"ATOMIC SPECTROSCOPY AND OPACITY"

- 3 Weeks Lecture Course
- Textbook: "Atomic Astrophysics and Spectroscopy"

-A.K. Pradhan and S.N. Nahar (Cambridge, 2011)

SULTANA N. NAHAR

Department of Astronomy

The Ohio State University

Columbus, Ohio, USA

Email: naharastronomy.ohio-state.edu

Web: www.astronomy.ohio-state.edu/∼nahar

Faculty of Science

Cairo University

Physics Department

Cairo University, Giza, Egypt

February 16 - March 7, 2013

Support: DOE, NSF, OSC, Cairo University

"ATOMIC SPECTROSCOPY AND OPACITY"

- **3 Weeks Lecture Course**
- **Textbook: "Atomic Astrophysics and Spectroscopy" (AAS) -A.K. Pradhan and S.N. Nahar (Cambridge, 2011)**

Lecture Topics:

Week 1:

- **Physics and Astronomy Connection**

i) Elements and Spectroscopy
ii) Opacity and Observations
iii) The Sun and Evolution of Spectroscopy
iv) Electron and Photon Distribution Functions
v) The Plasma Universe

- **Atomic Structure and Spectroscopy**

i) Hydrogen - Single electron energy and wave functions
ii) Quantum numbers n,l,m, s, parity
iii) Spectral lines - Rydberg formula

Week 2:

- **Atomic Structure, Computation with SUPERSTRUCTURE & Atomic Processes**

i) Multi-election Systems - Angular Sates
ii) Angular Couplings, Quantum Defects
iii) Hartee-Fock Approximation
iv) Central Field Approximations
v) Dirac Equation, Breit-Pauli Approximation, Dirac-Fock

Approximation
vi) Atomic Processes of Plasma Opacity

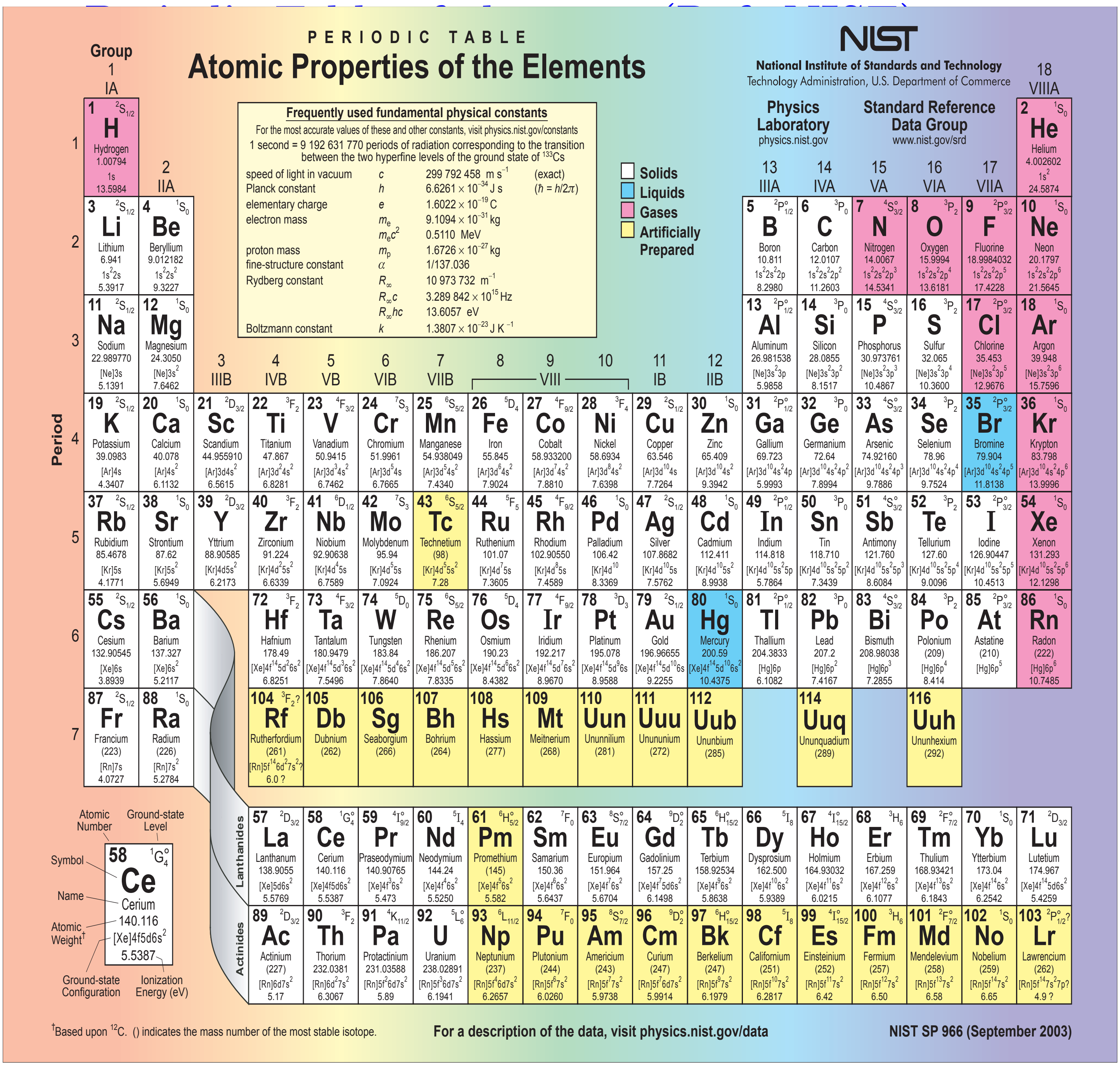
Week 3:

- **Plasma Opacity, R-matrix Calculations for Atomic Processes**

i) Autoionization and Resonances and Opacity
ii) Plasma Opacity
iii) Close-Coupling Approximation and R-matrix Method
iv) R-matrix Calculations

i) Elements and Spectroscopy:

ELEMENTS (Key Information)



• **Elements: Gases (pink), Solids (white),i Liquids (blu**
Artificially Prepared (yellow)

- **Abundant Elements: H (X - 90%, mass:70%), He (Y - 7%, mass:28%)**

- **Other elements (metals) (Z- 3%, mass: 2%): Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, S, Ar, Ca, Ti, Cr, Fe, Ni**
- Fusion cycle in a star usually ends at Fe (strongest nuclear force)

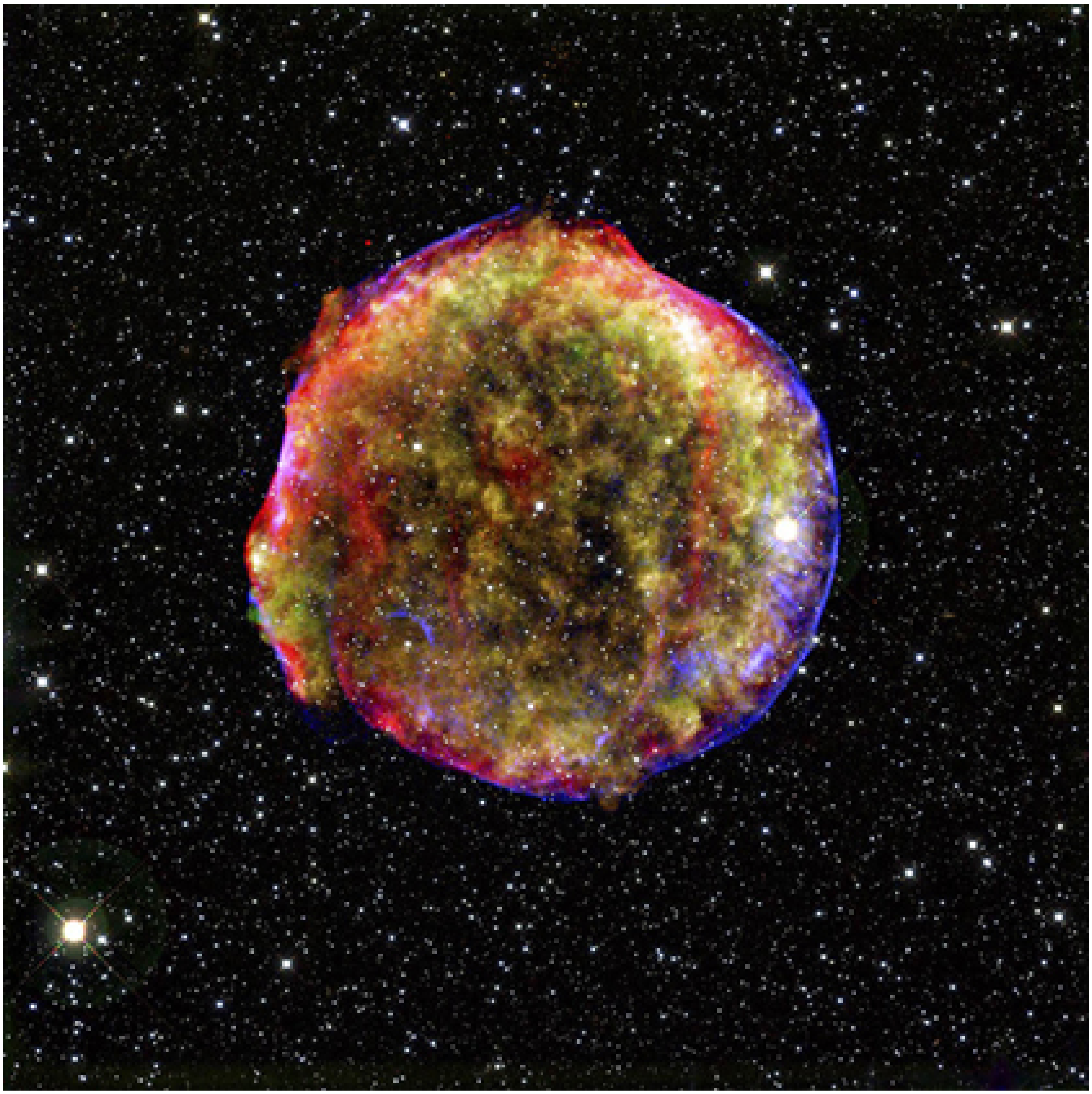
- **Study elements through spectroscopy**

- **Although constitute only 2% of the plasma, the metals are responsible for most of the spectral features**
- they crucially determine properties such as the plasma opacity that governs the transfer of radiation through the source

- **Heavier elements - Supernova explosion**
- **Solar system made from debris of supernova explosions**

TYCHO SUPERNOVA REMNANT IN CASSIOPI

Low Resolution Observation: Spitzer (red - Infrared - dust), Calar Alto (O, white stars), Chandra (X-rays - yellow, green - Expanding debris, blue - Ultra-energetic electrons)



SOLAR ABUNDANCES

Solar abundances (A_k, usually in log scale):

- **H - 90 % (by number), 70% (by mass fraction)**
- **He - 10 % (by number), 28 % (by mass)**
- **Metals - 2% (by mass). O (highest), C, N, Ne, Mg, Si, S, Ar, Fe**
- **Traditionally H abundance: $\log(A_H)$ = 12, other elements are scaled relative to it**
- **Table: A mixture of "standard" solar abundances (10% uncertainties, Seaton et al. 1994)**

Element (k)	Log A_k	A_k/A_H
H	12.0	1.0
He	11.0	1.00(-1)
C	8.55	3.55(-4)
N	7.97	9.33(-5)
O	8.87	7.41(-4)
Ne	8.07	1.18(-4)
Na	6.33	2.14(-6)
Mg	7.58	3.80(-5)
Al	6.47	2.95(-6)
Si	7.55	3.55(-5)
S	7.21	1.62(-5)
Ar	6.52	3.31(-6)
Ca	6.36	2.29(-6)
Cr	5.67	4.68(-7)
Mn	5.39	2.46(-7)
Fe	7.51	3.24(-5)
Ni	6.25	1.78(-6)

- **A supernova remnant:** an outer shimmering shell of expelled material, and a core skeleton of a once-massive star

- Heavy elements, beyond Iron, are generated from nuclear fusion during supernova explosions and are scattered into interstellar medium

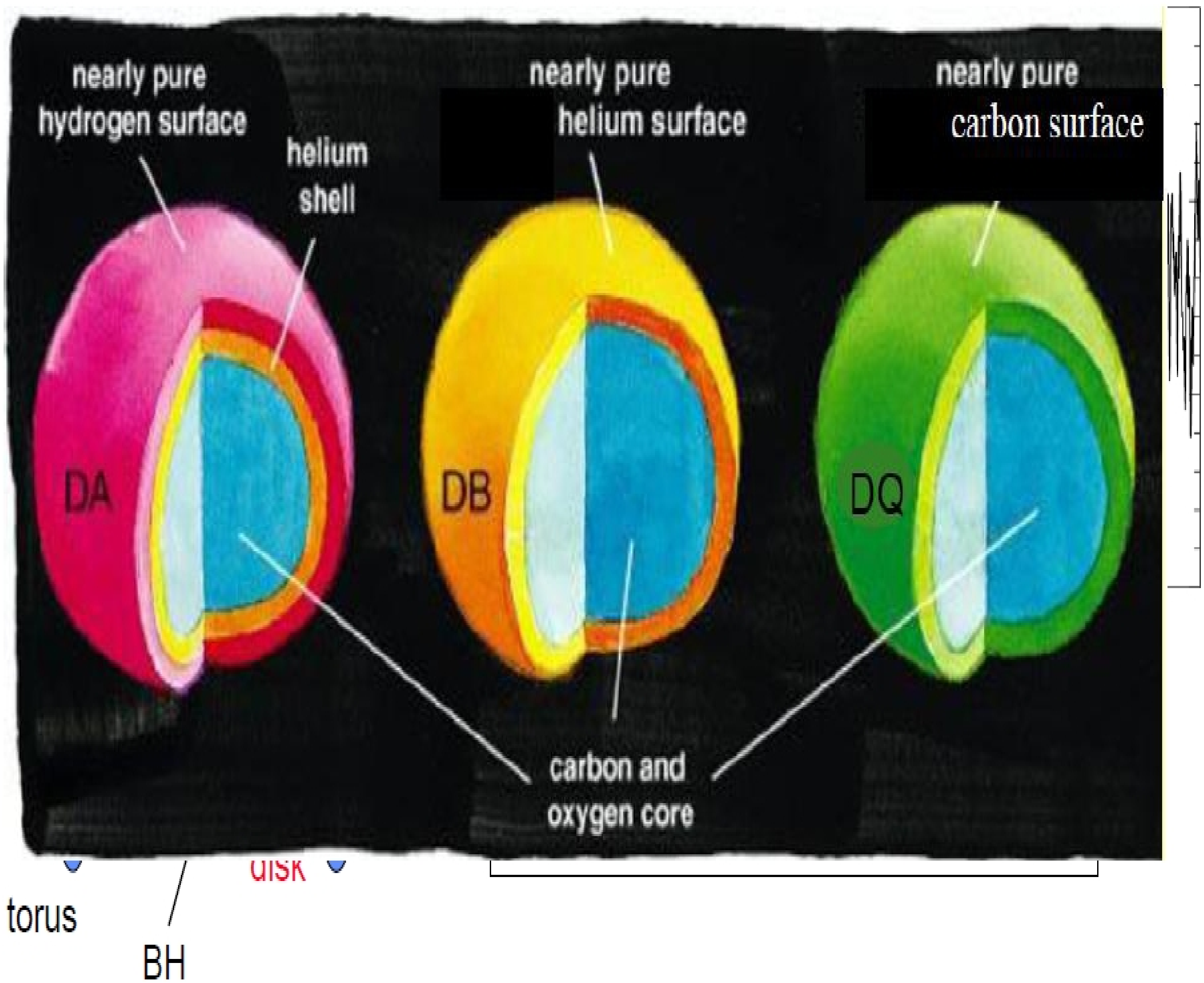
- Two pure H & He clouds, Pristine Clouds, detected first in 2010

- End of a star (98%): Below 1.4 solar mass (Chandra limit): Core becomes a white dwarf - diomond formation (electron repulsion equals gravity)

- Above 1.4 but below 4 solar mass: neutron star (electrons pressed to Neutron formation - largher gravity)

Larger mass - blackhole (extreme gravity)

White Dwarf stars -¿ cosmic clocks. The age of the universe is at least as big as the oldest stars in it. This principle can map the ages of galactic compoments



ii) Opacity and Observation
STUDYING ASTRONOMICAL OBJECTS

ASTRONOMICAL objects are studied in three ways:

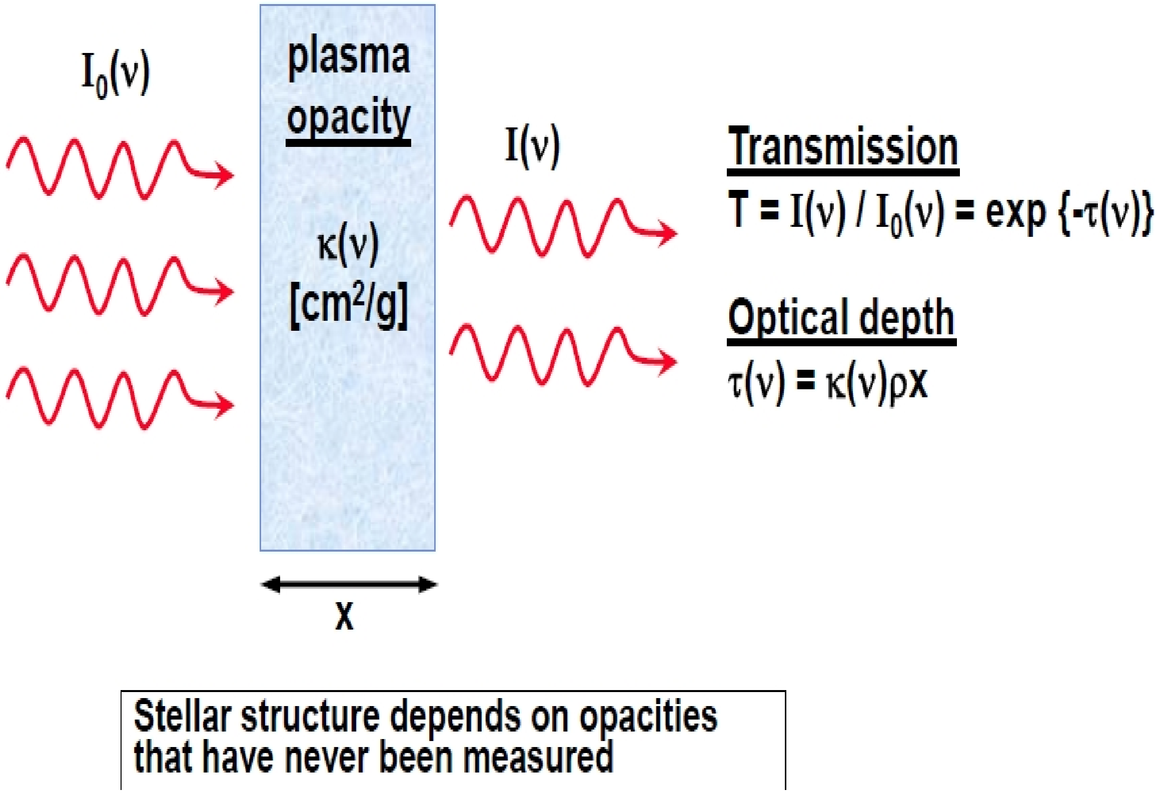
- **Imaging:** **- Beautiful pictures or images of astronomical objects, Stars, Nebulae, Active Galactic Nuclei (AGN), Blackhole Environments, etc**
→ Provides information of size and location of the objects

- **Photometry:** **Bands of Electromagnetic Colors ranging from X-ray to Radio waves**
→ macroscopic information and low resolution spectroscopy

- **Spectroscopy:** **Taken by spectrometer - Provides most of the detailed knowledge: temperature, density, extent, chemical composition, etc. of astronomical objects**

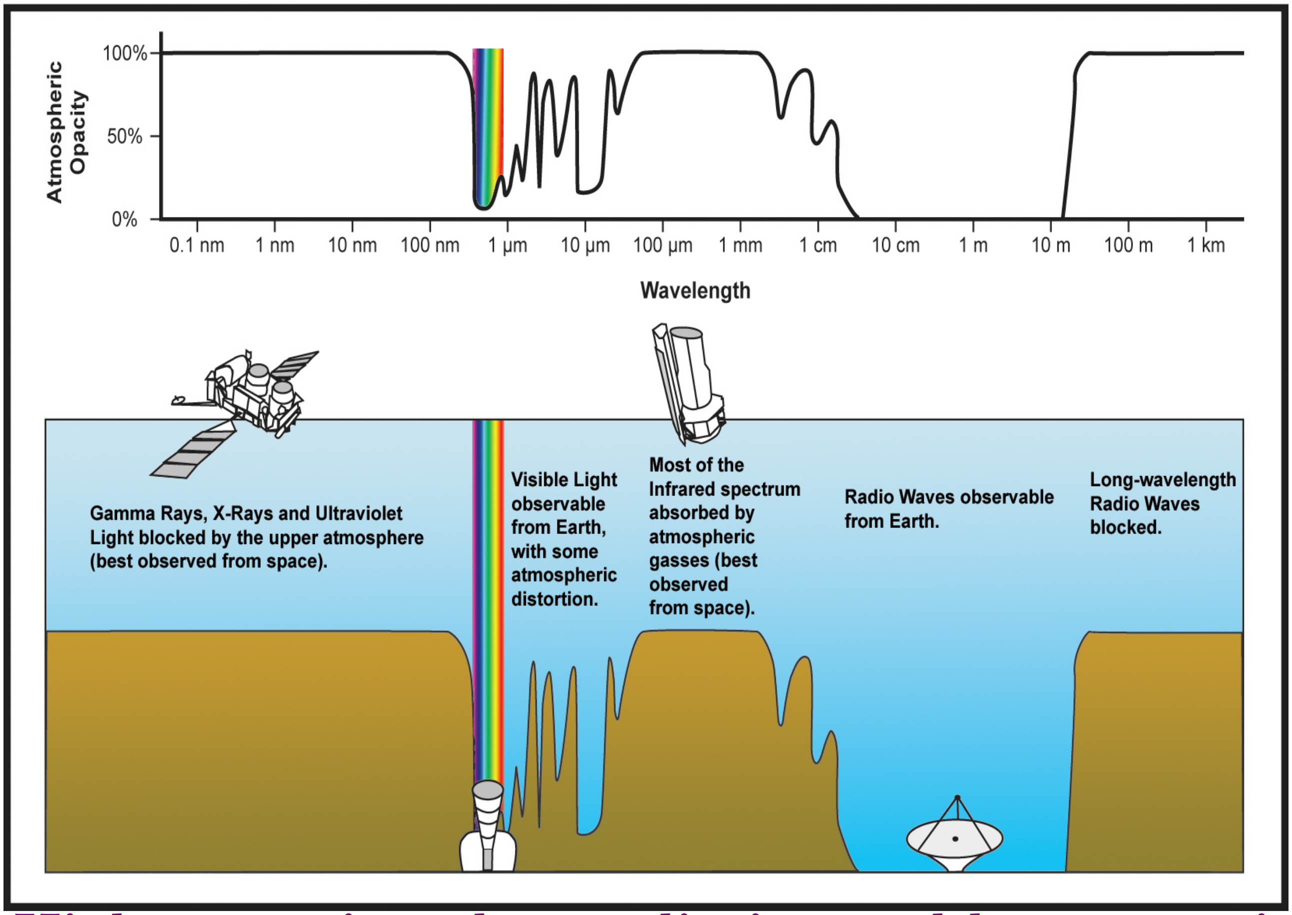
Spectroscopy is underpinned by Atomic & Molecular Physics

