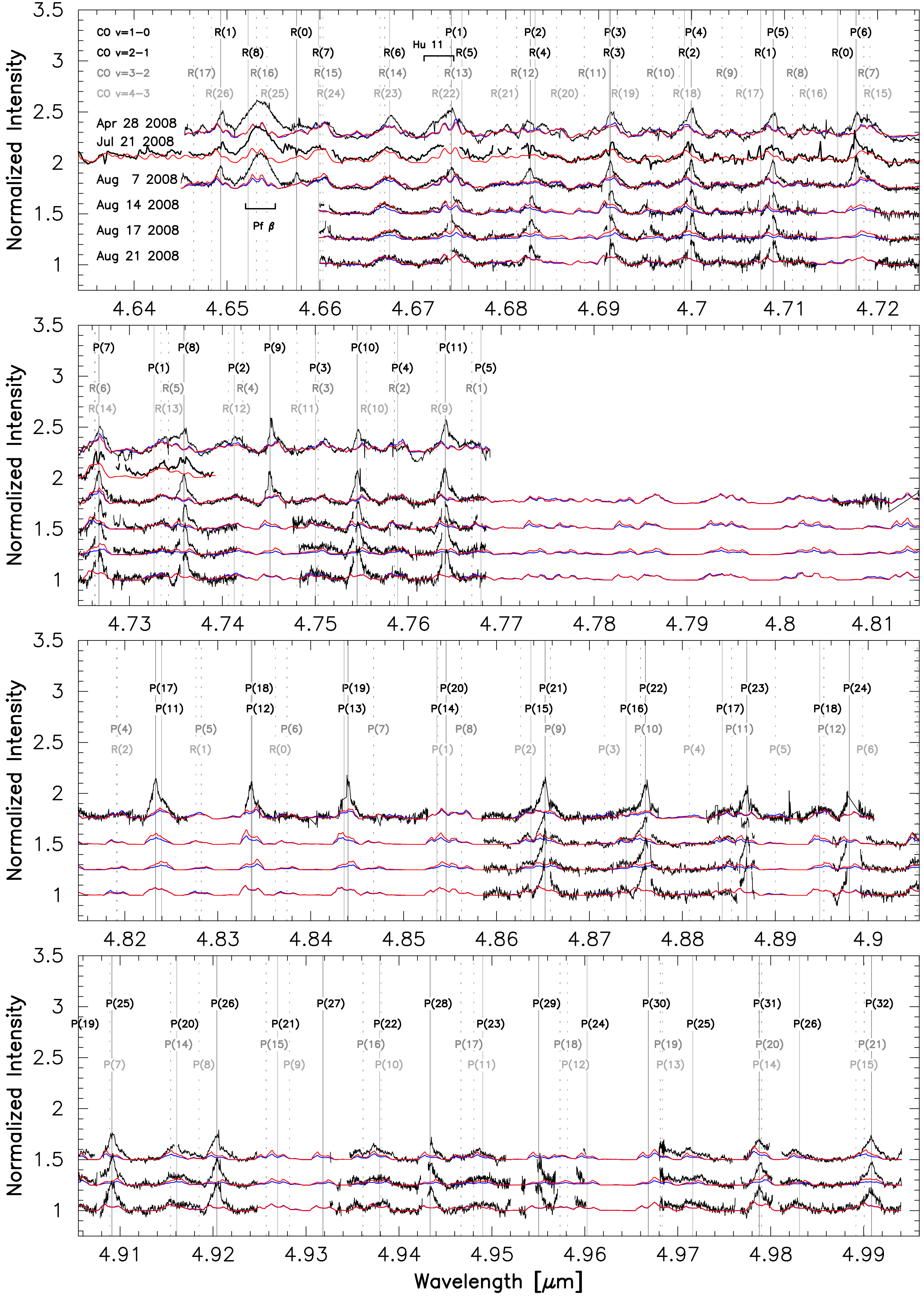
① Find sweet spot of CO J=1-0

HITRAN http://hitran.iao.ru

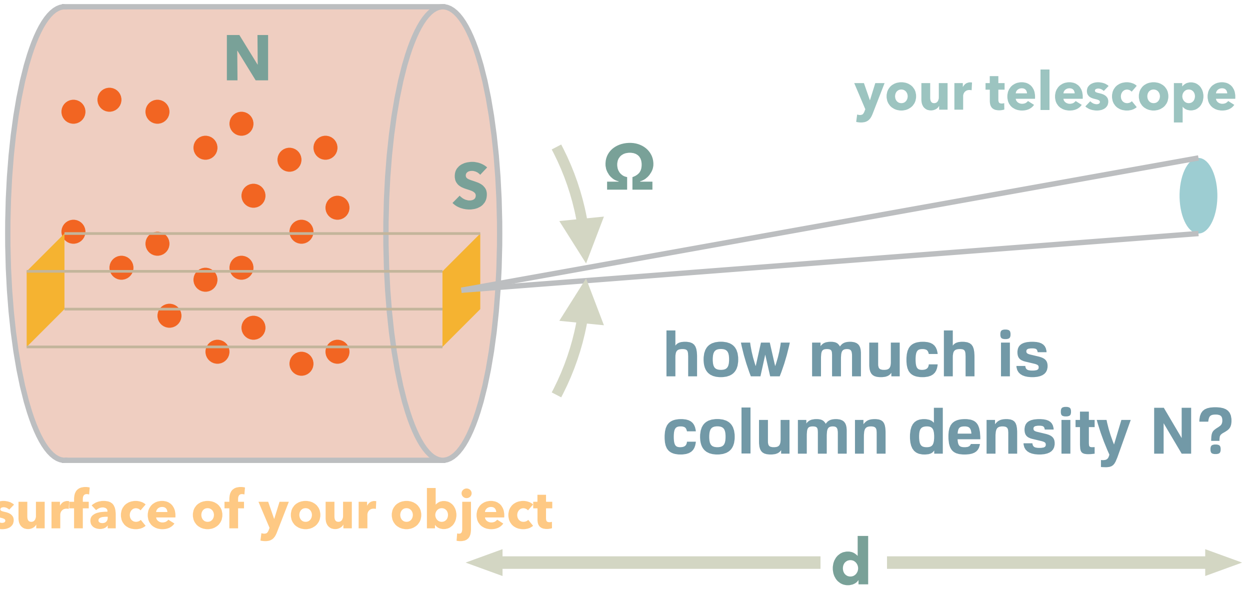


v=0-0	v=0-0
CO J=1-0	H_2 J=2-0
2-1	
3-1	C : 3e-11 [cm³ s⁻¹]

How to derive physical parameter from your observation?



emission

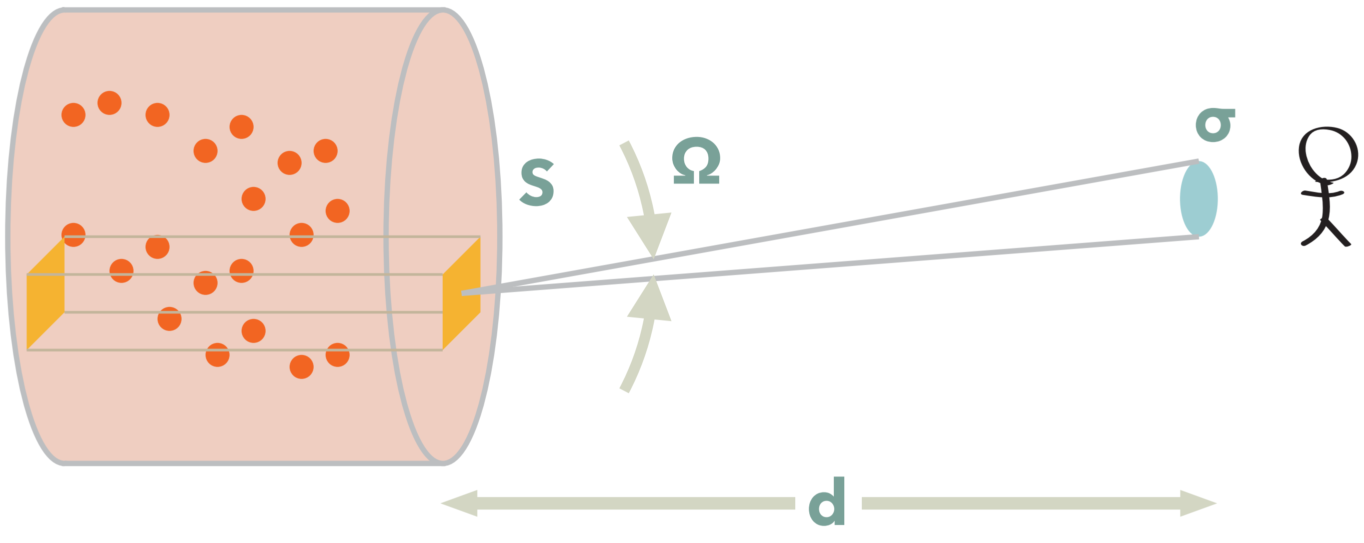


how much is
column density N?

