Physics 224
The Interstellar Medium

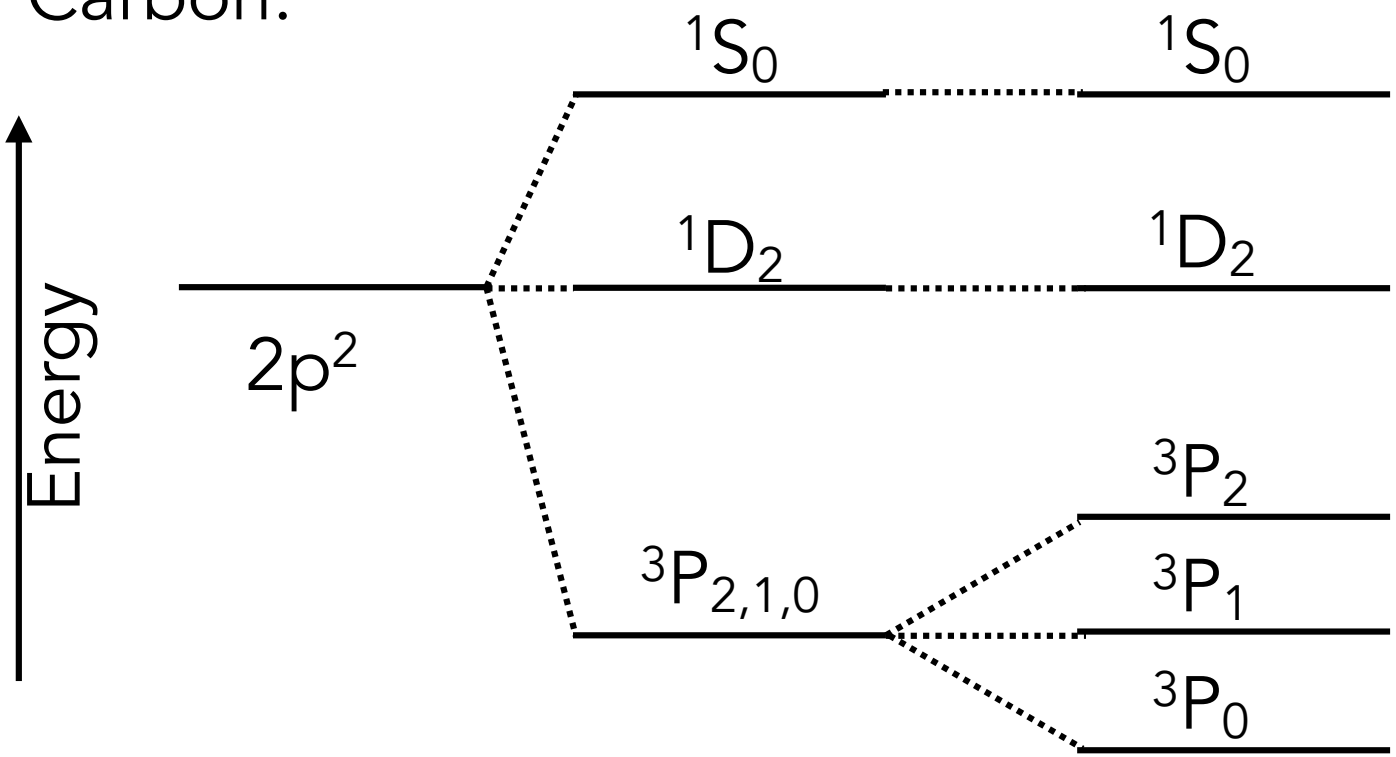
Lecture #5

- Part I: Energy Levels & Transitions in Atoms/ Molecules
- Part II: Radiative Transfer

Energy Levels ⟷ Terms

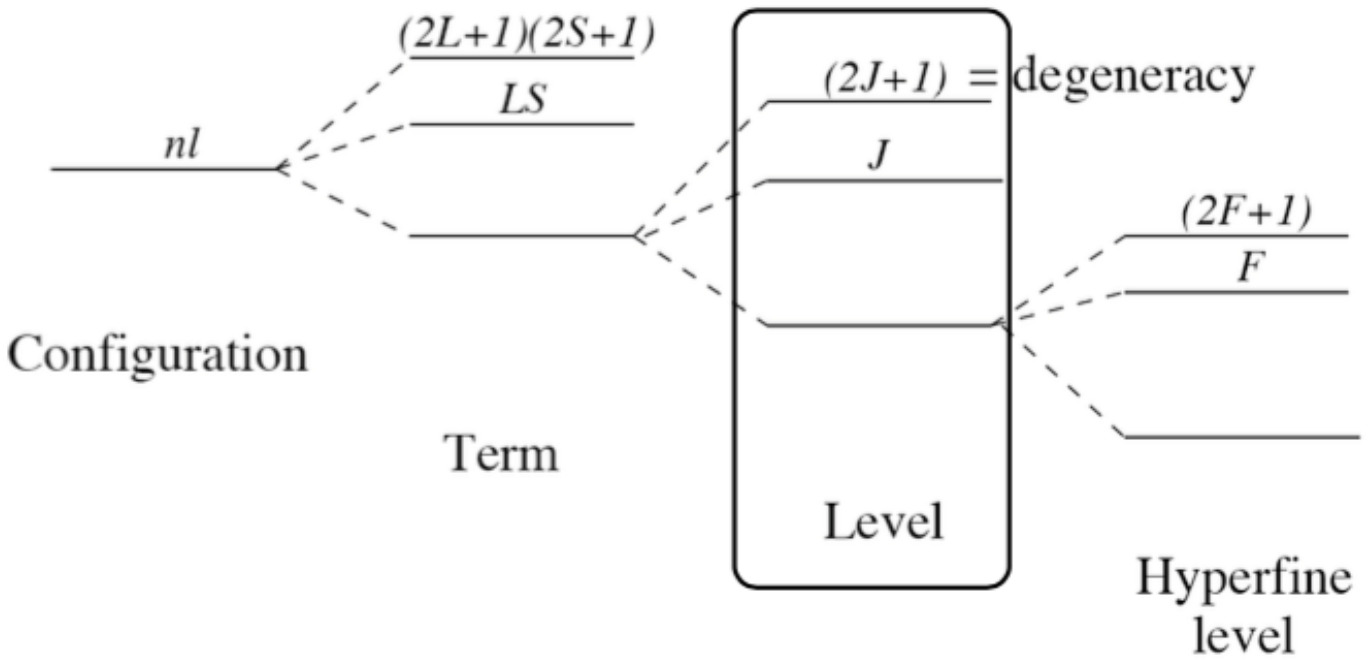
$$^{2S+1}\mathcal{L}_{J}^{p}$$

Carbon:



Type of Transition	Mechanism	Selection Rules
“allowed"	electric dipole	1) Parity must change 2) $\Delta L = 0, \pm 1$ 3) $\Delta J = 0, \pm 1$ but not $J=0 \rightarrow 0$ 4) only one e- wavefunction $\boldsymbol{nl}$ changes with $\Delta \boldsymbol{l} = \pm 1$ 5) $\Delta S = 0$
“semi-forbidden” or “intersystem”	electric dipole but with $\Delta S \neq 0$ from configuration mixing due to relativistic effects	same as “allowed” except violates #5
“forbidden"	magnetic dipole or electric quadrupole	violates at least one other selection rule other than #5

Fine and Hyperfine Structure Transitions



Fine & Hyperfine are "forbidden" parity doesn't change, $\Delta S \neq 0$

-fine structure transitions (transitions within a term, e.g. $^2P_{1/2}$ - $^2P_{3/2}$ 158μm line of [CII] within ^2P term)

-hyperfine structure transitions (transitions within a given level of a term caused by splitting due to interaction of electron & nuclear spin, e.g. HI 21 cm spin-flip transition)

Forbidden transitions are very important in astronomy!

Collisions populate the levels of the ground state

There is a low probability (B_{lu}) for forbidden transitions so the line is generally optically thin

When there is a radiative transition, that energy escapes! Very important for cooling!