OPACITY



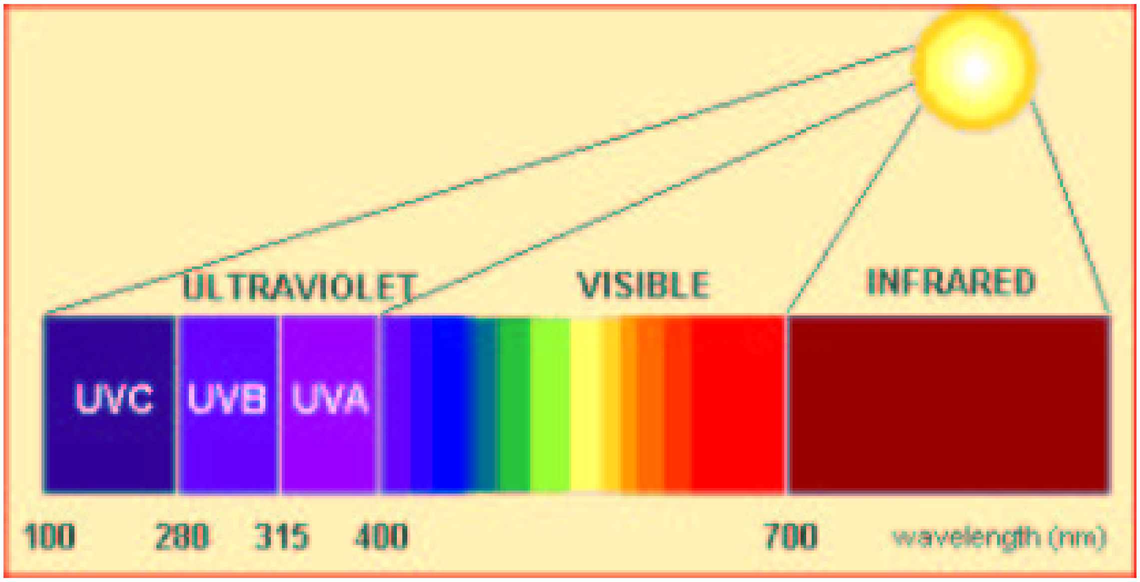
- Opacity is a measure of radiation transfer
- Higher opacity - less radiation and lower opacity - more radiation transfer

ATMOSPHERIC OPACITY
(www.ipac.caltech.edu/Outreach/Edu)



- Higher opacity - less radiation and lower opacity - more radiation reaching earths surface
- Opacity determines types of telescopes - earth based or space based
- Gamma, X-ray, UV are blocked while visible light passes through
- CO_2, H_2O vapor, other gases absorb most of the infrared frequencies
- Part of radio frequencies is absorbed by H_2O and O_2, and part passes through

iii) The Sun and Evolution of Spectroscopy

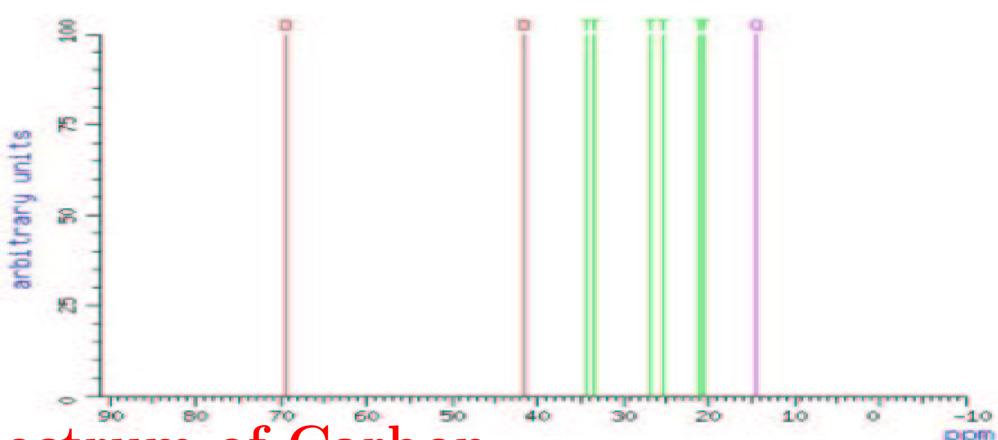


• Light is a mixture of colors - Spectrum: splitting of colors
For example: Rainbow is the spectrum of white sunlight

• Each atom gives out light with its own set of colors

• Spectrum is lines of colors, like the barcode on an item

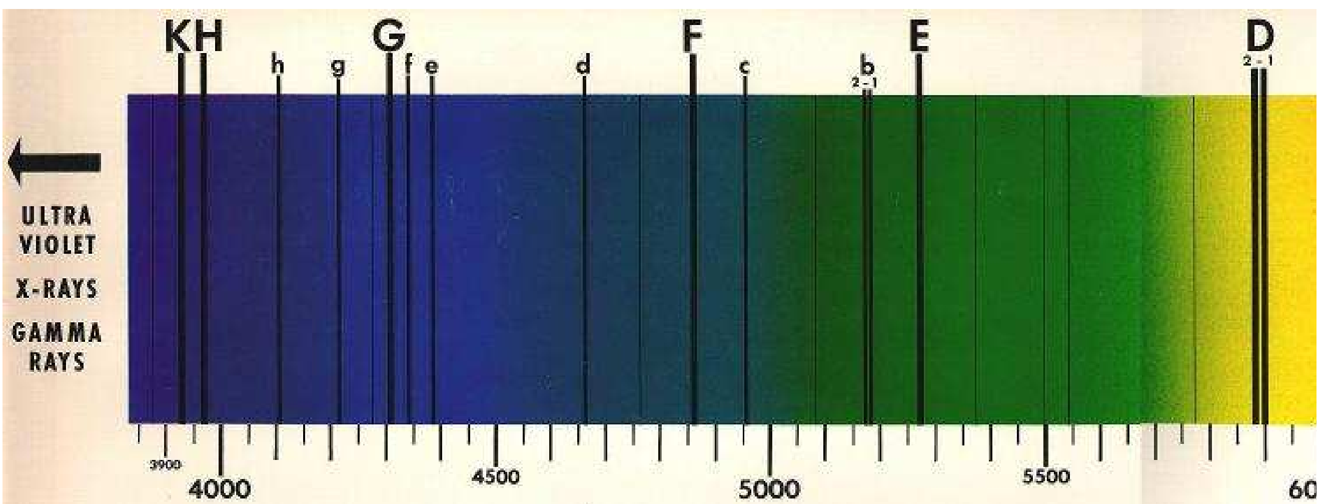
• The lines → key information of astronomical objects the blackhole or other astrophysical objects



Spectrum of Carbon

Solar Spectra: Absorption & Emission Lines

- Absorption line - by absorption of a photon as an electon jumps to a higher level
- Emission line - by emission of a photon as electron dumps to a lower level
- An absorption or emission line from the same two energy levels appear at the same energy position in the spectrum



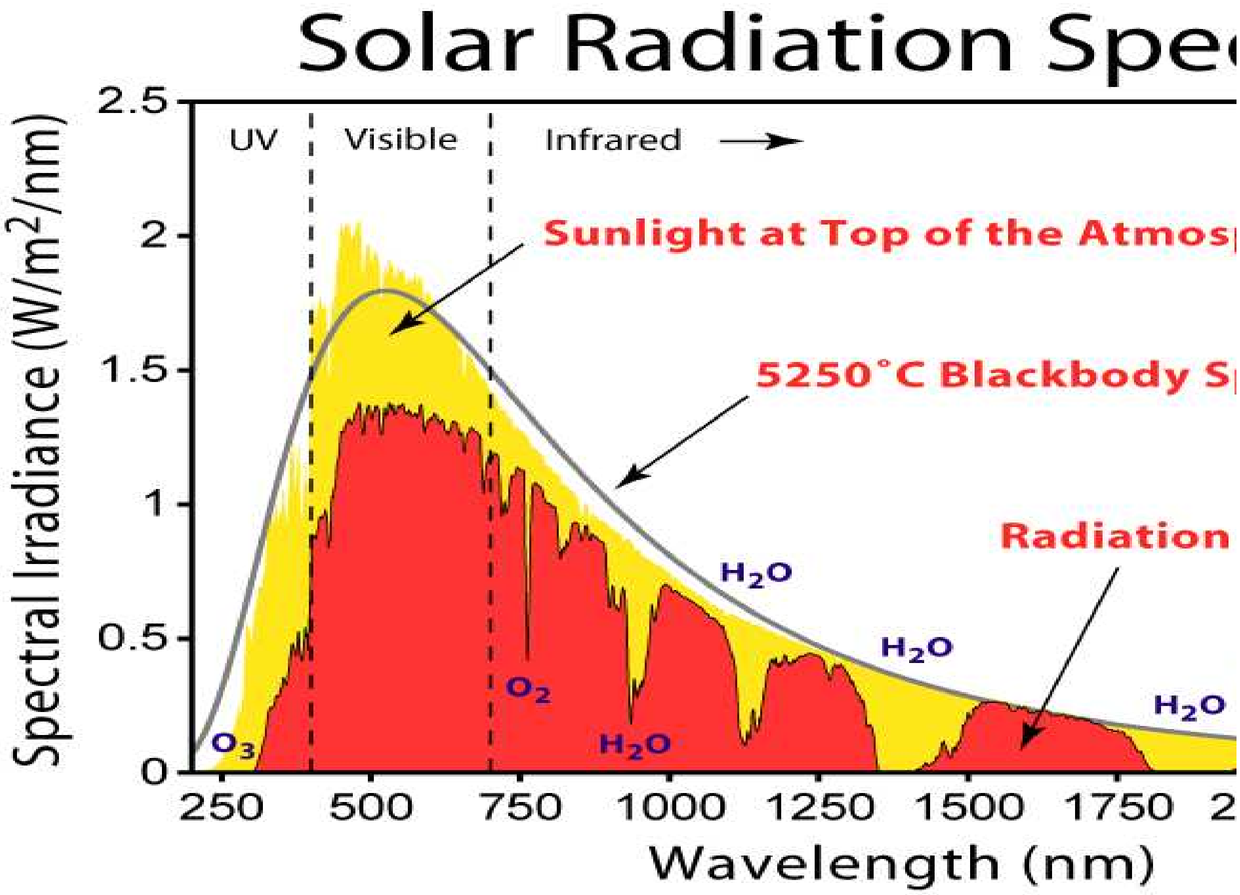
Fraunhofer lines (1815) in the Solar Spectrum

Used alphabet - no element assignment; Later spectoscopy with quantum mechanics: A (7594 Å,O), B (6867 Å,O) (air), C (6563 Å H), D1 & D2 (5896, 5890 Å Na, yellow sun), E(Fe I), G(CH), H $ K (Ca II)

[(Courtesy: Institute for Astronomy, University of Hawaii]

"SUNLIGHT" ON THE EARTH SURFACE

(http://globalwarmingart.com/wiki/Image:Solar_Spectrum_png)



- The Sun - Blackbody (constant T), gives out radiation in Planck distribution
- Solar surface $T_* = 5770\,\mathrm{K} \rightarrow$ peak blackbody emission - yellow $\sim$5500 Å.
- H_2O has inefficient absorption windows: 3 are molecular IR bands - J, H, and K bands
- Solar UV flux drops off rapidly by *ozone effect* preventing it to reach earth

iv) Electron and Photon Distribution Functions

• A plasma of charged particles and a radiation field of photons treated with two distribution functions, Planck and Maxwell

• 'Temperature' is defined through a radiation (photon) or the particle (electron) *energy distribution* → *kinetic* T defined from

$\mathbf{E = h\nu \sim kT, \text{ or } E = 1/2mv^2 = 3/2kT}$

• Consider a star ionizing a molecular cloud into a gaseous nebula
- The two objects, the star & the nebula, have different T distribution functions

• Energy of the radiation emitted by the star - Planck distribution function

• Energies of electrons in the surrounding ionized gas heated by the star - Maxwell distribution

PLANCK DISTRIBUTION FUNCTION

• **total energy emitted by an object s related to its T by the Stefan-Boltzmann Law**

$$\mathbf{E} = \sigma \mathbf{T^4} \tag{1}$$

$\sigma = 5.67 \times 10^{-8}$ **Watts/($\mathbf{m}^2$ $\mathbf{K}^4$)= Stefan constant**

• **Radiation of a star, a blackbody, is given by the Planck distribution function**

$$\mathbf{B_\nu(T_*)} = \frac{\mathbf{2h\nu^3}}{\mathbf{c^2}} \frac{\mathbf{1}}{\mathbf{exp(h\nu/kT_*) - 1}}, \tag{2}$$

T_* =***radiation temperature***, ν = **frequency of the photons.**

MAXWELL DISTRIBUTION FUNCTION

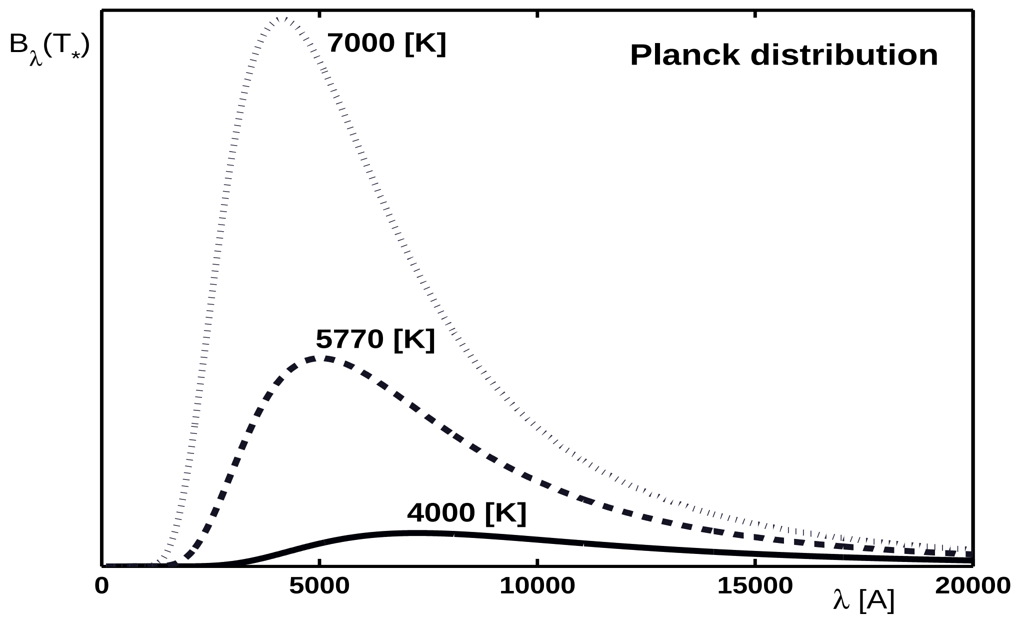
The charged particles in the plasma ionized by a star in an H II region has an *electron temperature* T_e **associated with the mean kinetic energy of the electrons** kT_e

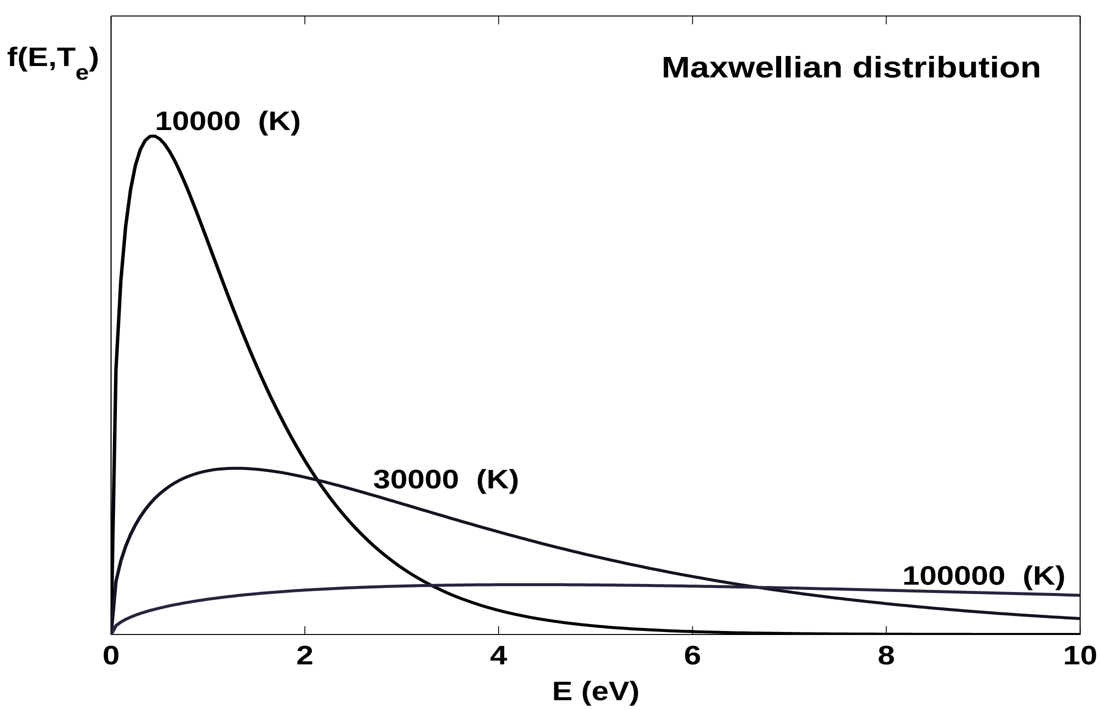
$$\frac{\mathbf{1}}{\mathbf{2}}\mathbf{mv^2} = \frac{\mathbf{3}}{\mathbf{2}}\mathbf{kT_e}. \tag{3}$$

The velocity (or energy) distribution of electrons is characterized by a Maxwellian function at temperature T_e,

$$\mathbf{f}(\mathbf{v}) = \frac{\mathbf{4}}{\sqrt{\pi}}\left(\frac{\mathbf{m}}{\mathbf{2kT}}\right)^{\mathbf{3/2}}\mathbf{v}^{\mathbf{2}}\mathbf{exp}\left(-\frac{\mathbf{mv}^{\mathbf{2}}}{\mathbf{2kT}}\right). \tag{4}$$

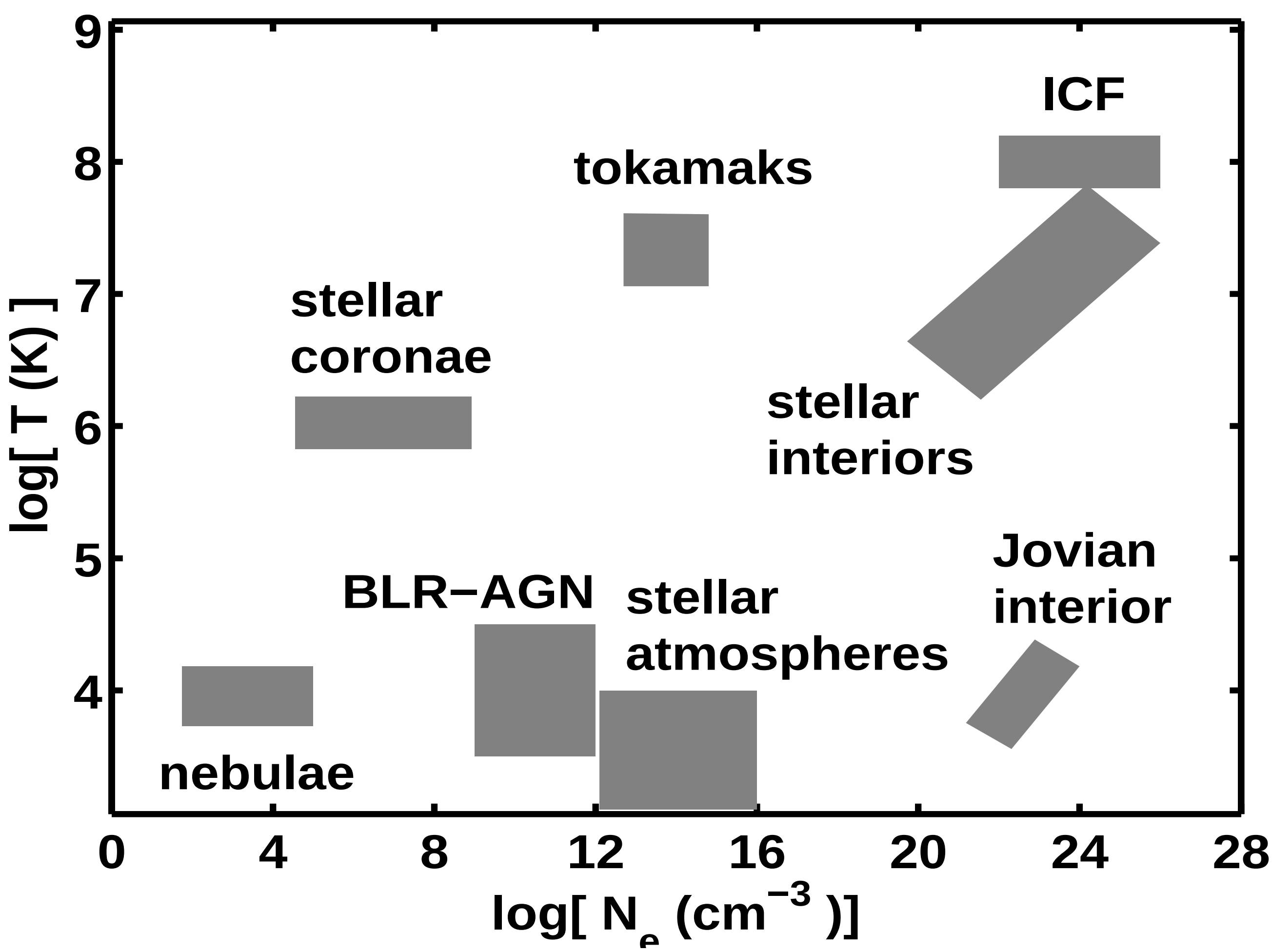
PLANCK & MAXWELL DISTRIBUTIONS





- **H II region (nebula): Ionized by black-body radiation of $T \sim$ 30000 - 40000 K , electron kinetic energy of Maxwellian distribution at $T_e \approx 10000 - 20000$ K**

v) The Plasma Universe
PLASMA COVERS VAST REGION (99%) IN T-ρ PHASE SPACE
(AAS, Pradhan & Nahar, 2011)