optically thin
no background

energy you received

$$E = N \frac{A_{21}}{4\pi} \cdot h\nu \, \Omega S$$

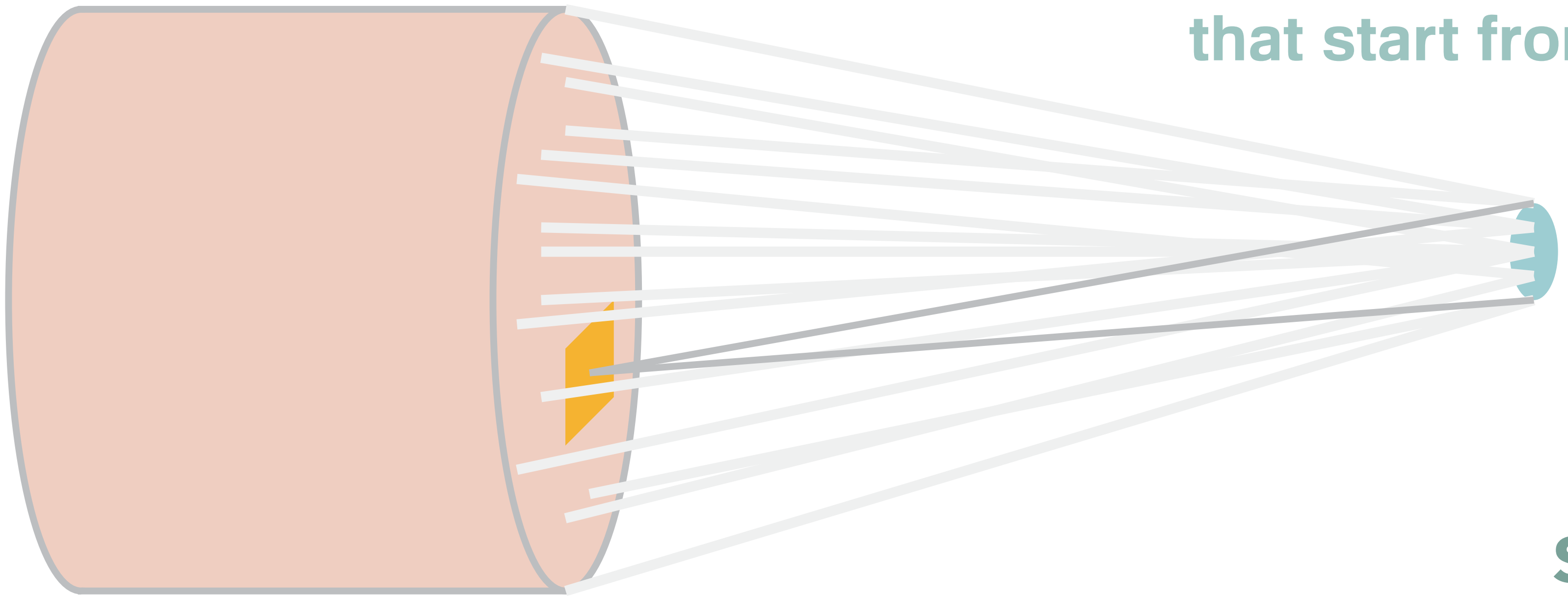


$$\Omega = \frac{\sigma}{d^2}$$

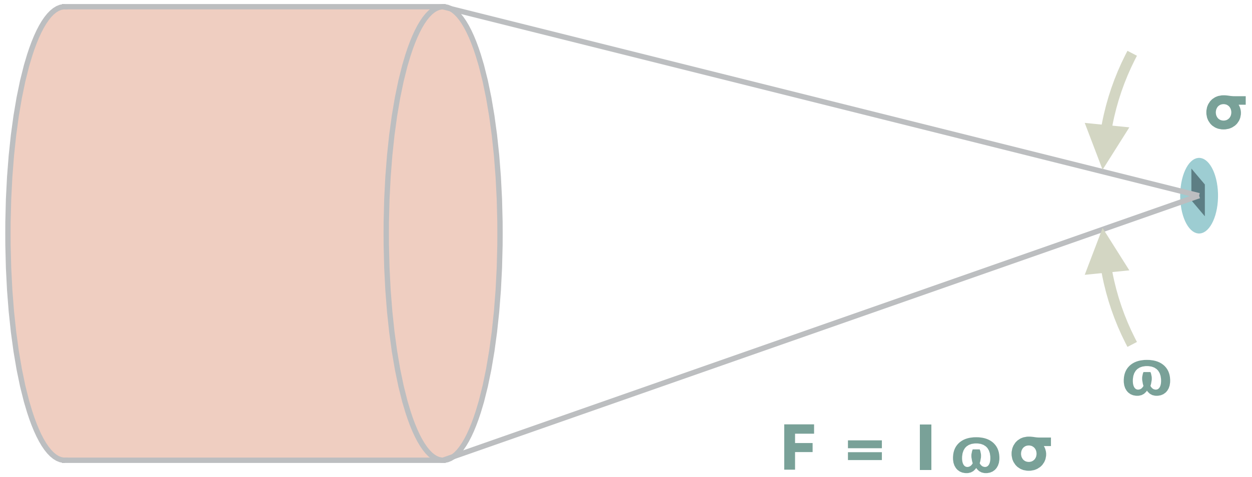
$$F = I\,\Omega\,S$$

draw all possible rays

that start from S and hit σ



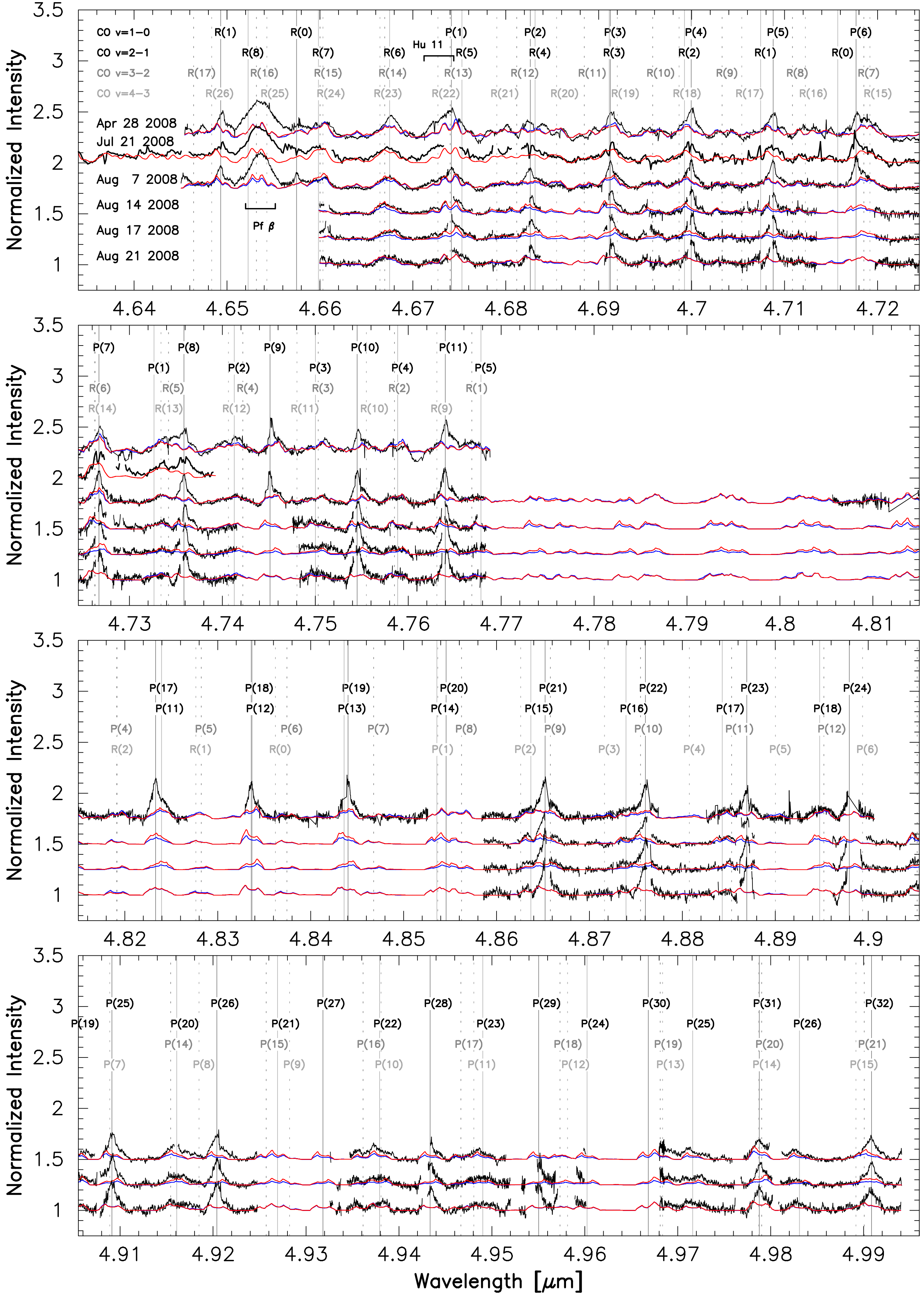
$$\varpi = \frac{S}{d^2}$$

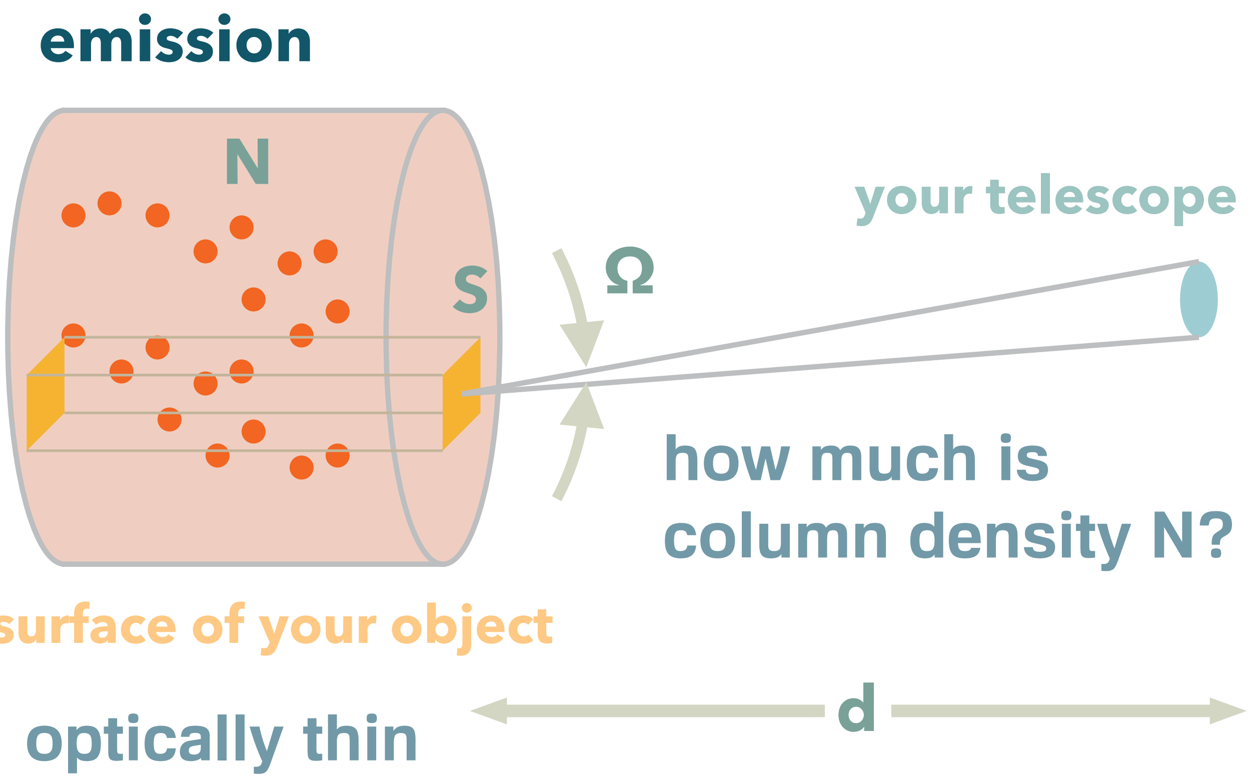


$$\Omega S = \frac{\sigma S}{d^2} = \varpi\,\sigma$$

$$F = I\,\varpi\,\sigma$$

How to derive physical parameter from your observation?





emission

your telescope

how much is column density N?

surface of your object

optically thin
no background

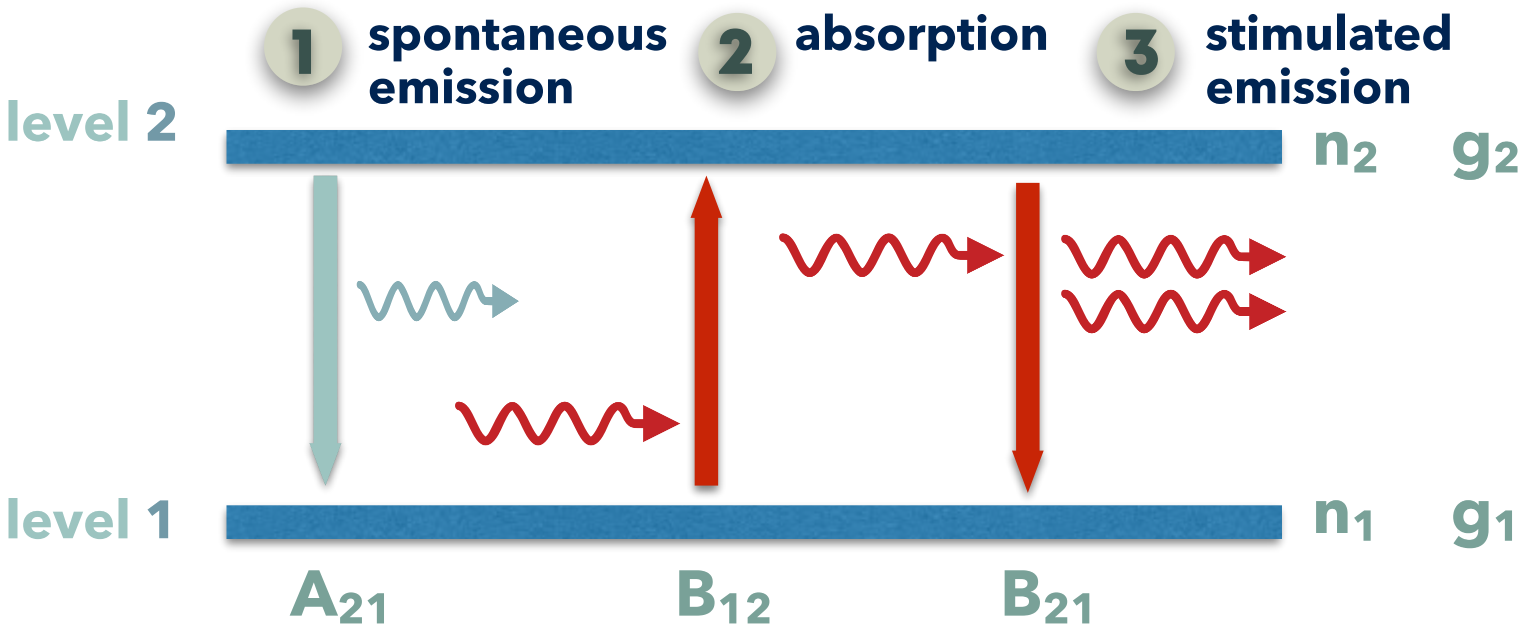
$$F = I \Omega S$$
$$= I \varpi \sigma$$

energy you received

$$E = N \frac{A_{21}}{4\pi} \cdot h\nu \, \Omega S$$

$$= N \frac{A_{21}}{4\pi} \cdot h\nu \, \varpi \sigma$$

absorption

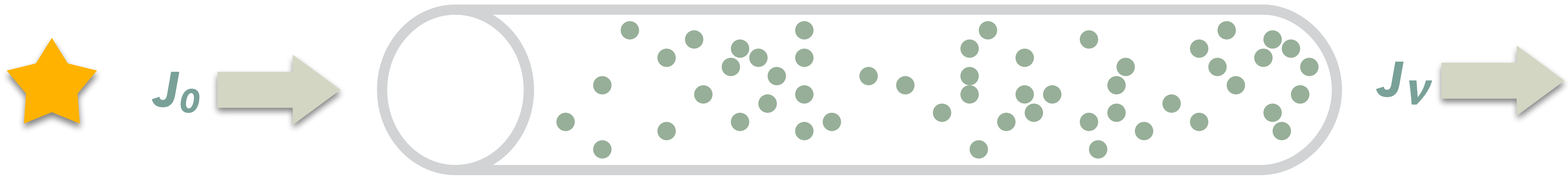


$h\nu >> kT \qquad n_2 << n_1$

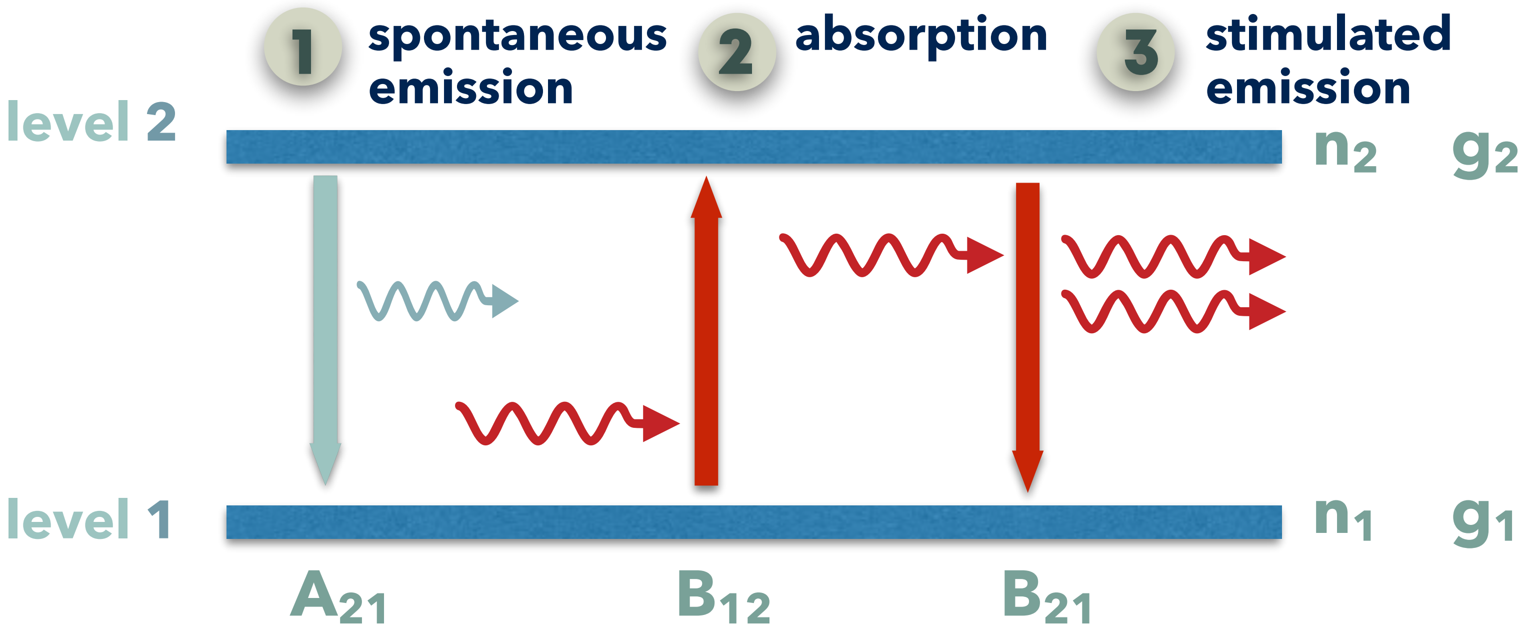
negative absorption negligible

$$\frac{A_{21}}{B_{21}} = \frac{2h\nu^3}{c^2}$$

$$B_{12} = \frac{g_2}{g_1} B_{21}$$



absorption



$h\nu >> kT$ $n_2 << n_1$

negative absorption negligible

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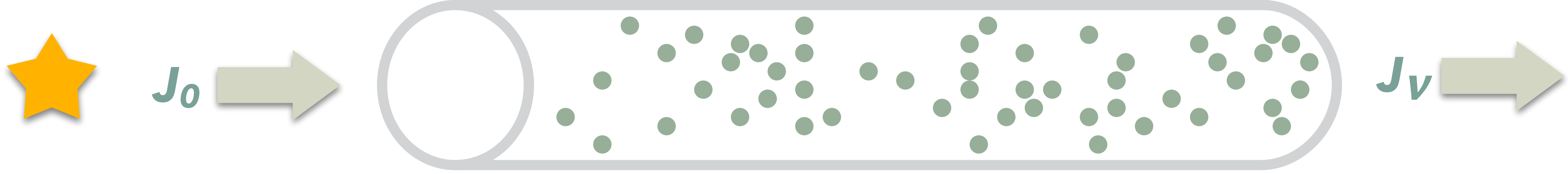