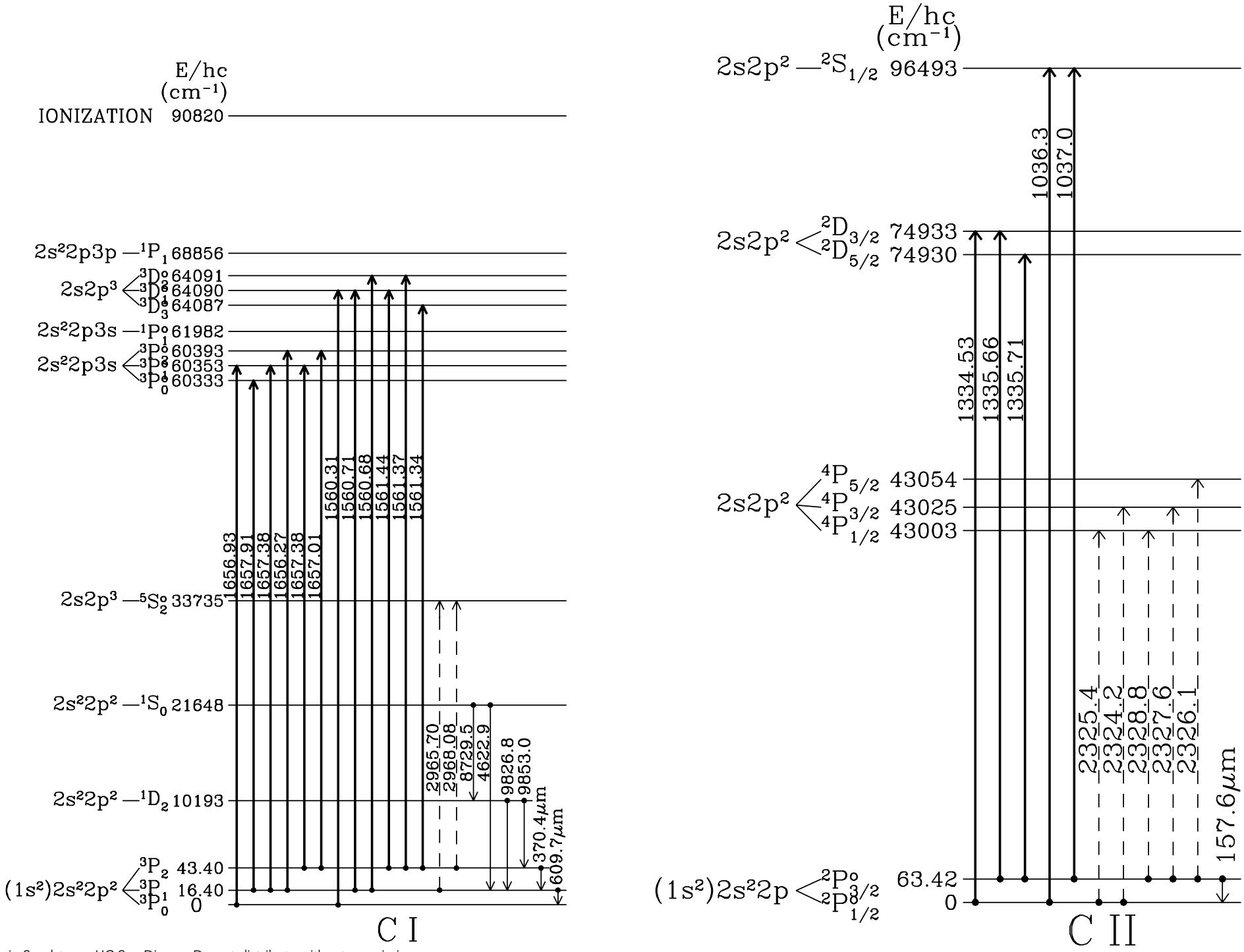
Ionization Potentials

	I→II	II→III	III→IV	IV→V	V→VI
1 H	13.598				
2 He	24.587	54.416			
3 Li	5.392	75.638	122.451		
4 Be	9.322	18.211	153.893	217.713	
5 B	8.298	25.154	37.930	259.368	340.217
6 C	11.260	24.383	47.887	64.492	392.077
7 N	14.534	29.601	47.448	77.472	97.888
8 O	13.618	35.116	54.934	77.412	113.896
9 F	17.422	34.970	62.707	87.138	114.240
10 Ne	21.564	40.962	63.45	97.11	126.21
11 Na	5.139	47.286	71.64	98.91	138.39
12 Mg	7.646	15.035	80.143	109.24	141.26
13 Al	5.986	18.828	28.447	119.99	153.71
14 Si	8.151	16.345	33.492	45.141	166.77
15 P	10.486	19.725	30.18	51.37	65.023
16 S	10.360	23.33	34.83	47.30	72.68
17 Cl	12.967	23.81	39.61	53.46	67.8
18 Ar	15.759	27.629	40.74	59.81	75.02
19 K	4.341	31.625	45.72	60.91	82.66
20 Ca	6.113	11.871	50.908	67.10	84.41
21 Sc	6.54	12.80	24.76	73.47	91.66
22 Ti	6.82	13.58	27.491	43.266	99.22
23 V	6.74	14.65	29.310	46.707	65.23
24 Cr	6.766	16.50	30.96	49.1	69.3
25 Mn	7.435	15.640	33.667	51.2	72.4
26 Fe	7.870	16.18	30.651	54.8	75.0
27 Co	7.86	17.06	33.50	51.3	79.5
28 Ni	7.635	18.168	35.17	54.9	75.5
29 Cu	7.726	20.292	36.83	55.2	79.9
30 Zn	9.394	17.964	39.722	59.4	82.6
31 Ga	5.999	20.51	30.71	64	
32 Ge	7.899	15.934	34.22	45.71	93.5

Can be ionized when H is neutral.

Carbon is the most abundant element that can be ionized when H is neutral.

	Notes	Important Lines
He	→ He II at 24.59 eV, → He III at 54.4 eV, H II regions can have both He I and He II, rarely He III	optical
C	C II can exist in regions with neutral H, fine structure transition in ground state $^2P_{3/2}$ -> $^2P_{1/2}$, requires 91 K to excite	[CII] 158 μm
N	N II in regions with ionized H, fine structure transitions in $^3P_{2,1,0}$ ground state easy to excite	[NII] far-IR and optical lines
O	O ionization potential very close to H, charge exchange reactions maintain O+/O and H+/H balance	[O I] [OIII] far-IR, [OII], [OIII] opt
Mg	7.6 eV ionization potential, mostly in Mg II no fine struct most Mg is depleted into dust grains	Mg II in UV
Si	8.1 eV ionization potential, mostly in Si II most Si is depleted into dust grains	[Si II] 35 μm
S	10.4 eV ionization potential, mostly in S II, not a major dust constituent, but no fine structure in $^4S_{3/2}$ ground state of S II	
Fe	almost entirely in dust (only ~few % in gas)	



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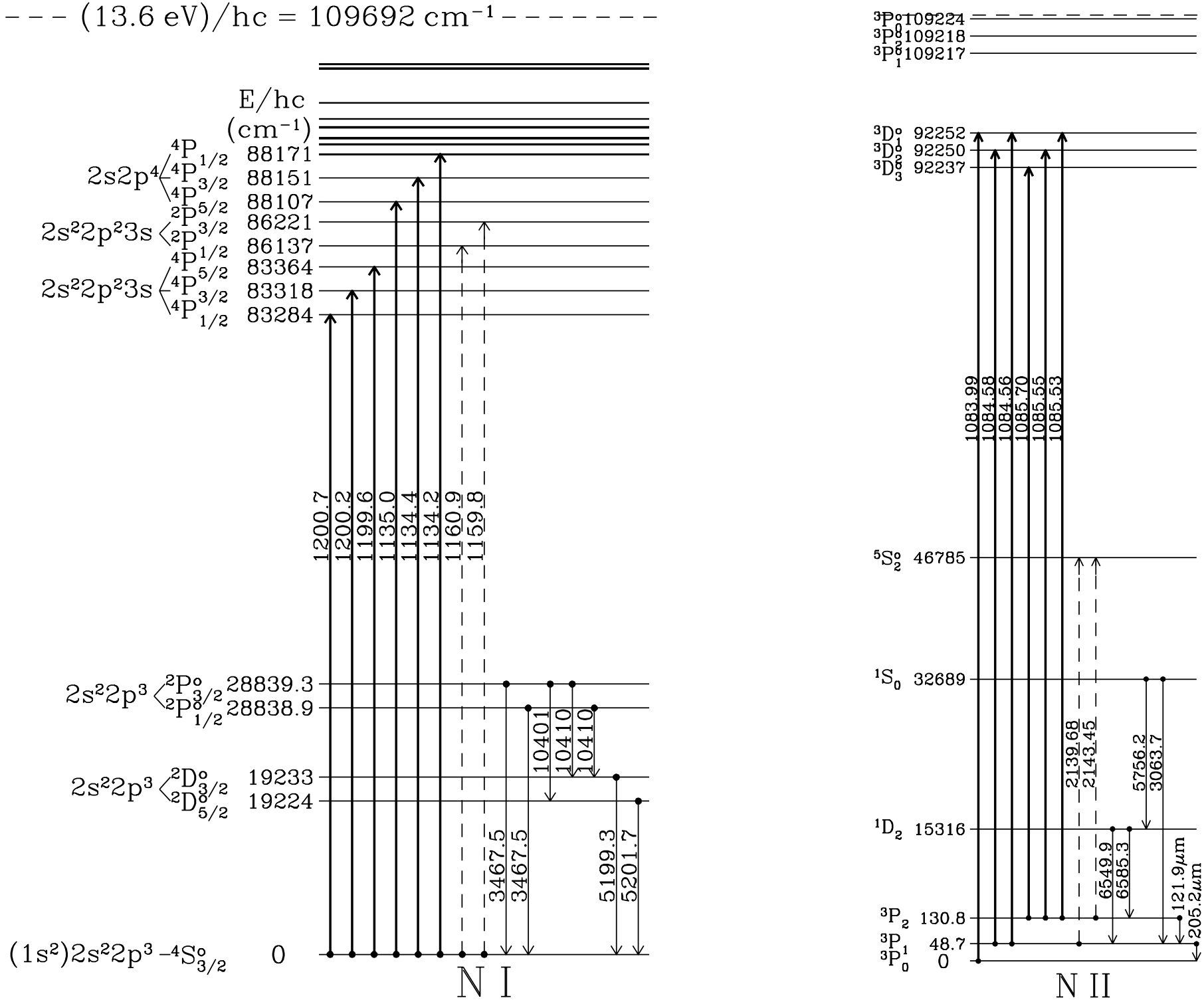

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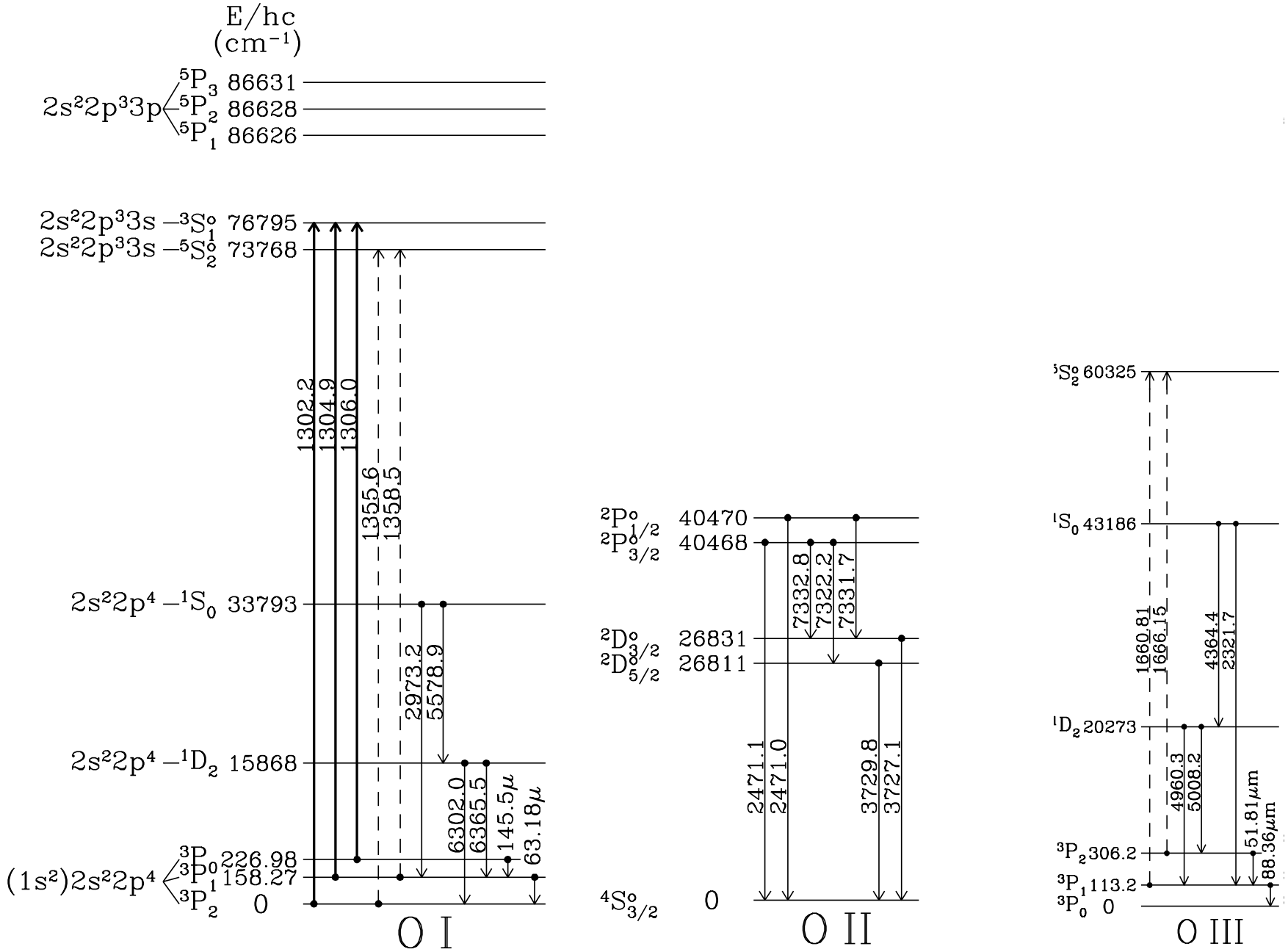

