Lecture 2

- The photoionization cycle
- Ionization calculations
- Level populations
- Critical densities, n_e^{cr}
- Transition probabilities/selection rules
- Excitation mechanisms for levels/lines

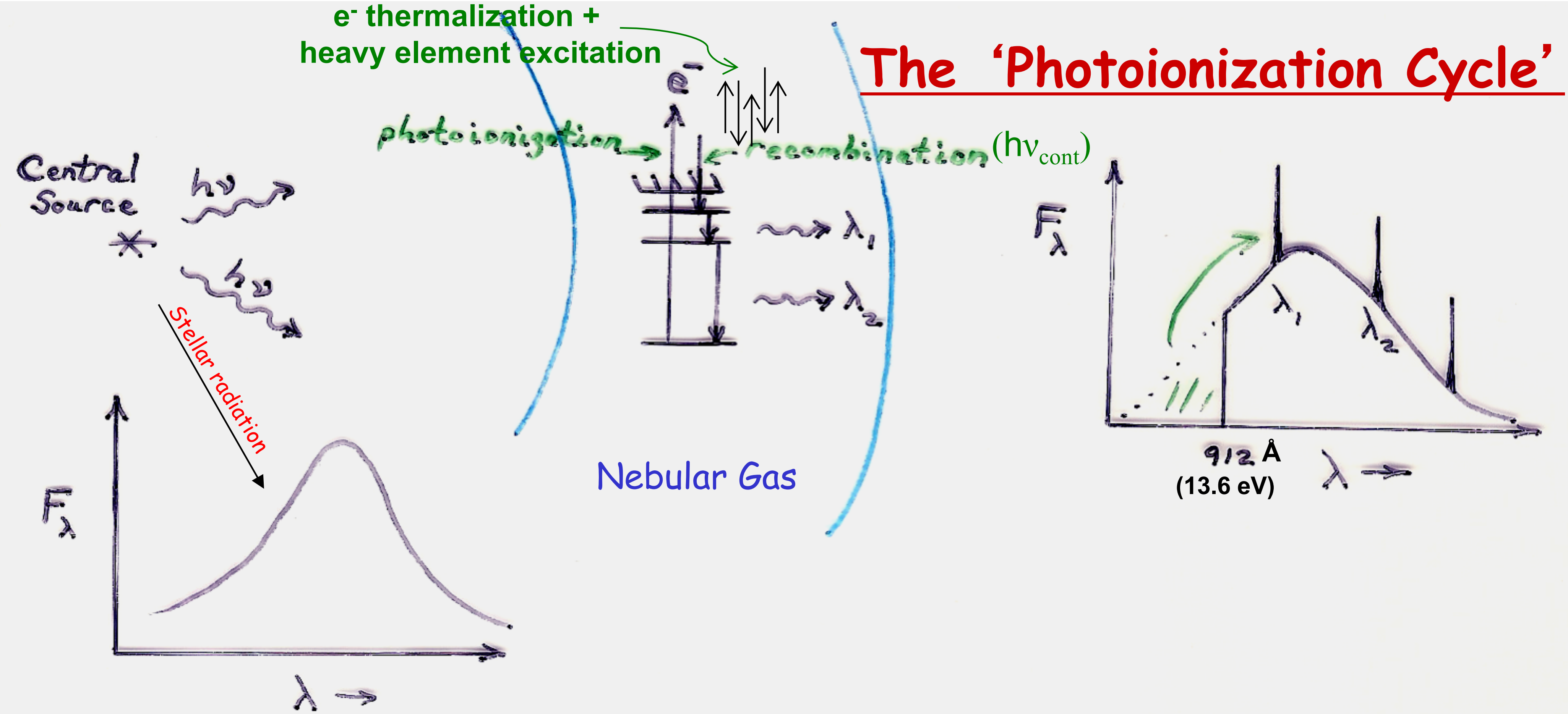
❖***Statistical Equilibrium*** is the concept that applies to processes, i.e., ionization, temperature, level populations, etc., that have arrived at a ***steady-state*** equilibrium that is determined by the interactions that create *(populate)* and that destroy (*de-populate*) that state.

-In a time-constant situation the ***rate equations*** define the balance that determines the values of parameters. For example, at each point in space where steady-state equilibrium applies

Ionization: No. of ionizations/(cm^3 sec) = No. of de-ionizations/(cm^3 sec)

Level population: No. of excitations/(cm^3 sec) = No. of de-excitations/(cm^3 sec)

Temperature: Rate of energy input/(cm^3 sec) = Rate of energy loss/(cm^3 sec)



1) UV (λ<912 Å) radiation is absorbed by neutral H° gas surrounding hot star, ionizing it (ISM timescale, t~10^3 yr)
2) Ejected e⁻ 'thermalizes' from collisns w other e⁻'s and ions (1 mo). Then, …….
3) Electron recapture (recombination) by H^+, typically to an excited level (after t~10^3 yrs)
4) Excited H° rapidly decays to ground state by emission of line radiation of Paschen, Balmer, Lyman ….series (t~10^{-7} sec)
5) Remains in ground state (t~10^3 yr) before process repeats

→ Net Result: Stellar UV radiation converted to H & He emission line+continuum radiation + hot gas

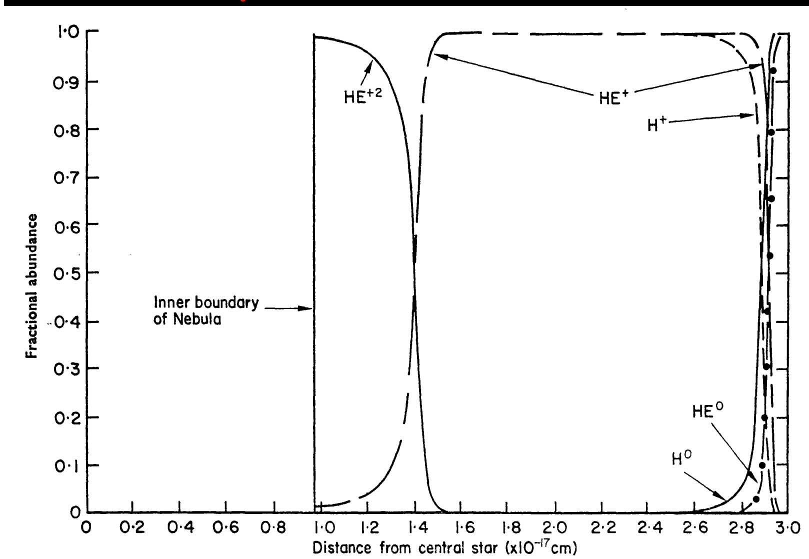
❖ 'Stromgren Sphere' Interpretation of Ionization Structure