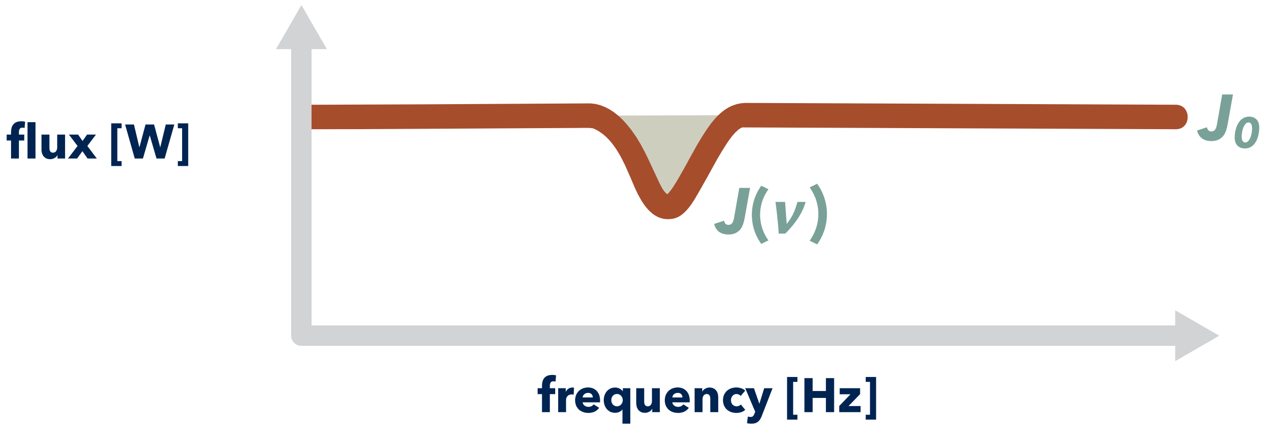
energy lost in absorption $$\Delta E = \overset{\text{number of transition}}{J_0 N_1 B_{12}} \cdot \overset{\text{energy absorbed in one transition}}{h\nu}$$

$$\Delta E = \int J_0 - J(\nu)\ d\nu$$

$$J_0 - J(\nu) = J_0 N_1 B_{12} \cdot h\nu$$

$$\frac{J_0 - J(\nu)}{J_0} = N_1 B_{12} \cdot h\nu$$

we do not need to know absolute flux



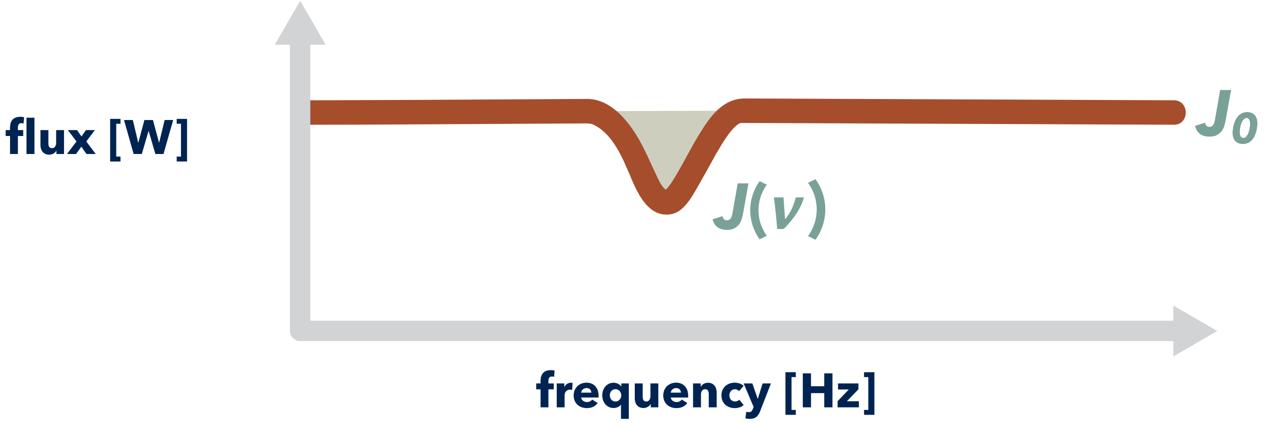
energy lost in absorption $\Delta E = J_0 N_1 B_{12} \cdot h\nu$

$$\Delta E = \int J_0 - J(\nu) \; d\nu$$

$$J_0 - J(\nu) = J_0 N_1 B_{12} \cdot h\nu$$

$$\frac{J_0 - J(\nu)}{J_0} = N_1 B_{12} \cdot h\nu$$

we do not need to know absolute flux



energy lost in absorption

$$\Delta E = J_0 N_1 B_{12} \cdot h\nu$$

$$\Delta E = \int J_0 - J(\nu) \; d\nu$$

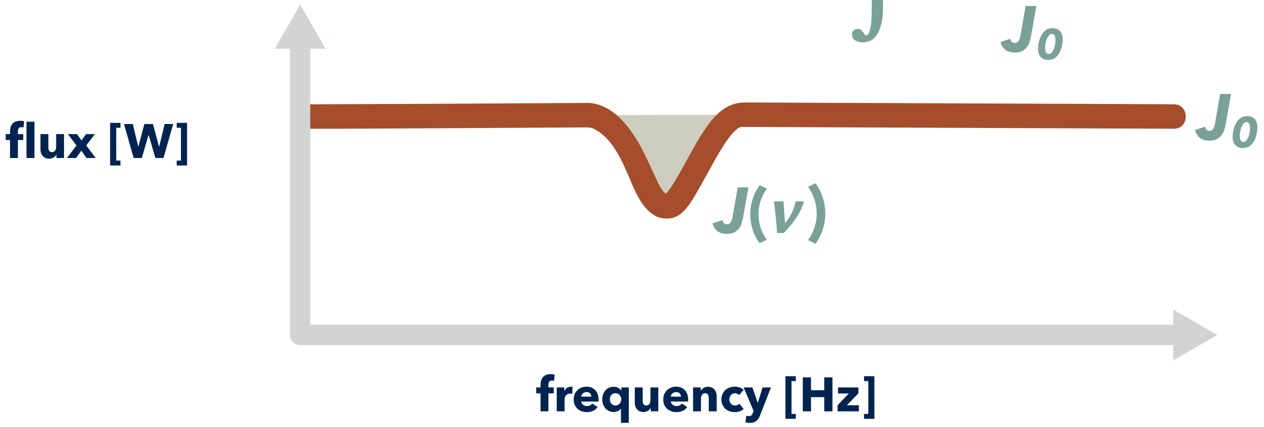
$$J_0 - J(\nu) = J_0 N_1 B_{12} \cdot h\nu$$

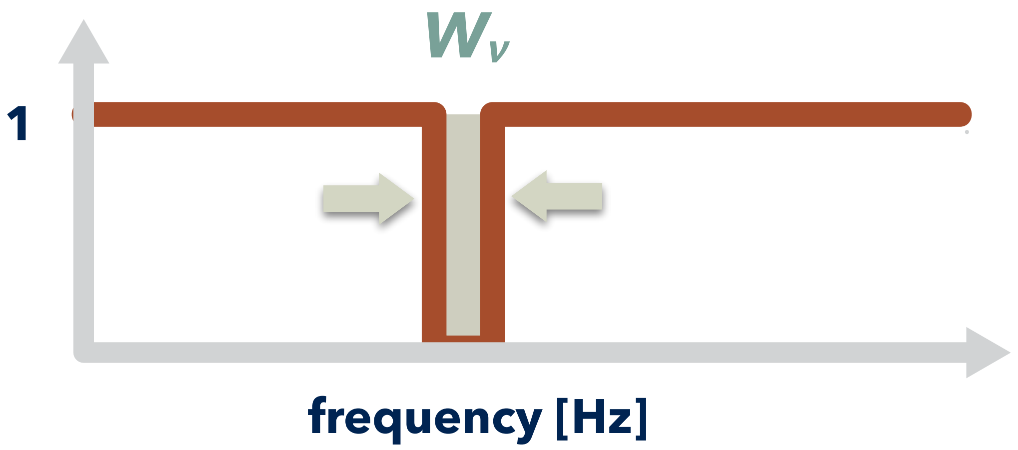
$$\frac{J_0 - J(\nu)}{J_0} = N_1 B_{12} \cdot h\nu$$

we do not need to know absolute flux

equivalent width

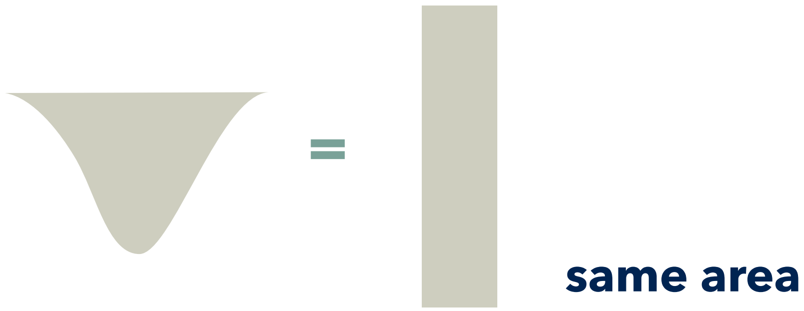
$$W_\nu = \int \frac{J_0 - J(\nu)}{J_0} d\nu$$





in the unit of

[Hz]
[cm-1]
[um]



energy lost in absorption

$$\Delta E = J_0 N_1 B_{12} \cdot h\nu$$

$$\Delta E = \int J_0 - J(\nu)\ d\nu$$

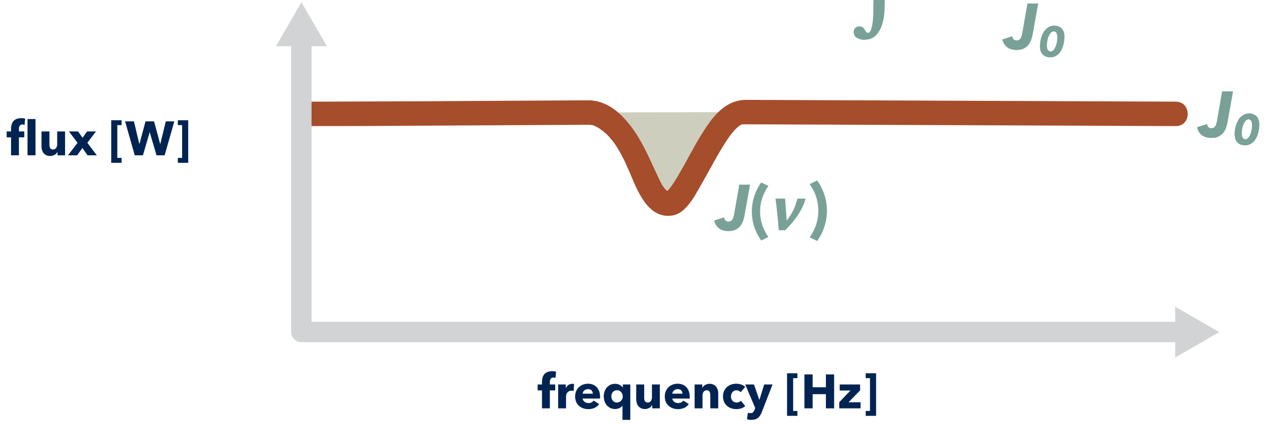
$$J_0 - J(\nu) = J_0 N_1 B_{12} \cdot h\nu$$

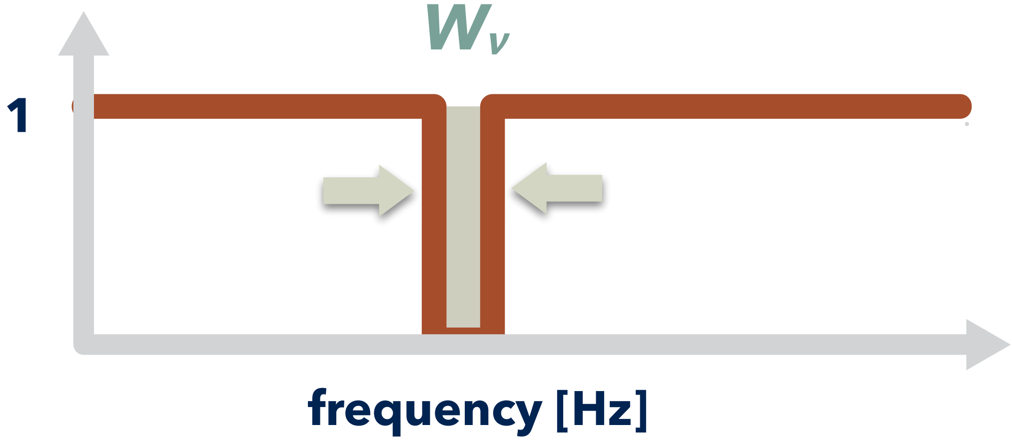
$$\frac{J_0 - J(\nu)}{J_0} = N_1 B_{12} \cdot h\nu$$

we do not need to know absolute flux

equivalent width

$$W_\nu = \int \frac{J_0 - J(\nu)}{J_0} d\nu$$





in the unit of

[Hz]
[cm-1]
[um]