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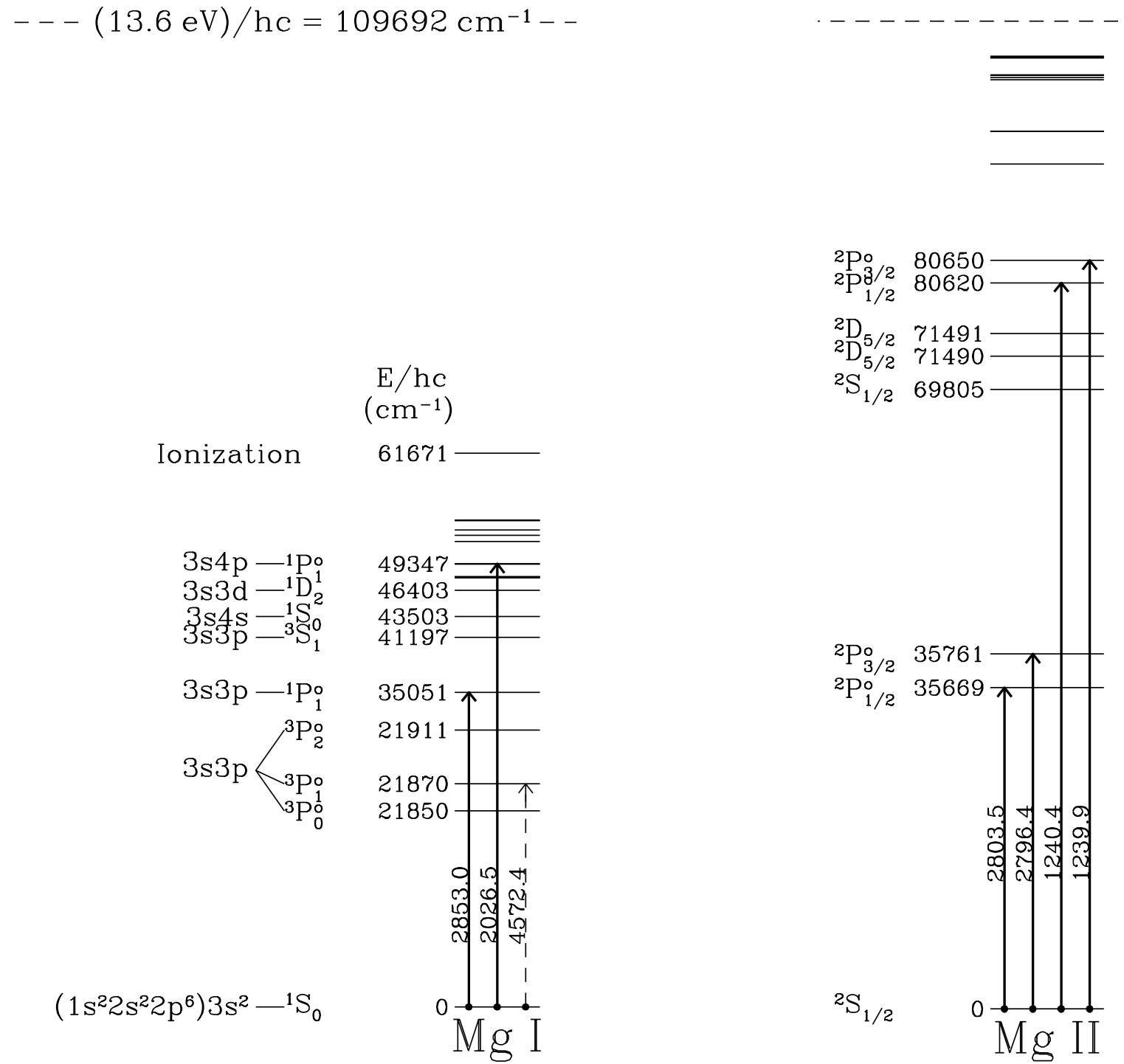

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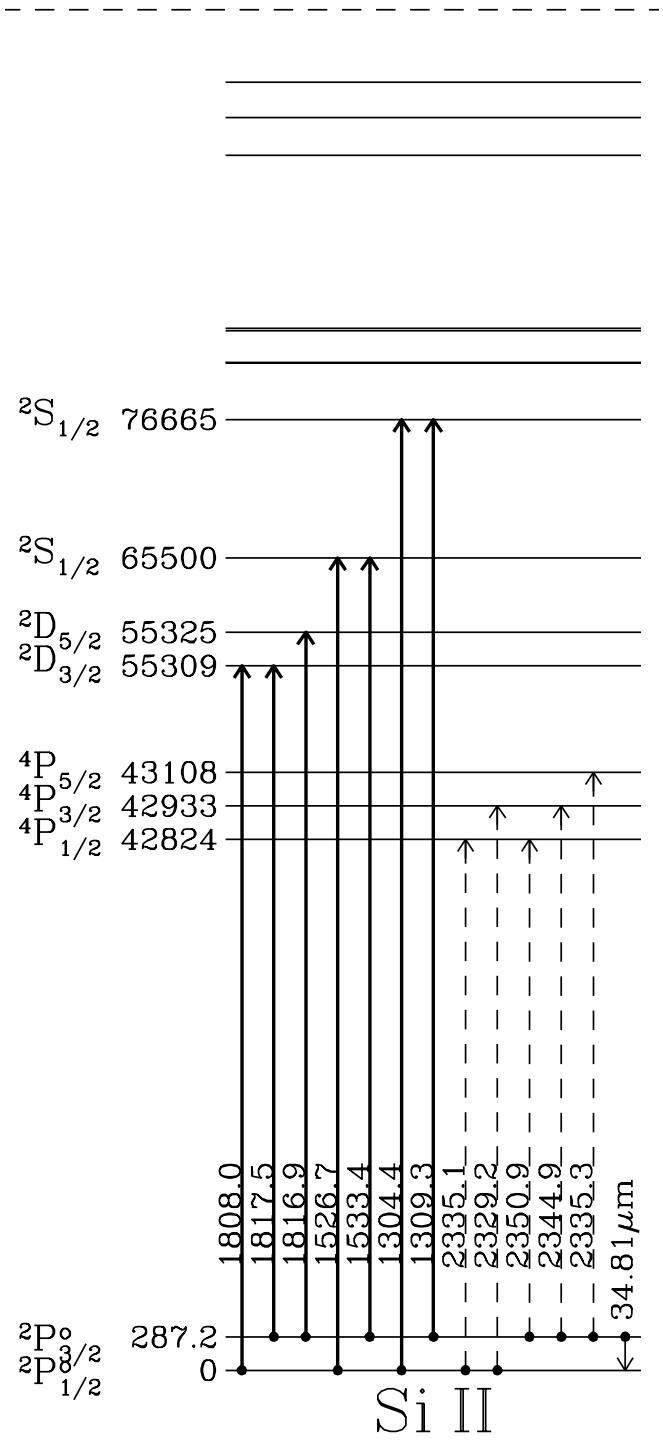