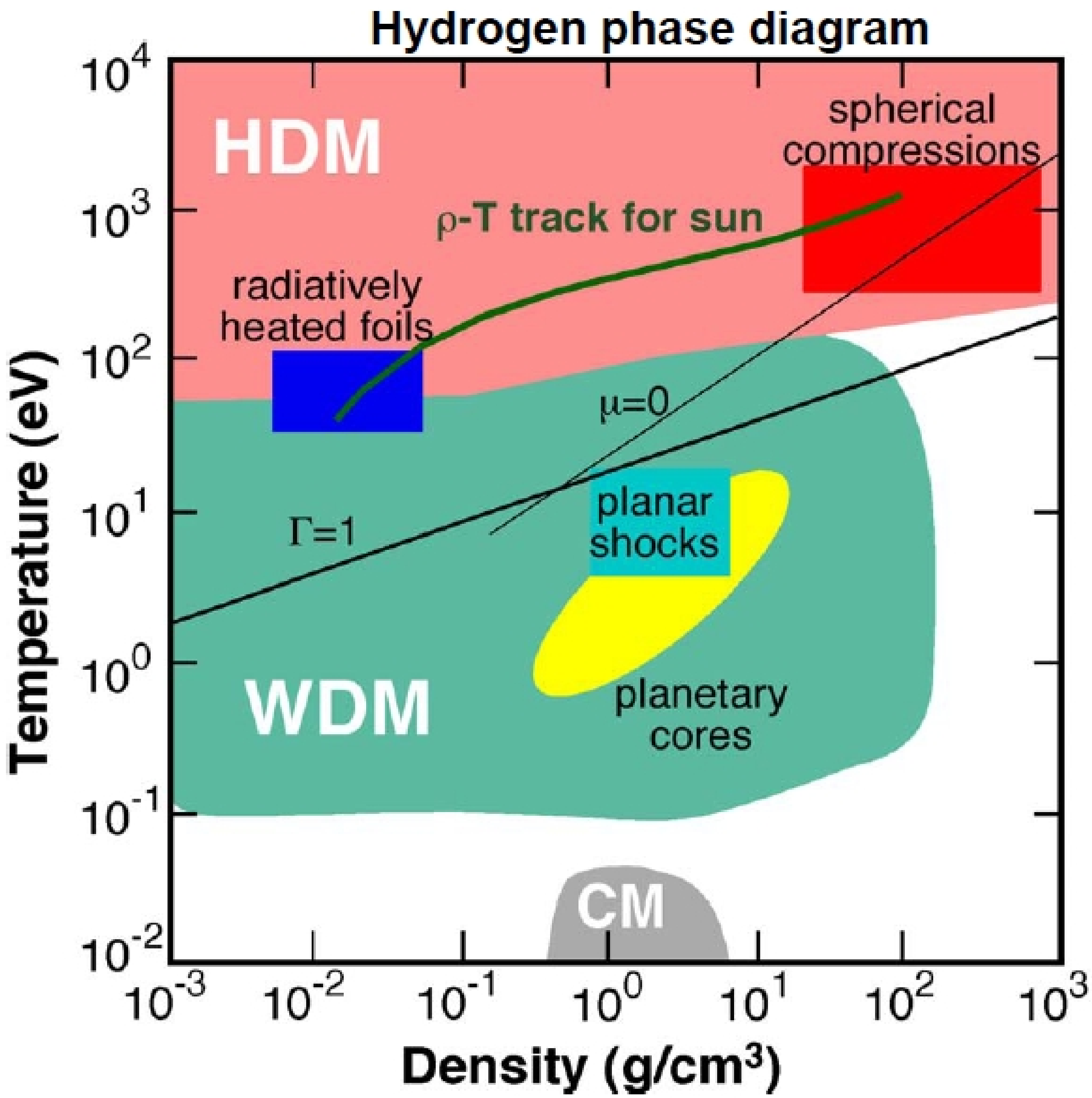


• Temperature-density regimes of plasmas in astrophysical objects - BLR-AGN ("broad-line regions) in active galactic nuclei", where many spectral features associated with the central massive black hole activity manifest themselves

• Laboratory plasmas - tokamaks (magnetic confinement fusion devices), Z-pinch machines (inertial confinement fusion (ICF) devices)

WARM & HOT DENSE MATTER

(HEDLP-FESAC report)



•

Hot Dense Matter (HDM):

- Sun's ρ-T track, Supernovae, Stellar Interiors, Accretion Disks, Blackhole environments
- Laboratory plasmas in fusion devices: inertial confinement
- laser produced (NIF) and Z pinches (e.g. Sandia), magnetic confinement (tokamaks)

• Warm Dense Matter (WDM):

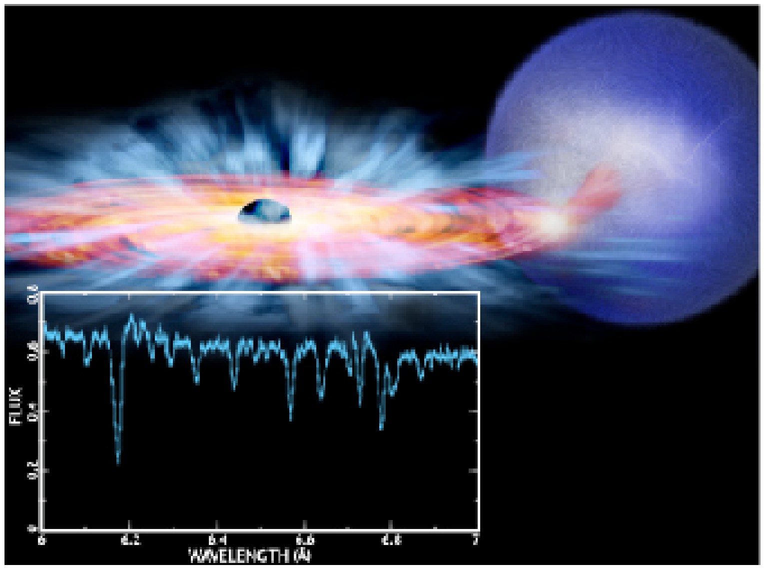
- cores of large gaseous planets

X-RAYS FROM A BLACKHOLE - CENTAURUS A GALAXY

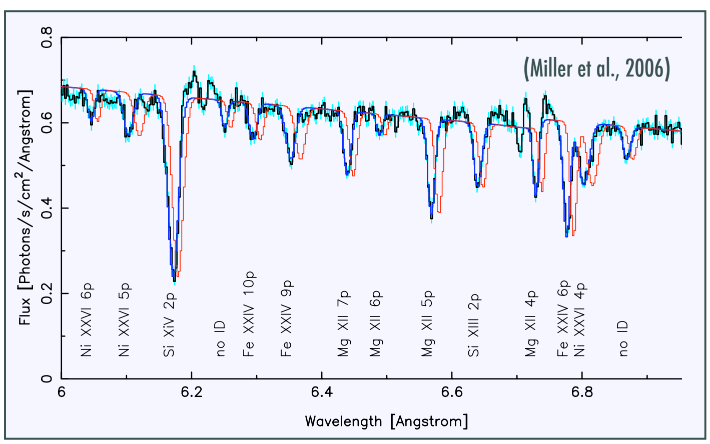
(Observed by Chandra space telescope)

- Photometric image: red - low-energy X-rays, green - intermediate-energy X-rays, and blue - the highest-energy X-rays. The dark green and blue bands are dust lanes that absorb X-rays.
- Highly energetic SUPERHOT ATOMS encircling the blackhole are in a plasma state & emit bright K_α X-rays
- Electrons are ripped off - highly charged state, e.g. He- & Li-like Ne,SI, S, Fe; - emit mainly K_α (1s - 2p) photons
- Sucked in materials are ejected as a jet (L & E conservation)
- Blasting from the black hole a jet of a billion solar-masses extending to 13,000 light years

SPECTRUM of the Wind near Blackhole: GRO J1655-40 Binary Star System



- **Materials from the large star is sucked into the companion blackhole** - form wind as they spiral to it

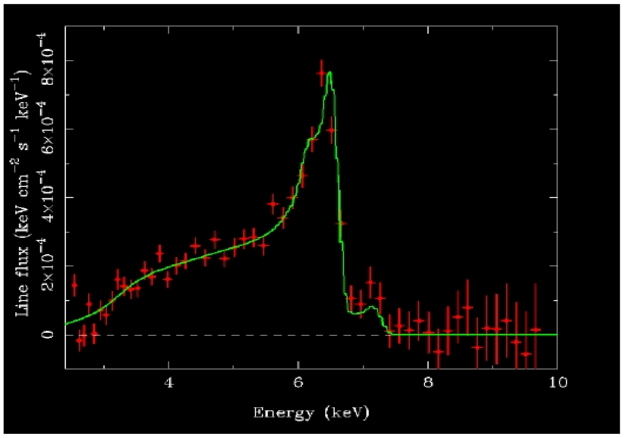


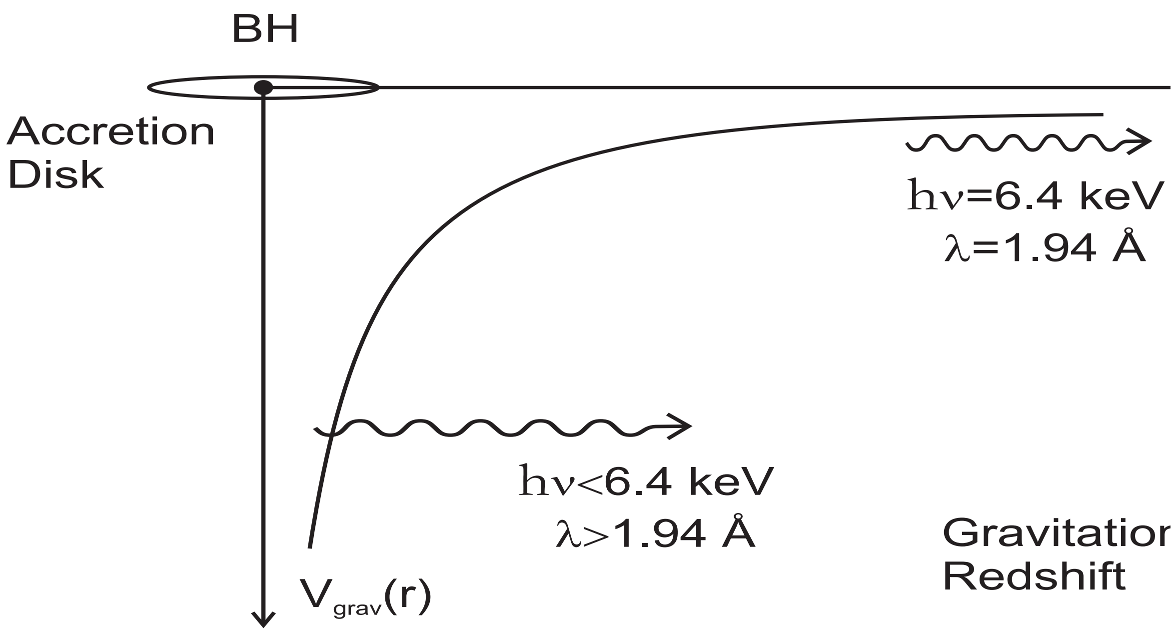
Spectrum: Highly charged Mg, Si, Fe, Ni lines

Red Spectrum - Elements in natural widths

Doppler Blue Shift - Wind is blowing toward us

Signature of a Blackhole



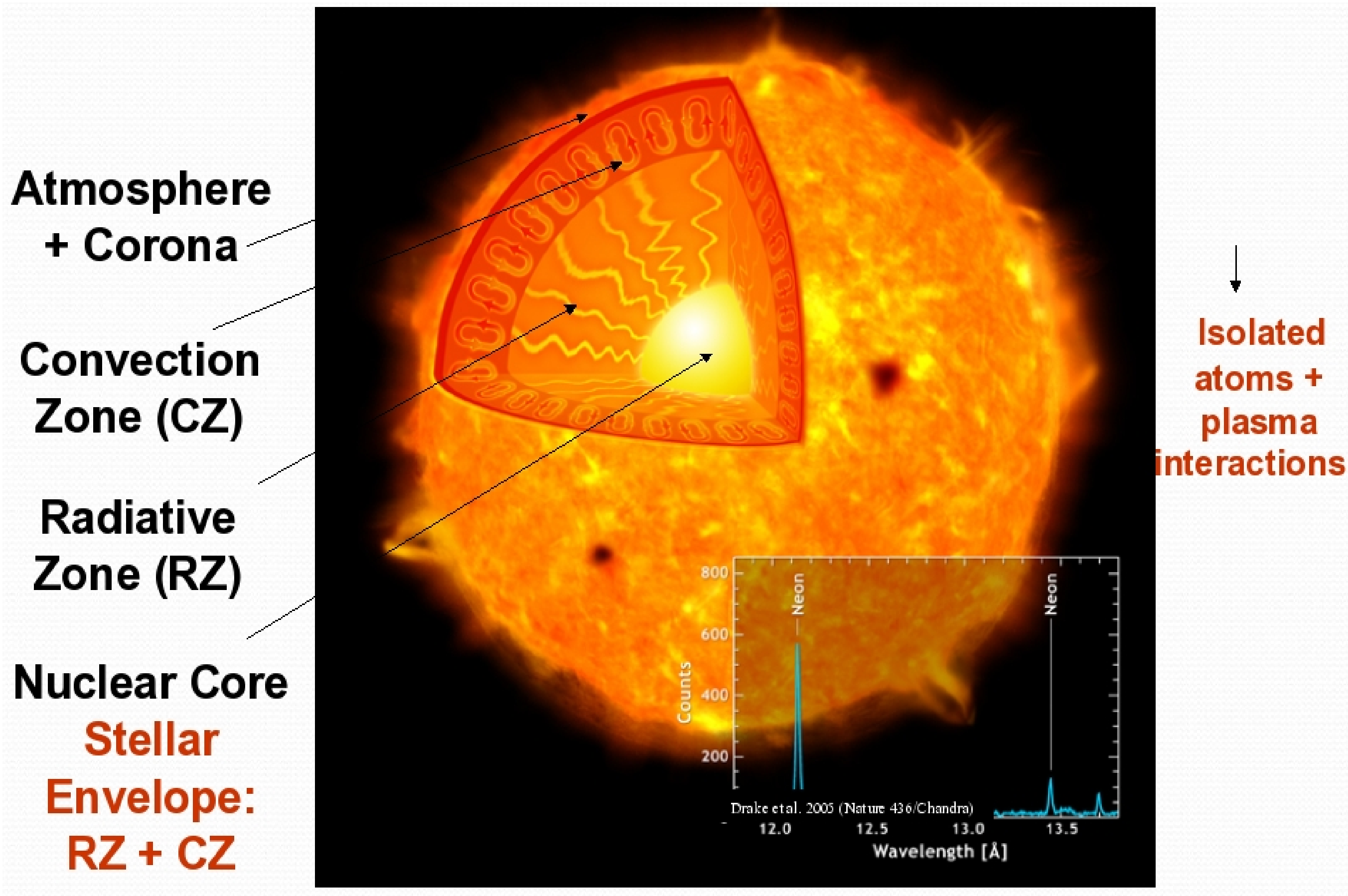


• The well-known K_α (1s-2p) transition array lines of iron near a black hole in Seyfert I galaxy MCG-6-30-15 6 (ASCA & Chandra obs)

• The maximum energy for a 1s-2p transition in iron is 6.4 keV. However, the large extension of the lines toward low energy means that the escaped photons have lost energies in the black hole.

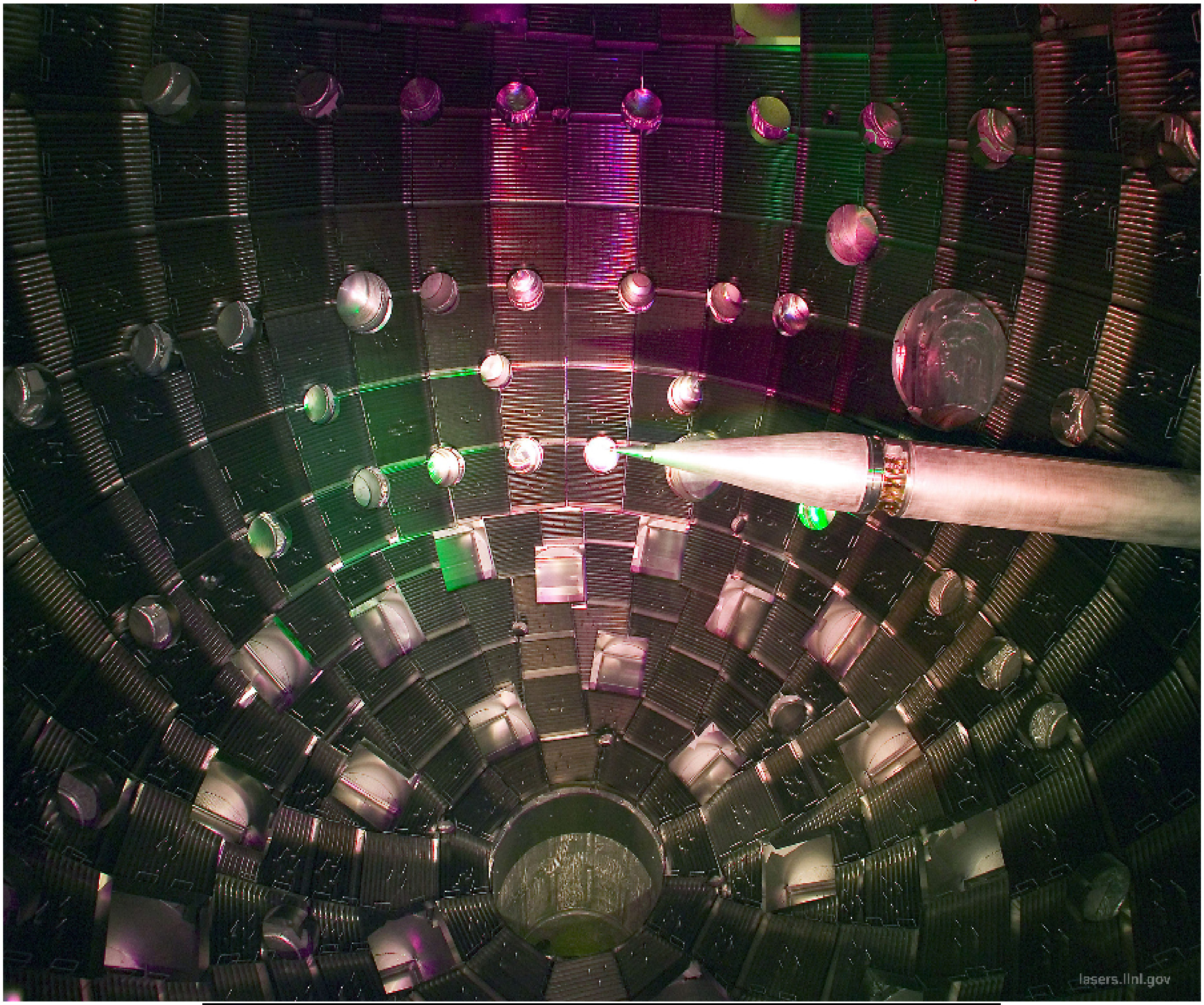
• Gravitational broadening of Fe K_α emission line from close vicinity of the black hole.

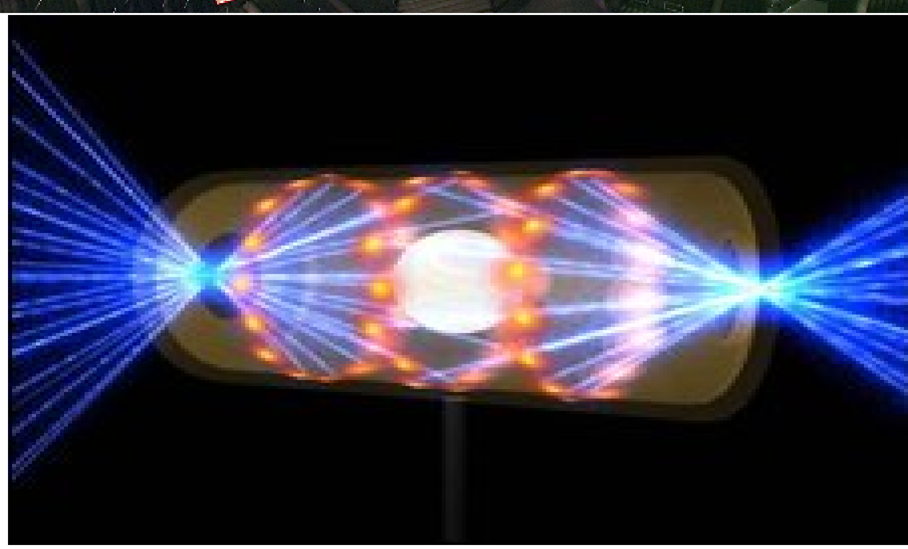
SOLAR ABUNDANCES & HED PLASMA



- Sun's interior - nuclear core to the end of convection zone beyond which the radiation escapes
- At the convection zone boundary, R_{CZ}, the temperature $T_e \sim$193 eV, density $n_e \sim 10^{23}/cm^3$ (HED - High Energy Density - Fe ions (Fe XVII-XIX))
- Takes over a million years for radiation created in the core (gamma rays) to travel to surface: Reason - OPACITY
- Although the most studied star, we can not explain all observations. Recent determination of solar abundances, from measurements and 3D hydro NLTE models, show 30-40% lower abundances of C, N, O, Ne, Ar than the standard abundances; contradict the accurate helioseismology data