column density

$$W_\nu = N_1 B_{12} \cdot h\nu$$

$$= N_1 \frac{g_2}{g_1} B_{21} \cdot h\nu$$

$$= N_1 \frac{g_2}{g_1} \frac{c^2}{2h\nu^3} A_{21} \cdot h\nu$$

$$\frac{A_{21}}{B_{21}} = \frac{2h\nu^3}{c^2}$$

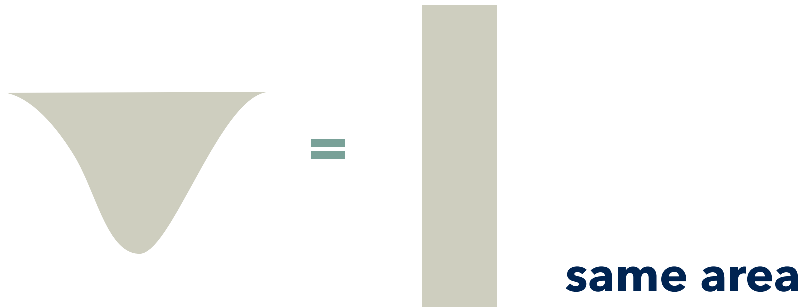
$$B_{12} = \frac{g_2}{g_1} B_{21}$$

$$A \propto u^2$$

depends only on quantum mechanics

calculated theoretically

can measure in lab



column density

$$W_\nu = N_1 \frac{g_2}{g_1} \frac{c^2}{2h\nu^3} A_{21} \cdot h\nu$$

$$N_1 = W_\nu \frac{g_1}{g_2} \frac{2h\nu^3}{c^2} \frac{1}{A_{21} \cdot h\nu}$$

literature / database

observed spectrum

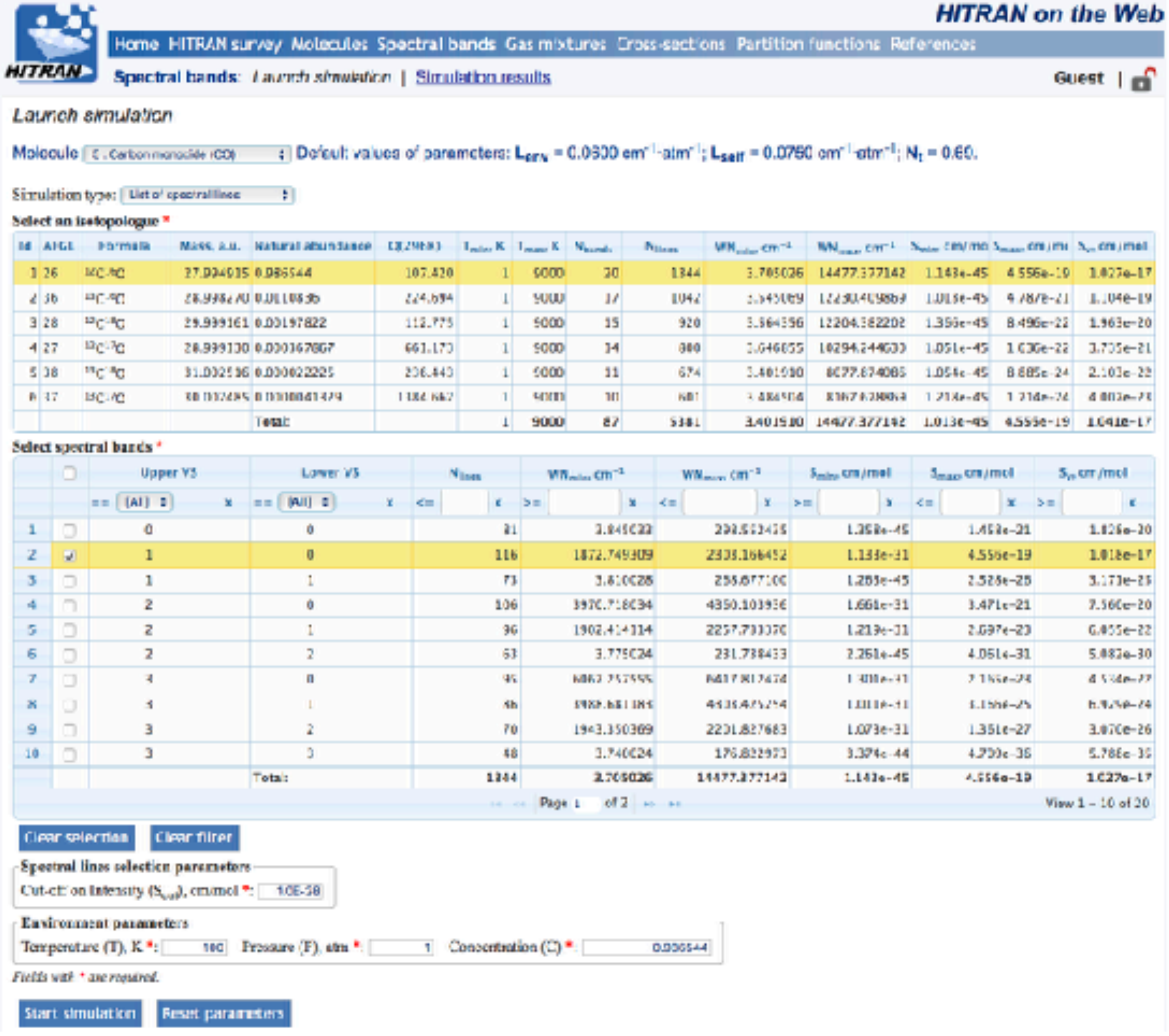
think **or literature / database**

conversion of $W_\nu \rightarrow W_\lambda$

$$\frac{W_\nu}{\nu} = \frac{W_\lambda}{\lambda}$$

dimensionless equivalent width

HITRAN	http://hitran.iao.ru
ExoMol	http://exomol.com



HITRAN on the Web

Home HITRAN survey Molecules Spectral bands Gas mixtures Cross-sections Partition functions References

Spectral bands: *Launch simulation* | Simulation results Guest |

Launch simulation

Molecule: 5. Carbon monoxide (CO) Default values of parameters: L_{air} = 0.0600 $cm^{-1}\cdot atm^{-1}$; L_{self} = 0.0760 $cm^{-1}\cdot atm^{-1}$; N_t = 0.60.

Simulation type: List of spectral lines

Select an isotopologue *

Id	AFGL	Formula	Mass, a.u.	Natural abundance	Q(296K)	T_{min}, K	T_{max}, K	N_{bands}	N_{lines}	WN_{min}, cm^{-1}	WN_{max}, cm^{-1}	S_{min} cm/mol	S_{max} cm/mol	S_Σ cm/mol
1	26	$^{12}C^{16}O$	27.994915	0.986544	107.420	1	9000	20	1344	3.705026	14477.377142	1.143e-45	4.556e-19	1.027e-17
2	36	$^{13}C^{16}O$	28.998270	0.0110836	224.694	1	9000	17	1042	3.543069	12230.409869	1.015e-45	4.787e-21	1.104e-19
3	28	$^{12}C^{18}O$	29.999161	0.00197822	112.775	1	9000	15	920	3.564356	12204.382202	1.356e-45	8.496e-22	1.963e-20
4	27	$^{12}C^{17}O$	28.999130	0.000367867	661.173	1	9000	14	880	3.646055	10294.244633	1.051e-45	1.030e-22	3.735e-21
5	38	$^{13}C^{18}O$	31.002516	0.0000222225	236.443	1	9000	11	674	3.401910	8077.674085	1.054e-45	8.885e-24	2.103e-22
6	37	$^{13}C^{17}O$	[illegible]	[illegible]	[illegible]	1	9000	10	681	[illegible]	[illegible]	1.214e-45	[illegible]	[illegible]
				Total:		1	9000	87	5381	3.401910	14477.377142	1.013e-45	4.556e-19	1.041e-17

Select spectral bands *

	☐	Upper VS	Lower VS	N_{lines}	WN_{min} cm^{-1}	WN_{max} cm^{-1}	S_{min} cm/mol	S_{max} cm/mol	S_Σ cm/mol
		== (All) x	== (All) x	<= x	>= x	<= x	>= x	<= x	>= x
1	☐	0	0	31	3.845022	298.552435	1.358e-45	1.452e-21	1.826e-20
2	☑	1	0	116	1872.749309	2333.166452	1.133e-31	4.556e-19	1.018e-17
3	☐	1	1	73	3.610028	255.677100	1.283e-45	2.528e-28	3.173e-25
4	☐	2	0	106	3970.718034	4350.103936	1.661e-31	3.471e-21	7.560e-20
5	☐	2	1	96	1902.414114	2257.733370	1.219e-31	2.697e-23	6.055e-22
6	☐	2	2	63	3.775024	231.738433	2.261e-45	4.051e-31	5.882e-30
7	☐	3	0	95	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
8	☐	3	1	56	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
9	☐	3	2	70	1943.350369	2201.827683	1.073e-31	1.351e-27	3.070e-26
10	☐	3	3	48	3.740024	176.822973	3.374e-44	4.700e-36	5.786e-35
			Total:	1344	3.705026	14477.377142	1.143e-45	4.556e-19	1.027e-17

Page 1 of 2 View 1 - 10 of 20

Clear selection Clear filter

Spectral lines selection parameters

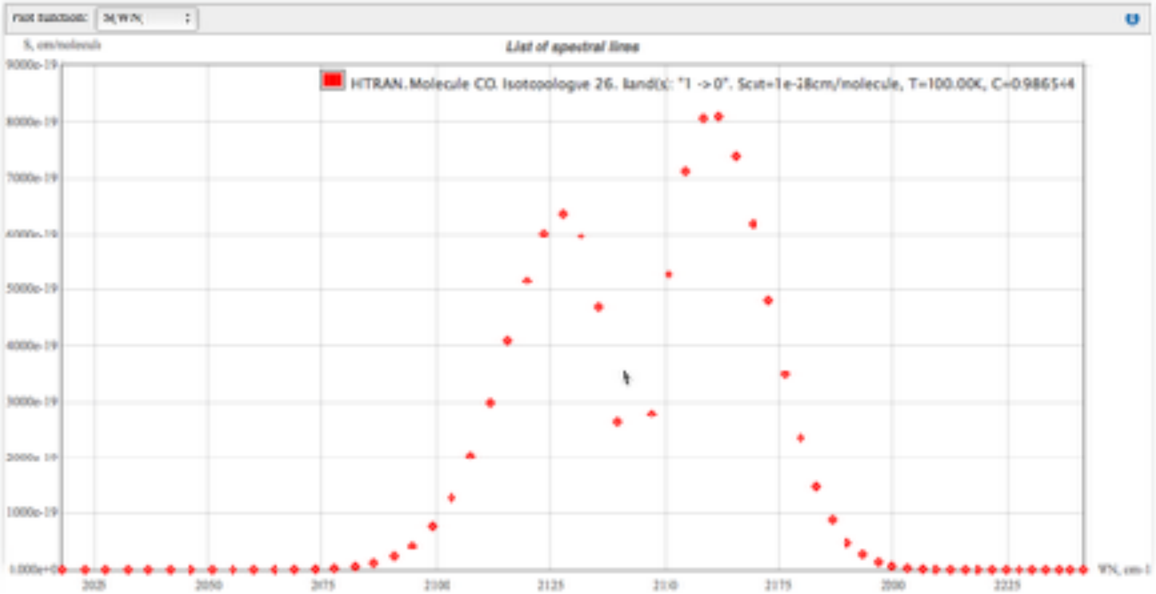
Cut-off on intensity (S_{cut}), cm/mol *: 1.0E-58