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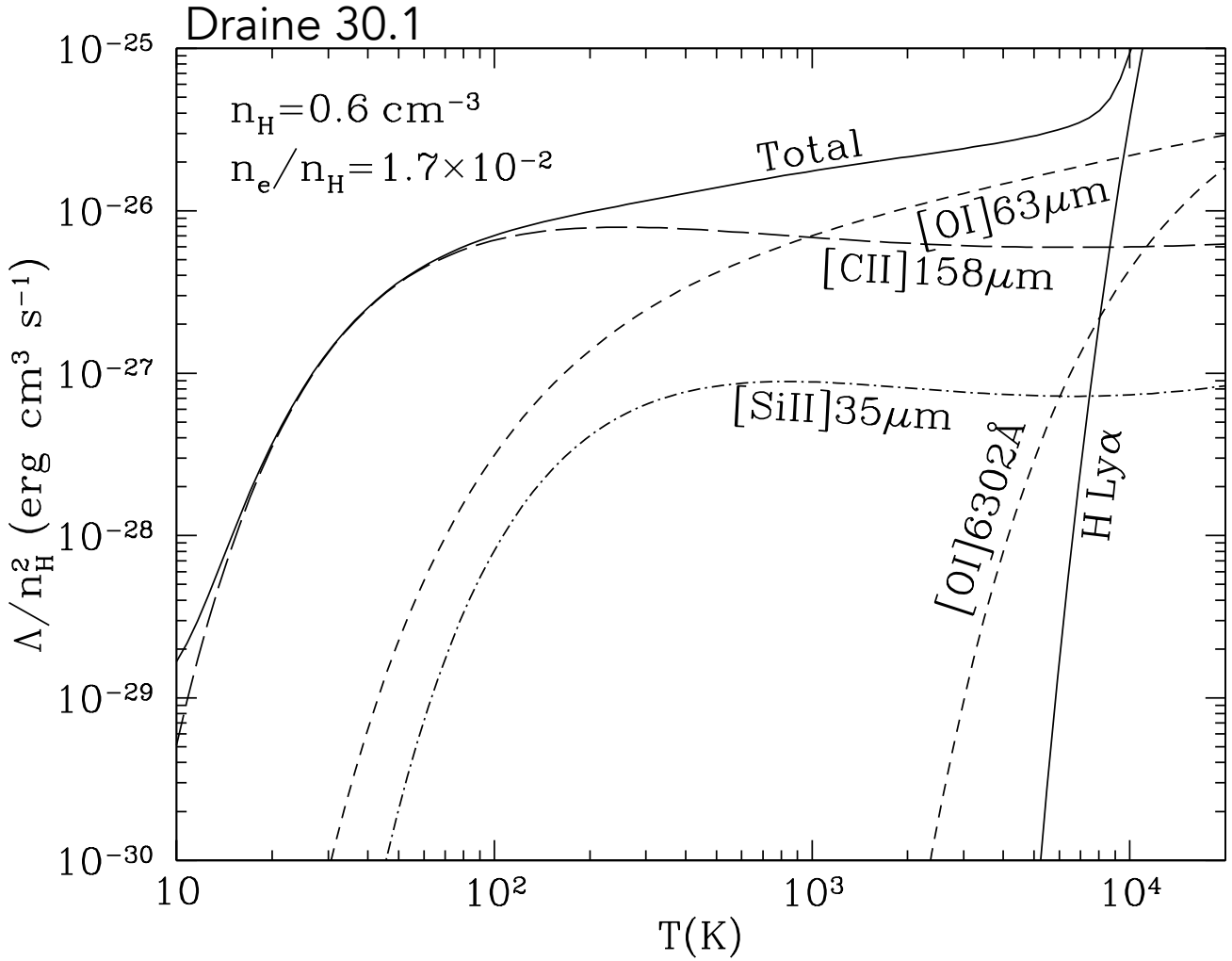
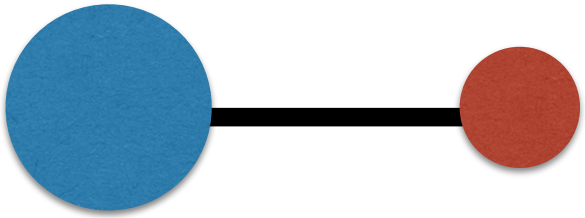
Emission lines from ions, atoms & molecules are critical for cooling ISM gas



Neutral Gas

Order of Magnitude Molecular Energy Levels

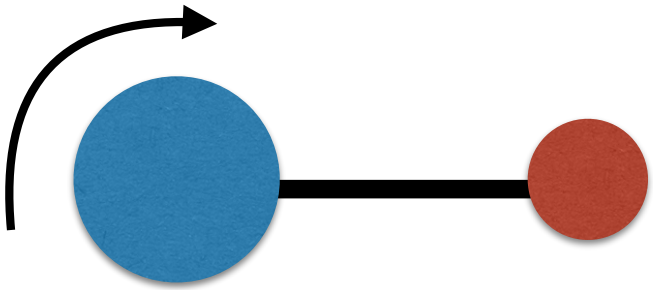
Cover diatomic molecules, read Draine ch 5 for more detailed info.



1) Electronic Transitions of e-

Order of Magnitude Molecular Energy Levels

Cover diatomic molecules, read Draine ch 5 for more detailed info.

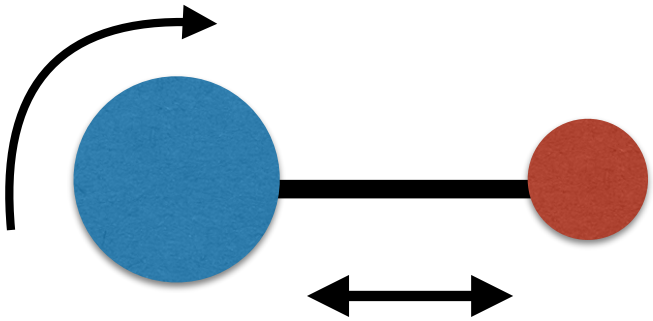


1) Electronic Transitions of e-

2) Rotational Transitions

Order of Magnitude Molecular Energy Levels

Cover diatomic molecules, read Draine ch 5 for more detailed info.



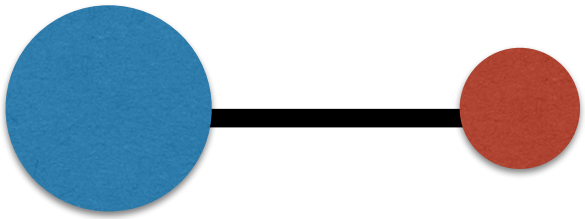
1) Electronic Transitions of e-

2) Rotational Transitions

3) Vibrational Transitions

Order of Magnitude Molecular Energy Levels

Typical energies

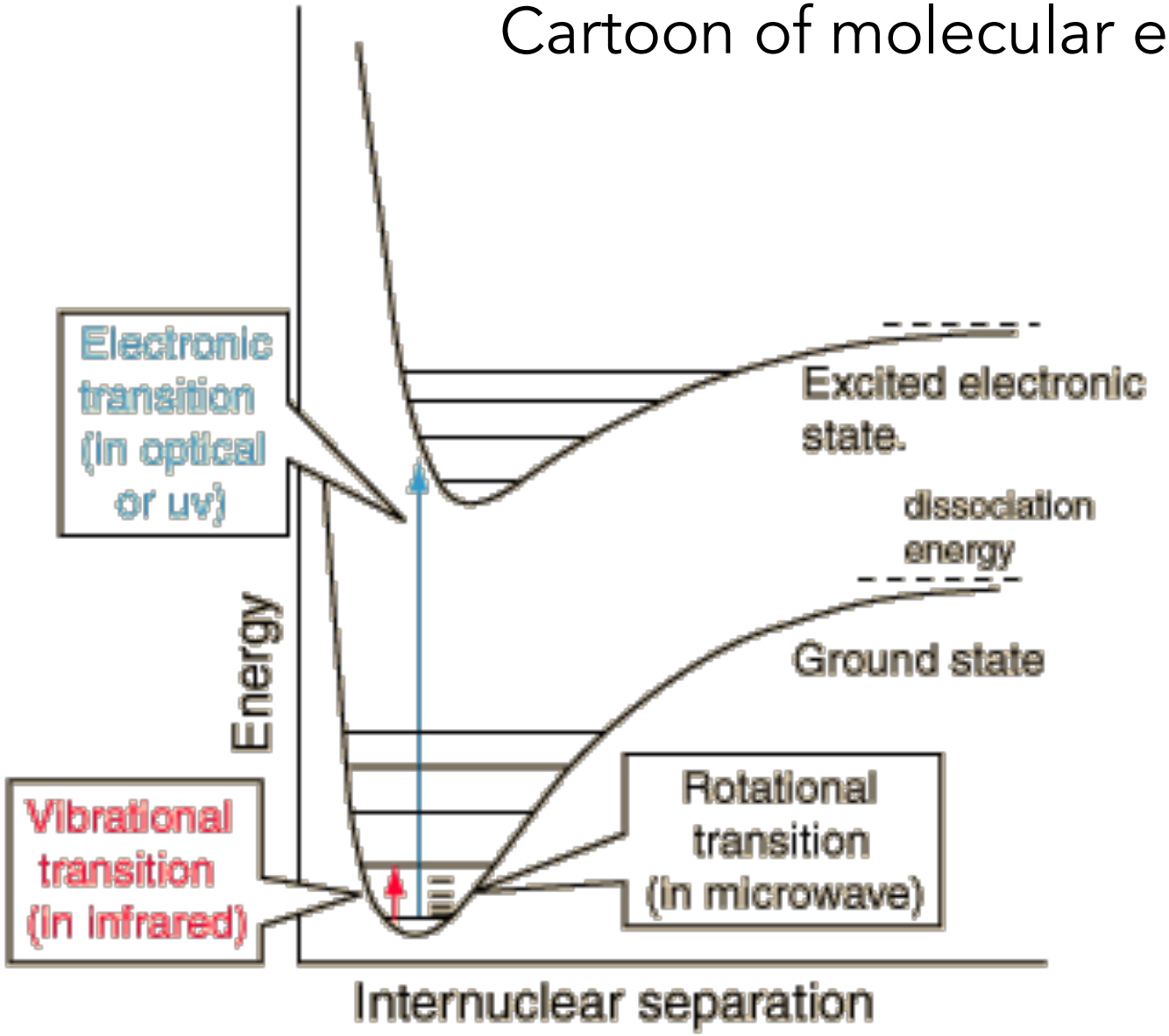


$$E \sim E_{rot} + E_{vib} + E_{el}$$

10^{-3}-10^{-2} eV 10^{-2}-10^{-1} eV 1-10 eV

Electrons move much more quickly than nuclei
so for rotation/vibration calculations we can average over
the electron transitions (Born-Oppenheimer approximation)