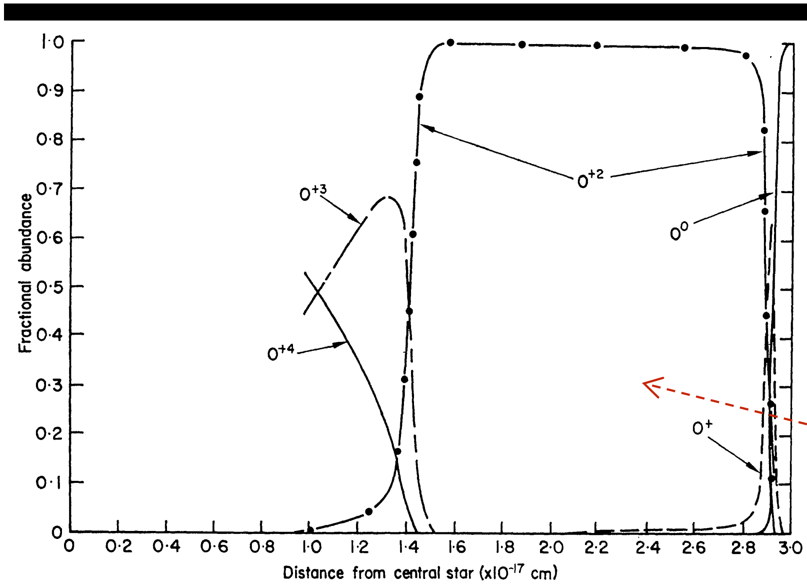
(Stromgren, B. 1939, ApJ, 89, 526)

(Independent variable: *r*)

Planetary Nebula: $J_\nu \propto B_\nu(T)$

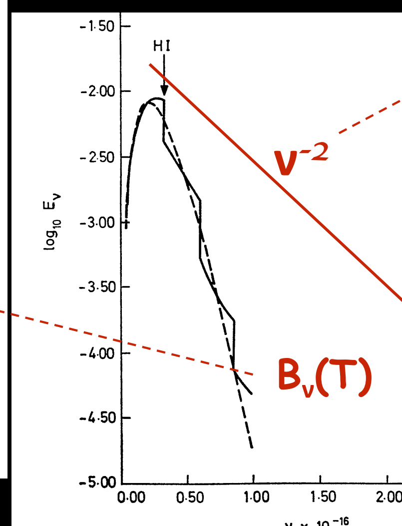
Crab Nebula: : $J_\nu \propto \nu^{-2}$

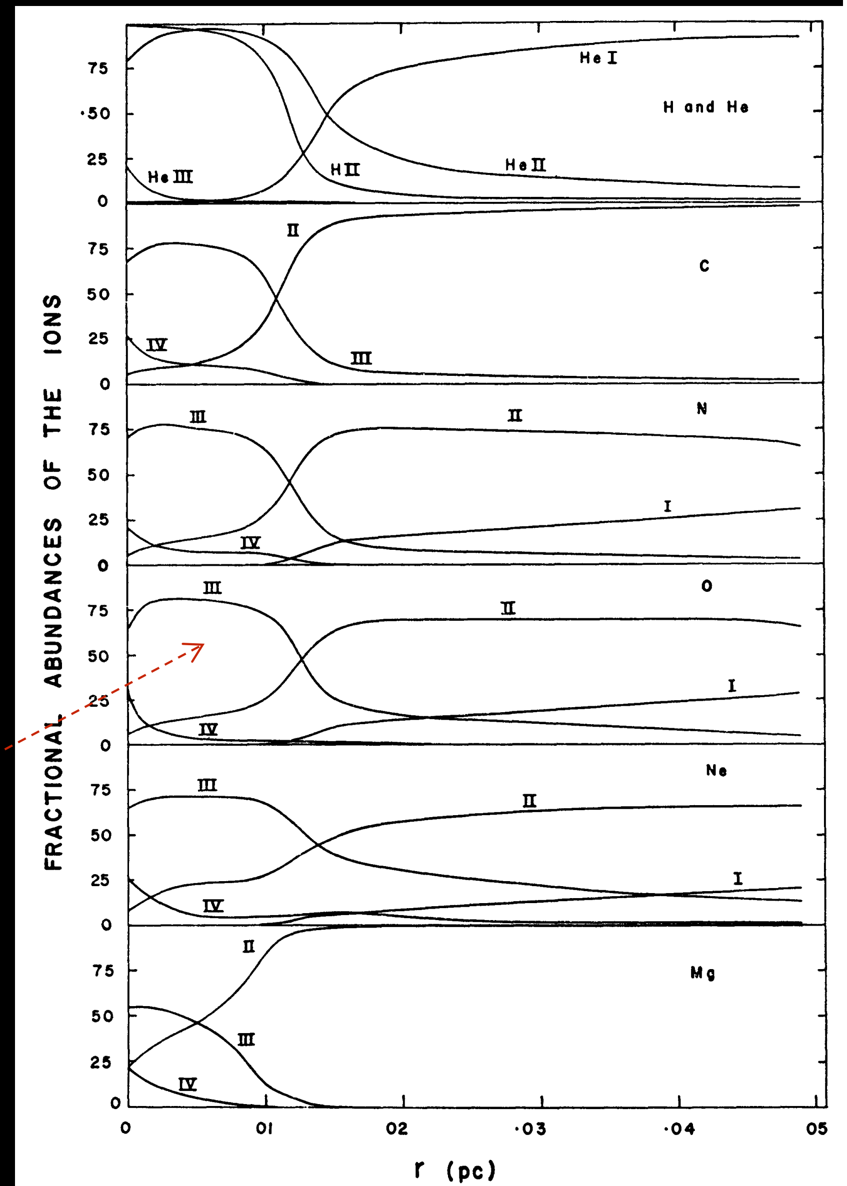




..... as in:

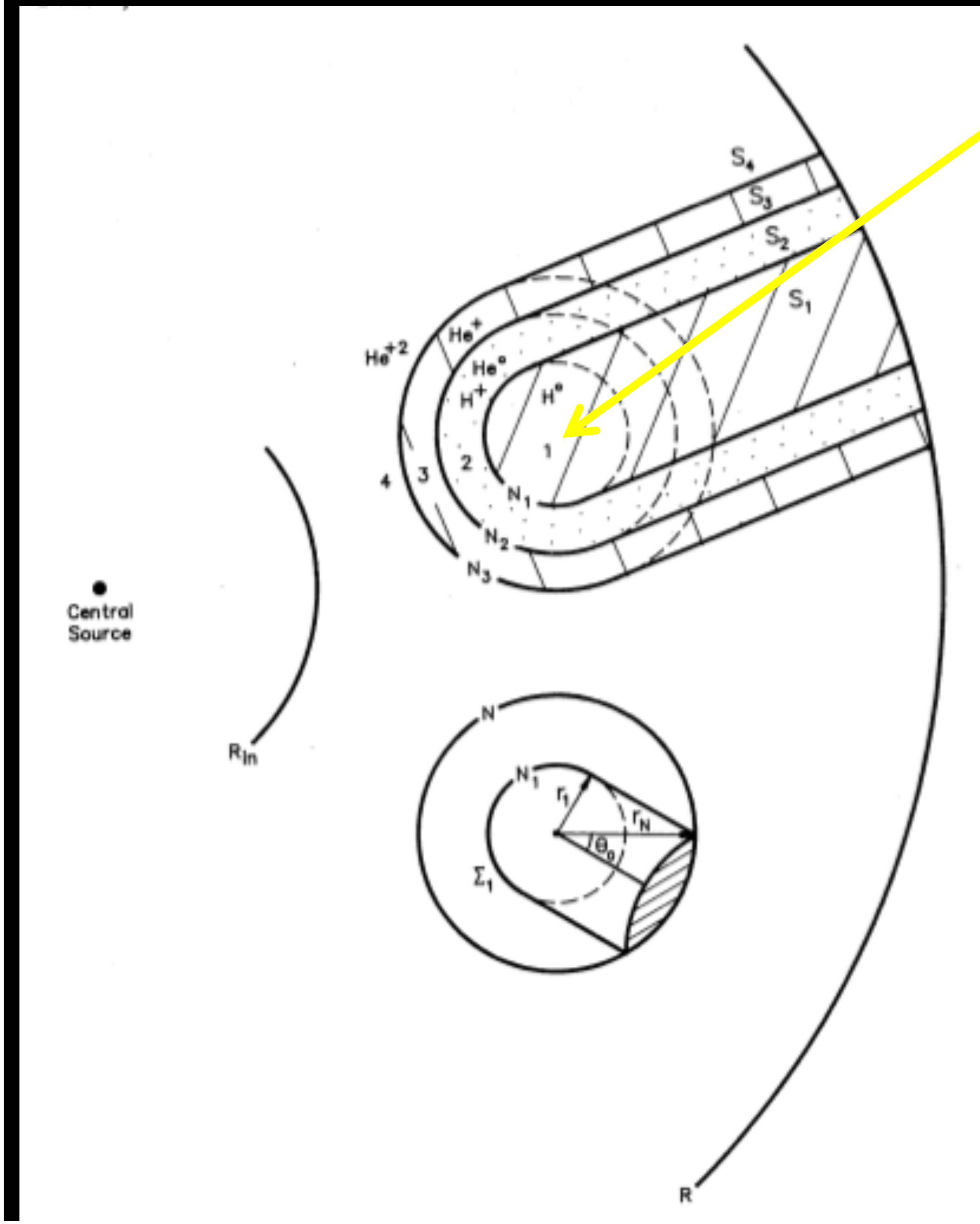
' CLOUDY'
(www.nublado.org)
or
'MAPPINGS'
(www.ifa.hawaii.edu/~kewley/Mappings/)
or
'ION'





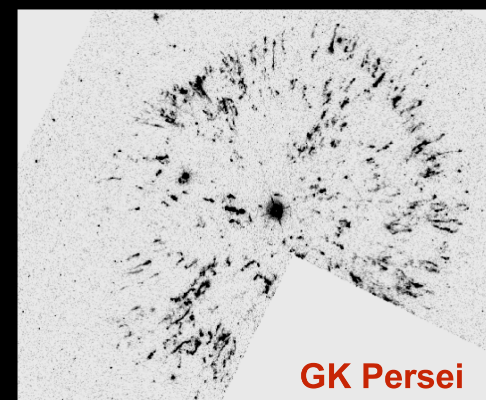
'Density Inhomogeneity' Interpretation of Ionization Structure

(Independent variable: *n*)