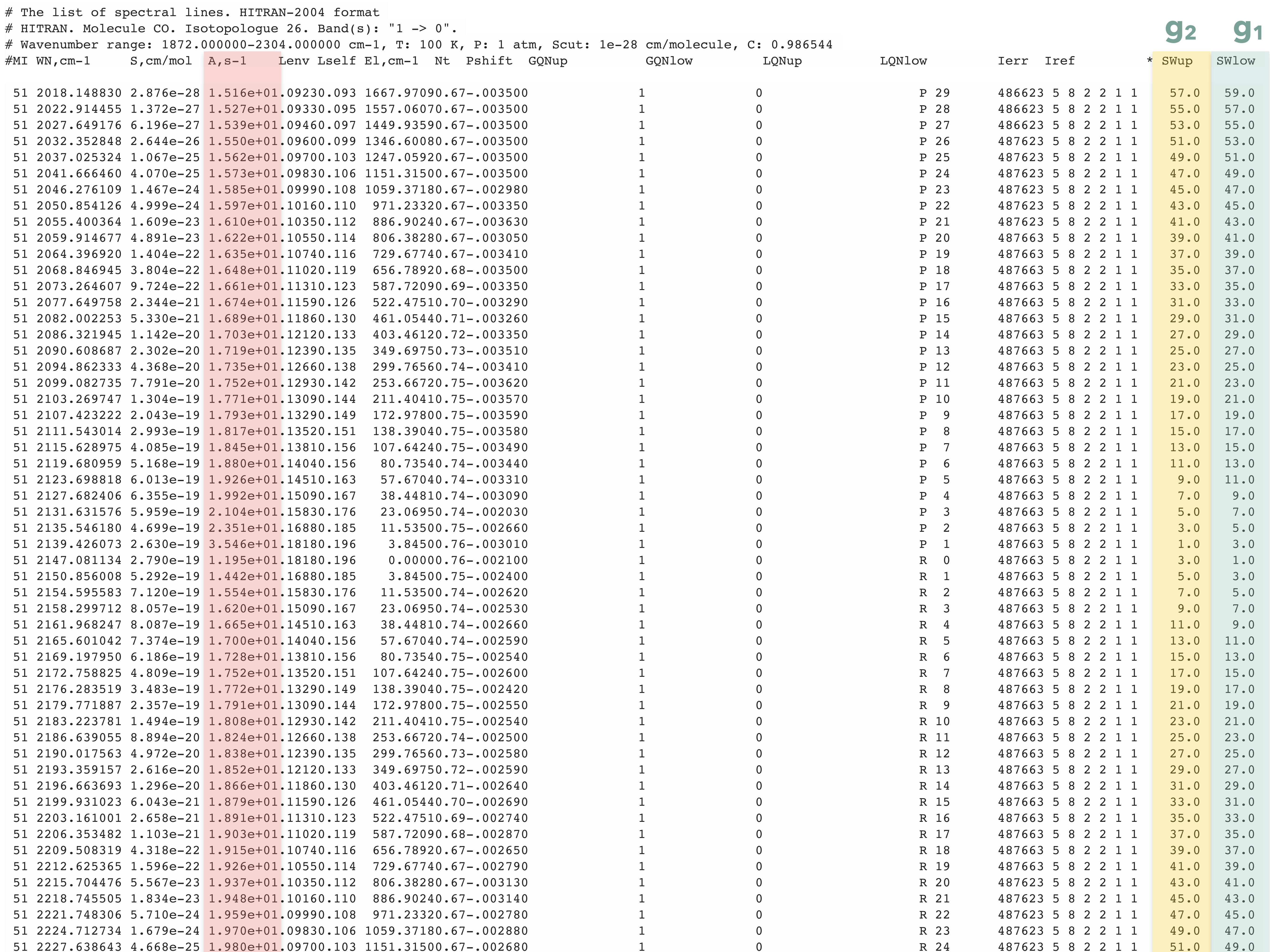
Environment parameters

Temperature (T), K *: 100 Pressure (P), atm *: 1 Concentration (C) *: 0.986544

*Fields with * are required.*

Start simulation Reset parameters





```
# The list of spectral lines. HITRAN-2004 format
# HITRAN. Molecule CO. Isotopologue 26. Band(s): "1 -> 0".
# Wavenumber range: 1872.000000-2304.000000 cm-1, T: 100 K, P: 1 atm, Scut: 1e-28 cm/molecule, C: 0.986544
#MI WN,cm-1     S,cm/mol  A,s-1    Lenv Lself El,cm-1  Nt  Pshift  GQNup          GQNlow         LQNup          LQNlow         Ierr  Iref         * SWup   SWlow

 51 2018.148830 2.876e-28 1.516e+01.09230.093 1667.97090.67-.003500              1              0                    P 29      486623 5 8 2 2 1 1    57.0   59.0
 51 2022.914455 1.372e-27 1.527e+01.09330.095 1557.06070.67-.003500              1              0                    P 28      486623 5 8 2 2 1 1    55.0   57.0
 51 2027.649176 6.196e-27 1.539e+01.09460.097 1449.93590.67-.003500              1              0                    P 27      486623 5 8 2 2 1 1    53.0   55.0
 51 2032.352848 2.644e-26 1.550e+01.09600.099 1346.60080.67-.003500              1              0                    P 26      487623 5 8 2 2 1 1    51.0   53.0
 51 2037.025324 1.067e-25 1.562e+01.09700.103 1247.05920.67-.003500              1              0                    P 25      487623 5 8 2 2 1 1    49.0   51.0
 51 2041.666460 4.070e-25 1.573e+01.09830.106 1151.31500.67-.003500              1              0                    P 24      487623 5 8 2 2 1 1    47.0   49.0
 51 2046.276109 1.467e-24 1.585e+01.09990.108 1059.37180.67-.002980              1              0                    P 23      487623 5 8 2 2 1 1    45.0   47.0
 51 2050.854126 4.999e-24 1.597e+01.10160.110  971.23320.67-.003350              1              0                    P 22      487623 5 8 2 2 1 1    43.0   45.0
 51 2055.400364 1.609e-23 1.610e+01.10350.112  886.90240.67-.003630              1              0                    P 21      487623 5 8 2 2 1 1    41.0   43.0
 51 2059.914677 4.891e-23 1.622e+01.10550.114  806.38280.67-.003050              1              0                    P 20      487663 5 8 2 2 1 1    39.0   41.0
 51 2064.396920 1.404e-22 1.635e+01.10740.116  729.67740.67-.003410              1              0                    P 19      487663 5 8 2 2 1 1    37.0   39.0
 51 2068.846945 3.804e-22 1.648e+01.11020.119  656.78920.68-.003500              1              0                    P 18      487663 5 8 2 2 1 1    35.0   37.0
 51 2073.264607 9.724e-22 1.661e+01.11310.123  587.72090.69-.003350              1              0                    P 17      487663 5 8 2 2 1 1    33.0   35.0
 51 2077.649758 2.344e-21 1.674e+01.11590.126  522.47510.70-.003290              1              0                    P 16      487663 5 8 2 2 1 1    31.0   33.0
 51 2082.002253 5.330e-21 1.689e+01.11860.130  461.05440.71-.003260              1              0                    P 15      487663 5 8 2 2 1 1    29.0   31.0
 51 2086.321945 1.142e-20 1.703e+01.12120.133  403.46120.72-.003350              1              0                    P 14      487663 5 8 2 2 1 1    27.0   29.0
 51 2090.608687 2.302e-20 1.719e+01.12390.135  349.69750.73-.003510              1              0                    P 13      487663 5 8 2 2 1 1    25.0   27.0
 51 2094.862333 4.368e-20 1.735e+01.12660.138  299.76560.74-.003410              1              0                    P 12      487663 5 8 2 2 1 1    23.0   25.0