CREATION OF HED PLASMA: NIF, LLNL

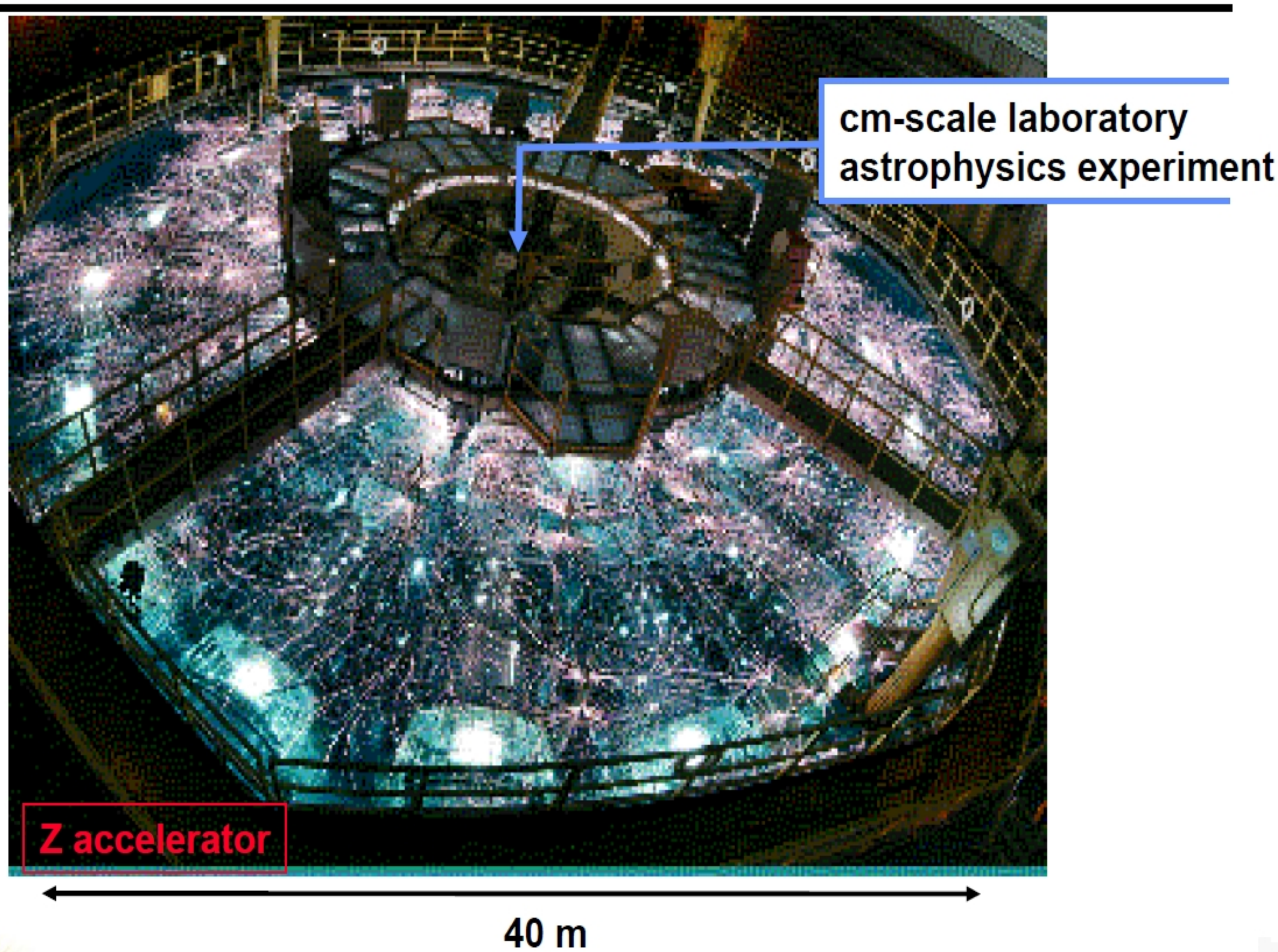


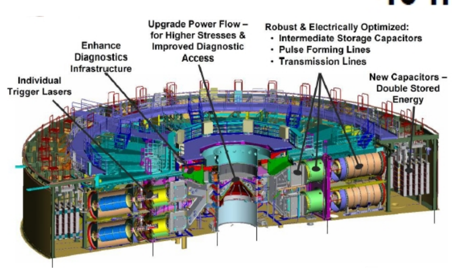


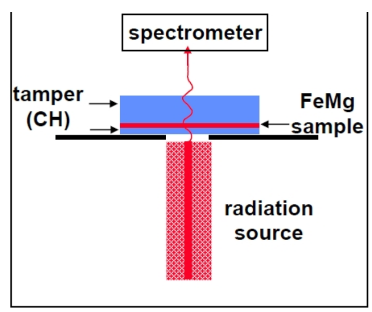
• **NIF: Pulses from 192 high-power lasers arrive (in 10^{-12}s of each other) (TOP, spike - target position) to center target (mm-size)- 1.875MJ shot (Bottom)**

HED PLASMA, Z PINCH, Sandia Natl lab

The 20million Amp current provided by the Z accelerator enables this research





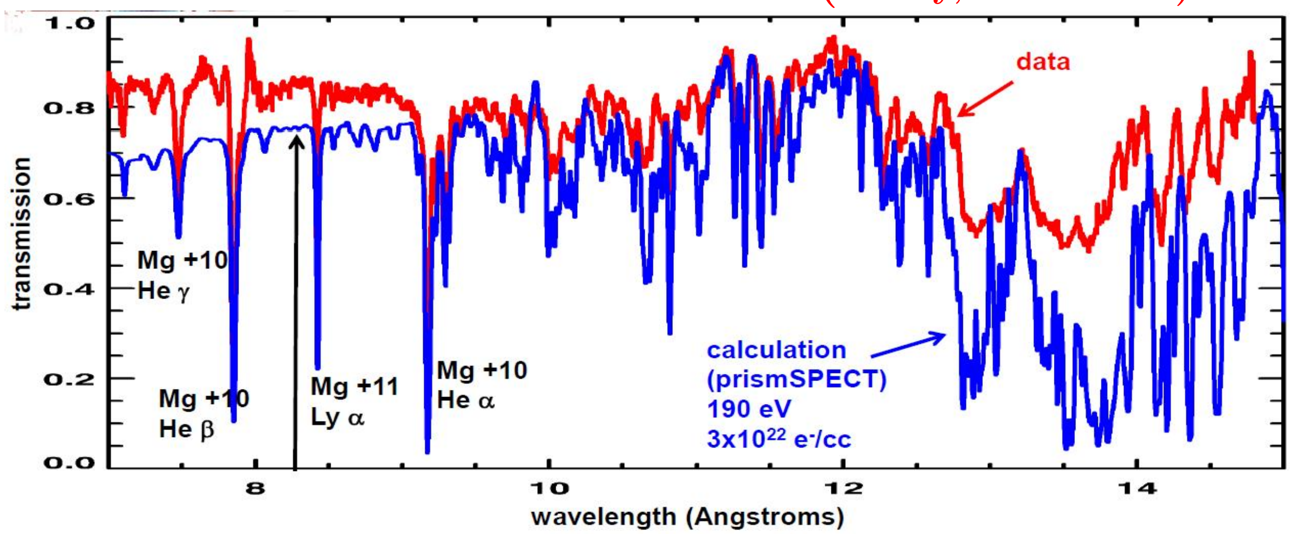


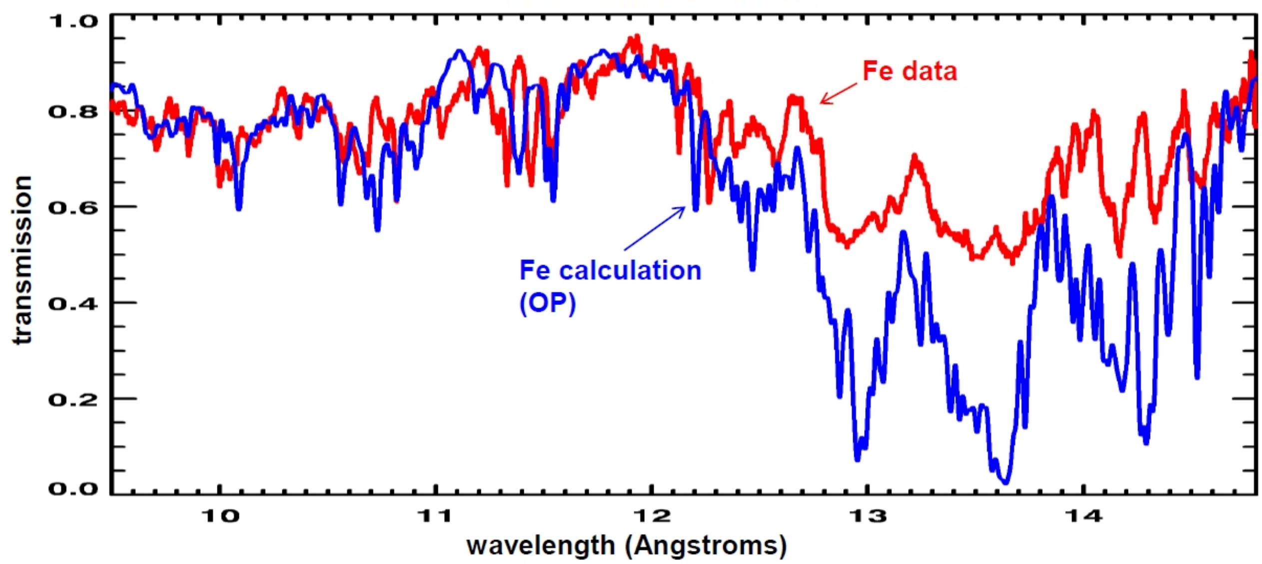
New Z
The refurbished Z delivers 24 million Amps to the load
50% increase in electrical energy for present day experiments

New sample design
Increasing the rear tamper thickness delays expansion onset
This leads to higher density and higher temperature

- **Magnetically driven z-pinch implosions convert electrical energy into radiation. Internal shock heating → X-rays - Energy: 1.5 MJ, Power: 200 TW (Latest: ∼ 27 Mamp)**
- **T_e ∼190 eV, density $n_e \sim 2.8 \times 10^{22}/cm^3$, similar to that at solar (R_{RZ})**

DISCREPANCY BETWEEN EXPERIMENTAL & THEORETICAL OPACITIES (Bailey, Sandia lab)





- **Z PINCH spectra, SNL: Plasma - $T_e \sim 193$ eV, Density $n_e \sim 10^{23}/cm^3$ - similar at solar R_{CZ}**
- **Observed (red), Calculated (blue). Top: Diagnostic lines, Bottom: Iron - Large differences Reason: OPACITY**
- **Serious discrepancies for Fe opacity**
- **Experimental n_e is wrong OR bound- free absorption (photoionization) is inaccurate**

"ATOMIC PROCESSES FOR ASTROPHYSICAL SPECTROSCOPY"

1. Photo-Excitation & De-excitation:

$$X^{+Z} + h\nu \rightleftharpoons X^{+Z*}$$

- An Electron jumps up or down to level, but does not leave the atom
- Fig:Top- Energy levels C I, C II

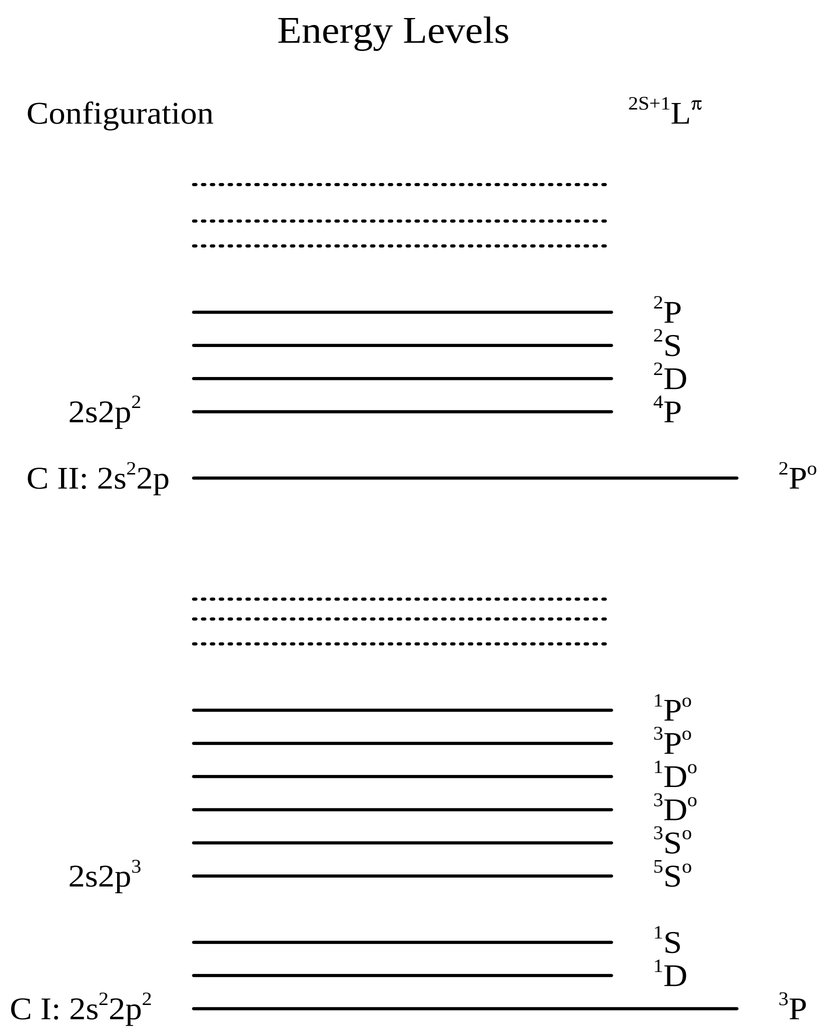
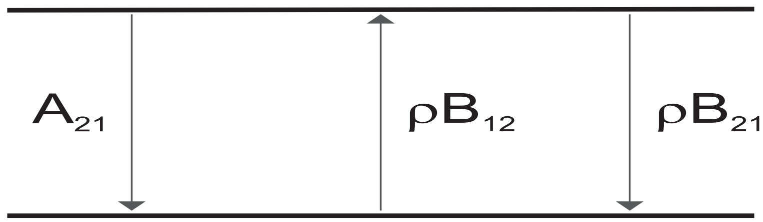


Photo-Excitation and Opacity



A_{21}- Spontaneous Decay
B_{21}- Stimulated Decay with a radiation field

- Intoduces absorption or emission lines
- Atomic quantities (constant numbers):

- Oscillator Strength (f)
- Radiative Decay Rate (A-value)

- Monochromatic opacity (κ_ν) depends on f_{ij}

$$\kappa_\nu(\mathbf{i} \longrightarrow \mathbf{j}) = \frac{\pi \mathbf{e^2}}{\mathbf{mc}} \mathbf{N_i f_{ij}} \phi_\nu \tag{5}$$

N_i = ion density in state i, ϕ_ν = profile factor

- κ includes thousands to millions of transitions

ALLOWED & FORBIDDEN TRANSITION

Determined by angular momentum selection rules

i) Allowed: Electric Dipole (E1) transitions
(Δ J = 0,$\pm$1, Δ L = 0,$\pm$1,$\pm$2; parity changes, same-spin & different spin or intercombination transition)

Forbidden:
ii) Electric quadrupole (E2) transitions
(Δ J = 0,$\pm$1,$\pm$2, parity does not change)

iii) Magnetic dipole (M1) transitions
(Δ J = 0,$\pm$1, parity does not change)

iv) Electric octupole (E3) transitions
(Δ J= $\pm$2, $\pm$3, parity changes)

v) Magnetic quadrupole (M2) transitions
(Δ J = $\pm$2, parity changes)

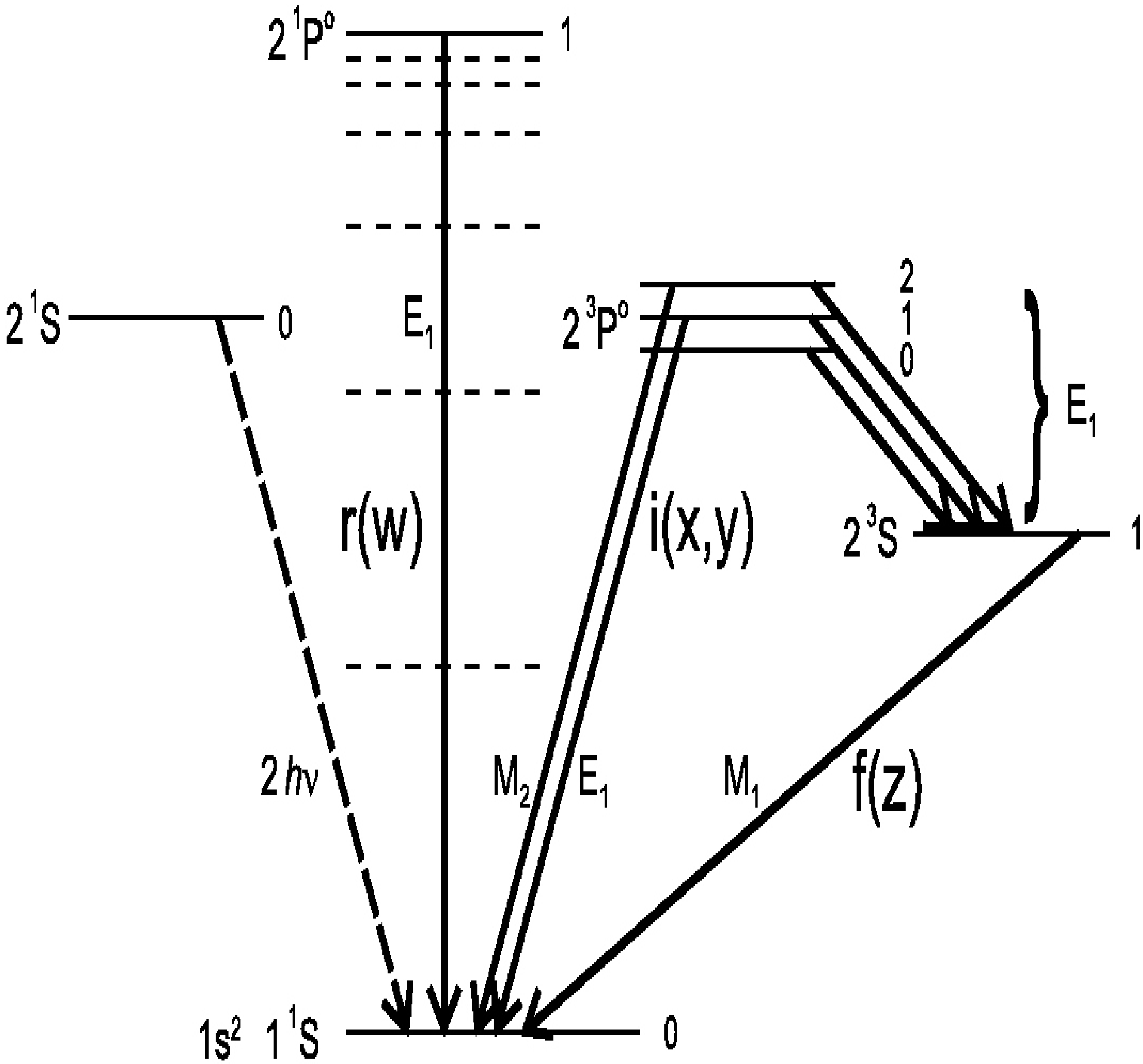
Allowed transitions >> Forbidden transitions

EX: ALLOWED & FORBIDDEN TRANSITIONS

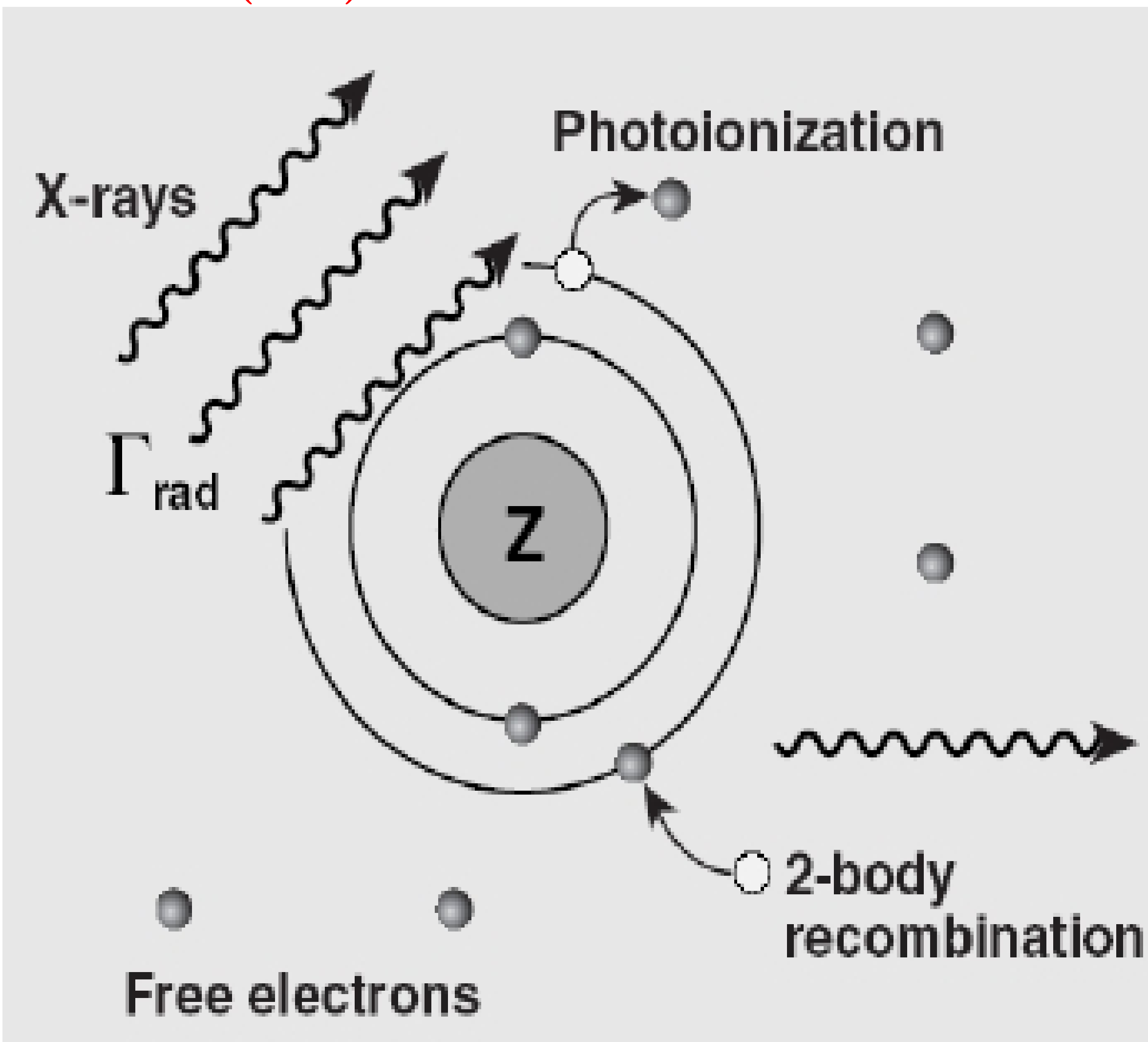
Diagnostic Lines of He-like Ions: w,x,y,z

w(E1) : $1s2p(^1P^o_1) - 1s^2(^1S_0)$ (Allowed Resonant)
x(M2) : $1s2p(^3P^o_2) - 1s^2(^1S_0)$ (Forbidden)
y(E1) : $1s2p(^3P^o_1) - 1s^2(^1S_0)$ (Intercombination)
z(M1) : $1s3s(^3S_1) - 1s^2(^1S_0)$ (Forbidden)

NOTE: 1s-2p are the K_α transitions



2 & 3. PHOTOIONIZATION (PI) & RECOMBINATION (RC):



Examples:

- **Photoionization - in absorption spectra**
- **Recombination - in emission spectra**

2 & 3. PHOTOIONIZATION (PI) & RECOMBINATION (RC): Inverse Processes

i) Direct Photoionization (PI) & Radiative Recombination (RR) (1-step Bound-Continuum transitions):

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons X^{+Z+1}} + \epsilon$$

ii) Autoionization (AI) & Dielectronic recombination (DR) (2-steps with intermediate autoionizing state):

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons (X^{+Z-1})^{**} \rightleftharpoons X^{+Z+1}} + \epsilon$$

More exactly,

$$\mathbf{e + X^{+Z} \leftrightarrow (X^{+Z-1})^{**}} \leftrightarrow \begin{cases} e + X^{+Z} & \text{AI} \\ X^{+Z-1} + h\nu & \text{DR} \end{cases}$$