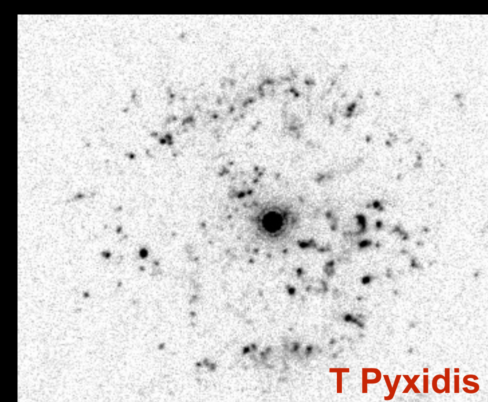


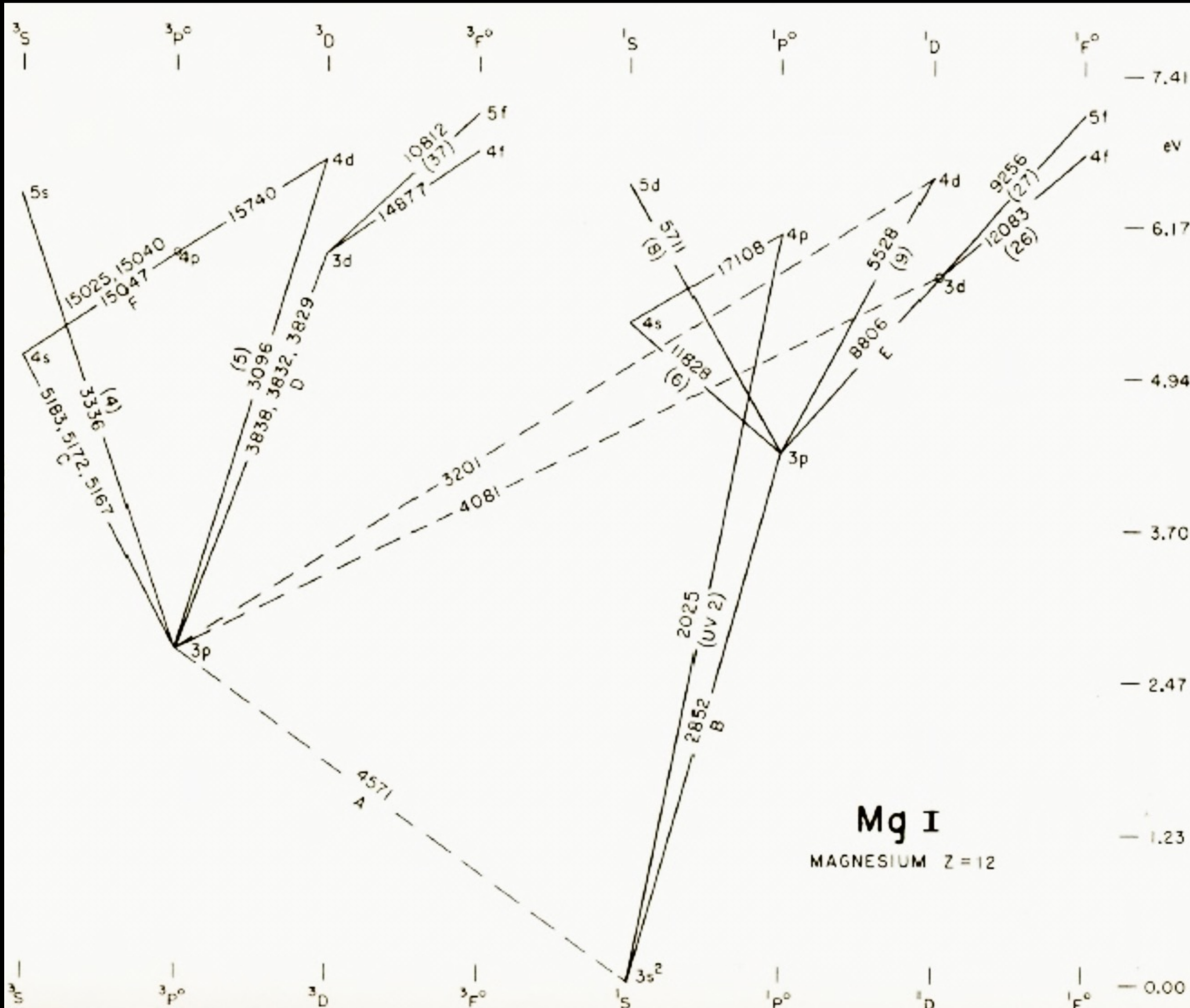
$n(r) \propto n_o \, r^{-\gamma}$

Complex geometry, so not yet successfully modeled in detail . . . . . .

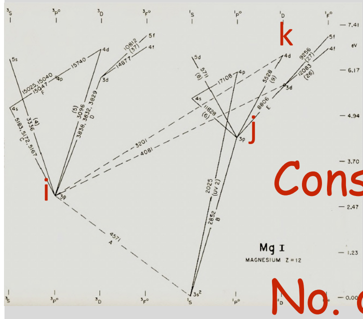

GK Persei


NGC 7293 'Helix'


T Pyxidis



Mg I
MAGNESIUM Z = 12
eV
7.41
6.17
4.94
3.70
2.47
1.23
0.00
4571
A
2852
B
2025
(UV 2)
5183, 5172, 5167
C
3838, 3832, 3829
D
8806
E
15025, 15040
15047
F
3336
(4)
3096
(5)
3201
4081
15740
14877
10812
(37)
5711
(8)
11828
(6)
17108
5528
(9)
9256
(27)
12083
(26)



Level Populations

Consider rate of radiative & collisional interactions into/out of excited level j.

No. of radiative (de-)excitations out of level j/(cm^{3}sec) = $n_j\,(A_{ji} + \cancel{B_{ji}J_{ji}})$ ignore

No. of radiative excitations into level j/(cm^{3}sec) = $n_1 B_{1j} J_{1j}$

No. of collisional excitations, de-excitations into j/(cm^{3}sec) = $\sum_k n_e n_k \langle\sigma_{kj}^{de\text{-}exc}(v)\, v\rangle$

No. of collisional excitations, de-excitations out of j/(cm^{3}sec) = $\sum_k n_e n_j \langle\sigma_{jk}^{exc}(v)\, v\rangle$

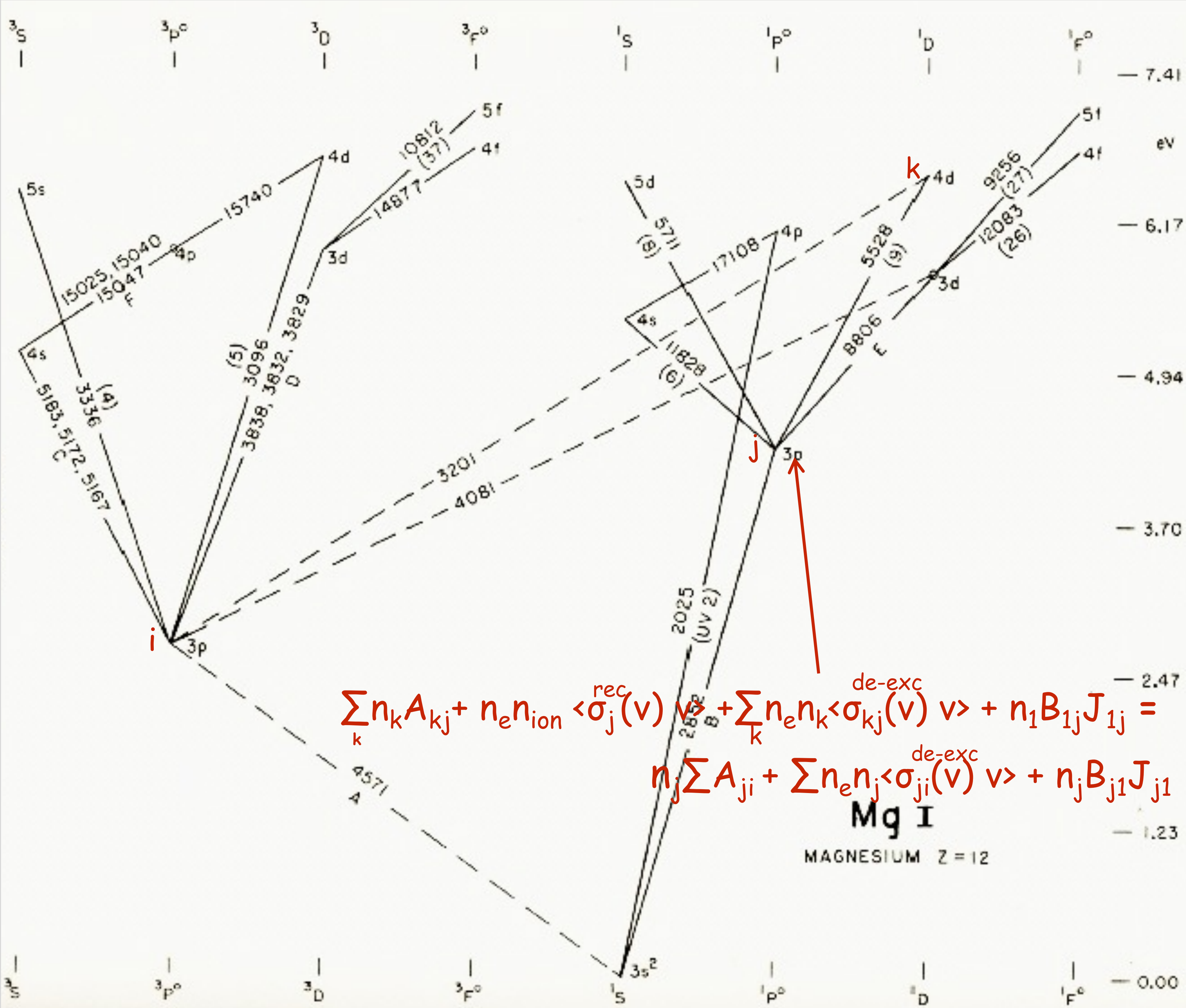
No. of electron recombinations into level j/(cm^{3}sec) = $n_e n_{ion} \langle\sigma_j^{rec}(v)\, v\rangle$