 51 2099.082735 7.791e-20 1.752e+01.12930.142  253.66720.75-.003620              1              0                    P 11      487663 5 8 2 2 1 1    21.0   23.0
 51 2103.269747 1.304e-19 1.771e+01.13090.144  211.40410.75-.003570              1              0                    P 10      487663 5 8 2 2 1 1    19.0   21.0
 51 2107.423222 2.043e-19 1.793e+01.13290.149  172.97800.75-.003590              1              0                    P  9      487663 5 8 2 2 1 1    17.0   19.0
 51 2111.543014 2.993e-19 1.817e+01.13520.151  138.39040.75-.003580              1              0                    P  8      487663 5 8 2 2 1 1    15.0   17.0
 51 2115.628975 4.085e-19 1.845e+01.13810.156  107.64240.75-.003490              1              0                    P  7      487663 5 8 2 2 1 1    13.0   15.0
 51 2119.680959 5.168e-19 1.880e+01.14040.156   80.73540.74-.003440              1              0                    P  6      487663 5 8 2 2 1 1    11.0   13.0
 51 2123.698818 6.013e-19 1.926e+01.14510.163   57.67040.74-.003310              1              0                    P  5      487663 5 8 2 2 1 1     9.0   11.0
 51 2127.682406 6.355e-19 1.992e+01.15090.167   38.44810.74-.003090              1              0                    P  4      487663 5 8 2 2 1 1     7.0    9.0
 51 2131.631576 5.959e-19 2.104e+01.15830.176   23.06950.74-.002030              1              0                    P  3      487663 5 8 2 2 1 1     5.0    7.0
 51 2135.546180 4.699e-19 2.351e+01.16880.185   11.53500.75-.002660              1              0                    P  2      487663 5 8 2 2 1 1     3.0    5.0
 51 2139.426073 2.630e-19 3.546e+01.18180.196    3.84500.76-.003010              1              0                    P  1      487663 5 8 2 2 1 1     1.0    3.0
 51 2147.081134 2.790e-19 1.195e+01.18180.196    0.00000.76-.002100              1              0                    R  0      487663 5 8 2 2 1 1     3.0    1.0
 51 2150.856008 5.292e-19 1.442e+01.16880.185    3.84500.75-.002400              1              0                    R  1      487663 5 8 2 2 1 1     5.0    3.0
 51 2154.595583 7.120e-19 1.554e+01.15830.176   11.53500.74-.002620              1              0                    R  2      487663 5 8 2 2 1 1     7.0    5.0
 51 2158.299712 8.057e-19 1.620e+01.15090.167   23.06950.74-.002530              1              0                    R  3      487663 5 8 2 2 1 1     9.0    7.0
 51 2161.968247 8.087e-19 1.665e+01.14510.163   38.44810.74-.002660              1              0                    R  4      487663 5 8 2 2 1 1    11.0    9.0
 51 2165.601042 7.374e-19 1.700e+01.14040.156   57.67040.74-.002590              1              0                    R  5      487663 5 8 2 2 1 1    13.0   11.0
 51 2169.197950 6.186e-19 1.728e+01.13810.156   80.73540.75-.002540              1              0                    R  6      487663 5 8 2 2 1 1    15.0   13.0
 51 2172.758825 4.809e-19 1.752e+01.13520.151  107.64240.75-.002600              1              0                    R  7      487663 5 8 2 2 1 1    17.0   15.0
 51 2176.283519 3.483e-19 1.772e+01.13290.149  138.39040.75-.002420              1              0                    R  8      487663 5 8 2 2 1 1    19.0   17.0
 51 2179.771887 2.357e-19 1.791e+01.13090.144  172.97800.75-.002550              1              0                    R  9      487663 5 8 2 2 1 1    21.0   19.0