The doubly excited state "autoionizing state" introduces resonances

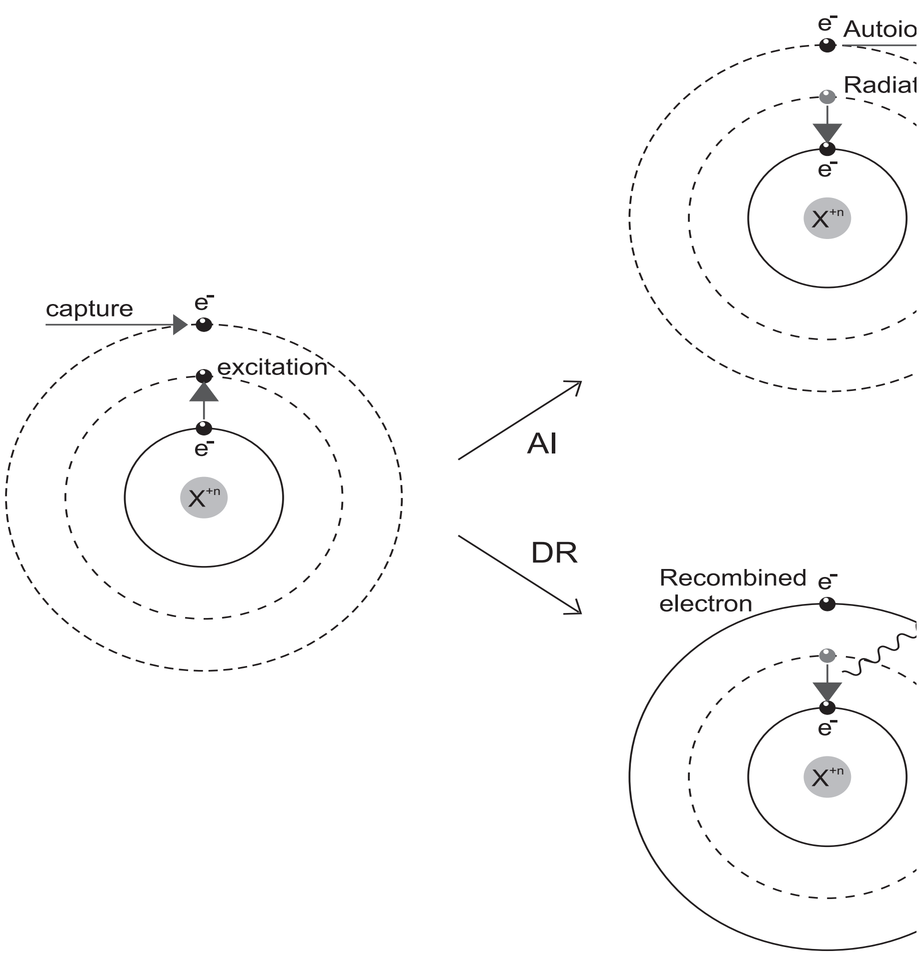
• i & ii Energetic electron leaves/combines the atom

• Photoionization Cross Sections (σ_{PI})

• Recombination Cross Sections (σ_{RC}) & Rate Coefficients (α_{RC})

- Show features with energy

Fig. Photoionization, Autoionization, Recombination:



- Incoming electron energy - excites the core and binds the electron to an higher excited leve - short lived Quasi-bound, doubly excited state (AI)
- outer electron goes free when core drops down
- core drops down with emssion of a photon -outer electron becomes bound (DR)

ELECTRON-ION COLLISIONS:

1. Electron-impact excitation (EIE):

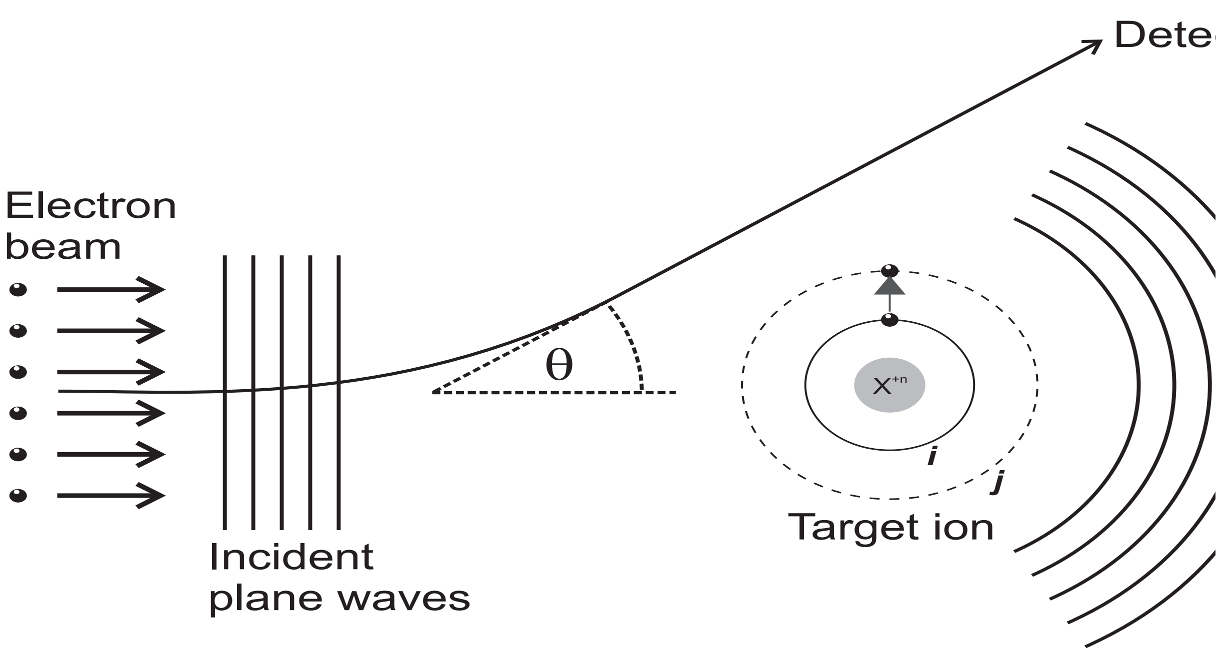
$$e + X^{+Z} \rightarrow e' + X^{+Z*} \rightarrow e' + X^{+Z} + h\nu$$

- - Light is emitted as the excitation decays
- show most common lines in astrophysical spectra
- diagnostic forbidden lines
- Scattered electron shows features with energy

•Can go through an autoionizing state

• Atomic quantity: *Collision Strength* (Ω)

Fig. Excitation by electron impact:



2. Electron-impact Ionization (EII, important, but may not emit photon):

$$\mathbf{e + X^{+Z} \rightarrow e' + e" + X^{+Z+1}}$$

- **Atomic parameters:**

Ionization cross section ($\sigma_{\mathbf{EII}}$)
Ionizatin strength ($\mathbf{S_{EII}}$)
(often available experimentally)

THEORY

("Atomic Astrophysics and Spectroscopy", (AAS) Pradhan and Nahar, Cambridge 2011)

Hamiltonian: For a multi-electron system, the relativistic Breit-Pauli Hamiltonian is:

$$\mathbf{H}_{\rm BP} = \mathbf{H_{NR}} + \mathbf{H}_{\rm mass} + \mathbf{H}_{\rm Dar} + \mathbf{H}_{\rm so} +$$

$$\frac{1}{2}\sum_{i\neq j}^{N}[g_{ij}(so + so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}$$

where the non-relativistic Hamiltonian is

$$\mathbf{H_{NR}} = \left[\sum_{i=1}^{N}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N}\frac{2}{r_{ij}}\right\}\right] \qquad (6)$$

the Breit interaction is

$$\mathbf{H_B} = \sum_{i>j}[g_{ij}(so + so') + g_{ij}(ss')] \qquad (7)$$

and one-body correction terms are

$$\mathbf{H_{mass}} = -\frac{\alpha^2}{4}\sum_i p_i^4, \mathbf{H_{Dar}} = \frac{\alpha^2}{4}\sum_i \nabla^2\left(\frac{Z}{r_i}\right), \mathbf{H_{so}} =$$

$$\frac{\mathbf{Ze^2\hbar^2}}{\mathbf{2m^2c^2r^3}}\mathbf{L.S}$$

Wave functions and energies are obtained solving:

$$\mathbf{H\Psi = E\Psi}$$

- $\mathbf{E < 0} \rightarrow$ **Bound (e+ion) states** Ψ_B
- $\mathbf{E \geq 0} \rightarrow$ **Continuum states** Ψ_F

Transition Matrix elements with a Photon

Dipole operator: $\mathbf{D} = \sum_i \mathbf{r}_i$:

$< \Psi_B||\mathbf{D}||\Psi_{B'} >$ $\rightarrow$ **Photo-excitation & De-excitation**

$< \Psi_B||\mathbf{D}||\Psi_F >$ $\rightarrow$ **Photoionization**

Matrix element is reduced to generalized line strength

$$\mathbf{S} = \left| \left\langle \mathit{\Psi}_\mathbf{f} \middle| \sum_{\mathbf{j=1}}^{\mathbf{N+1}} \mathbf{r_j} \middle| \mathit{\Psi}_\mathbf{i} \right\rangle \right|^{\mathbf{2}} \tag{8}$$

Oscillator Strength, Photoionization, Recombination all are related to S

Evaluation of the transition matrix element with a radiation field is non-trivial because of the exponential operator $e^{i\mathbf{k.r}}$ describing the field

$$e^{i\mathbf{k.r}} = 1 + i\mathbf{k.r} + [i\mathbf{k.r}]^2/2! + \ldots, \tag{9}$$

- **Various terms in the exponential expansion corresponds to various multipole transitions. The first term gives the electric dipole transitions E1, 2nd term E2 and M1, ...**
- **The slection rules arise from the angular algebra of the transition matrices.**

• The exponential factor $e^{i\mathbf{k}.\mathbf{r}}$ in the transition matrix element gives the spatial dependence of the incident wave.
An electron at a distance from the nucleus is of the order of Bohr radius, 10^{-8} cm.
The magnitude of the wave vector k is $2\pi/\lambda$. For visible light k is of the order of 10^5 cm^{-1}
→ the wavelength is much larger than the size of an atom
Retaining only the term unity in the first expansion, leads to the ***electric dipole approximation***:
$\mathbf{e^{ik.r}} \approx \mathbf{1}$.

f-, S, A-VALUES FOR VARIOUS TRANSITIONS

Allowed electric dipole (E1) transtitions

The oscillator strength (f_{ij}) and radiative decay rate (A_{ji}) for the bound-bound transition are

$$\mathbf{f_{ij}} = \left[\frac{\mathbf{E_{ji}}}{\mathbf{3g_i}}\right]\mathbf{S}, \quad \mathbf{A_{ji}(sec^{-1})} = \left[\mathbf{0.8032 \times 10^{10}}\frac{\mathbf{E_{ji}^3}}{\mathbf{3g_j}}\right]\mathbf{S} \qquad (10)$$

i) Same spin multipliciy dipole allowed (Δ j=0,$\pm$1, $\Delta L = 0$, $\pm$1, $\pm$2, ΔS = 0, parity π changes)
ii) Intercombination (Δ j=0,$\pm$1, $\Delta L = 0$, $\pm$1, $\pm$2, ΔS $\neq$ 0, π changes)

Forbidden transitions

i) Electric quadrupole (E2) transitions (Δ J = 0,$\pm$1,$\pm$2, parity does not change)

$$\mathbf{A_{ji}^{E2}} = \mathbf{2.6733 \times 10^3 \frac{E_{ij}^5}{g_j} S^{E2}(i,j)}\ \mathrm{s}^{-1}, \qquad (11)$$

ii) Magnetic dipole (M1) transitions (Δ J = 0,$\pm$1, parity does not change)

$$\mathbf{A_{ji}^{M1} = 3.5644 \times 10^4 \frac{E_{ij}^3}{g_j} S^{M1}(i,j)\ s^{-1}}, \tag{12}$$

iii) Electric octupole (E3) transitions (Δ J= $\pm$2, $\pm$3, parity changes)

$$\mathbf{A_{ji}^{E3} = 1.2050 \times 10^{-3} \frac{E_{ij}^7}{g_j} S^{E3}(i,j)\ s^{-1}}, \tag{13}$$

iv) Magnetic quadrupole (M2) transitions (Δ J = $\pm$2, parity changes)

$$\mathbf{A_{ji}^{M2} = 2.3727 \times 10^{-2} s^{-1} \frac{E_{ij}^5}{g_j} S^{M2}(i,j)}. \tag{14}$$

<u>LIEFTIME:</u>

The lifetime of a level can be obtained from the A-values,

$$\tau_k(\mathbf{s}) = \frac{\mathbf{1}}{\sum_i \mathbf{A_{ki}(s^{-1})}}. \tag{15}$$

Photoionization & Recombination cross section:

Photoionization cross section is given by

$$\sigma_{\mathbf{PI}}(\mathbf{K}\alpha,\nu) = \frac{4\pi^2\mathbf{a_o^2}\alpha}{\mathbf{3}}\frac{\mathbf{E_{ij}})}{\mathbf{g_k}}\mathbf{S} \tag{16}$$

In central-field approximation, the photoionization cross section in length form is given by,

$$\sigma_{\mathbf{L}} = \frac{4\pi^2\alpha\omega_{\mathbf{ij}}}{\mathbf{3}}\frac{\mathbf{1}}{\mathbf{2l_i+1}}\left[\mathbf{l_i}\left|\mathbf{R}_{\mathbf{n_il_i}}^{\mathbf{n_j,l_i+1}}\right|^{\mathbf{2}} + (\mathbf{l_i+1})|\mathbf{R}_{\mathbf{n_il_i}}^{\mathbf{n_j,l_i-1}}]\right]. \tag{17}$$

A general expression for the photoionization cross section of level n of a hydrogenic system is (Seaton 1959)

$$\sigma_{\mathbf{n}} = \frac{\mathbf{64}\pi\alpha\mathbf{a_o^2}}{\mathbf{3}\sqrt{\mathbf{3}}}\left(\frac{\omega_{\mathbf{n}}}{\omega}\right)^{\mathbf{3}}\frac{\mathbf{ng}(\omega,\mathbf{n},\mathbf{l},\mathbf{Z})}{\mathbf{Z^2}}, \tag{18}$$

where

$$\omega > \omega_{\mathbf{n}} = \frac{\alpha^{\mathbf{2}}\mathbf{mc^2}}{\mathbf{2\hbar}}\frac{\mathbf{Z^2}}{\mathbf{n^2}}, \tag{19}$$

and $g(\omega, n, l, Z)$ is the bound-free Gaunt factor which is approximately unity at near-threshold energies. A more detailed expression for photoionization of a state nl is

$$\sigma_{\mathbf{nl}} = \frac{\mathbf{512}\pi^{\mathbf{7}}\mathbf{m_e^{10}}}{\mathbf{3}\sqrt{\mathbf{3}}\mathbf{ch^6}}\frac{\mathbf{g}(\omega,\mathbf{n},\mathbf{l},\mathbf{Z})\mathbf{Z^4}}{\mathbf{n^5}\omega^{\mathbf{3}}} \tag{20}$$

The photoionization cross section can be approximated by using hydrogenic wavefunctions that yield

the Kramer's formula,

$$\sigma_{\mathbf{PI}} = \frac{\mathbf{8}\pi}{\mathbf{3^{1.5}c}} \frac{\mathbf{1}}{\mathbf{n^5}\omega^{\mathbf{3}}} \tag{21}$$

This is sometimes used to extrapolate photoionization cross sections in the high-energy region, where other features have diminished contribution with a relatively smooth background. However, it is not accurate.

Since the spin does not change in a dipole transiton, and $S_i = S_j$, the angular algebra remains the same for both the bound-bound and bound-free transitions. So we have the same selection rules for photoionization,

$$\begin{array}{l} \Delta L = L_j - L_i = 0, \pm 1, \;\; \Delta M = M_{L_j} - M_{L_i} = 0, \pm 1, \\ \Delta l = l_j - l_i = \pm 1. \end{array} \tag{22}$$

The length photoionization cross section is,

$$\begin{array}{l} \sigma_L = \frac{\pi^2 c^2}{n_\omega \omega_{ij}^2} T_{ij} \\ = \frac{4\pi^2 \alpha}{3} \omega_{ij} \sum_{l_j = l_i \pm 1} \sum_{L_j} (2L_j + 1) \frac{(l_i + l_j + 1)}{2} W^2(l_i L_i l_j L_j; L_1 1) | \\ < n_j l_j | r | n_i l_i > |^2 \end{array} \tag{23}$$

With $\alpha = e^2/(\hbar c)$ the cross section is in units of a_o^2 and the constant in the equation is $\frac{4\pi^2 a_o^2 \alpha}{3} =$ 2.689 Megabarns,

abbreviated as Mb $= 10^{-18}$ **cm**^{2} **The radial integral**

$$< \mathbf{n_j l_j | r | n_i l_i} >= \int_0^\infty \mathbf{R_{n_j l_j} r R_{n_i l_i} r^2 dr}, \tag{24}$$

involves an exponentially decaying initial bound state wavefunction, and an oscillating continuum free-electron wavefunction as a plane wave. The bound state wavefunctions are normalized to $| < i|i > |^2$**=1, and free state wavefunctions are normalized per unit energy**

Recombination cross section, σ_{RC}**, from principle of detailed balance:**

$$\sigma_{\mathbf{RC}} = \sigma_{\mathbf{PI}} \frac{\mathbf{g_i}}{\mathbf{g_j}} \frac{\mathbf{h^2} \omega^2}{\mathbf{4\pi^2 m^2 c^2 v^2}}. \tag{25}$$

The recombination rate coefficient:

$$\alpha_{\mathbf{RC}}(\mathbf{T}) = \int_0^\infty \mathbf{v f(v)} \sigma_{\mathbf{RC}} \mathbf{dv}, \tag{26}$$

$\mathbf{f(v,T)} = \frac{\mathbf{4}}{\sqrt{\pi}} (\frac{\mathbf{m}}{\mathbf{2kT}})^{\mathbf{3/2}} \mathbf{v^2 e^{-\frac{mv^2}{2kT}}}$ **= Maxwellian velocity distribution function**

Recombination Rate Coefficient in terms of photoelectron energy is

$$\alpha_{\mathbf{RC}}(\mathbf{E}) = \mathbf{v} \sigma_{\mathbf{RC}}$$

Total α_{RC} $\rightarrow$ ***Contributions from infinite number of recombined states***

• Radiative & Dielectronic Recombinations are inseparable in nature

UNIFIED TREATMENT FOR ELECTRON-ION RECOMBINATION

(Nahar & Pradhan, 1992, 1994, Zhang, Nahar, Pradhan, 1999)

EXISTING METHODS: $\alpha_{\mathbf{RC}} = \alpha_{\mathbf{RR}} + \alpha_{\mathbf{DR}}$

UNIFIED METHOD: Total α_{RC} - subsumes RR and DR including interference effects

• Considers infinite number of recombined states:
i) Group (A) Low-n Bound States ($n \le n_o \sim$ 10):
σ_{RC} are obtained from σ_{PI} which includes autoionizing resonances. Hence subsumes both RR & DR
ii) Group (B) High-n States ($n_o \le n \le \infty$):
These densely packed highly excited states, dominated by DR process, are treated through DR theory (Bell & Seaton 1985, Nahar & Pradhan 1994) in close-coupling approximation

• Advantages of the "Unified method":

• Self-consistent treatment for photoionization & recombination - use of same wavefunction

• Provides "level-specific" recombination rate coefficients & photoionization cross sections for a large number of bound levels

Ionization Fractions in Astrophysical Plasma Equilibria: Unified Treatment of Photoionization & Electron-Ion Recombination

i) Plasma in Coronal Equilibrium:

Electron-Impact Ionization (EII) is balanced by Electron Ion Recombination:

$$\mathbf{N(z-1)S_{EII}(z-1) = N(z)\alpha_{RC}(z)}$$

$S_{EII}(z-1)$ = total EII rate coefficient, α_{RC} = total recombination rate coefficient

ii) Plasma in Photoionization Equilibrium:

With a radiation flux J_ν, photoionization is balanced by electron-ion recombination:

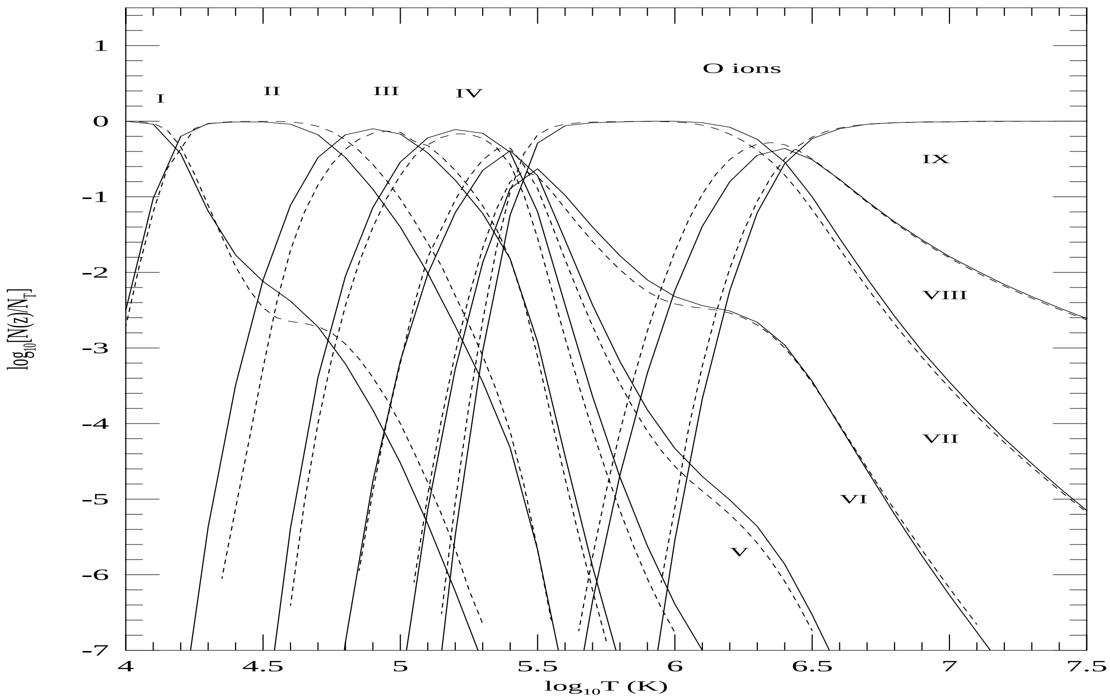
$$\mathbf{N(z)\int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{h\nu}\sigma_{PI}(z,\nu)d\nu = N_e N(z+1)\alpha_{RC}(z,T_e)}$$

ν_o = Ionization potential of the ion, σ_{PI} = Ground state photoionization cross sections