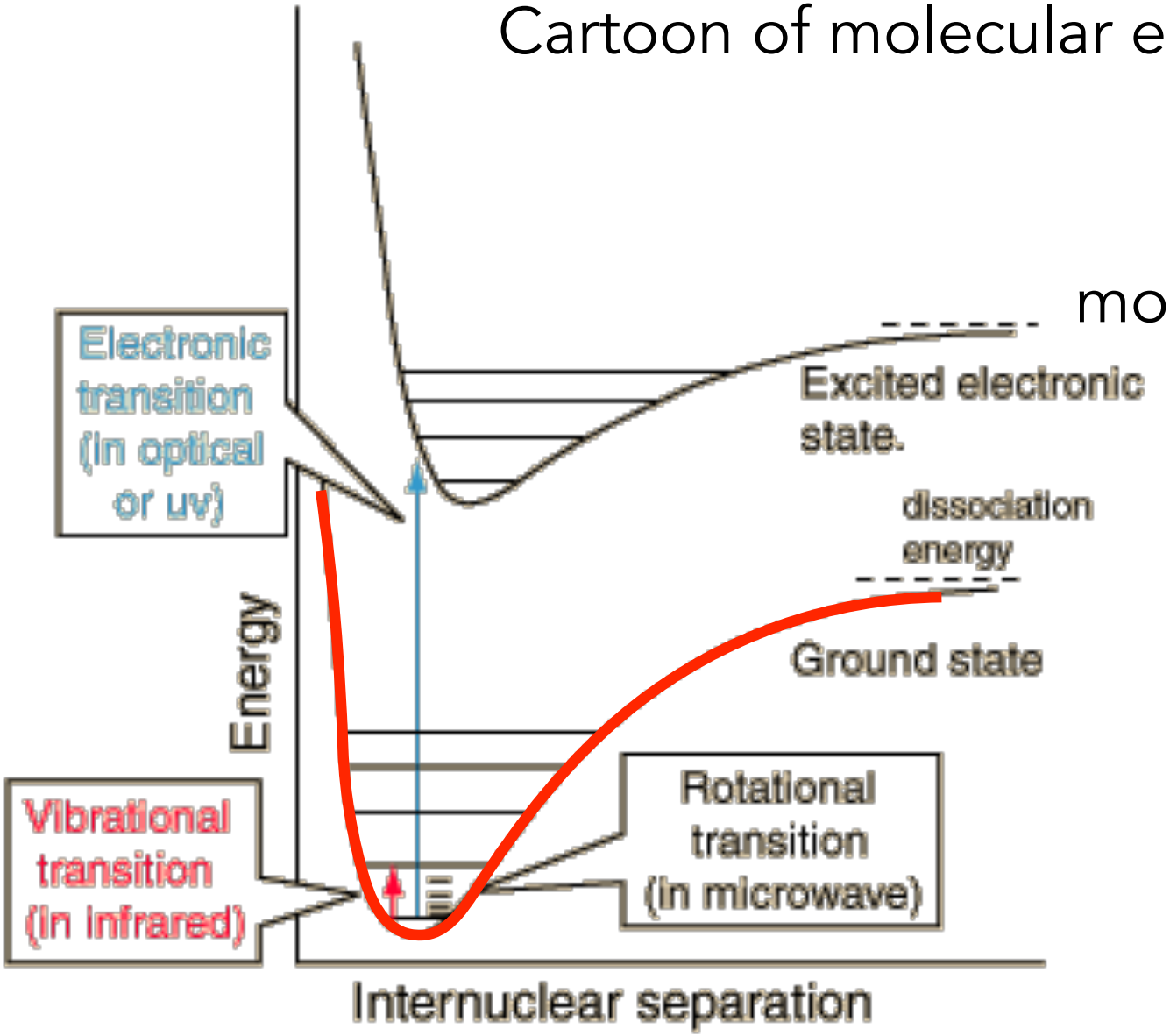
Cartoon of molecular energy levels



http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Cartoon of molecular energy levels

Basic structure of molecule sets this curve



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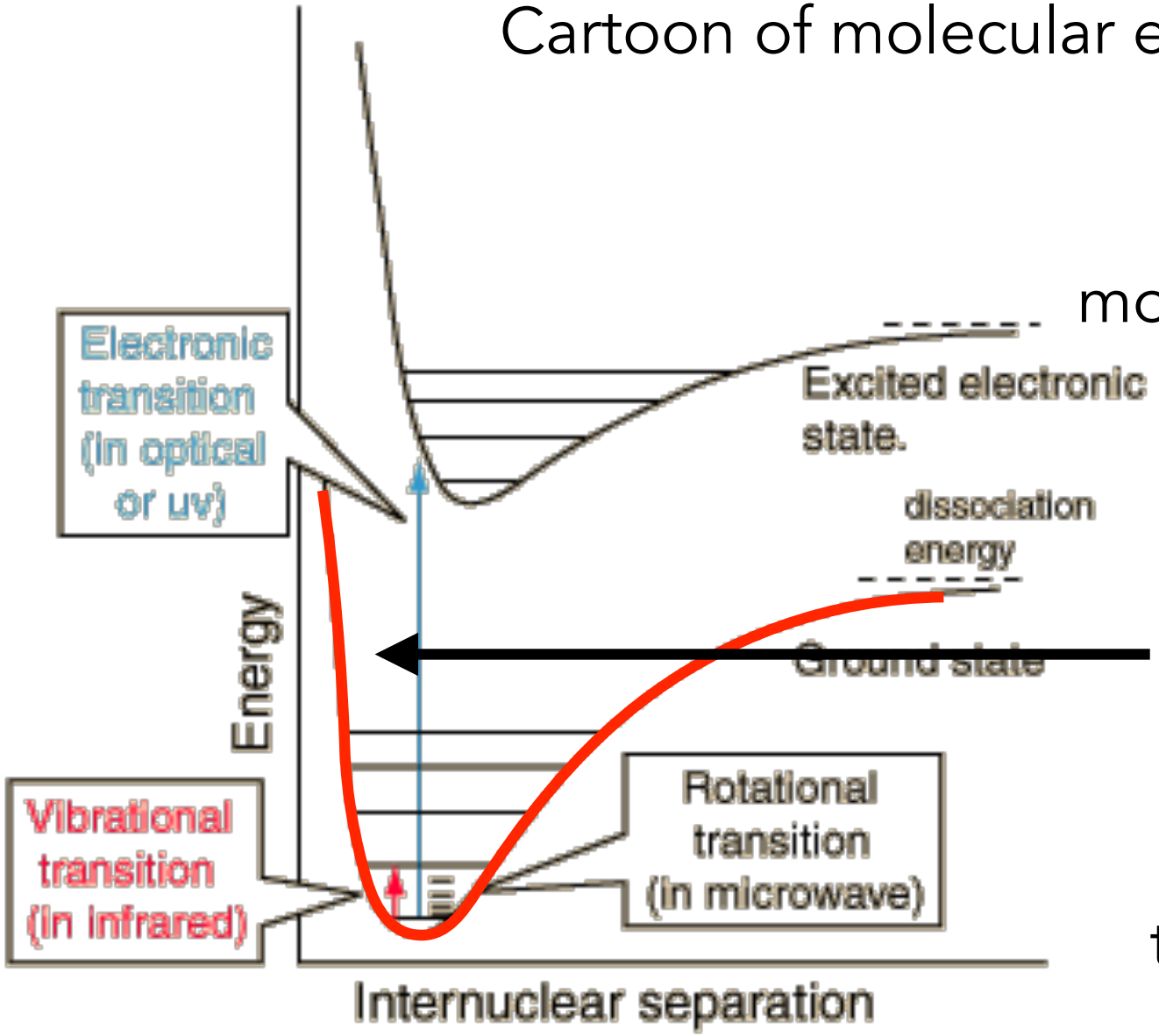

Basic structure of molecule sets this curve

If nuclei get too close together the repel each other, so energy required to make to get R->0 is large.

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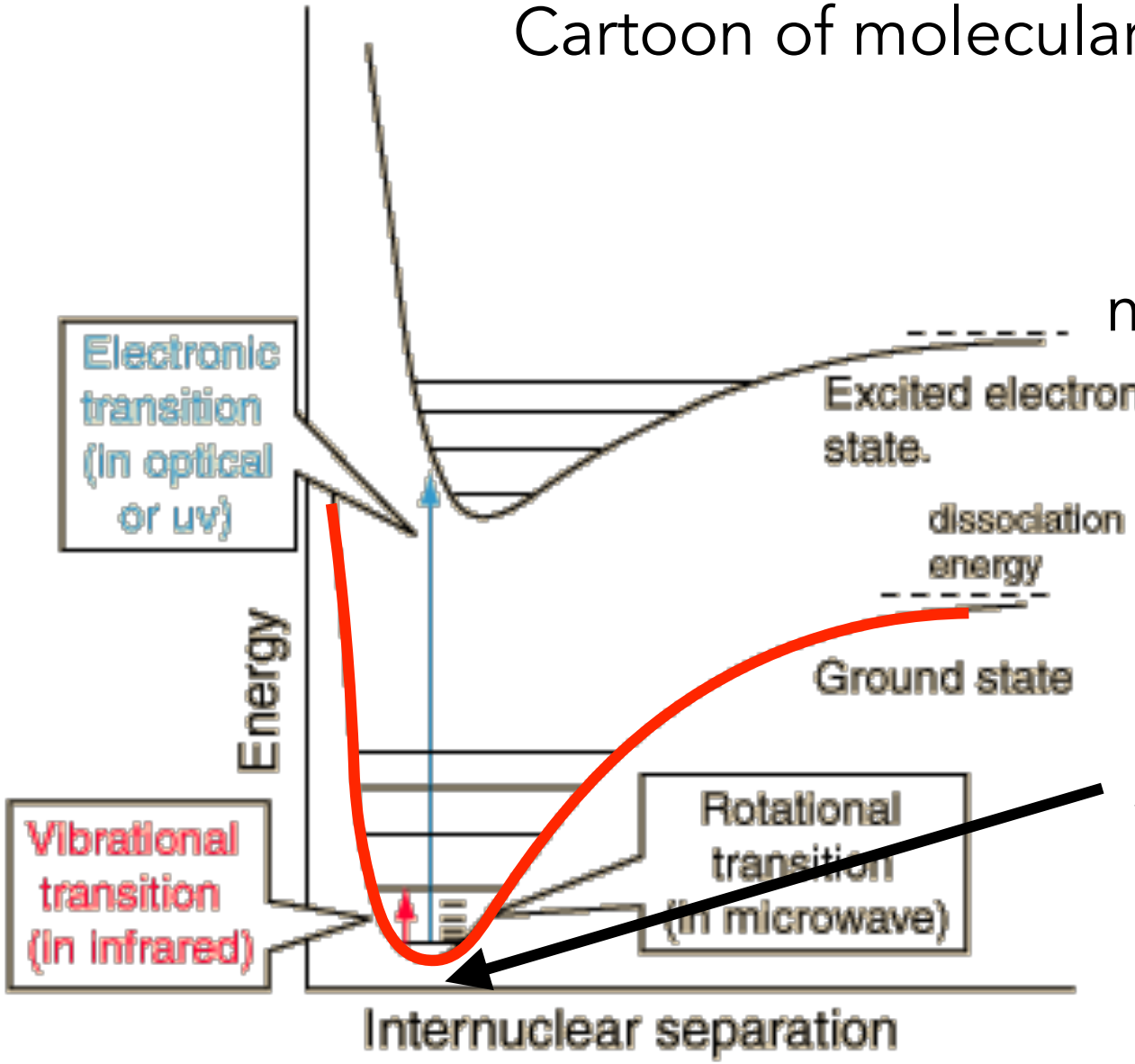
Cartoon of molecular energy levels