- **Statistical equilibrium** for level j that determines its population (and therefore the intensity of its line emission) is determined by the condition that:

Rate into level j/(cm^3 sec) = Rate out of level j/(cm^3 sec)

$$\sum_{k>j} n_k A_{kj} + n_e n_{ion} \langle\sigma_j^{rec}(v)\, v\rangle + \sum_k n_e n_k \langle\sigma_{kj}^{(de\text{-})exc}(v)\, v\rangle + n_1 B_{1j} J_{1j} = n_j \sum A_{ji} + \sum_{i<j} n_e n_j \langle\sigma_{ji}^{de\text{-}exc}(v)\, v\rangle + n_j B_{j1} J_{j1}$$

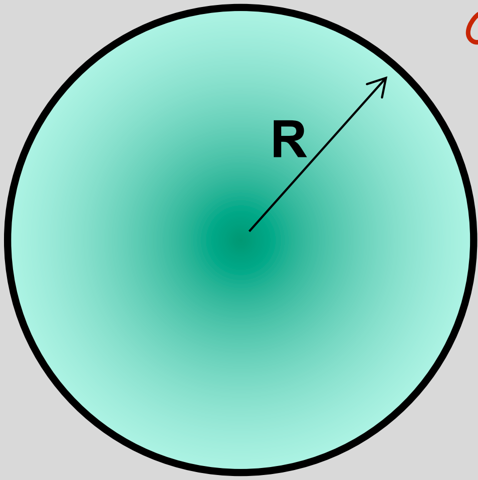
Resonance line scattering



$$\sum_k n_k A_{kj} + n_e n_{ion} \langle \sigma_j^{rec}(v)\, v \rangle + \sum_k n_e n_k \langle \sigma_{kj}^{de\text{-}exc}(v)\, v \rangle + n_1 B_{1j} J_{1j} =$$

$$n_j \sum A_{ji} + \sum n_e n_j \langle \sigma_{ji}^{de\text{-}exc}(v)\, v \rangle + n_j B_{j1} J_{j1}$$

Emission-Line Coefficients



Consider simplified situation where only one process populates a level and simple radiative decay de-populates it.

Let j_{21}=emission coefficient of transition 2->1 of some ion
F_{21} = observed flux of line from object at distance d

Luminosity of object in line 2->1, $L_{21} = \int_{vol} (4\pi j_{21})\, dV$ (if optically thin)

$$= 16\pi^2 \int_0^R j_{21}(r)\, r^2\, dr \quad \text{(if sph symm)}$$

$$= 4\pi d^2 F_{21}$$

$$\therefore\ F_{21} = 1/d^2 \int j_{21}\, dV = 4\pi/d^2 \int_0^R j_{21}(r)\, r^2\, dr$$

$$\text{where } j_{21} = n_2 A_{21} h\nu_{21}/4\pi = h\nu_{21}/4\pi \times \left\{ \begin{array}{ll} n_e n_{i+1} \langle \sigma_2^{rec}(v)\, v \rangle & \text{recombination} \\ n_e n_i \langle \sigma_{12}^{exc}(v)\, v \rangle & \text{collisional excitation} \\ n_1 B_{12} J_{12} & \text{resonance fluorescence} \end{array} \right.$$

Temperature Dependence of Collision Rates

The dependence of collision rates on electron temperature T_e and the different values of cross sections means that simplifications can be made in solving the level population equations.

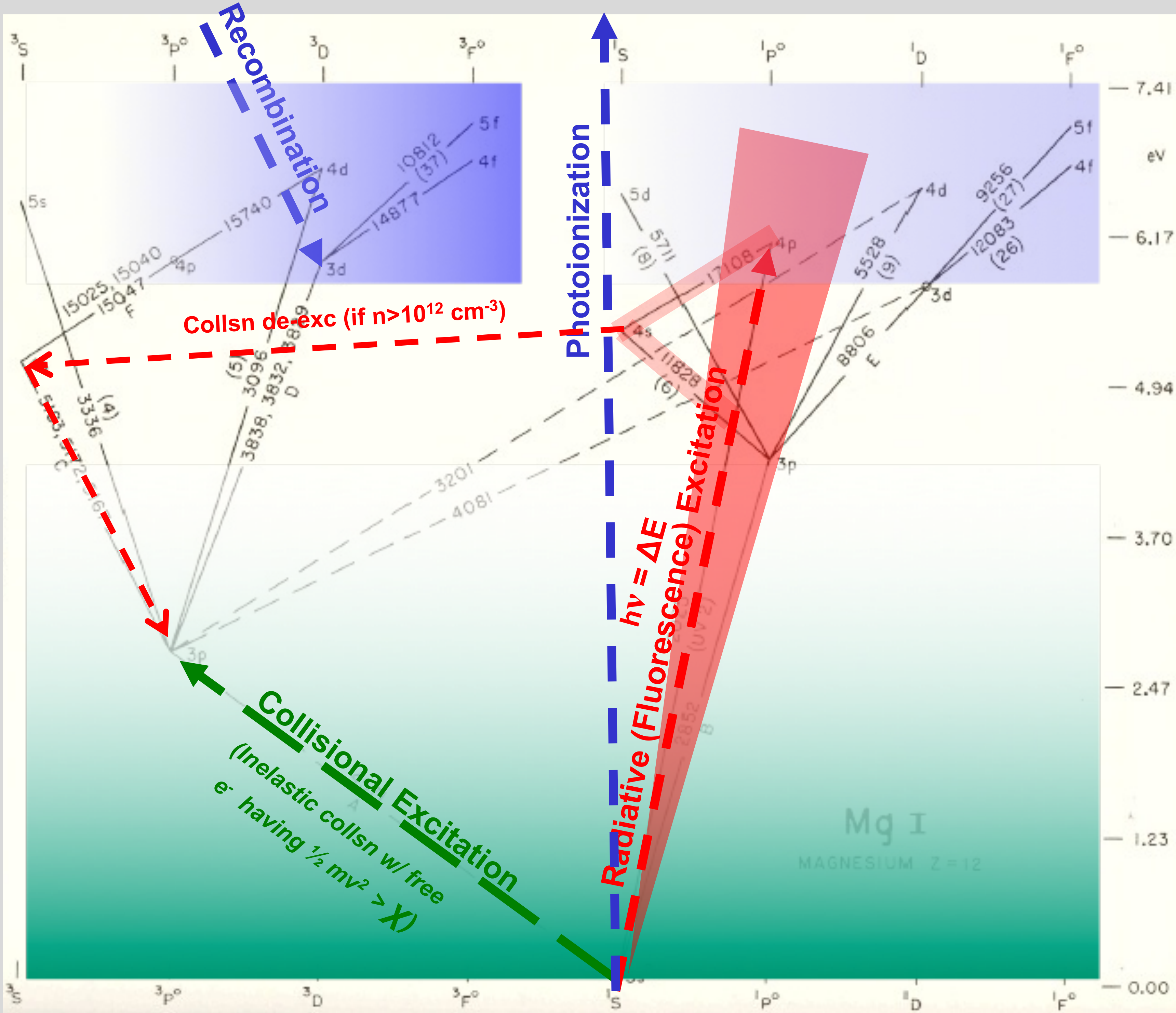
where $\langle \sigma_{ji}^{exc}(v)\, v \rangle = \int_{v_o}^{\infty} \sigma_{ji}^{exc}(v)\, v \times 4/\sqrt{\pi}\, (m/2kT_e)^{3/2}\, v^2 \exp(-mv^2/2kT_e)\, dv$