 51 2183.223781 1.494e-19 1.808e+01.12930.142  211.40410.75-.002540              1              0                    R 10      487663 5 8 2 2 1 1    23.0   21.0
 51 2186.639055 8.894e-20 1.824e+01.12660.138  253.66720.74-.002500              1              0                    R 11      487663 5 8 2 2 1 1    25.0   23.0
 51 2190.017563 4.972e-20 1.838e+01.12390.135  299.76560.73-.002580              1              0                    R 12      487663 5 8 2 2 1 1    27.0   25.0
 51 2193.359157 2.616e-20 1.852e+01.12120.133  349.69750.72-.002590              1              0                    R 13      487663 5 8 2 2 1 1    29.0   27.0
 51 2196.663693 1.296e-20 1.866e+01.11860.130  403.46120.71-.002640              1              0                    R 14      487663 5 8 2 2 1 1    31.0   29.0
 51 2199.931023 6.043e-21 1.879e+01.11590.126  461.05440.70-.002690              1              0                    R 15      487663 5 8 2 2 1 1    33.0   31.0
 51 2203.161001 2.658e-21 1.891e+01.11310.123  522.47510.69-.002740              1              0                    R 16      487663 5 8 2 2 1 1    35.0   33.0
 51 2206.353482 1.103e-21 1.903e+01.11020.119  587.72090.68-.002870              1              0                    R 17      487663 5 8 2 2 1 1    37.0   35.0
 51 2209.508319 4.318e-22 1.915e+01.10740.116  656.78920.67-.002650              1              0                    R 18      487663 5 8 2 2 1 1    39.0   37.0
 51 2212.625365 1.596e-22 1.926e+01.10550.114  729.67740.67-.002790              1              0                    R 19      487663 5 8 2 2 1 1    41.0   39.0
 51 2215.704476 5.567e-23 1.937e+01.10350.112  806.38280.67-.003130              1              0                    R 20      487623 5 8 2 2 1 1    43.0   41.0
 51 2218.745505 1.834e-23 1.948e+01.10160.110  886.90240.67-.003140              1              0                    R 21      487623 5 8 2 2 1 1    45.0   43.0
 51 2221.748306 5.710e-24 1.959e+01.09990.108  971.23320.67-.002780              1              0                    R 22      487623 5 8 2 2 1 1    47.0   45.0
 51 2224.712734 1.679e-24 1.970e+01.09830.106 1059.37180.67-.002880              1              0                    R 23      487623 5 8 2 2 1 1    49.0   47.0
 51 2227.638643 4.668e-25 1.980e+01.09700.103 1151.31500.67-.002680              1              0                    R 24      487623 5 8 2 2 1 1    51.0   49.0
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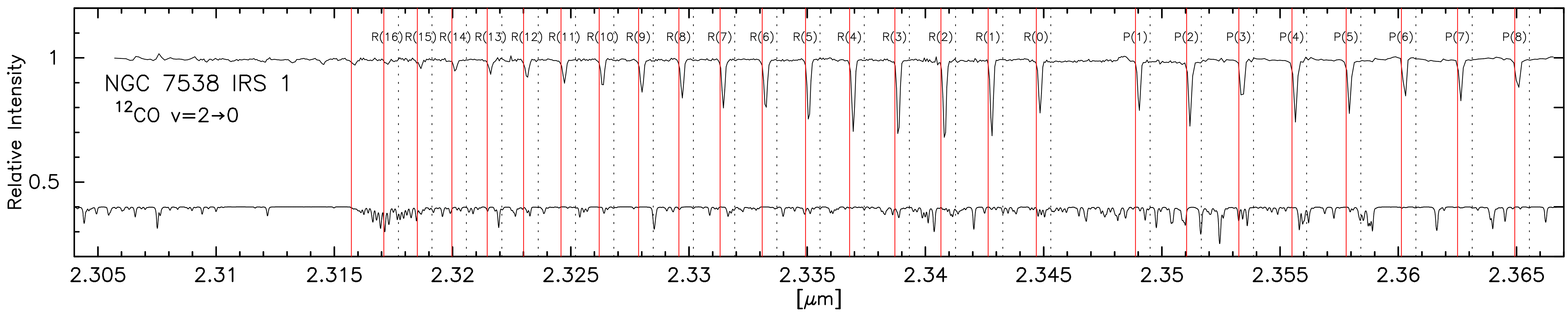
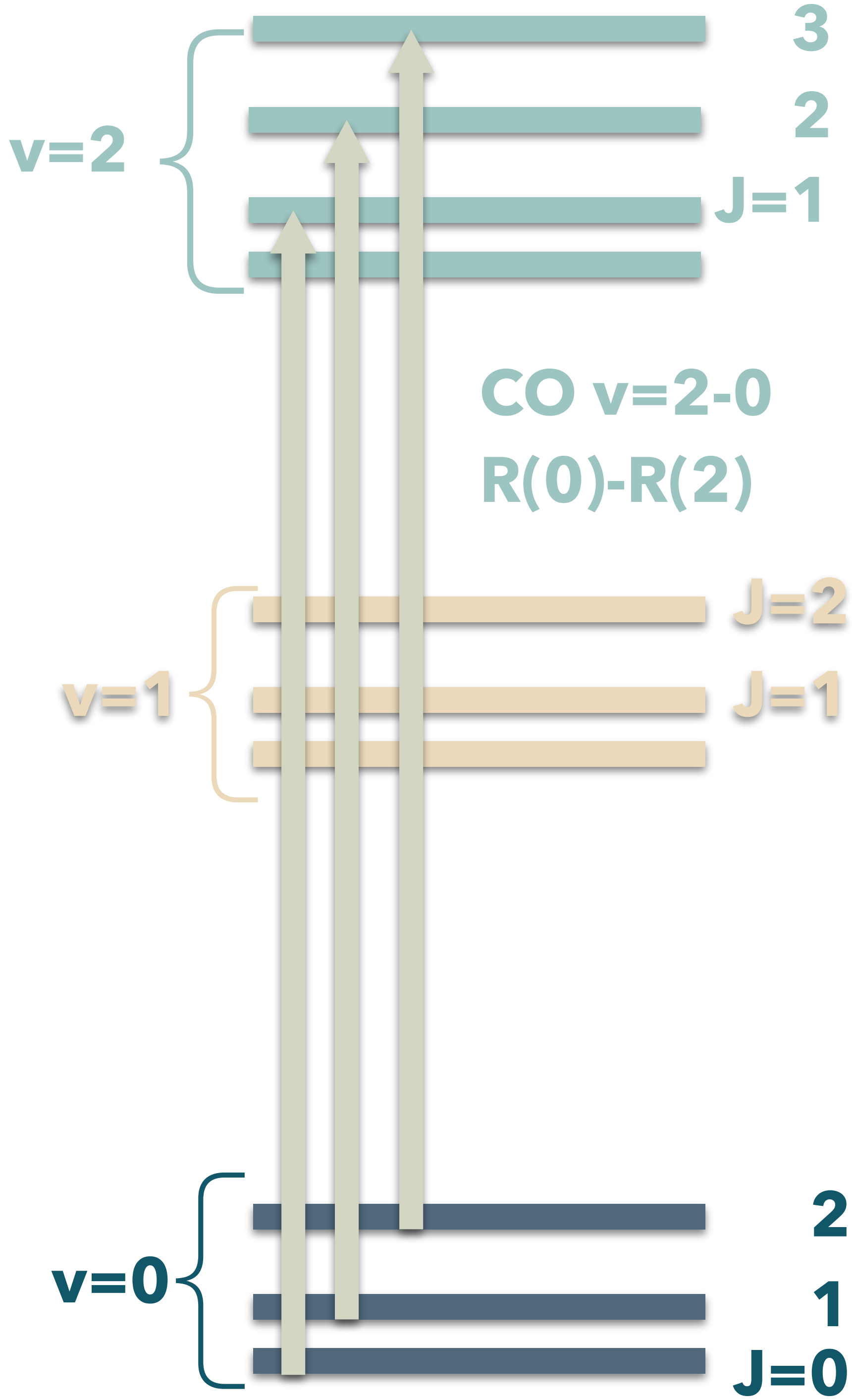
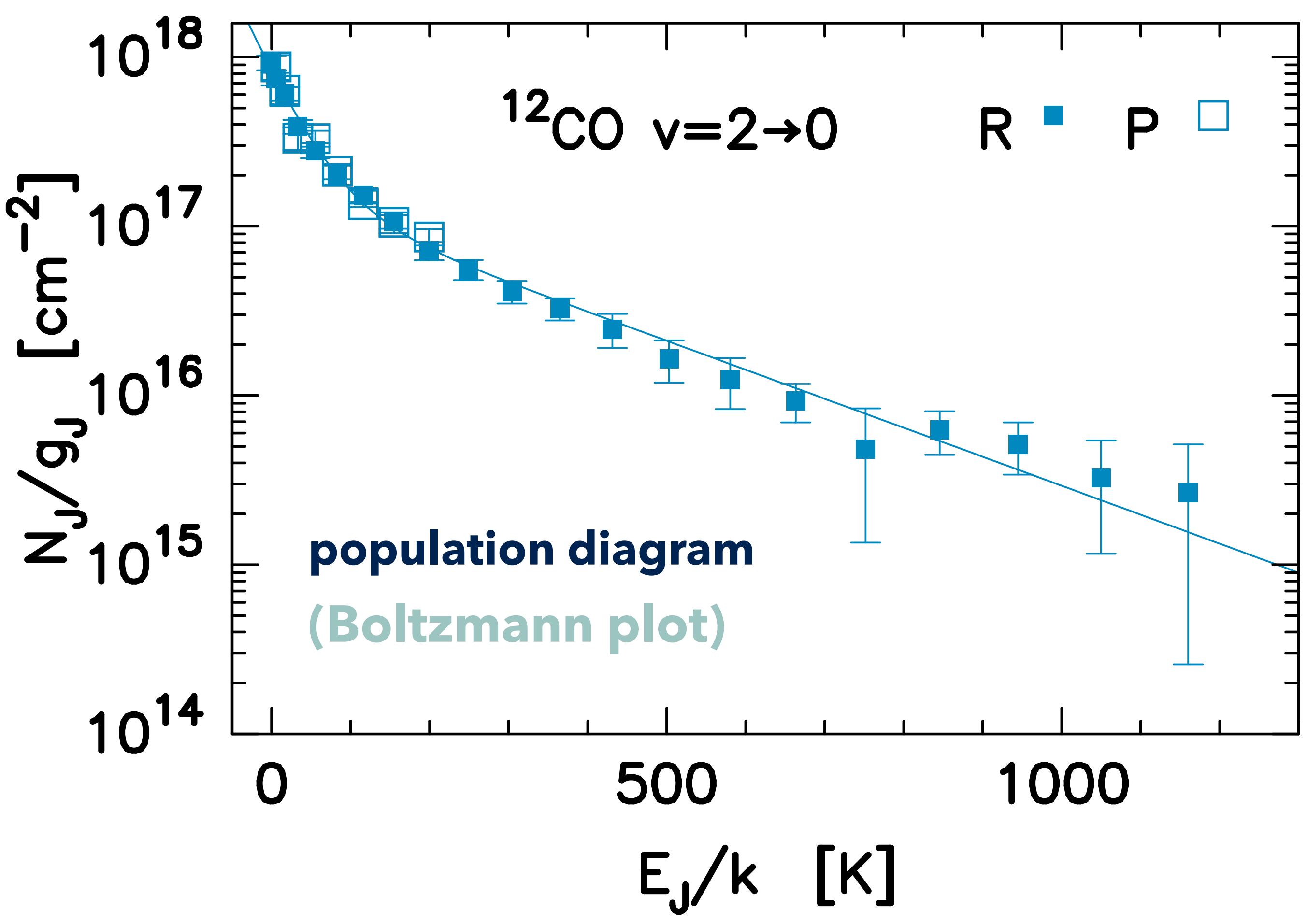




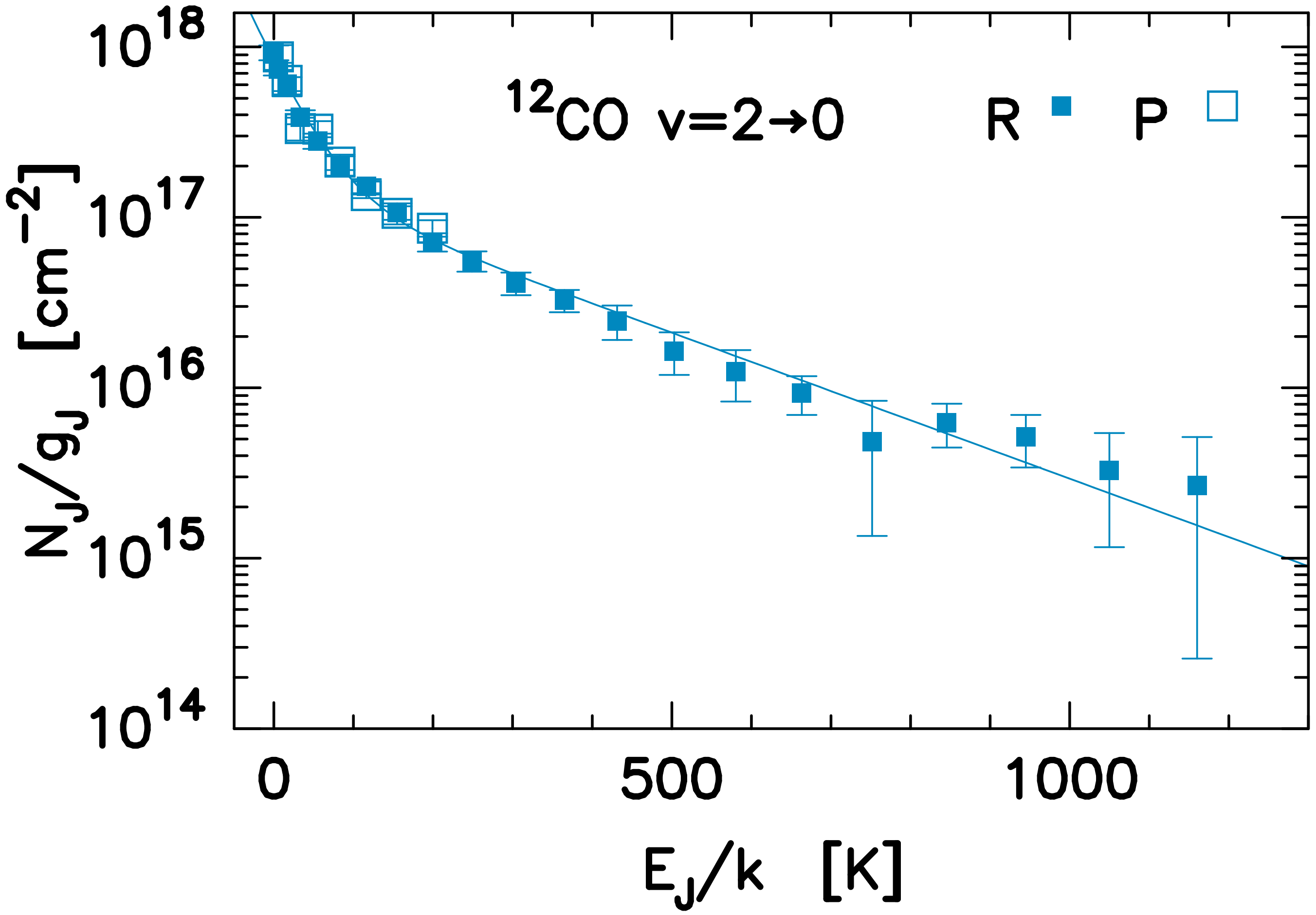
level column density **of lower levels**

$$N_1 = W_\nu \frac{g_1}{g_2} \frac{2h\nu^3}{c^2} \frac{1}{A_{21} \cdot h\nu}$$



population diagram

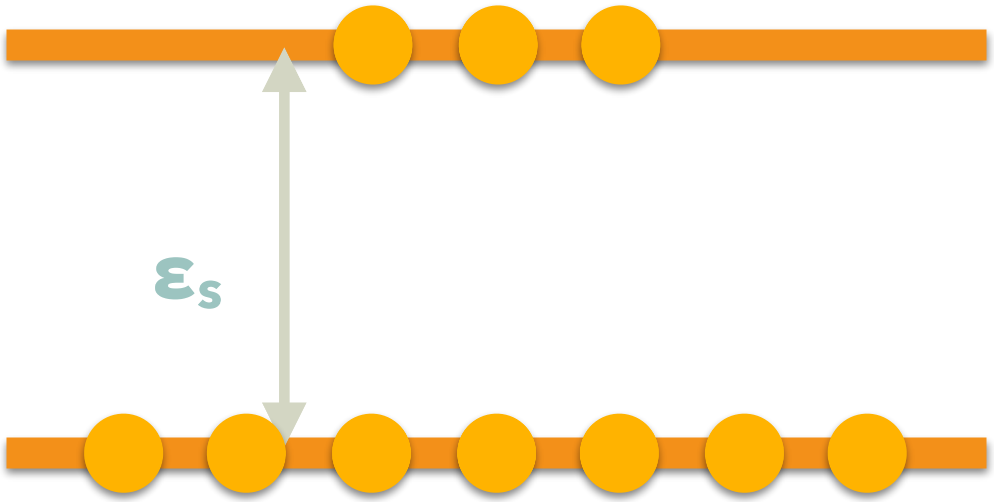
(Boltzmann plot)



probability that a system in the energy level ε_s is proportional to

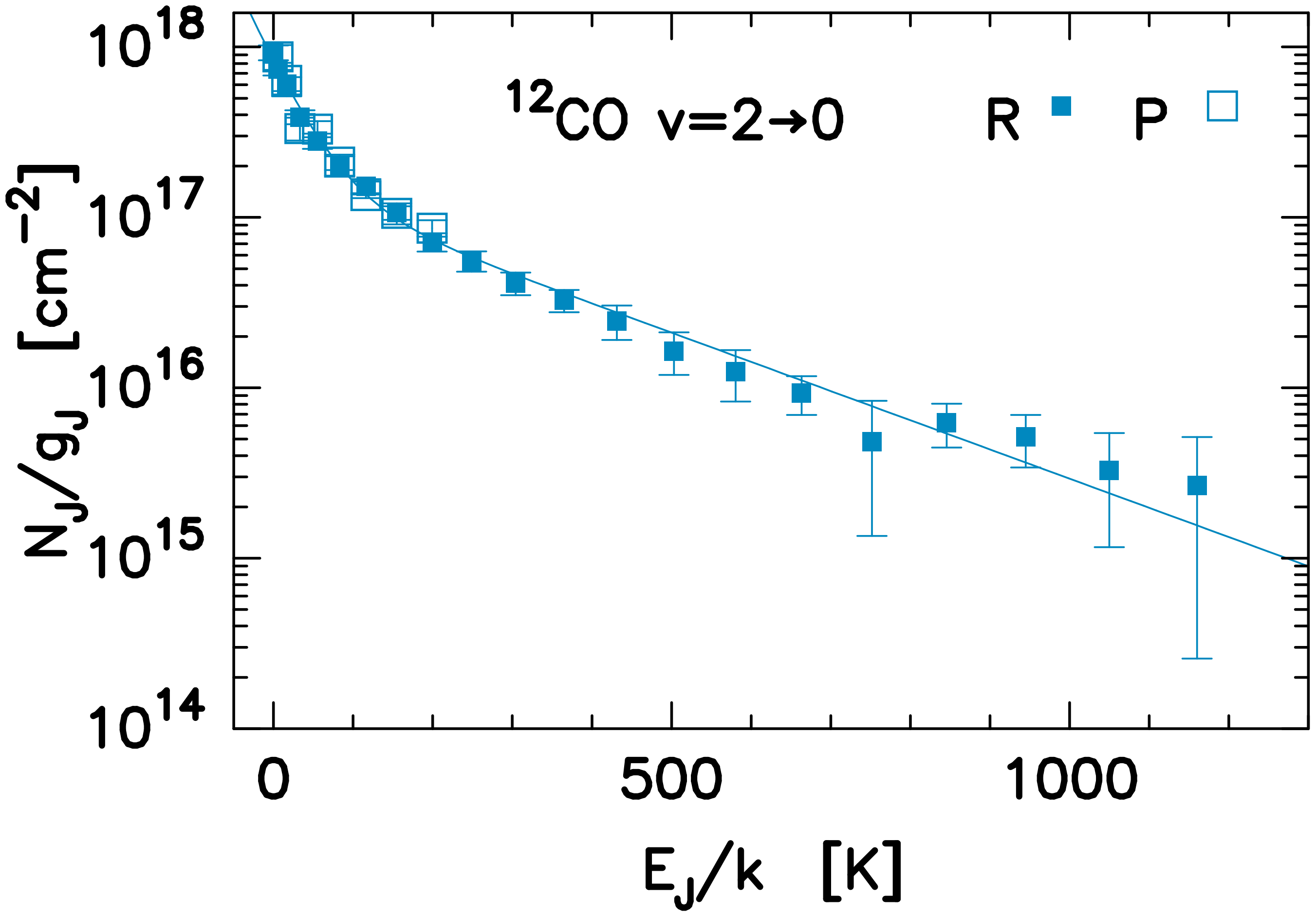
$$p \propto \exp(-\frac{\varepsilon_s}{\tau})$$

kT



ε_s [K]	lower level	upper level
0.5 kT	1	0.61
1 kT	1	0.37
2 kT	1	0.14

kT **definition of temperature**



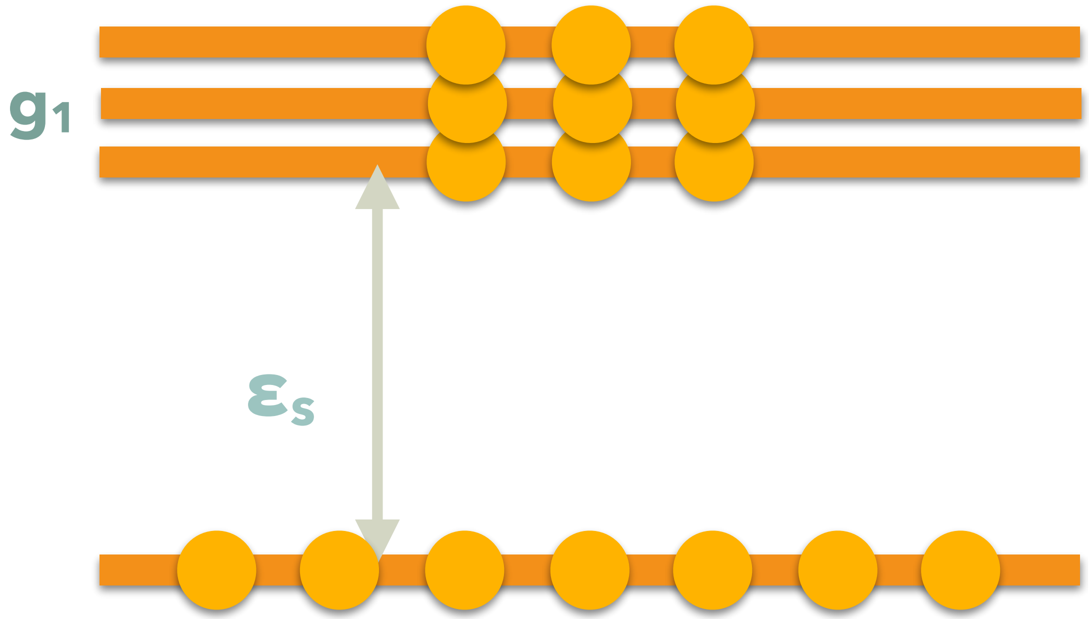
probability that a system in the energy level ε_s is proportional to

$$p \propto \exp(-\frac{\varepsilon_s}{\tau})$$

When a level is degenerated, all states are treated equally

$$p \propto g_1 \exp(-\frac{\varepsilon_s}{\tau})$$

Boltzmann distribution