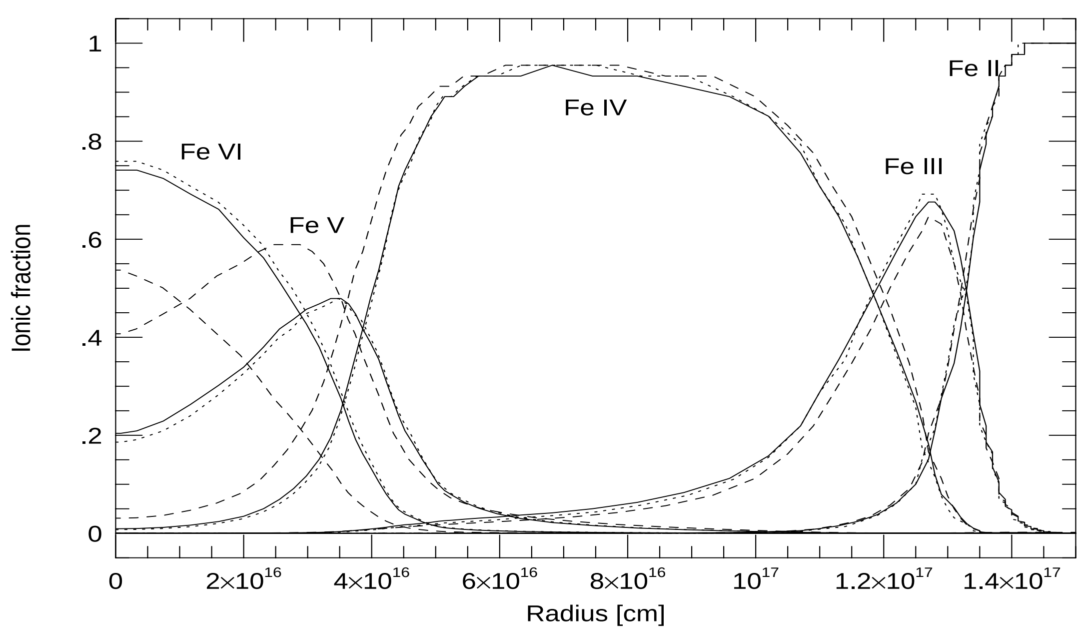
Accurate ionization fractions, N_i/N, requires

- **Unified treatment of *total* (RR+DR) rate coefficient**
- **Self-consistency between these inverse processes**

Ionization Fractions at Coronal Equibrium: O-ions (Nahar 1998)



Iron Ionization Fractions at Photoionization Equilibrium in a typical PNe: Fe IV dominates in most of the nebula, Fe V fraction is reduced by half (Nahar & Bautista 1995)



EIE:

Scattering matrix $\mathbf{S}_{SL\pi}(i,j)$ is obtained from the wave function phase shift. The EIE collision strength is

$$\Omega(S_iL_i - S_jL_j) =$$
$$\frac{1}{2}\sum_{SL\pi}\sum_{l_il_j}(2S+1)(2L+1)|S_{SL\pi}(S_iL_il_i - S_jL_jl_j)|^2$$

The effective collision strength $\Upsilon(T)$ is the Maxwellian averaged collision strength:

$$\Upsilon(T) = \int_0^\infty \Omega_{ij}(\epsilon_j)e^{-\epsilon_j/kT}d(\epsilon_j/kT) \qquad (27)$$

The excitation rate coefficient $q_{ij}(T)$ is

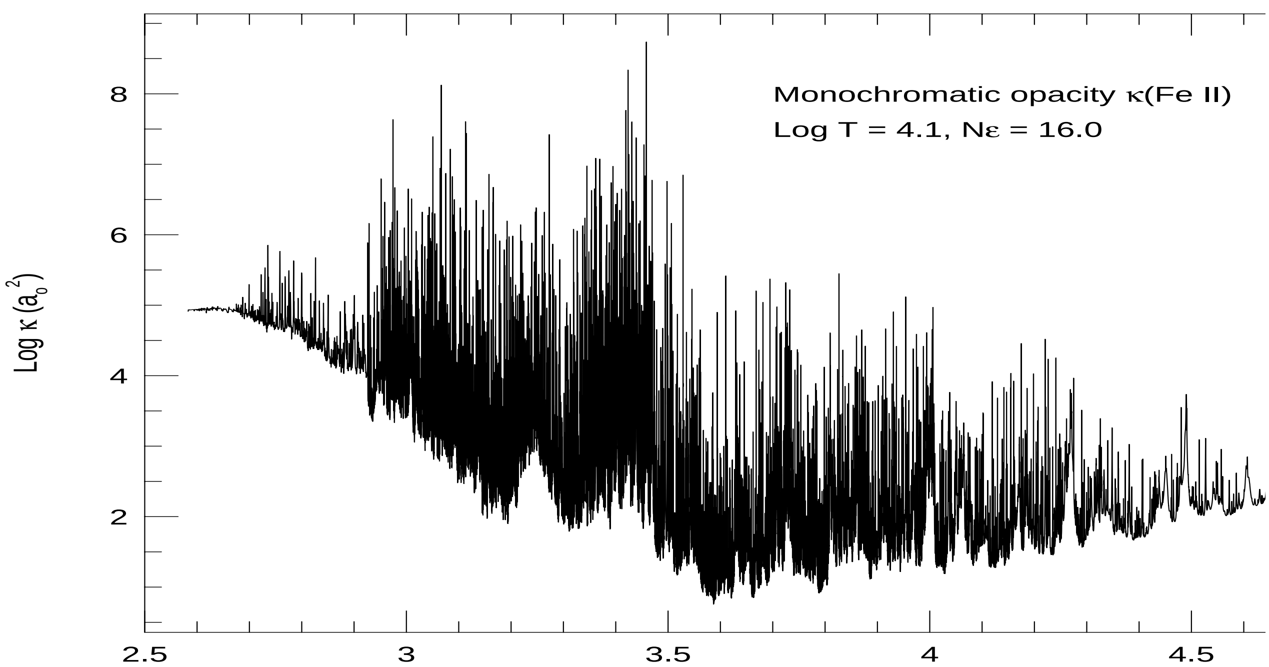
$$q_{ij}(T) = \frac{8.63\times10^{-6}}{g_iT^{1/2}}e^{-E_{ij}/kT}\Upsilon(T)\ \mathrm{cm^3s^{-1}} \qquad (28)$$

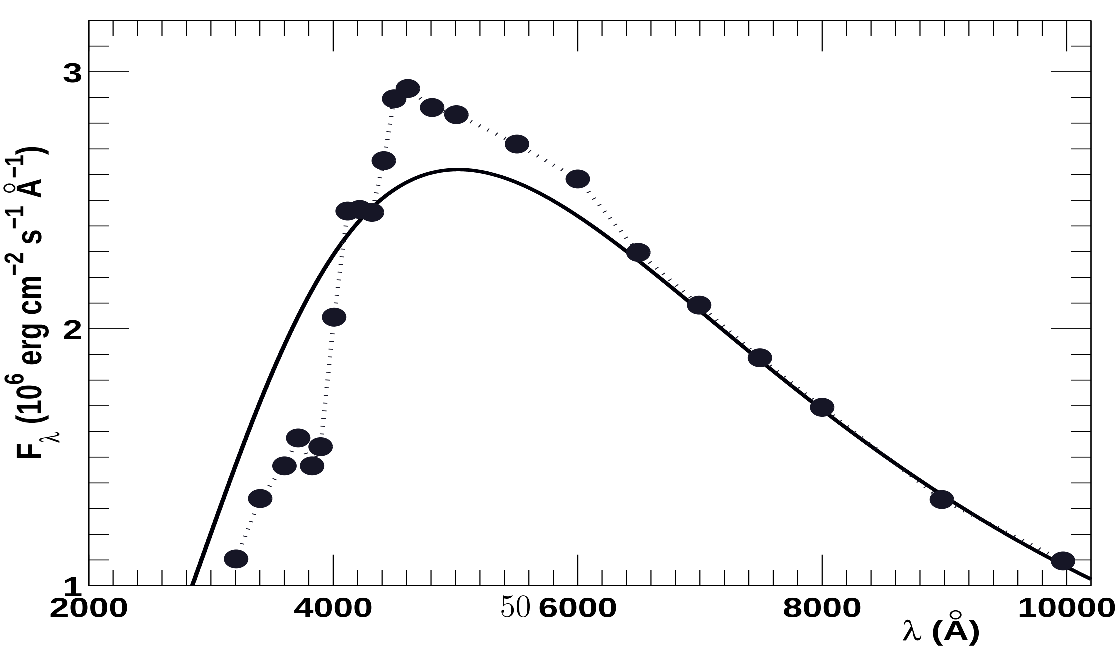
$E_{ij} = E_j - E_i$ **and** $E_i < E_j$ **in Rydbergs**

Monochromatic Opacities κ_ν of Fe II:

(Nahar & Pradhan 1993)

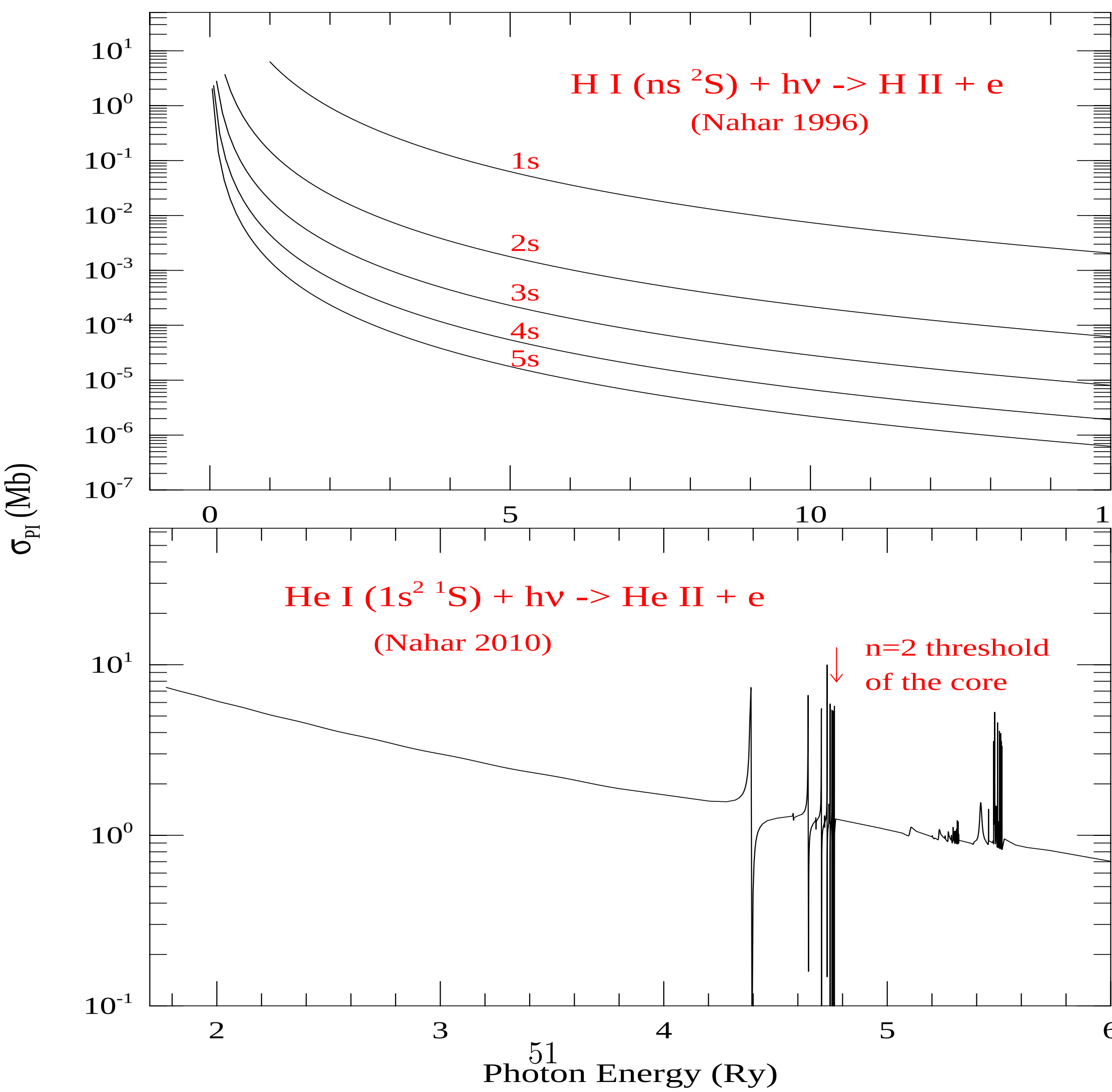
TOP: Complex structure in monochromatic opacity of Fe II at the Z-bump temperature and density Bottom: The high opacity in 2-3.5 region indicates the absorption by Fe I and Fe II in the solar blackbody radiation.



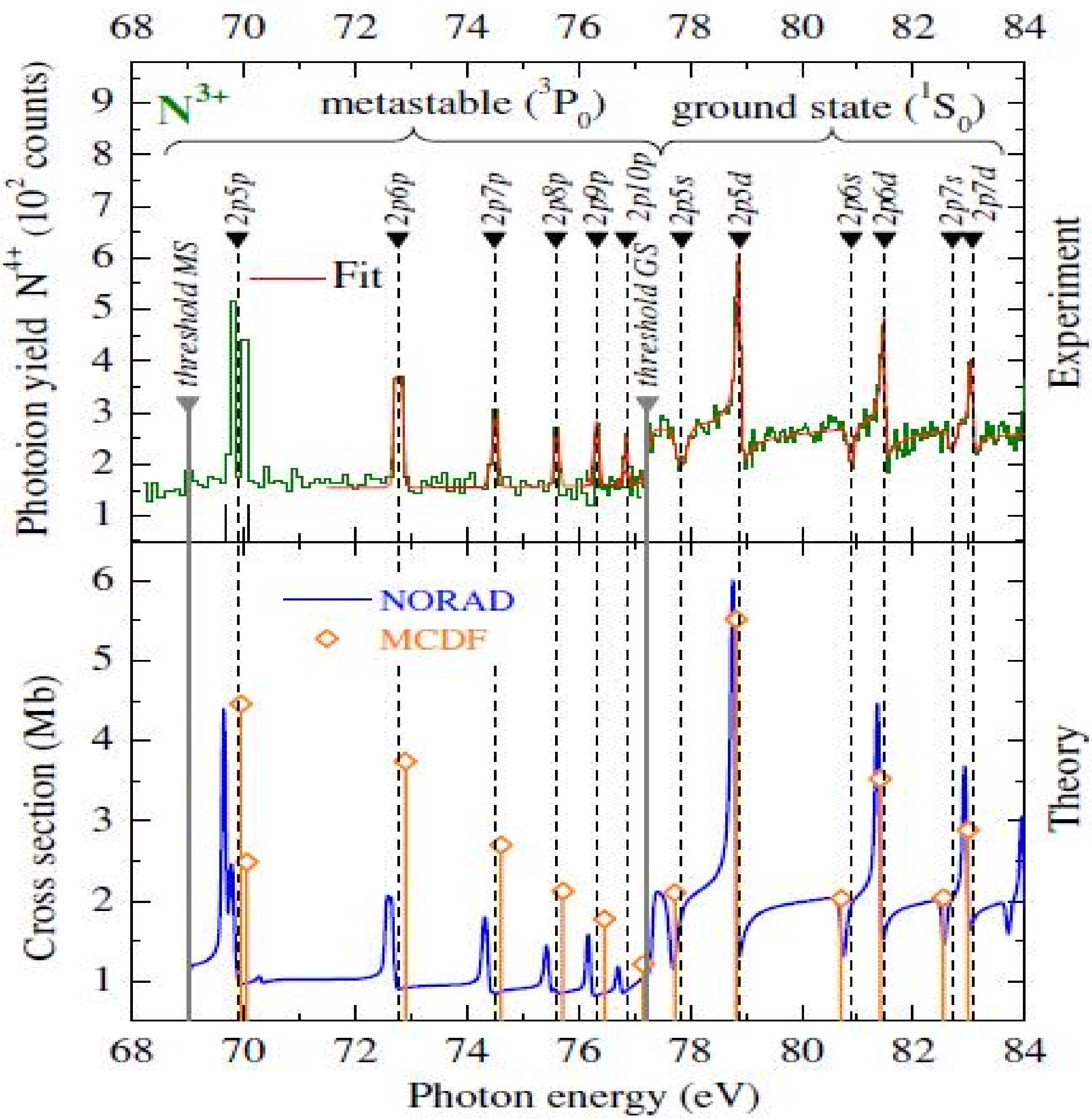


PHOTOIONIZATION

- An atom/ion with more than 1 electron will have resonances in σ_{PI}
- Earlier calculations for photoionization cross sections under the Opacity Project considered low-lying resonances
- Core excitations to higher states during photoionization are thought to be weaker and behave hydrogenic
- Fine structure introduce new features that can not be obtained in LS coupling
- New calculations under the Iron Project are showing new and dominating features not studied before - these are expected to resolve some longstanding problems



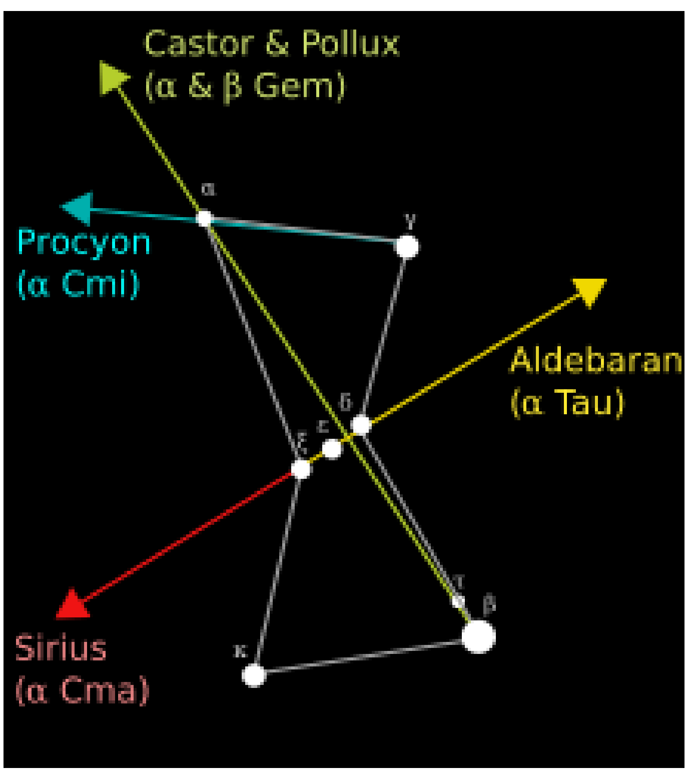
• Physics Experiment: Photoionization cross sections of N IV:
TOP: measured at synchrotron facility BESSY II by Simon et al (2010)
BOTTOM: Comparison with NORAD-Atomic-Data (Nahar & Praadhan 1997, blue). MCDF (Orange drop lines)



Photometric Image: Orion Constellation

Red gaseaous nebula in the background - "Orion Nebula" (reddish patch) below the belt of 3 stars (on the sword)

Below: Imaginary figure - "Orion the Hunter"



Determination of Abundance of Elements

Orion Nebula - Birthplace of Stars

[Composed by images from Spitzer & Hubble]

- Orion Nebula $\sim$ 1500 Lyr away, closest cosmic cloud to us
- Center bright & yellow gas - illuminated ultraviolet (UV) radiation

Images: Spitzer - Infrared (red & orange) C rich molecules - hydrocarbons, Hubble - optical & UV (swirl green) of H, S

- Small dots - infant stars; over 1000 young stars
- Detected lines of O II, O III

Determination of Abundance of Elements

• **Longstanding problems on determination of abudances of elements - lack of accurate atomic data**

• **One is Oxygen abundance in Nebular plasmas Ex: Planetary Nebula (PNe) K 4-55 (below)**

• **Planetary nebula (PNe): last stage of a star**

• **Has condensed central star: very high T $\sim$ 100,000 K ($>>$ T $\leq$ 40,000 K of a typical star)**

• **Envelope: thin gas radiatively ejected & illuminated by radiation of the central star: red (N), blue (O)**

• **Common lines of low ionization states: O III and O II - low density and low T**

Determination of OXYGEN Abundance:

- **Collisionally Excited Lines (CEL):**

e + O III → O III* → O III + hν

- **Recombination lines (REL):**

e + O III → O II + hν

- **The intensity of a CEL of ion X_I due to transition between *a* and *b* (*Atomic Astrophysics and Spectroscopy*, Pradhan & Nahar, 2011)**

$$\mathbf{I_{ba}(X_i, \lambda_{ba}) = \frac{h\nu}{4\pi} n_e n_{ion} q_{ba}} \tag{29}$$

q_{ba} **- EIE rate coeffcient in cm^3/sec. Hence population of a level b can be written as**

$$\mathbf{N(b) = n_{ion} q_{ba} = \frac{1}{n_e}\frac{4\pi}{h\nu} I_{ba}} \tag{30}$$

The abundance, $\mathbf{n(X)/n(H)}$ of the element, X, with respect to H, can be obtained from the intensity I

$$\mathbf{I(X_i, \lambda_{ba}) = \frac{h\nu}{4\pi} A_{ba} \frac{N(b)}{\sum_j N_j(X_i)} \frac{n(X_i)}{n(X)} \left[\frac{n(X)}{n(H)}\right] n(H)}$$

A_{ba} **- radiative decay rate, sum over N_j - total populations of all excited levels, $N(b)/\sum_j N_j(X_i)$ - population fraction, (obtained**

from a radiative -collisional model), $\frac{n(X_i)}{n(X)}$ - ionization fraction (come from photoionization model code)

- **Similarly abundance can obtaioned from the intensity of a REL from emissivity**

$$\epsilon(\lambda_{\mathbf{pj}}) = \mathbf{N_e N(X^+)}\alpha_{\mathbf{eff}}(\lambda_{\mathbf{pj}})\mathbf{h}\nu_{\mathbf{pj}}[\mathrm{arg\ cm^{-1}s^{-1}}]$$

intensity, cascade matrix, and formula similar to that of CEL but for REL

Problem: $\mathbf{N_e N(O\ III) q_{EIE}} < \alpha_{\mathbf{R}}(\mathbf{T})\mathbf{N_e N(O\ II)}$

•ONE SOLUTION: Recombination rate for (e + O III)→O II - higher at low T

Close-Coupling (CC) Approximation & the R-matrix method

- **CC approximation:**
- **Ion treated as a (N+1) electron system:**

- a target or the ion core of N electrons and
- an additional interating (N+1)th electron:

- **Total wavefunction expansion is:**

$$\mathbf{\Psi_E(e+ion) = A\sum_{i}^{N}\chi_i(ion)\theta_i + \sum_{j} c_j\Phi_j(e+ion)}$$

$\chi_i \rightarrow$ **target ion or core wavefunction**
$\theta_i \rightarrow$ **interacting electron wavefunction (continuum or bound)**
$\Phi_j \rightarrow$ **correlation functions of (e+ion)**

- **The complex resonant structures in the atomic processes are included through channel couplings.**
- **Substitution of Ψ_E(e+ion) in $H\Psi_E = E\Psi_E$ results in a set of coupled euqations**
- **Coupled equations are solved by R-matrix method**

Close-Coupling Approximation

The wavefunction is an expansion:

$$\mathbf{\Psi_E(e + ion) = A \sum_i^N \chi_i(ion)\theta_i + \sum_j c_j \Phi_j(e + ion)}$$

$\chi_i \rightarrow$ **core ion wavefunction,** $\Phi_j \rightarrow$ **correlation functions**

$\theta_i \rightarrow$ **interacting electron wavefunction (continuum or bound)**