collisional excitation $\longrightarrow \propto \sigma_o^{exc}\, T_e^{-1/2} \exp(-\chi_{exc}/kT_e)$ with $\sigma_{ji}(v)=\sigma_o(v_o/v)^2$

& e^- energy threshold $\frac{1}{2}mv_o^2 = \chi_{exc}$

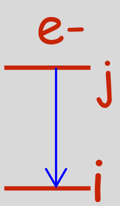
collisional de-excitation $\longrightarrow \approx 10^{-8}\, (10^4/T_e)^{1/2}$ for $\sigma_o = 10^{-16}\, cm^2$

$v_o = 0$ (de-excitation)



Recombination
Photoionization
Collsn de-exc (if n>10^12 cm^-3)
hν = ΔE
Radiative (Fluorescence) Excitation
Collisional Excitation
(Inelastic collsn w/ free
e- having ½ mv² > X)
Mg I
MAGNESIUM Z=12
eV
7.41
6.17
4.94
3.70
2.47
1.23
0.00

'Critical Density' for Transitions



Consider radiative vs. collisional de-excitation of excited level j.

No. of radiative de-excitations/(cm^{3}sec) = $n_j\,A_{ji}$

No. of collisional de-excitations/(cm^{3}sec) = $n_e n_j \langle \sigma_{ji}^{\text{de-exc}}(v)\, v \rangle$

The 'critical density', n_e^c, of level j is the density above which collisional de-excitations dominate radiative decay (so emission from that level weakens w.r.t. transitions from other levels):

$$\mathbf{n_e^c} = A_{ji} / \langle \sigma_{ji}^{\text{de-exc}}(v) v \rangle$$

where $\langle \sigma_{ji}^{\text{de-exc}}(v)\, v \rangle = \int_{v_0}^{\infty} \sigma_{ji}(v)\, v \times 4/\sqrt{\pi}\, (m/2kT_e)^{3/2}\, v^2 \exp(-mv^2/2kT_e)\, dv$

$\propto \sigma_o^{\text{de-exc}}\, T_e^{-1/2} \exp(-mv_o^2/2kT_e)$ with $\sigma_{ji}(v)=\sigma_o(v_o/v)^2$

v_o= e^- velocity excitation threshold

$\sim 10^{-8}\,(10^4/T_e)^{1/2}$ for $\sigma_o = 10^{-16}$ cm^2

$v_o = 0$ (de-excitation)

$\rightarrow\ \therefore\ \mathbf{n_e^c} \propto 10^8 A_{ji}$ cm^{-3}

Transition Probabilities

• From quantum mechanics ***time dependent perturbation theory***, the probability (='expectation value') P_{AB} of a system making a transition from state $A \rightarrow B$

$$P_{AB} \propto \left[\int \psi_B^* H_{int} \psi_A \, dV \right]^2 \qquad \text{because } H\psi = ih\,(\partial\psi/\partial t)$$

where H is the Hamiltonian of a charged particle in an electromagnetic field:

$$H = 1/2m\,(\underline{p} - e/c\,\underline{A})^2 + e\varphi \qquad [= H_{particle} + H_{interaction} + H_{field}]$$

• For multiple electrons this becomes

$$H = 1/2m\,(\underline{p} - e/c\,\underline{A})^2 + e\varphi + \sum e^2/4\pi\varepsilon_o r_{ij} + \sum(\,)\,\underline{\mathbf{s}}\bullet\underline{\boldsymbol{\ell}} + \sum(\,)\,\underline{\mathbf{s}}\bullet\underline{\mathbf{s}}$$

Large for Z<10 [H-Ne] → 'L-S Coupling'

For plane EM wave

$$\underline{A} = A_o\, e^{i(\underline{k\bullet r} \pm \omega t)} \propto A_o\,[1 + ik\bullet r - |k\bullet r|)^2 + \ldots\ldots]$$

where $kr \sim 2\pi a_o/\lambda \sim 10^{-3}$ for optical wavelengths (="long wavelength approximation")

Transition Selection Rules

- Radiative transitions between energy states are governed by 'selection rules' that are required for

$$P_{AB} \propto [\int \psi_B^* H_{int} \psi_A \, dV]^2$$

where $P_{n\ell m \to n'\ell' m'} \propto [\int \psi^*_{n'\ell' m'} (-e/m \, \underline{p}.\underline{A}_o \, e^{i(kr-\omega t)} \psi_{n\ell m}) \, dV]^2$ and $\underline{p} = m\dot{\underline{r}} = 2\pi i/h$ **[Hr – rH]**

$\propto [\int A_o(er + e(kr)^2 + \ldots\ldots) \, dV]^2$ **=** 0 from orthogonality relationships, except when

('Permitted')

('Forbidden')