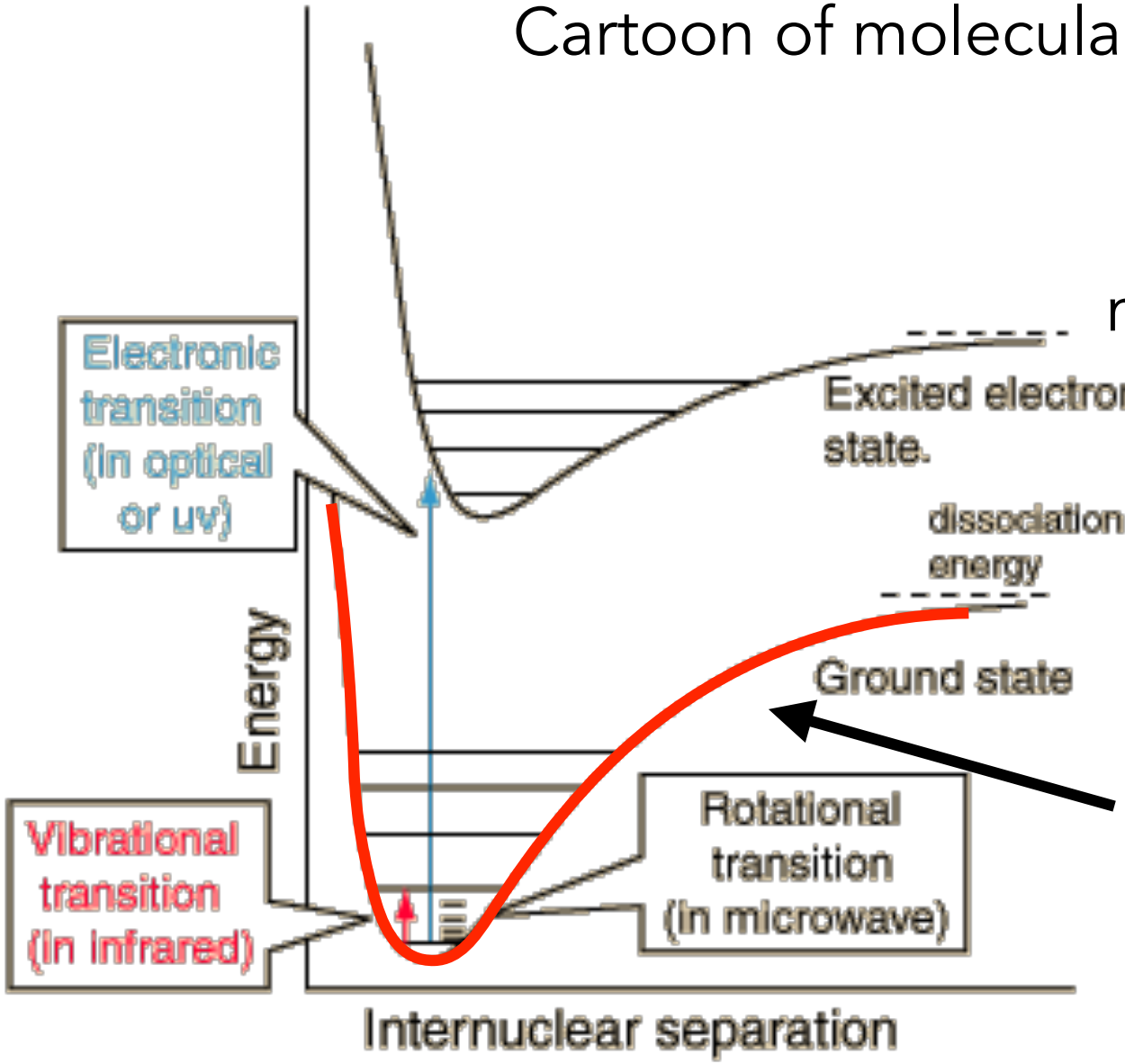


Basic structure of molecule sets this curve

Minimum separation set by the properties of the specific molecular bond.

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Cartoon of molecular energy levels

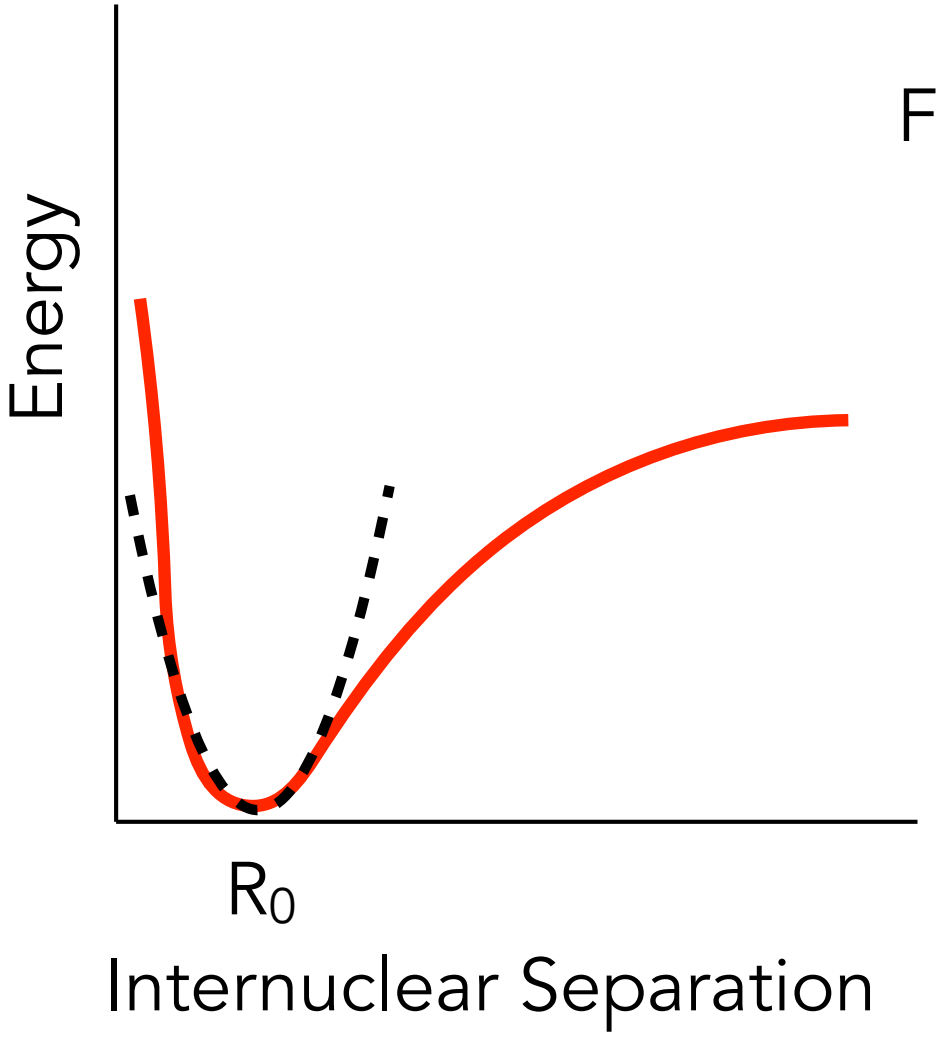


Basic structure of molecule sets this curve

R^{-6} long range attraction from van der Waal's force (fluctuations in electric dipole in one nucleus induces electric dipole in other nucleus)

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Can be approximated as a simple harmonic oscillator around R_0



Potential energy:

$$V(r) = V(R_0) + 1/2\ k\ (r - R_0)^2$$

k = "spring constant"
related to molecular bond

Fundamental Frequency of oscillator:

$$\omega = (k/m_r)^2$$

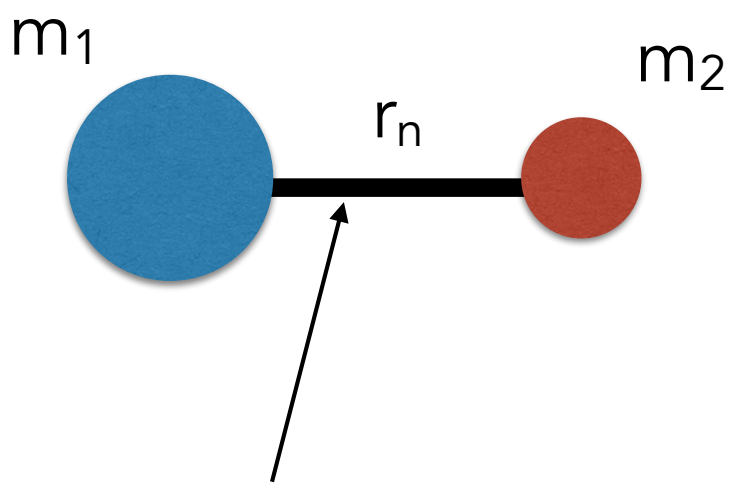
$$m_r = m_1m_2/(m_1+m_2)$$

Vibrational Energy Levels:

$$E_{vib} = \hbar\omega(v + 1/2)$$

v = vibrational quantum number

Rotational Transitions



Moment of intertia:

$$I = m_r r_n^2$$

reduced mass:

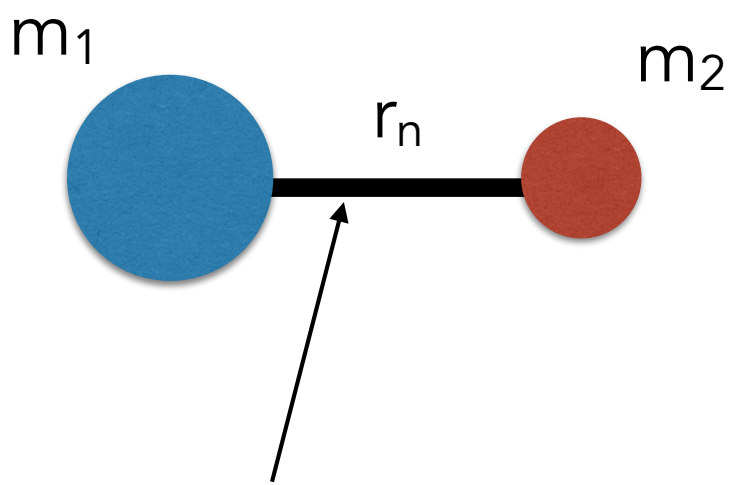
$$m_r = m_1 m_2/(m_1+m_2)$$

Rotational Energy Levels:

$$E_{rot} = \frac{J(J+1)\hbar^2}{2m_r r_n^2}$$

J = rotational quantum number

Rotational Transitions



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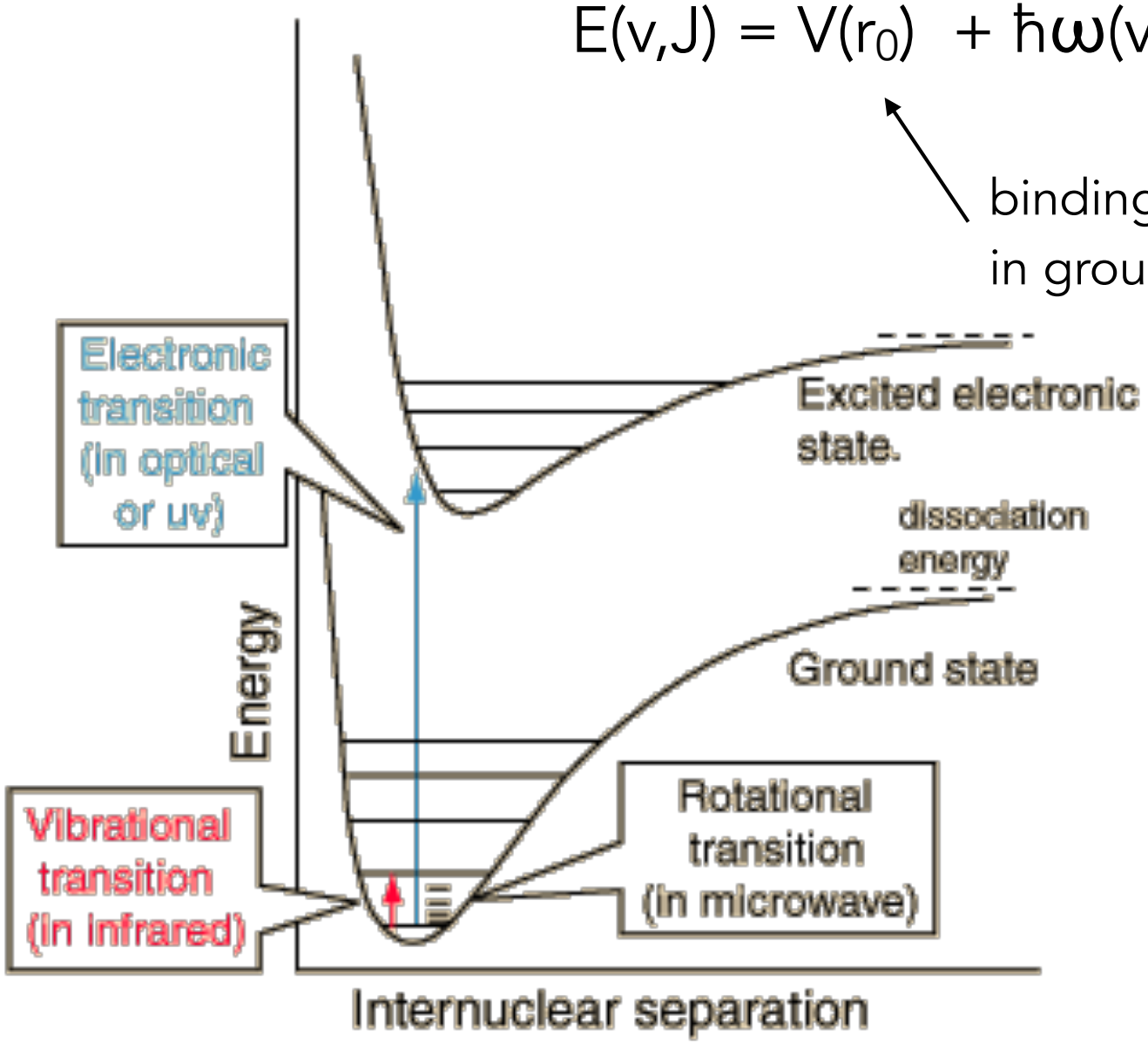
Define $B_v = \dfrac{\hbar^2}{2m_r r_n^2} = 2.1 \times 10^{-3} (m_H/m_r) (1\ \text{Å}/r_n)^2\ \text{eV}$

"rotational constant"

Total Energy:

$$E(v,J) = V(r_0) + \hbar\omega(v + 1/2) + B_vJ(J+1)$$

binding energy in ground state



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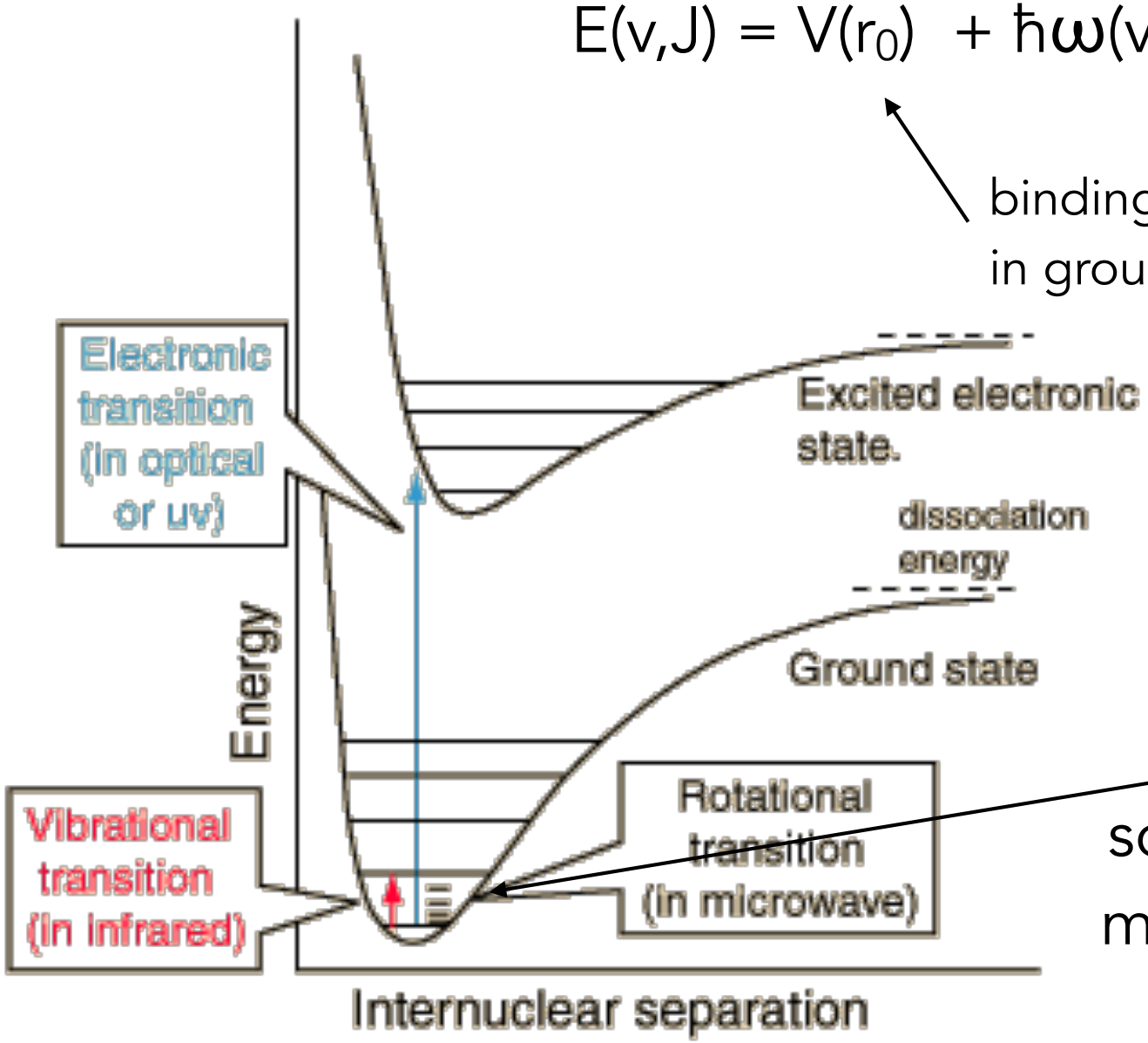
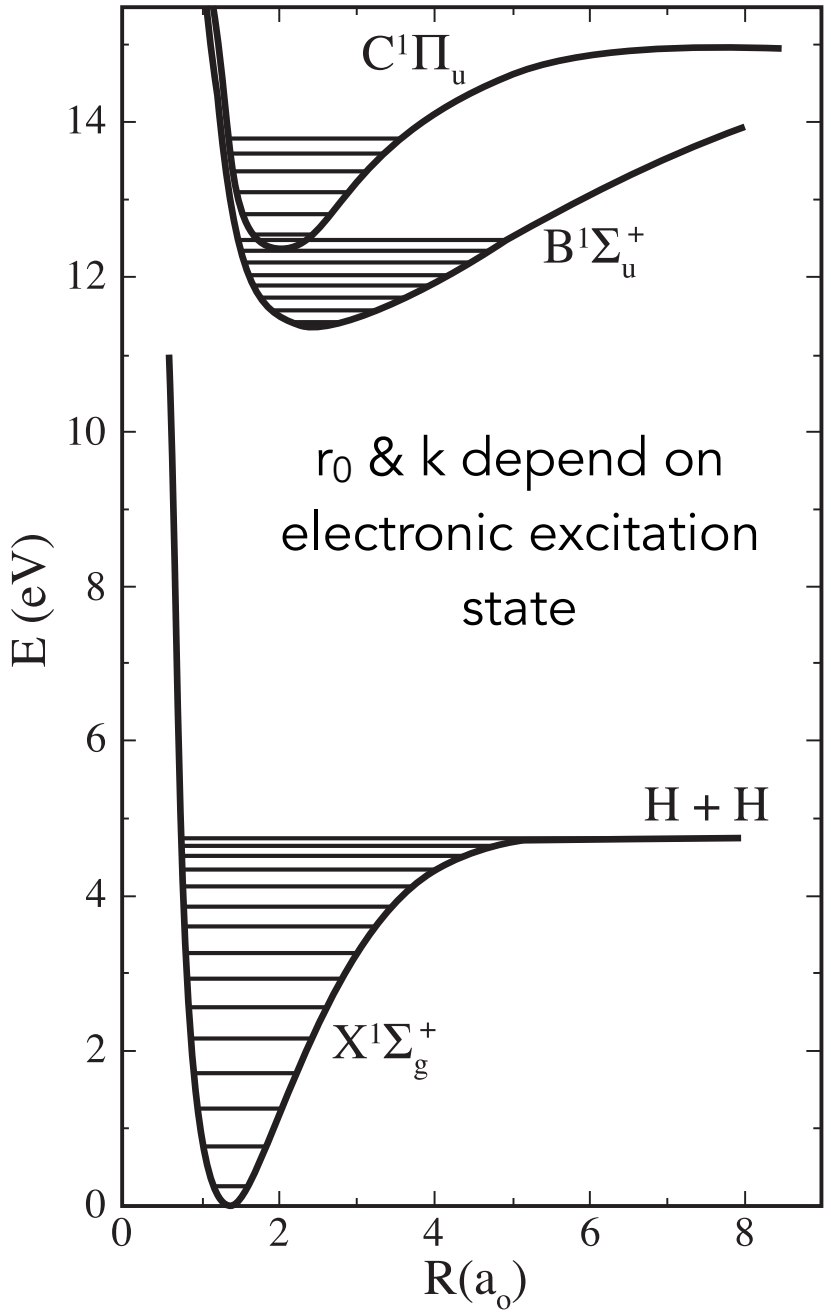