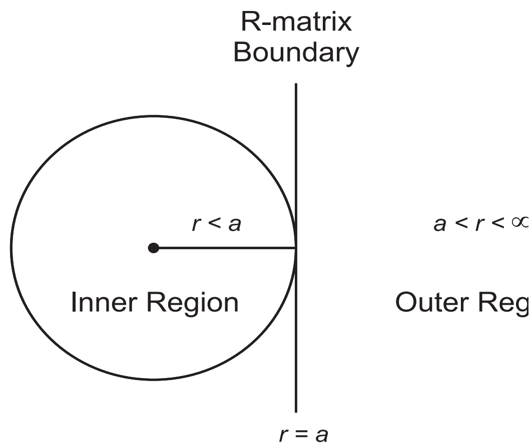
- **Resonant Structures - manifested through channel couplings**

Table (Example of $\mathbf{\Psi_E}$): Levels and energies (E_t) of the core O III in wave function expansion of O II; SS - calculated energies and NIST - observed energies

	Level	J_t	E_t(Ry) NIST	E_t(Ry) SS
1	$1s^22s^22p^2(^3P)$	0	0.0	0.
2	$1s^22s^22p^2(^3P)$	1	0.0010334	0.0011497
3	$1s^22s^22p^2(^3P)$	2	0.0027958	0.003384
4	$1s^22s^22p^2(^1D)$	2	0.18472	0.21215
5	$1s^22s^22p^2(^1S)$	2	0.39352	0.38420
6	$1s^22s2p^3(^5S^o)$	2	0.54972	0.46200
7	$1s^22s2p^3(^3D^o)$	3	1.0938	1.12584
8	$1s^22s2p^3(^3D^o)$	2	1.0940	1.12576
9	$1s^22s2p^3(^3D^o)$	1	1.0941	1.12573
10	$1s^22s2p^3(^3P^o)$	2	1.2975	1.32510
11	$1s^22s2p^3(^3P^o)$	1	1.2975	1.32500
12	$1s^22s2p^3(^3P^o)$	0	1.2976	1.32495
13	$1s^22s2p^3(^1D^o)$	2	1.7045	1.83934
14	$1s^22s2p^3(^3S^o)$	1	1.7960	1.89708
15	$1s^22s2p^3(^1P^o)$	1	1.9178	2.02463
16	$1s^22s2p3s(^3P^o)$	0	2.4354	2.33186
17	$1s^22s2p3s(^3P^o)$	1	2.4365	2.33300
18	$1s^22s2p3s(^3P^o)$	2	2.4388	2.33186
19	$1s^22s2p3s(^1P^o)$	1	2.4885	2.40908

R-matrix Method

Substitution of Ψ_E(e+ion) in $H\Psi_E = E\Psi_E$ → a set of coupled equations - solved by the R-matrix method



• Divide the space in two regions, the inner and the outer regions, of a sphere of radius r_a with the ion at the center. r_a is large enough for to include the electron-electron interaction potential. Wavefunction at $r > r_a$ is Coulombic due to perturbation

• In the inner region, the radial part $F_i(r)/r$ of the outer electron wave function (θ) is expanded in terms of a basis set, called the R-matrix basis,

$$\mathbf{F_i = \sum a_k u_k}$$

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + V(r) + \epsilon_{lk}\right] u_{lk} + \sum_n \lambda_{nlk} P_{nl}(r) = 0. \tag{31}$$

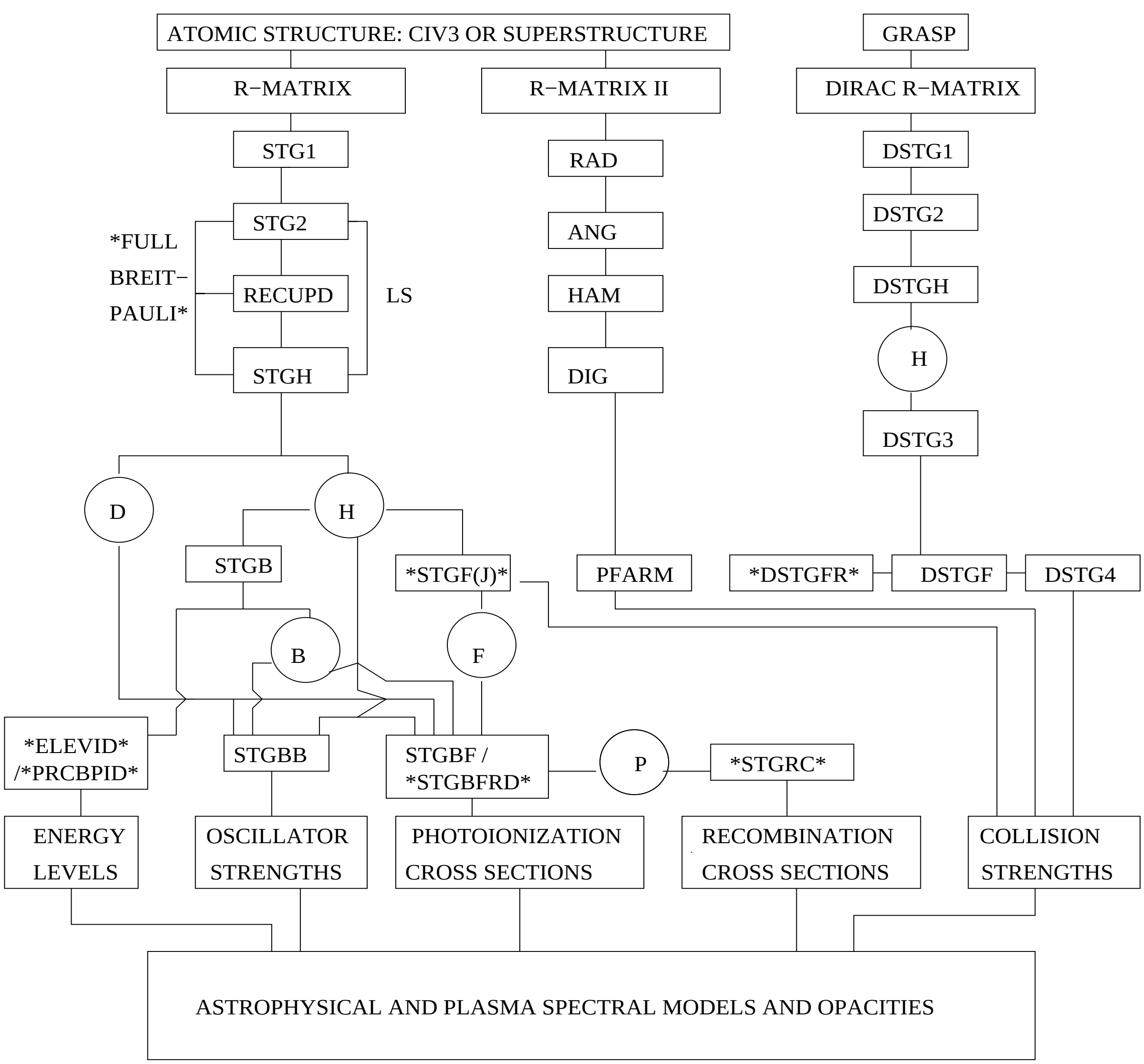
and is made continuous at r_a with the Coulomb functions outside r_a

R-Matrix Codes For Large-Scale Atomic Calculations at the Ohio Supercomputer Center

VARIOUS COMPUTATIONAL STAGES

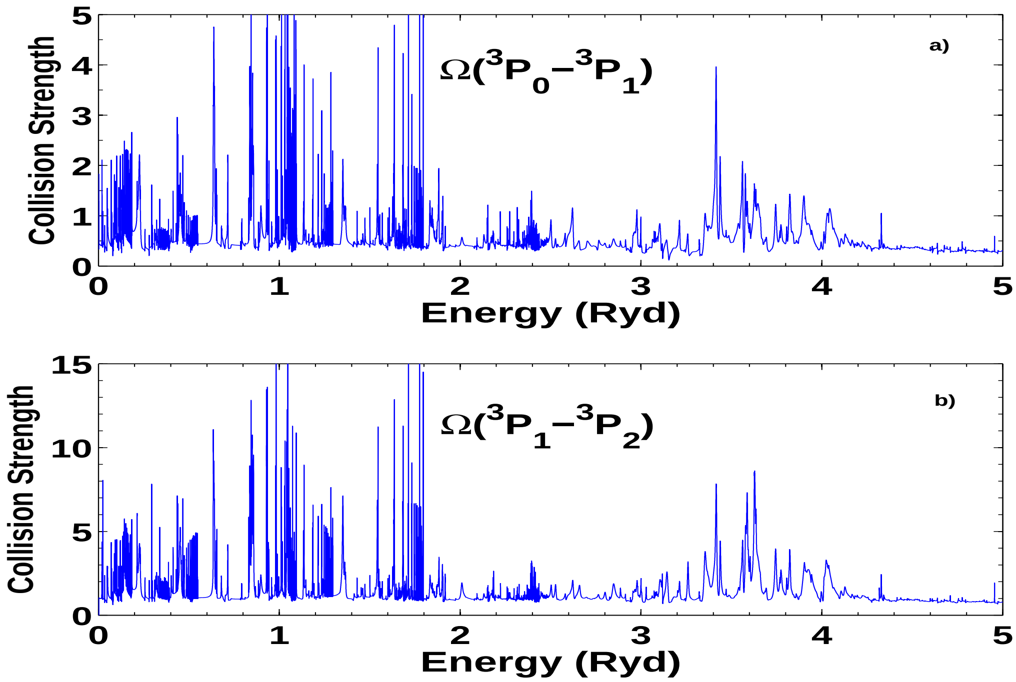
- **R-matrix calculations cen proceed in 3 branches - 1) LS coupling & relativistic Breit-Pauli, 2) LS coupling R-matrix II for Large configuration interaction, 3) DARC for Full Dirac relativistic**
- **Results - 1) Energy Levels, 2) Oscillator Strengths, 3) Photoionization Cross sections, 4) Recombination Rate Coefficients, 5) Collision Strengths; - Astrophysical Models**

THE R−MATRIX CODES AT OSU

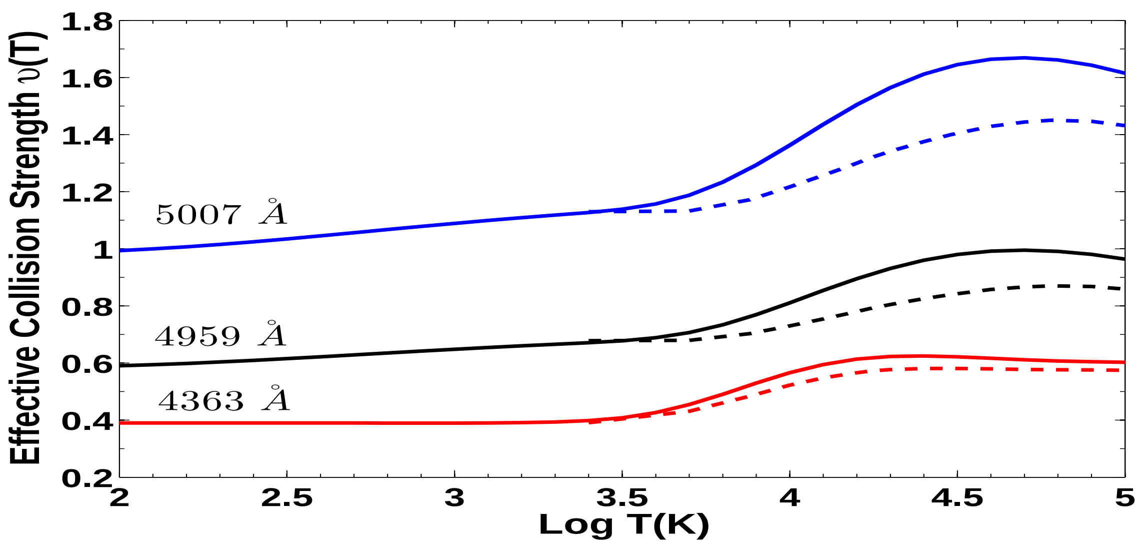


ELECTRON IMPACT EXCITATIONS (EIE)

• Fig Collision strengths Ω (EIE) of O III: $2p^2(^3P_0 - ^3P_1)$ $(88\mu m)$ and $2p^2(^3P_1 - ^3P_2)$ $(52\mu m)$ (IR) (Palay et al 2012)
• The near threshold resonances are seen for the first time

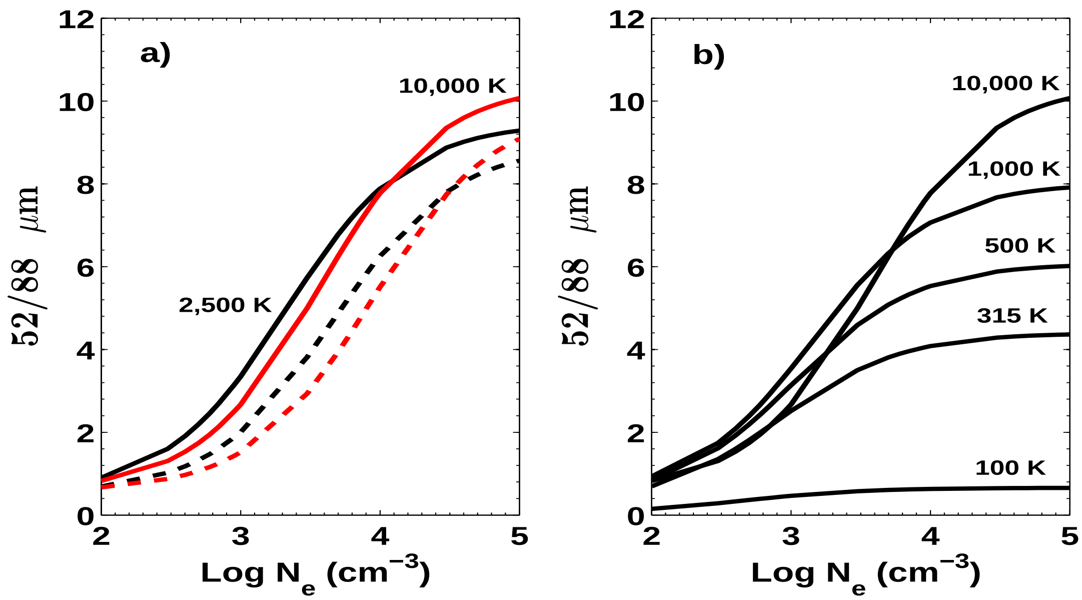


• Fig Effective Ω(T) of 3 optical lines; Solid: BPRM (present), Dashed: R-matrix(LS) (Aggarwal & Keenan)
• Differences to affect T and density diagnostics

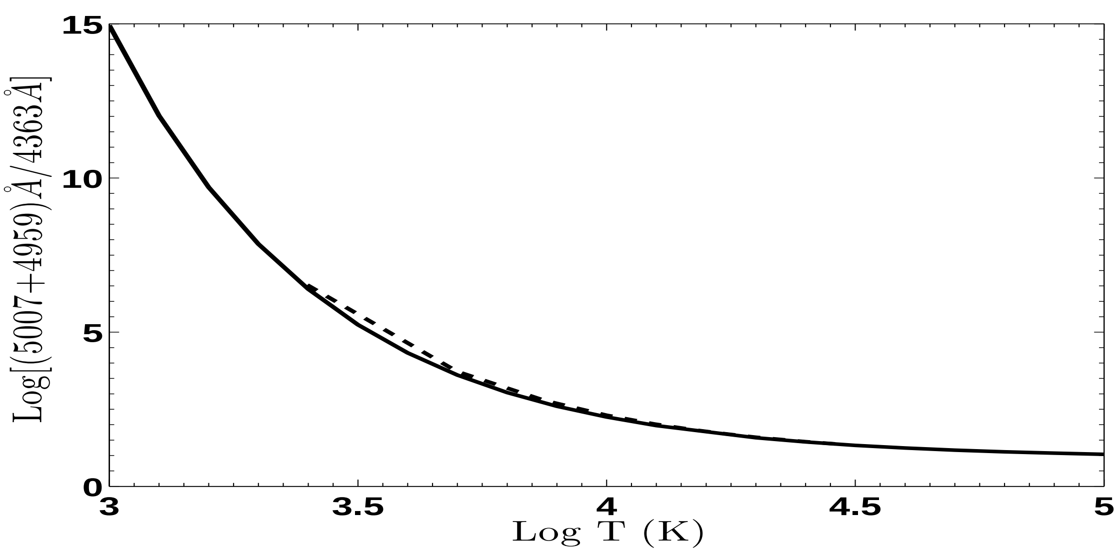


LINE RATIO: DENSITY & T DIAGNOSTICS

• Intensity ratio of two observed lines can be compared to the calculated curves for density (ρ) & T diagnostics
• Fig Significant FS effect on ρ diagnostics, 100 - 10,000 K



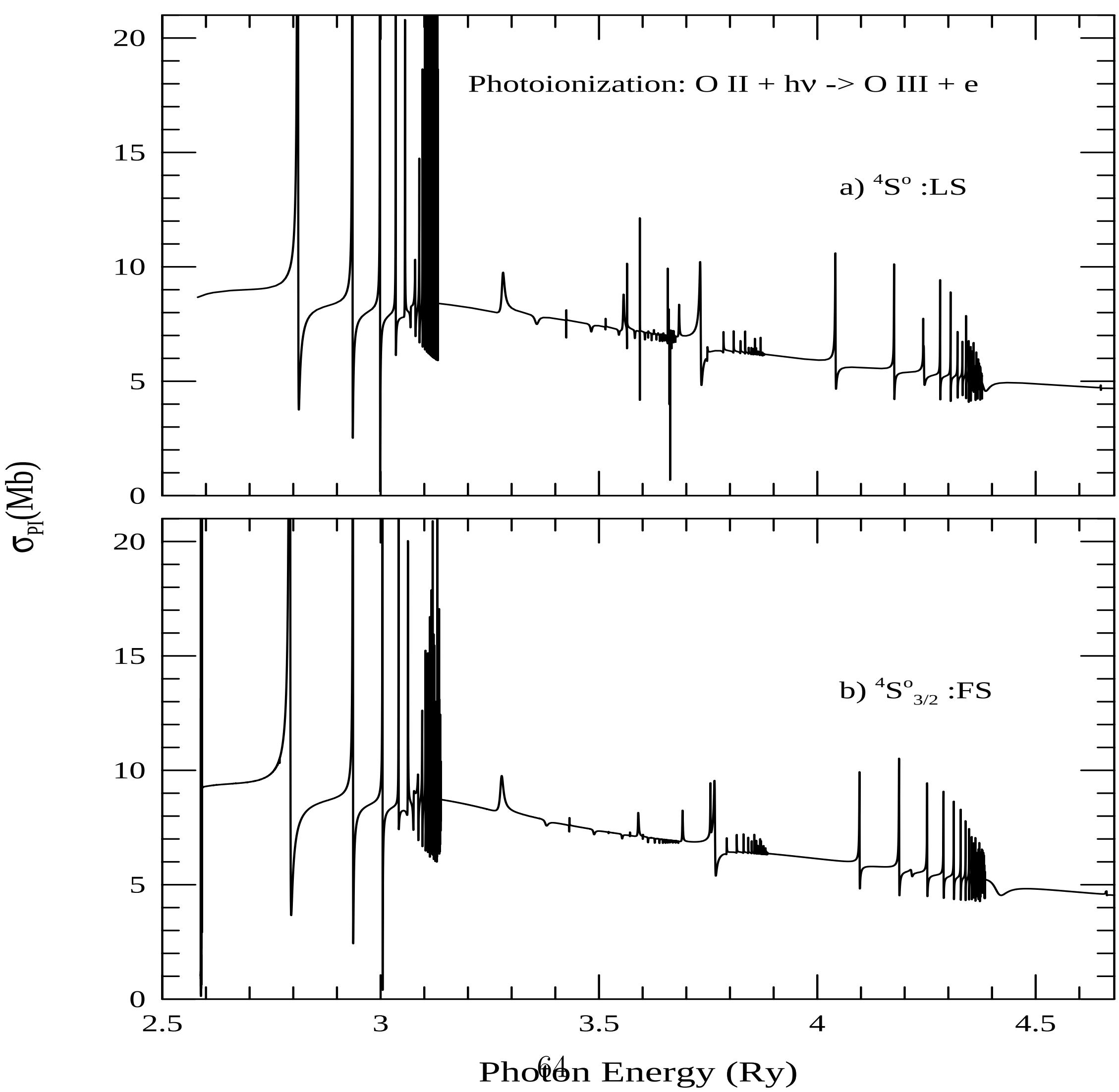
• Blended line ratio with T at $N_e = 10^3 cm^{-3}$. The diagnostic indicates considerable rise in low T region



Fine Structure Effects on Low Z ion: O II

(Nahar et al. 2010)

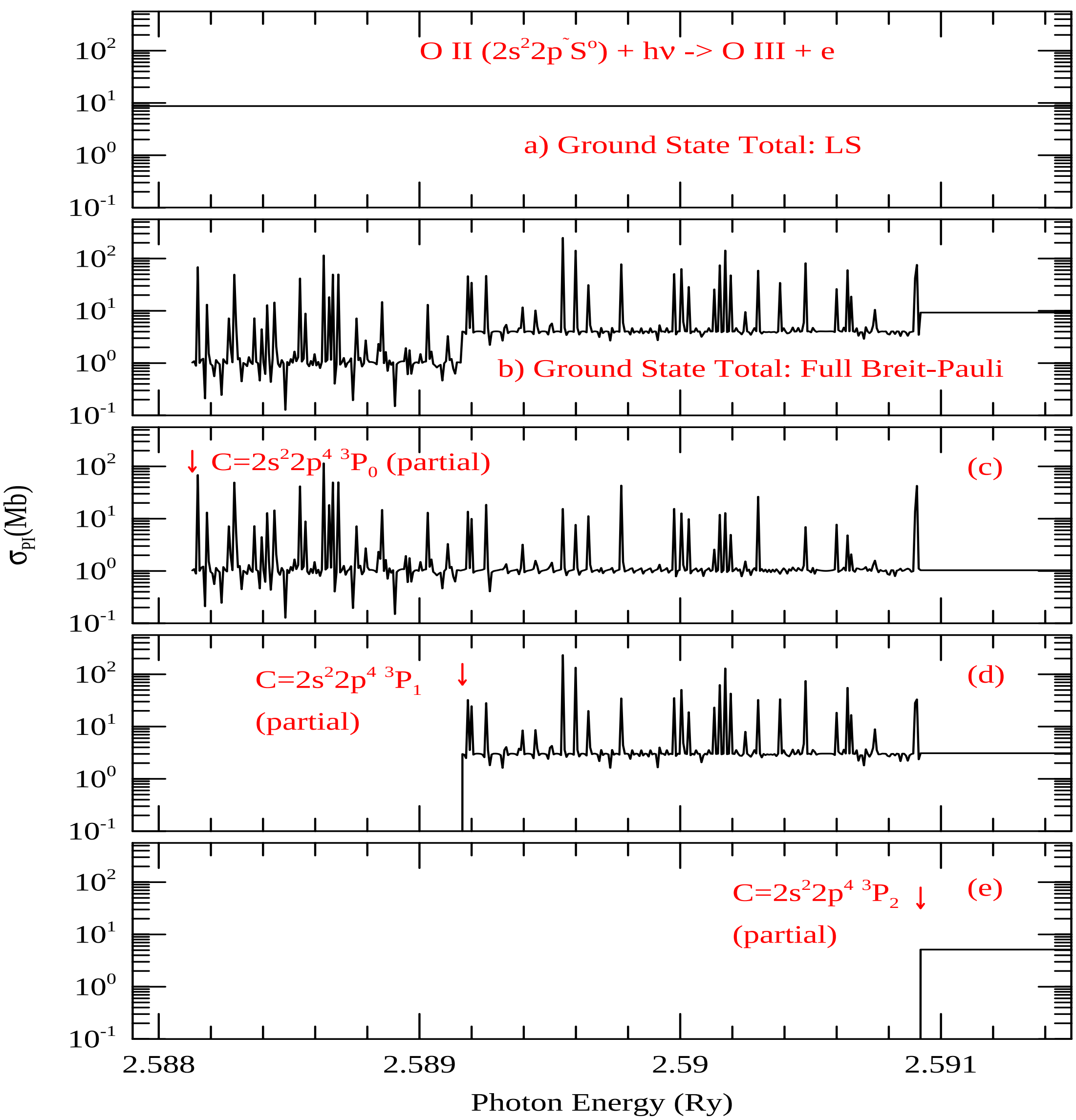
- Previous study of $\sigma_{\rm PI}$ for O II in LS coupling R-matrix (Nahar 2004) showed good agreement with experiment (ALS: Covington et al. 2001)
- However, problem remained with O II abundance at low T astrophysical plasmas
- σ_{PI} in fine structure (FS) is very similar to that in LS coupling except the resonant structure at the threshold
- The new low energy features in $\sigma_{\rm PI}$(FS) should narrow down the discrepancy