$$\frac{n_1}{g_1} \propto \exp(-\frac{E_J}{kT})$$

counting from J=0

$E_0 = BJ(J+1)=0$

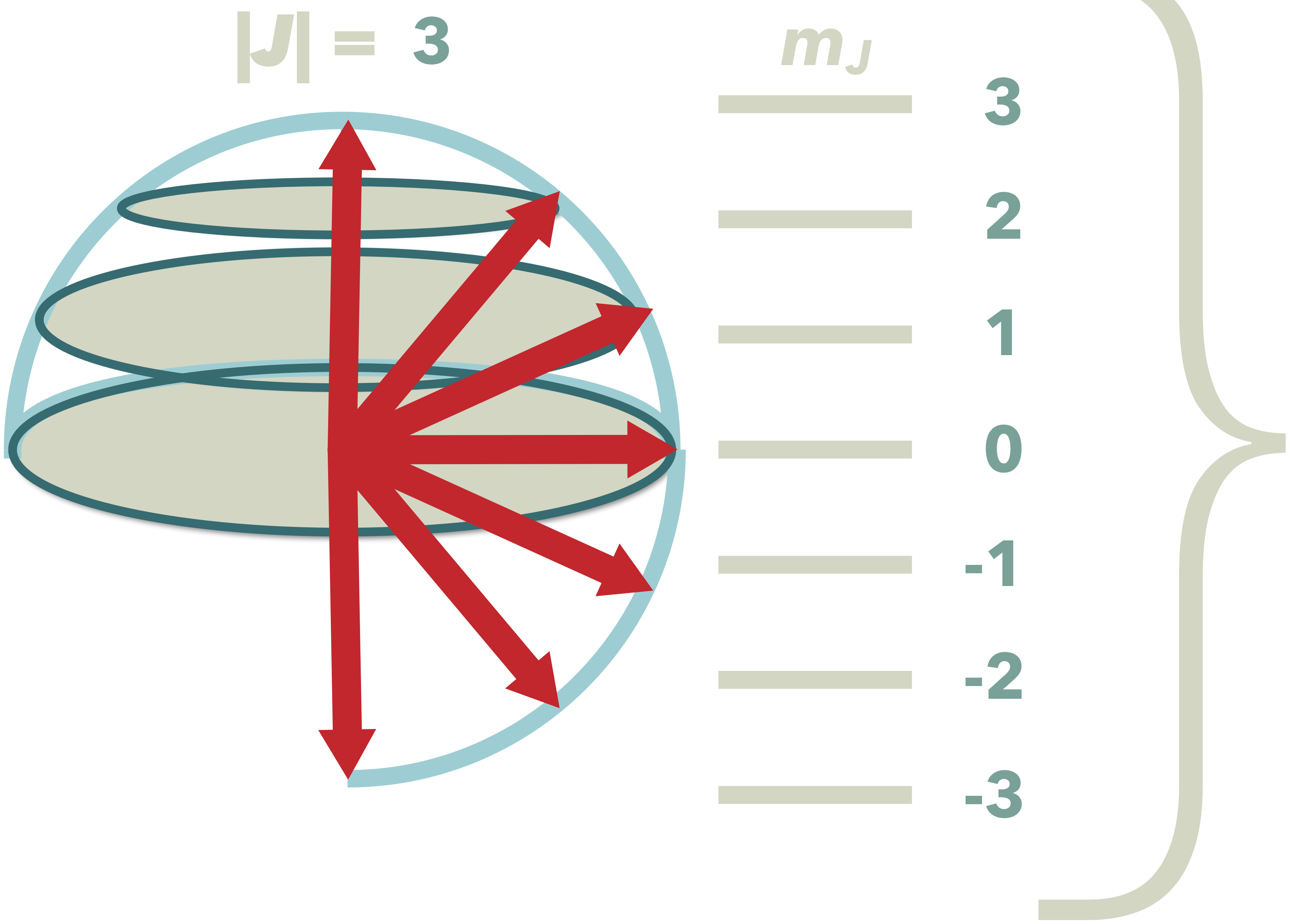
$g_0 = 1$

$$\frac{n_0}{g_0} \propto \exp(-\frac{E_0}{kT}) = 1$$

1890- LMU Physik

statistical weight (degeneracy)

$^{12}C^{16}O$



$|J| = 3$

m_J

3

2

1

0

-1

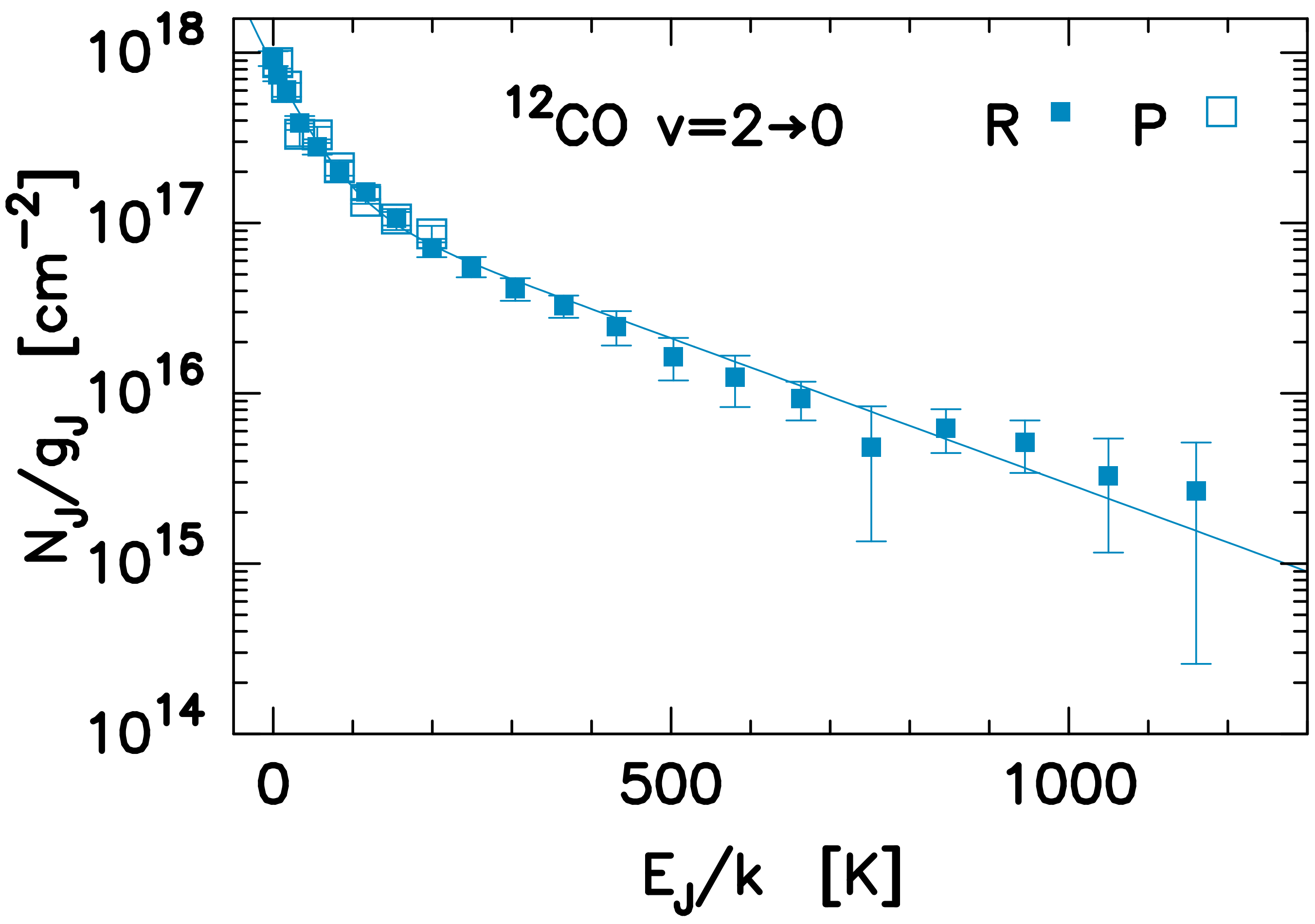
-2

-3

7

$g_J = 2J + 1$

⭐ will learn later



$$\frac{n_J}{g_J} \propto \exp\left(-\frac{E_J}{kT}\right)$$ ①

$$\frac{n_0}{g_0} \propto \exp\left(-\frac{E_0}{kT}\right) = 1$$ ②

divide ① / ②

$$\frac{n_J}{g_J} = n_0 \exp\left(-\frac{E_J}{kT}\right)$$ ③

take ln of ③

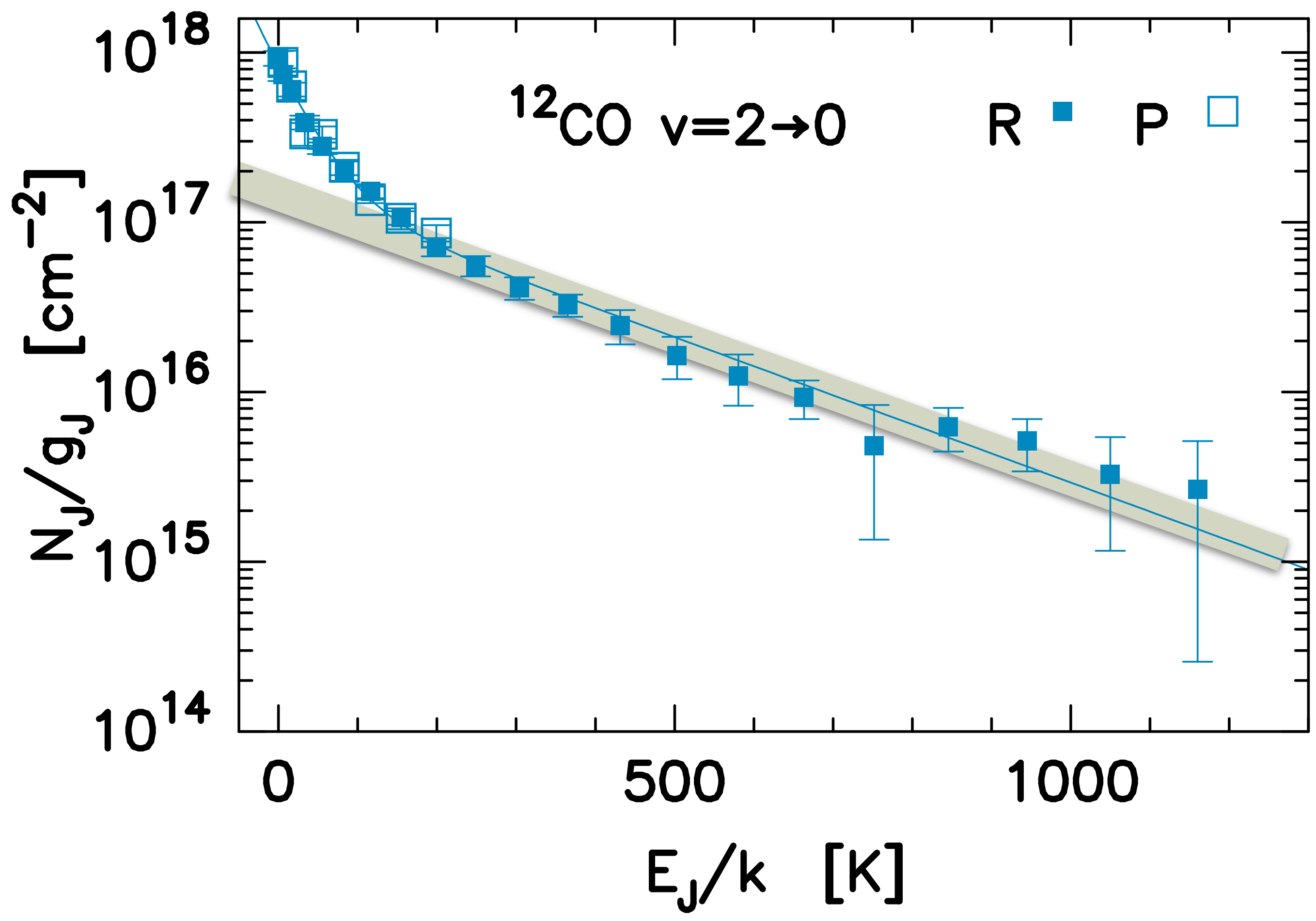
$$\ln\frac{n_J}{g_J} = \ln n_0 - \frac{E_J}{kT}$$

a?

b?

$$Y = b - a\,X$$

$$X = \frac{E_J}{k}$$



$$\frac{n_J}{g_J} \propto \exp(- \frac{E_J}{kT})$$ ①

$$\frac{n_0}{g_0} \propto \exp(- \frac{E_0}{kT}) = 1$$ ②

divide ① / ②

$$\frac{n_J}{g_J} = n_0 \exp(- \frac{E_J}{kT})$$ ③

take ln of ③

$$\ln \frac{n_J}{g_J} = \ln n_0 - \frac{E_J}{kT}$$

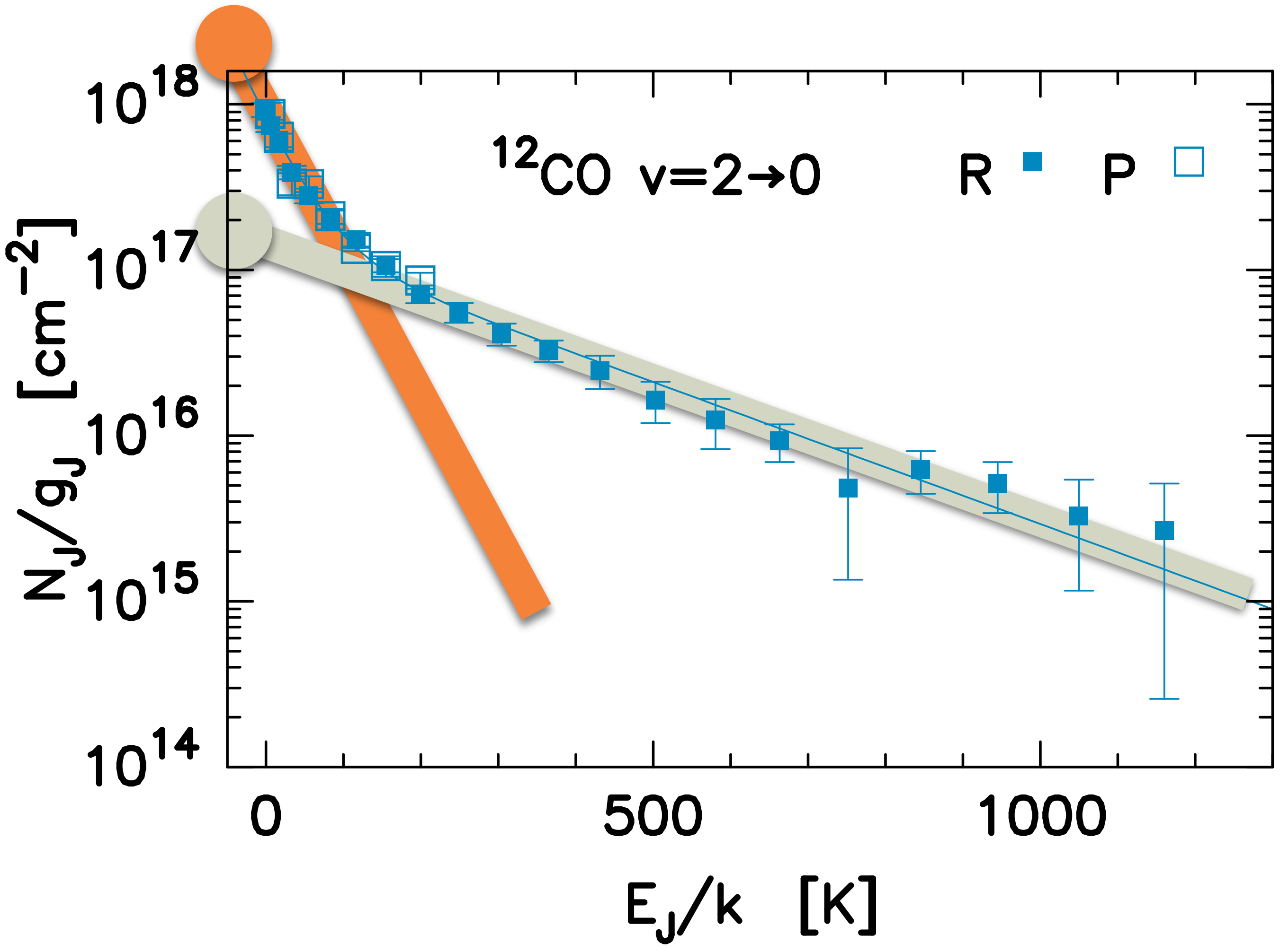
$$a = - \frac{1}{T}$$

$$b = \ln n_0$$

$$Y = b - a X$$

$$X = \frac{E_J}{k}$$

plot $\frac{n_J}{g_J}$ **as a function of** $\frac{E_J}{k}$



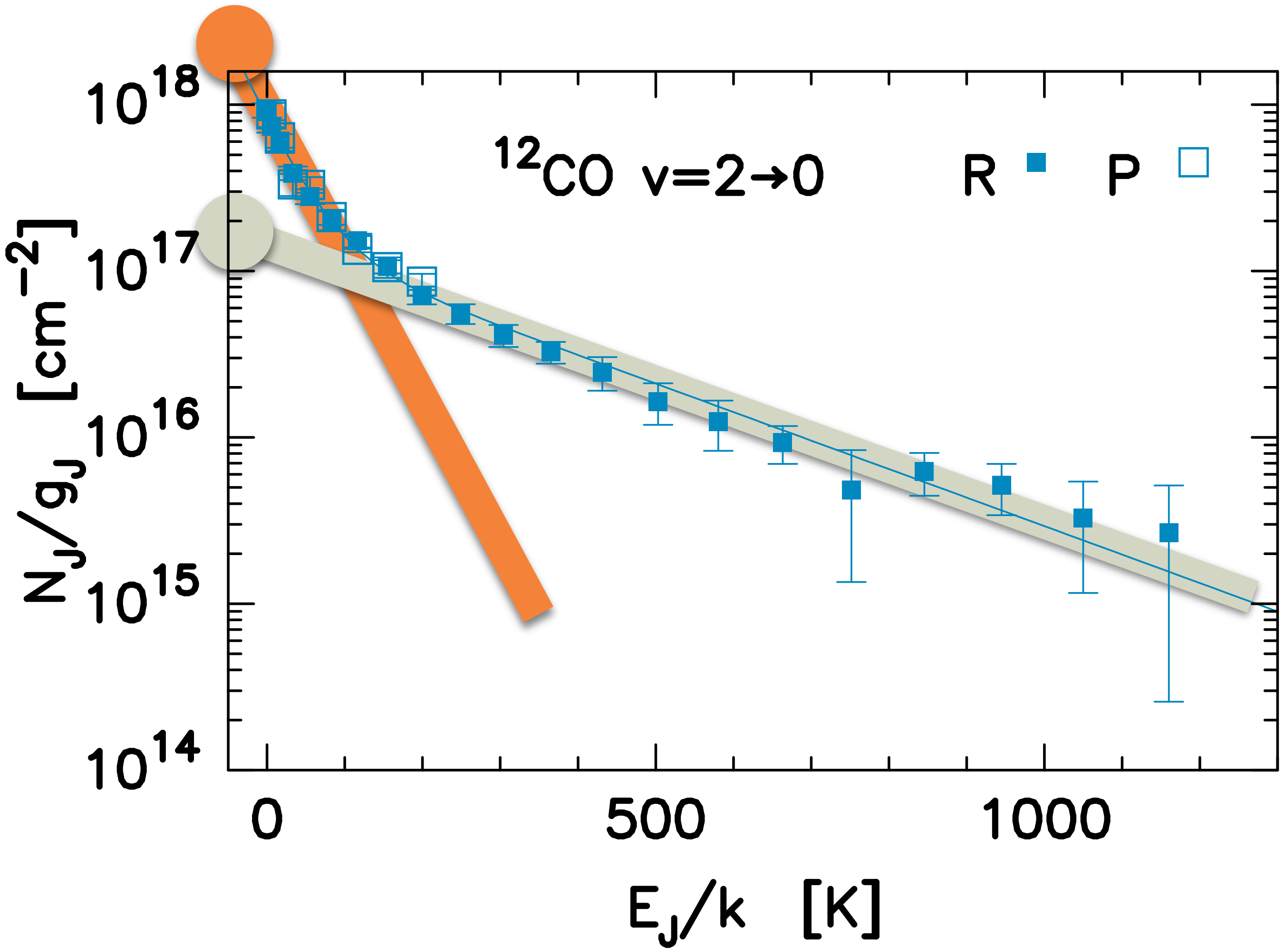
$$\ln \frac{n_J}{g_J} = \ln n_0 - \frac{E_J}{kT}$$

$$Y = b - a\, X$$

plot $\frac{n_J}{g_J}$ as a function o f $\frac{E_J}{k}$

What can we tell?

1. gas is thermalized or not
2. how many components?
3. excitation temperature T_{ex}
4. N_0
5. N_{total}
6. $n(H_2)$ volume density (as opposed to column)



total column density

$$\frac{N_J}{g_J} = N_0 \exp(- \frac{E_J}{kT})$$

$$N_{total} = \sum_J N_J$$

$$= \sum_J N_0 \; g_J \; \exp(-\frac{E_J}{kT})$$

$$= N_0 \sum_J g_J \; \exp(-\frac{E_J}{kT})$$

partition function weighted sum of g_J

$$Q(T) = \sum_J g_J \; \exp(-\frac{E_J}{kT})$$

“function” more like normalization factor

$$N_{total} = N_0 \, Q(T)$$

$$\frac{N_J}{g_J} = \frac{N_{total}}{Q(T)} \exp(- \frac{E_J}{kT})$$

$$\frac{n_J}{g_J} \propto \exp(- \frac{E_J}{kT})$$

Exercise today

1 Find sweet spot of CO J=1-0

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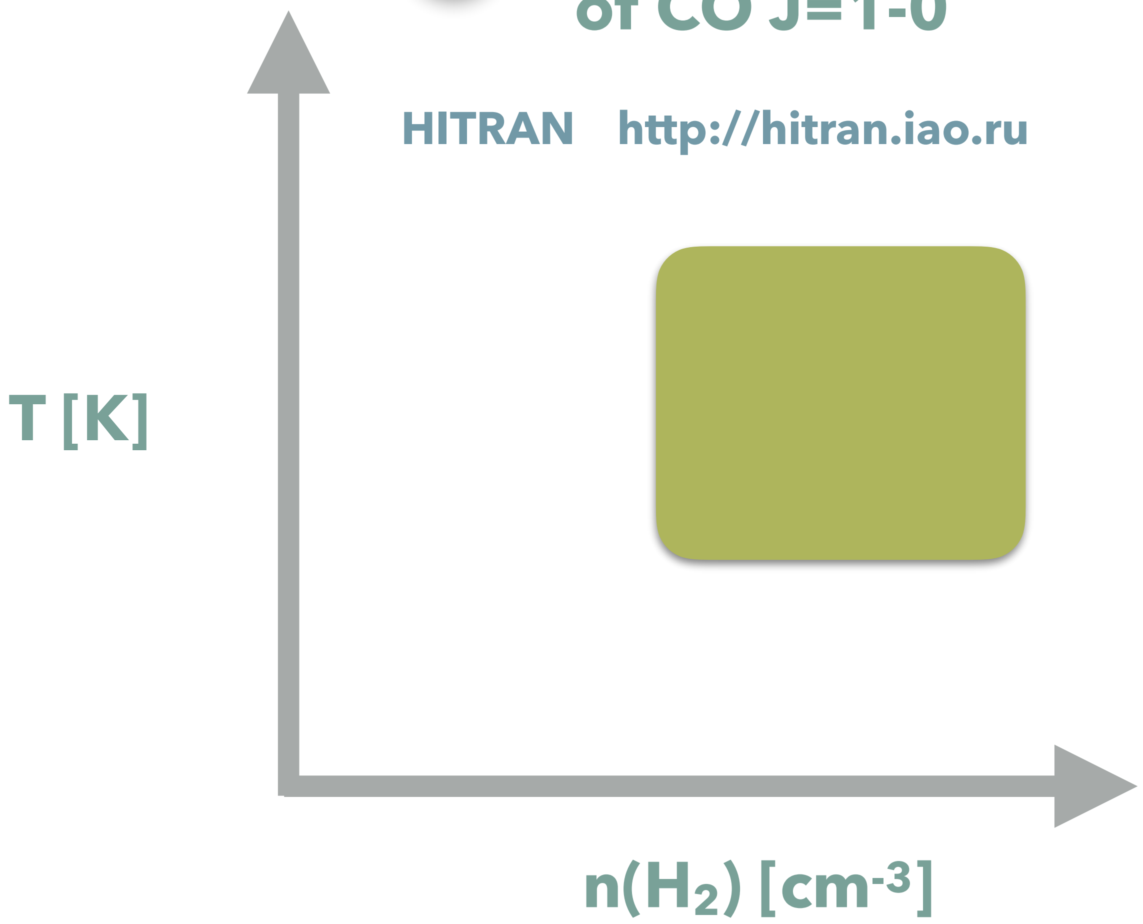

$$n_{cr} = \frac{A_{21}}{C_{21}}$$

$[s^{-1}]$

$[cm^3\ s^{-1}]$

$[cm^{-3}]$

C : 3e-11 $[cm^3\ s^{-1}]$

collisional rate coefficient

1 molecules has to exist

$$n_X > 10^{-10} \times n_{H2}$$

2 a molecular line prove medium that is about

$$n_{H2} \sim n_{cr}$$

3 medium has to be warm about

$$kT \sim \Delta E$$

Exercise today

$$n_{cr} = \frac{A_{21}}{C_{21}}$$

$[s^{-1}]$

$[cm^3\ s^{-1}]$

$[cm^{-3}]$

C : 3e-11 $[cm^3\ s^{-1}]$

collisional rate coefficient

1 **Find sweet spot of CO J=1-0**

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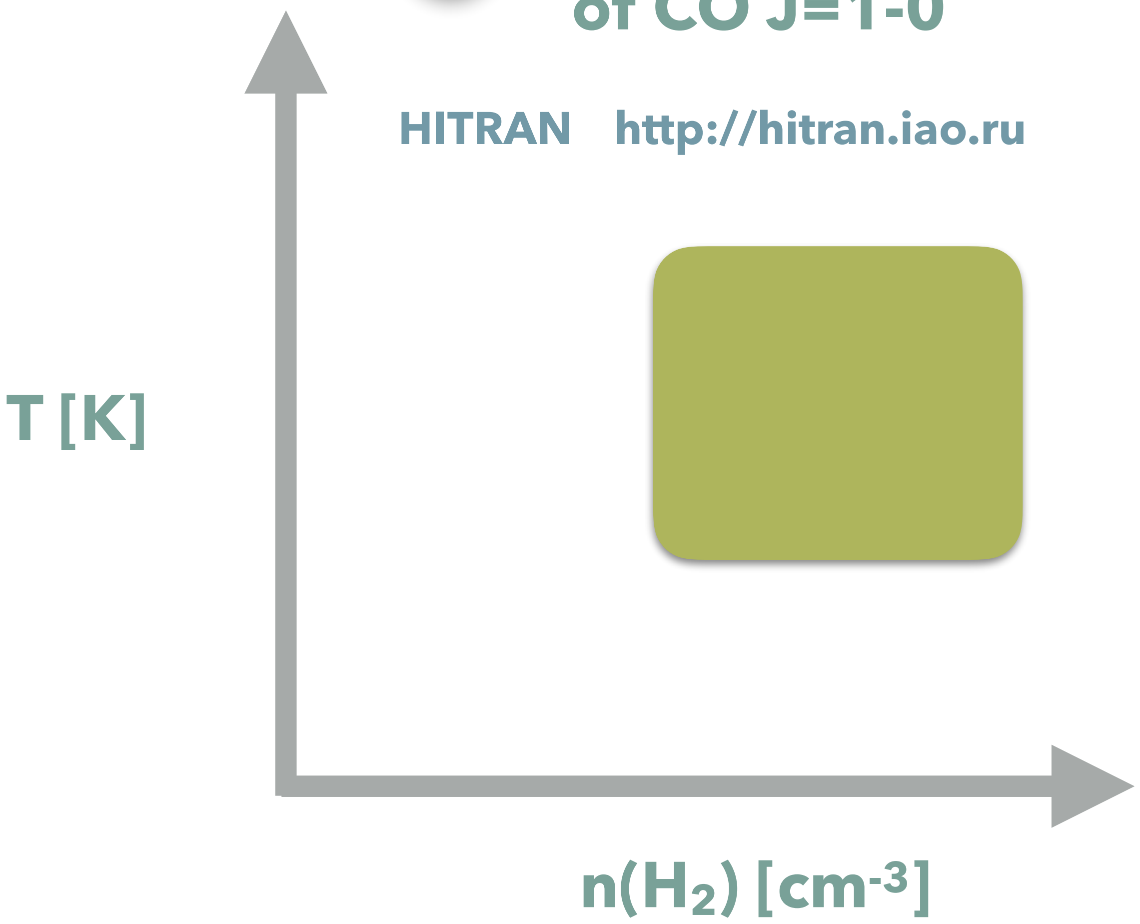

1 molecules has to exist

$$n_X > 10^{-10} \times n_{H2}$$

2 a molecular line prove medium that is about

$$n_{H2} \sim n_{cr}$$

3 medium has to be warm about

$$kT \sim \Delta E$$

```
#MI  WN,cm-1 A,s-1 El,cm-1  SWup  SWlow  GQNup  GQNlow  LQNup  LQNlow
 51     3.8450 7.203e-08      0.0000      3.0     1.0              0              0                R  0
 51     7.6899 6.911e-07      3.8450      5.0     3.0              0              0                R  1
 51    11.5345 2.497e-06     11.5350      7.0     5.0              0              0                R  2
```

$k=1.38 \times 10^{-16}$ [erg /K]

$h=6.63 \times 10^{-27}$ [erg s]

will discuss choice of seminar topics in next class