Generally:

$\hbar\omega >> B_v$

so rotational levels are more closely spaced in energy

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html



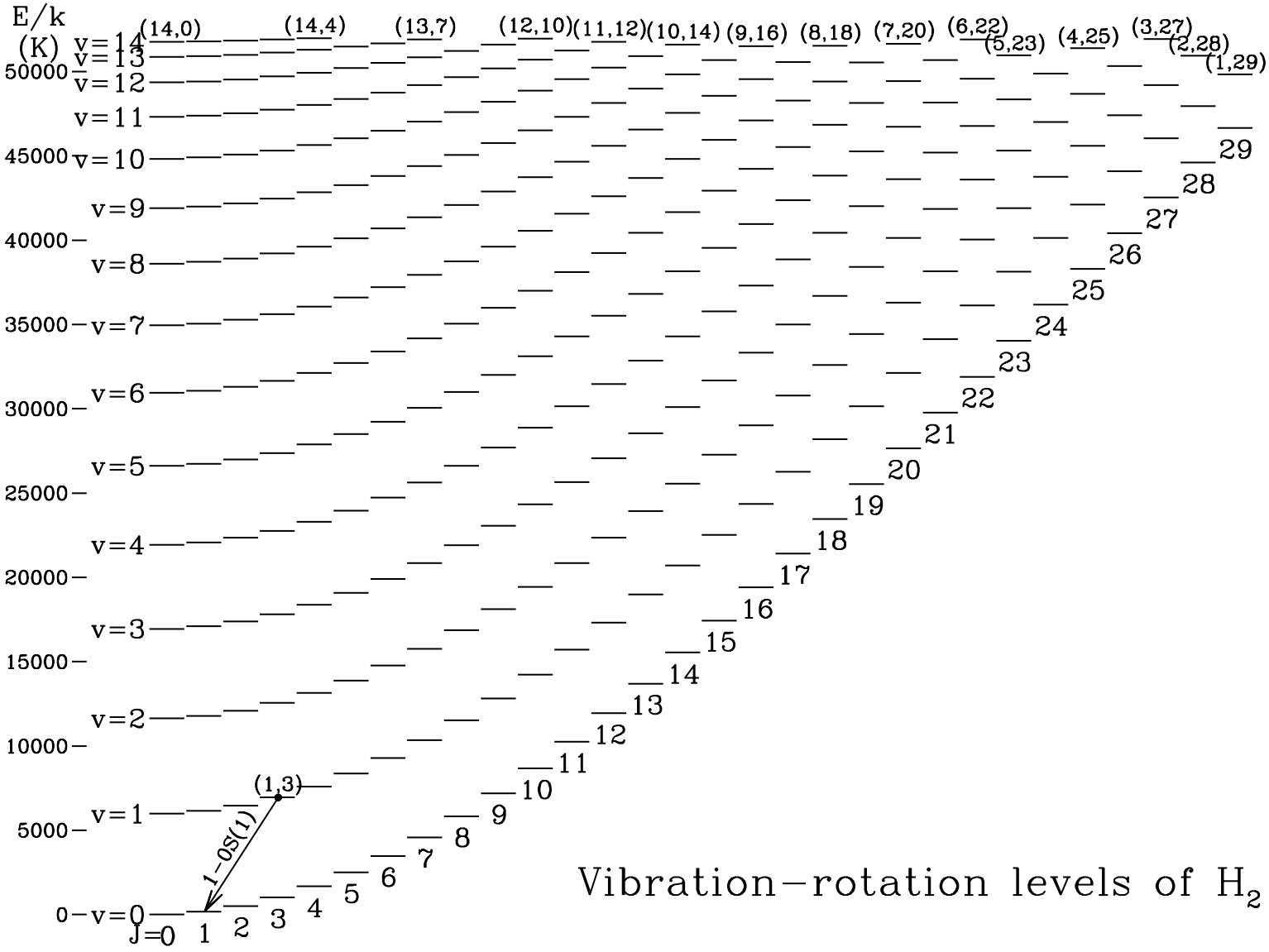
r_0 & k depend on electronic excitation state

H_2 Molecule

Additional wrinkle for H_2:
protons, like electrons,
can't share same quantum state

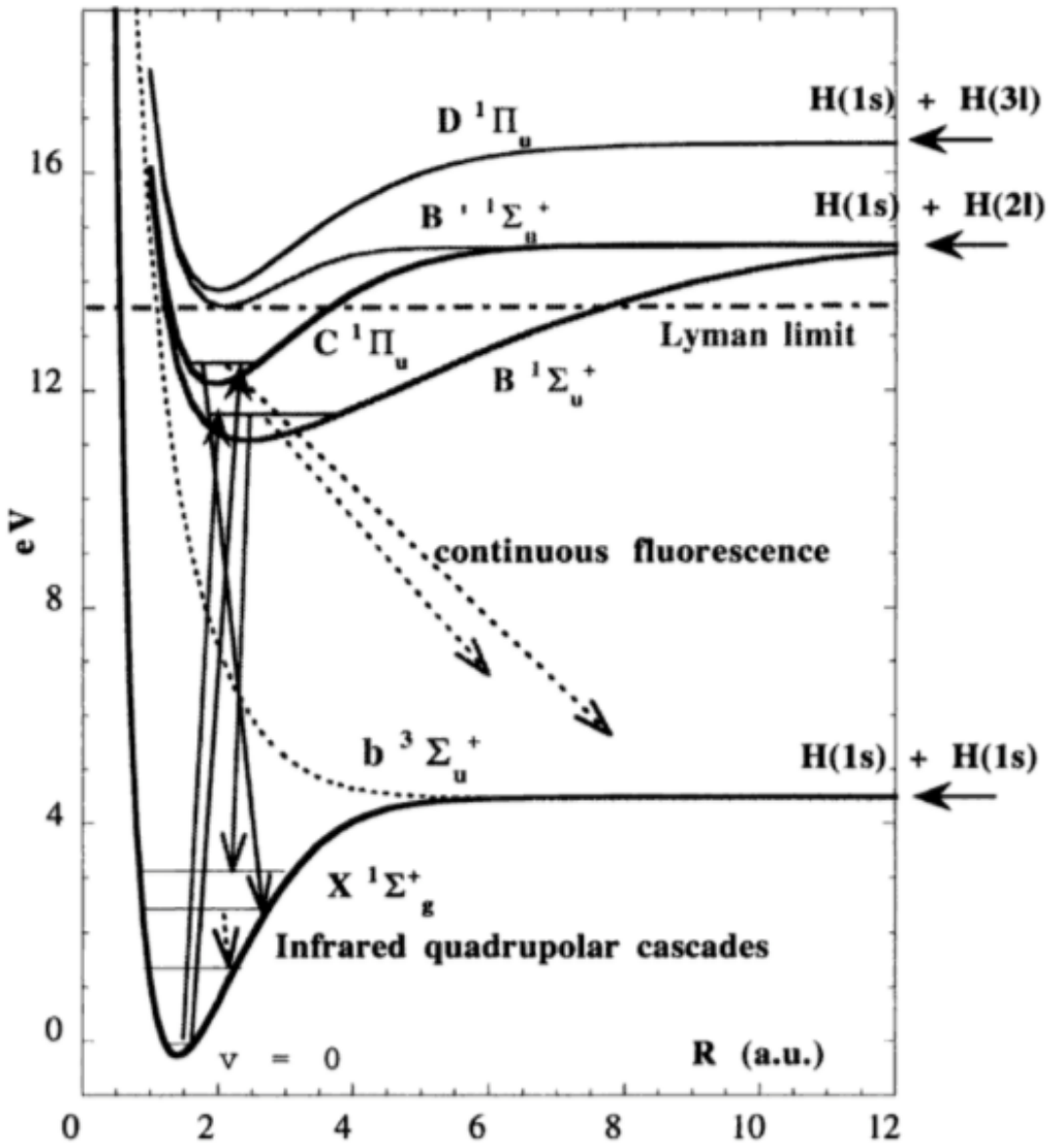
If total proton spin is 1,
rotational number J must be even.
-> "para-H_2" J=0,2,4…

If total proton spin is 0
rotational number J must be odd.
-> "ortho-H_2" J=1,3,5…



Vibration−rotation levels of H_2

Only $\Delta J = 0, \pm 2$ are possible to stay para-para or ortho-ortho



Combes & Pineau des-Forets 2000

Lots of interesting ways for H_2 to de-excite after getting into an electronic excited level.

Some involve dissociating some involve rotational cascades.

Will come back to H_2 when we get to molecular gas.

Radiative Transfer

Motions of individual particles

On scales ≫ mean free path for collisions

↓

Fluid dynamics

Propagation of individual photons

On scales ≫ λ

↓

Radiative Transfer

Transport Phenomena: https://en.wikipedia.org/wiki/Transport_phenomena