Electric Dipole ($A \sim 10^7$ sec^{-1})

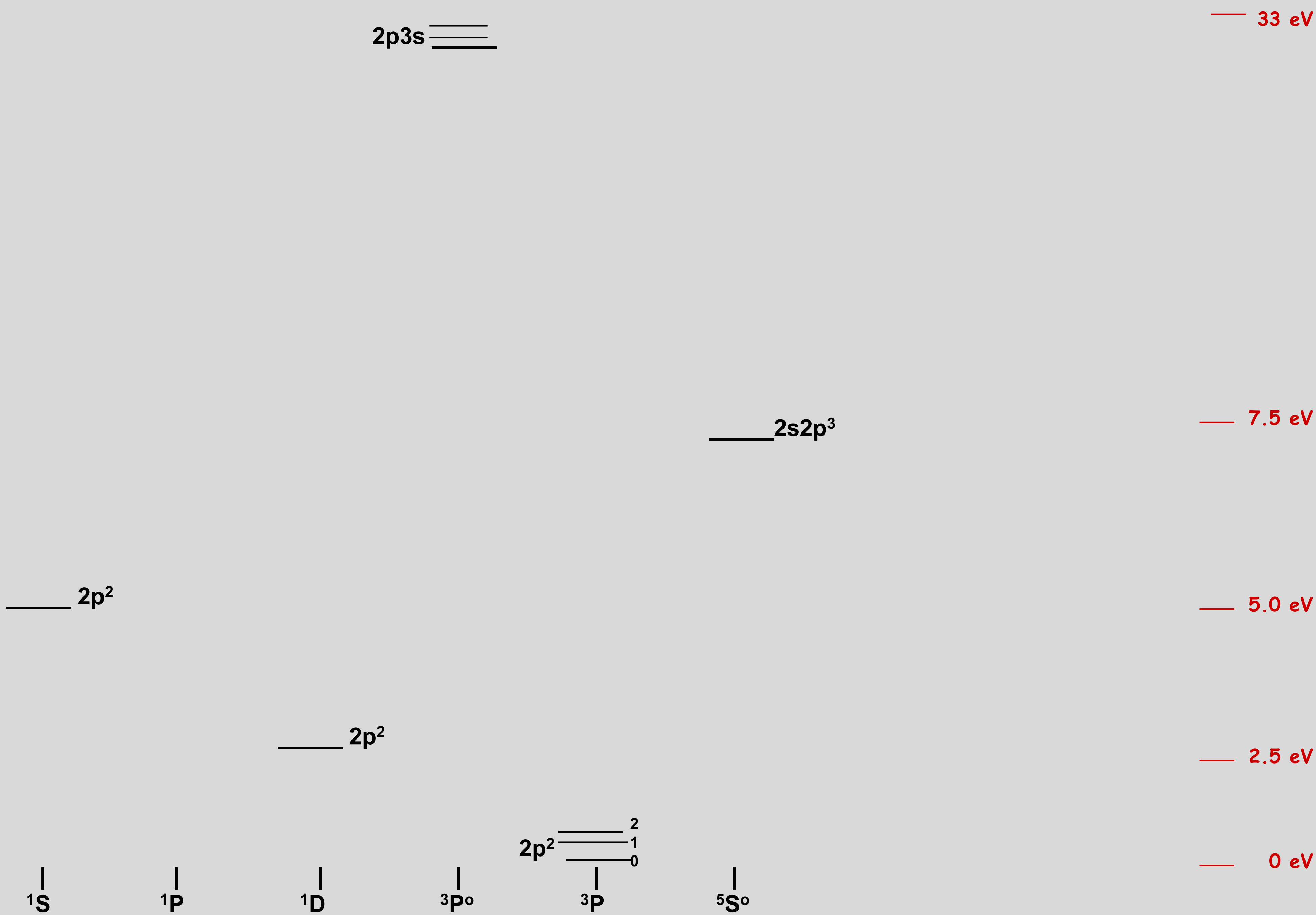
1. One electron jumps in (n, ℓ); others don't change. Δn = arbitrary
2. Parity must change: $\Delta\ell = \pm 1$
3. $\Delta L = 0, \pm 1$
4. $\Delta S = 0$ *(L-S rule only)*
5. $\Delta J = 0, \pm 1$

Magnetic Dipole ($A \sim 10^2$ sec^{-1})

1. No electrons jump in (n, ℓ)
2. Parity does not change: $\Delta\ell = 0$
3. $\Delta L = 0, \pm 1$
4. $\Delta S = 0$ *(L-S rule only)*
5. $\Delta J = 0, \pm 1$

Note: A multiplet consists of those lines between allowable J-values for a given ^{2S+1}L spectroscopic configuration

Atomic Energy Levels: O III ($1s^2 2s^2 2p^2$)



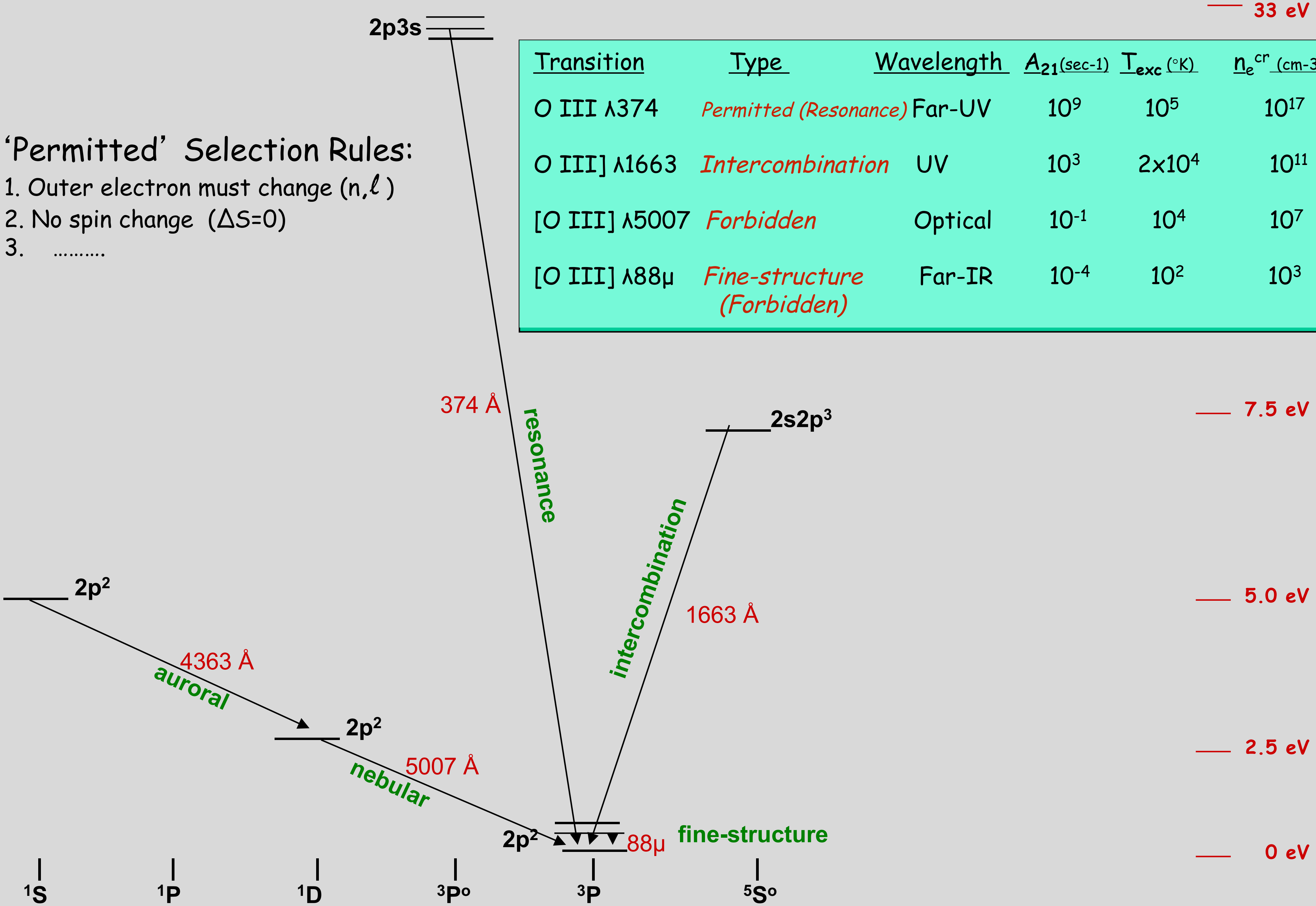
Bashkin & Stoner. 1975, Atomic Energy Levels (North Holland)

Atomic Energy Levels: O III ($1s^2 2s^2 2p^2$)

Transition	Type	Wavelength	A_{21} (sec-1)	T_{exc} (°K)	n_e^{cr} (cm-3)
O III λ374	*Permitted (Resonance)*	Far-UV	10^9	10^5	10^{17}
O III] λ1663	*Intercombination*	UV	10^3	2×10^4	10^{11}
[O III] λ5007	*Forbidden*	Optical	10^{-1}	10^4	10^7
[O III] λ88μ	*Fine-structure (Forbidden)*	Far-IR	10^{-4}	10^2	10^3

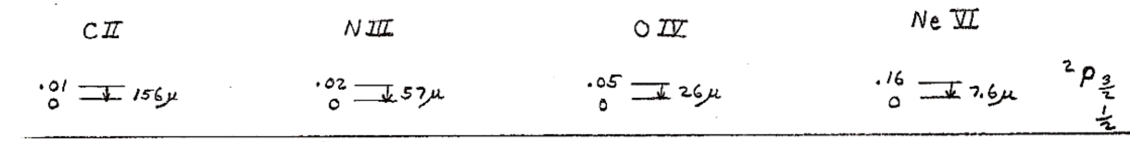
'Permitted' Selection Rules:

1. Outer electron must change (n,ℓ)
2. No spin change ($\Delta S=0$)
3. ……….

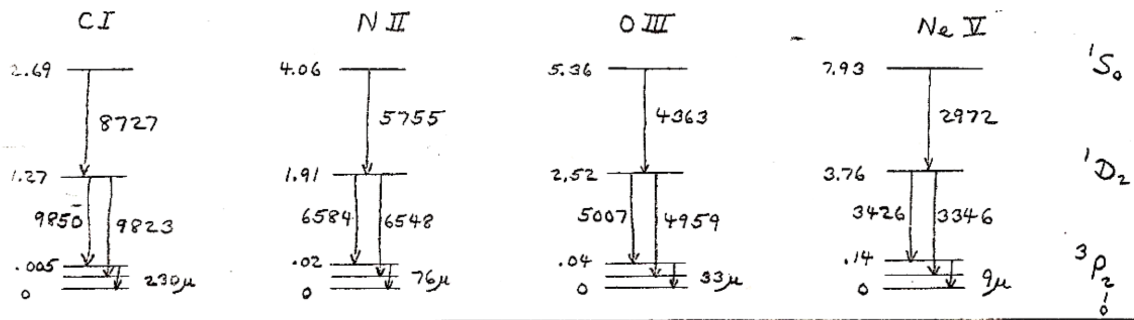


Low-lying Levels of Heavy Elements

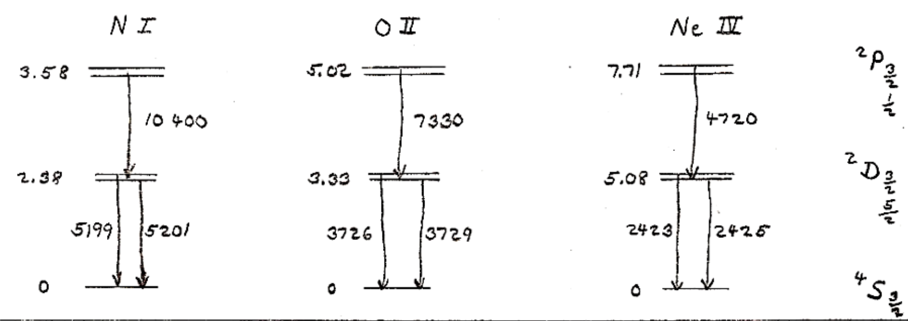
Electron Configuration: $2p$ Terms: ^2P



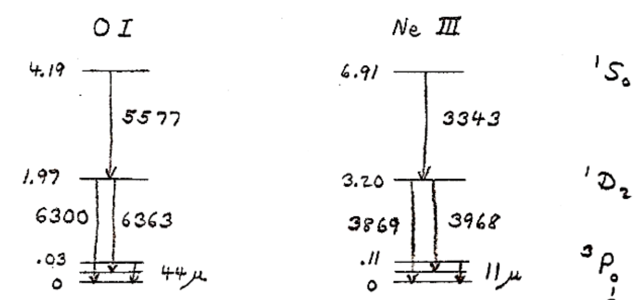
Electron Configuration: $2p^2$ Terms: ^3P, ^1D, ^1S



Electron Configuration: $2p^3$ Terms: ^4S, ^2D, ^2P



Electron Configuration: $2p^4$ Terms: ^3P, ^1D, ^1S



Electron Configuration: $2p^5$ Terms: ^2P