GROUND STATE PHOTOIONIZATION OF O II:

- **Photoionization of Ground state $^4S^o$ of O II in small energy region near threshold**
- **Panel a) (Top) Photoionization in LS coupling - no structure in the region (Nahar 2004)**
- **Panel b) Total σ_{PI}, of the ground level $^4S^o_{3/2}$: i) filled with resonant structures, ii) background shifts (Nahar et al. 2010)**
- **Panels c,d,e) Partial photoionization into fine structure components $2p^2\ ^3P_{0,1,2}$ of O III, arrows → ionization thresholds.**

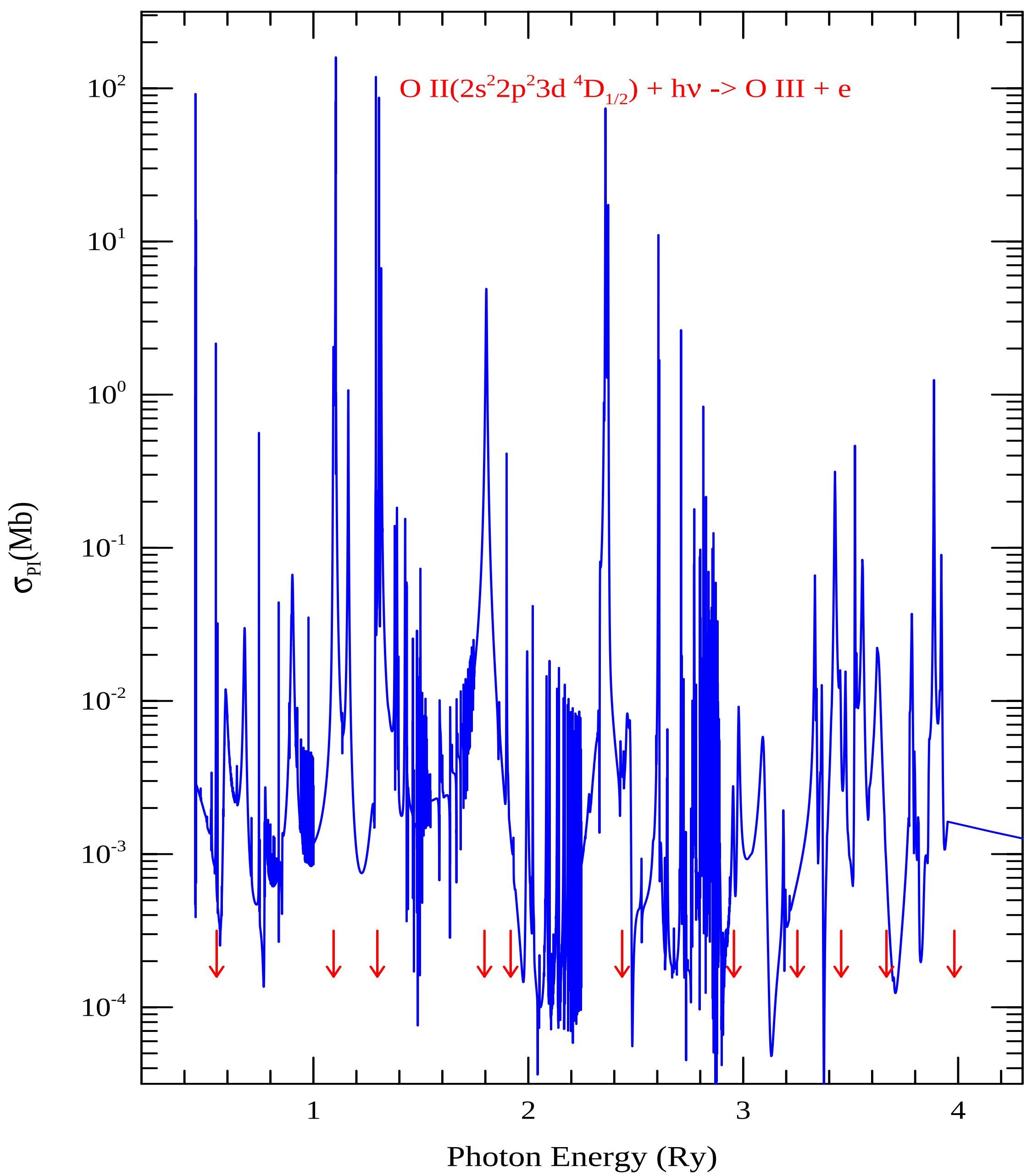
Photoionization Cross sections of O II



PHOTOIONIZATION OF O II: PEC RESONANCES

- PEC (Photo- Excitation-of-Core) resonances appear photoionization of single electron valence excited levels
- Figure shows that PEC resonances are strong and enhance the background cross sections by orders of magnitude
- These PEC resonances will affect photoionization and recombination rates of plasmas

Photoionization of O II: PEC Resonances

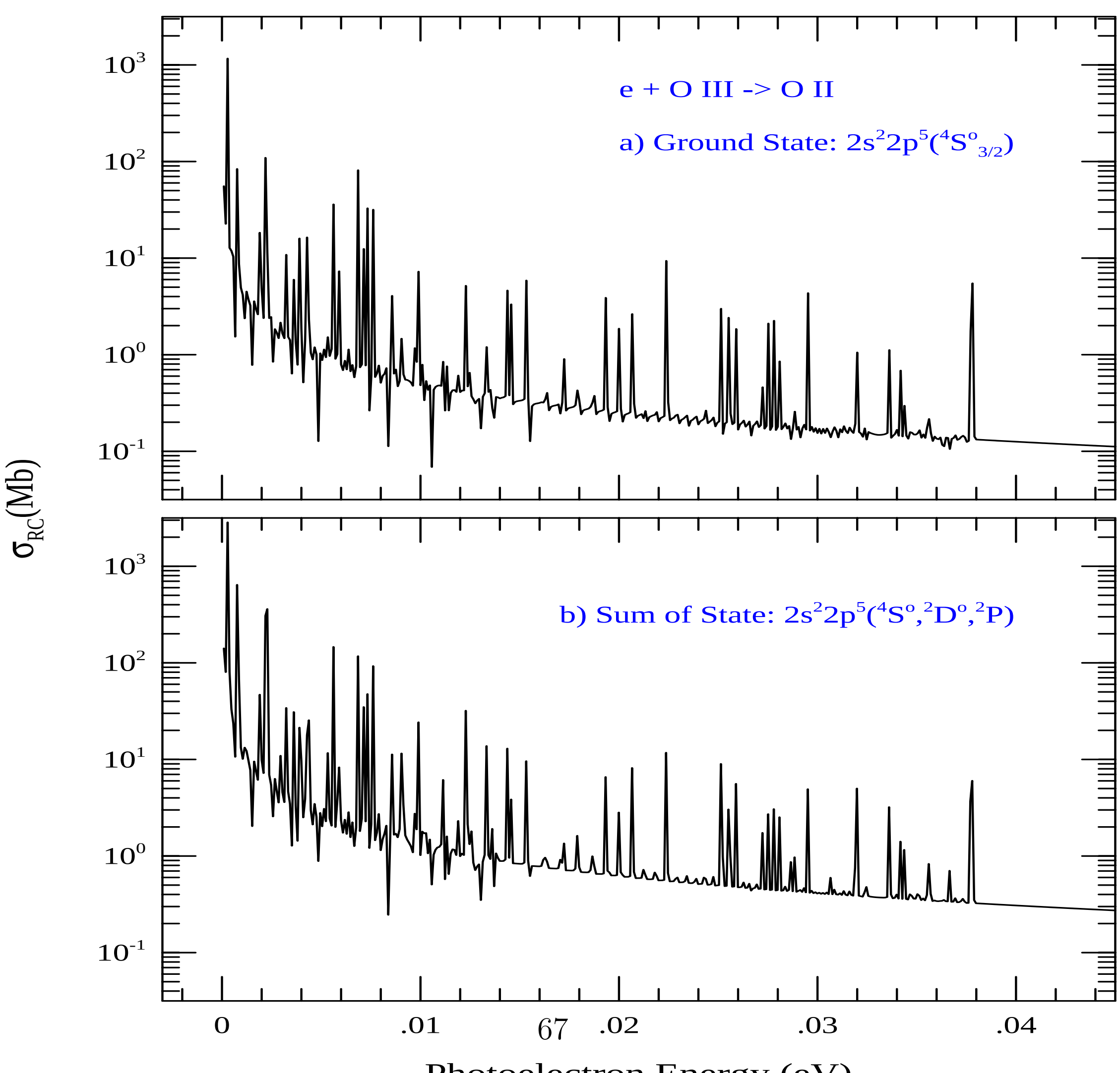


New RECOMBINATION CROSS SECTION AT LOW T: O II

(Nahar et al. 2010)

- Recombination cross section σ_{RC} show many resonances at very low energy
- Recombination rate from these will increase the recombination rate
- Higher recombination rate will decrease the oxygen abundance and hence will resolve or narrow down the existing gap in nebular problem

Recombination Cross Sections of O II

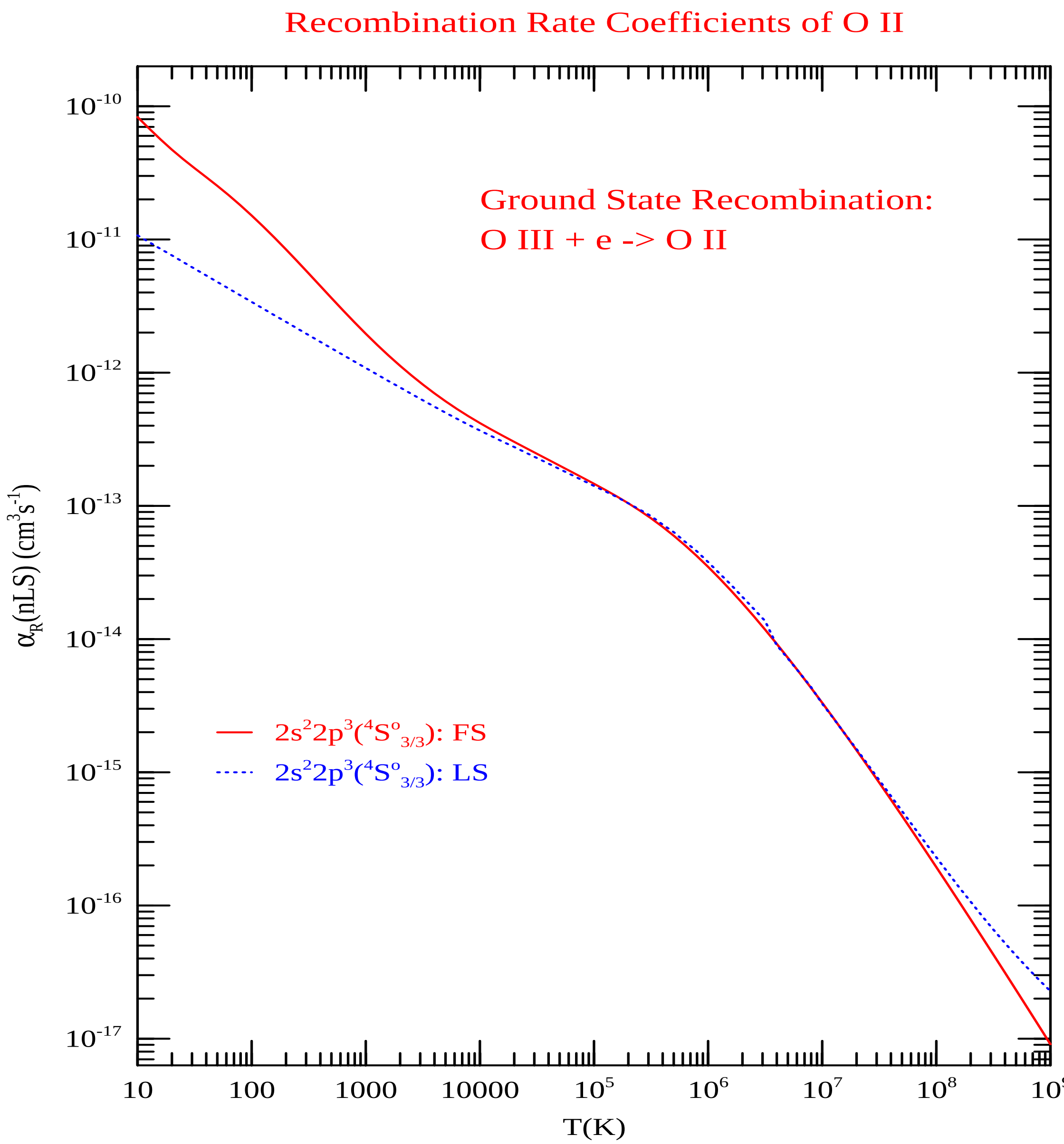


O II: Ground State RECOMBINATION (RR+DR):

• Fig: Recombination rate coefficients (RRC) α_{RC}(T) for the ground state

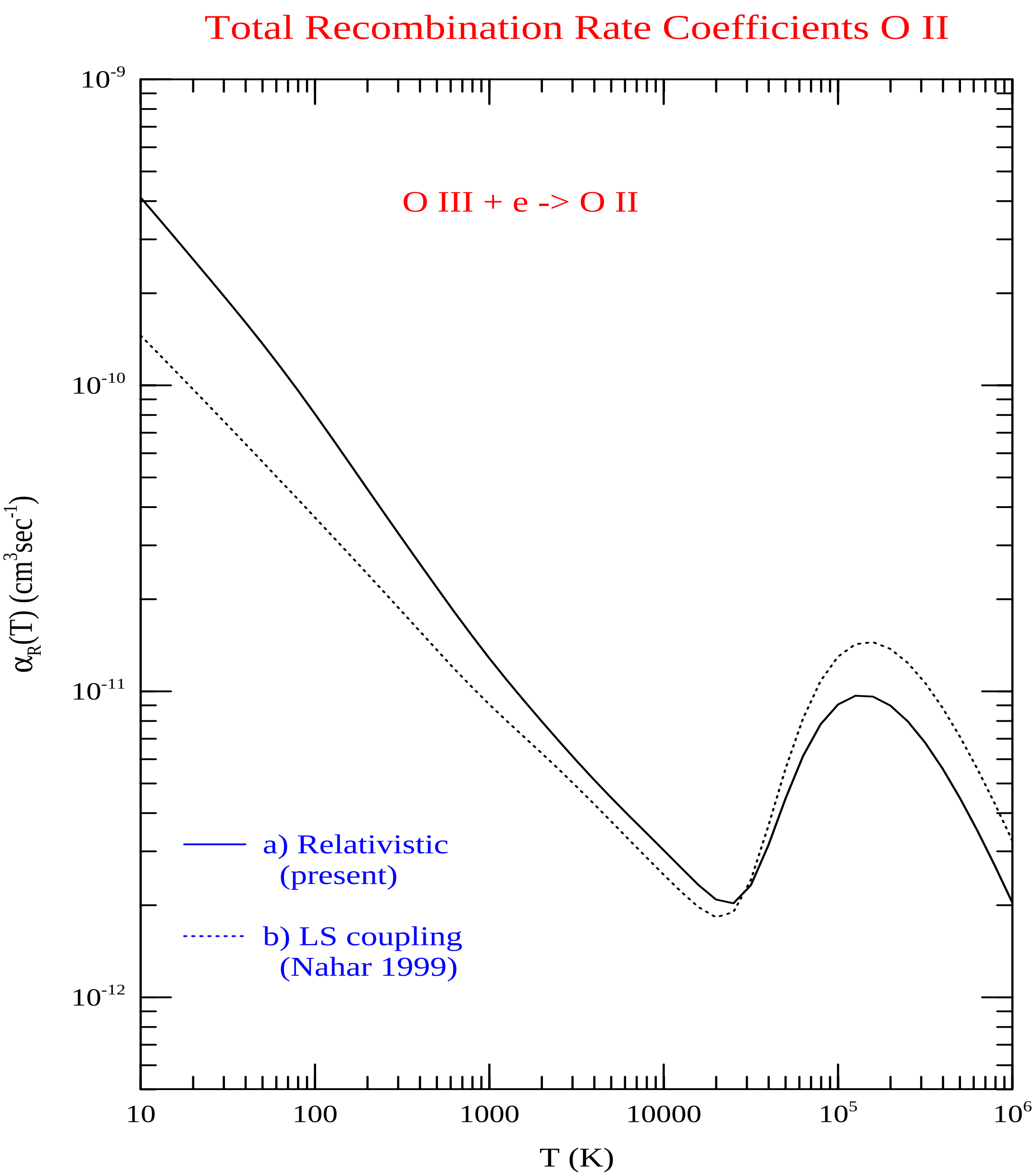
• Fine structure effects have increased RRC considerably at low temperatre

• This indicates lower abundance of oxygen

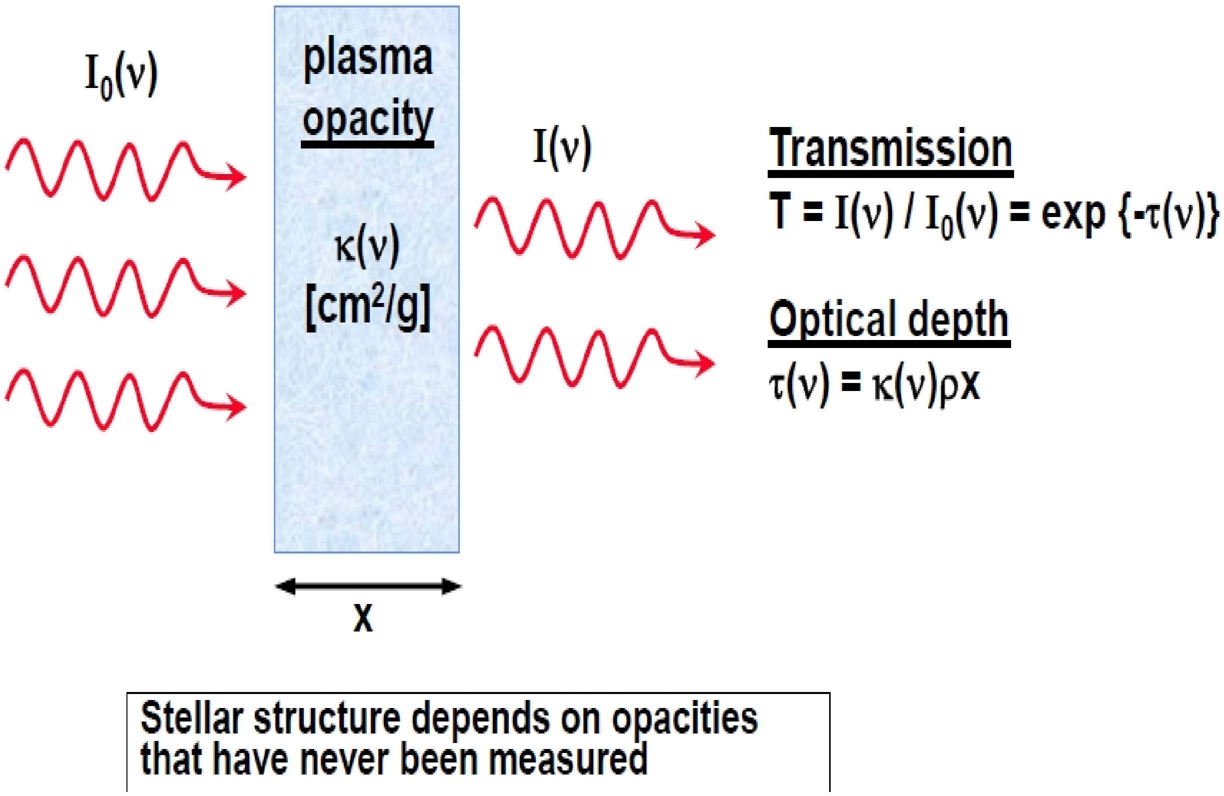


O II: TOTAL RECOMBINATION (RR+DR):

- **Fig: Total recombination rate coefficients (RRC) α_{RC}(T)**
- **Fine structure effects have increased RRC considerably, by 2.8 times around 10 K and 2.2 at 100 K,**
- **The high temperature DR peak has been reduced some. The reason could be some radiation damping effect included in the present work. The resolution of the narrow fine structure resonances could also affect the decrease.**



PLASMA OPACITY



- Opacity is a fundamental quantity for plasmas - it determines radiation transport in plasmas
- Opacity is the resultant effect of repeated absorption and emission of the propagating radiation by the constituent plasma elements.
- Microscopically opacity depends on two radiative processes: i) photo-excitation (bound-bound transition) & ii) photoionization (bound-free transition)
- The total $\kappa(\nu)$ is obtained from summed contributions of all possible transitions from all ionization stages of all elements in the source.
- Calculation of accurate parameters for such a large number of transitions has been the main problem for obtaining accurate opacities.

The OPACITY Project & The IRON Project

AIM: Accurate Study of Atoms & Ions, Applications to Astronomy

• International Collaborations: France, Germany, U.K., U.S., Venezuela, Canada, Belgium

• Earlier opacities were incorrect by factors of 2 to 5 → inaccurate stellar models → initiation of the Opacity Project in 1981

•THE OPACITY PROJECT - OP (1981 - 2006):
• Studied radiative atomic processes for (E, f, $\sigma_{\rm PI}$)
• Elements: H to Fe
• Calculated opacities of astrophysical plasmas

• THE IRON PROJECT - IP (1993 -): collisional & radiative processes of Fe & Fe peak elements

• RMAX: Under IP, study X-ray atomic astrophysics

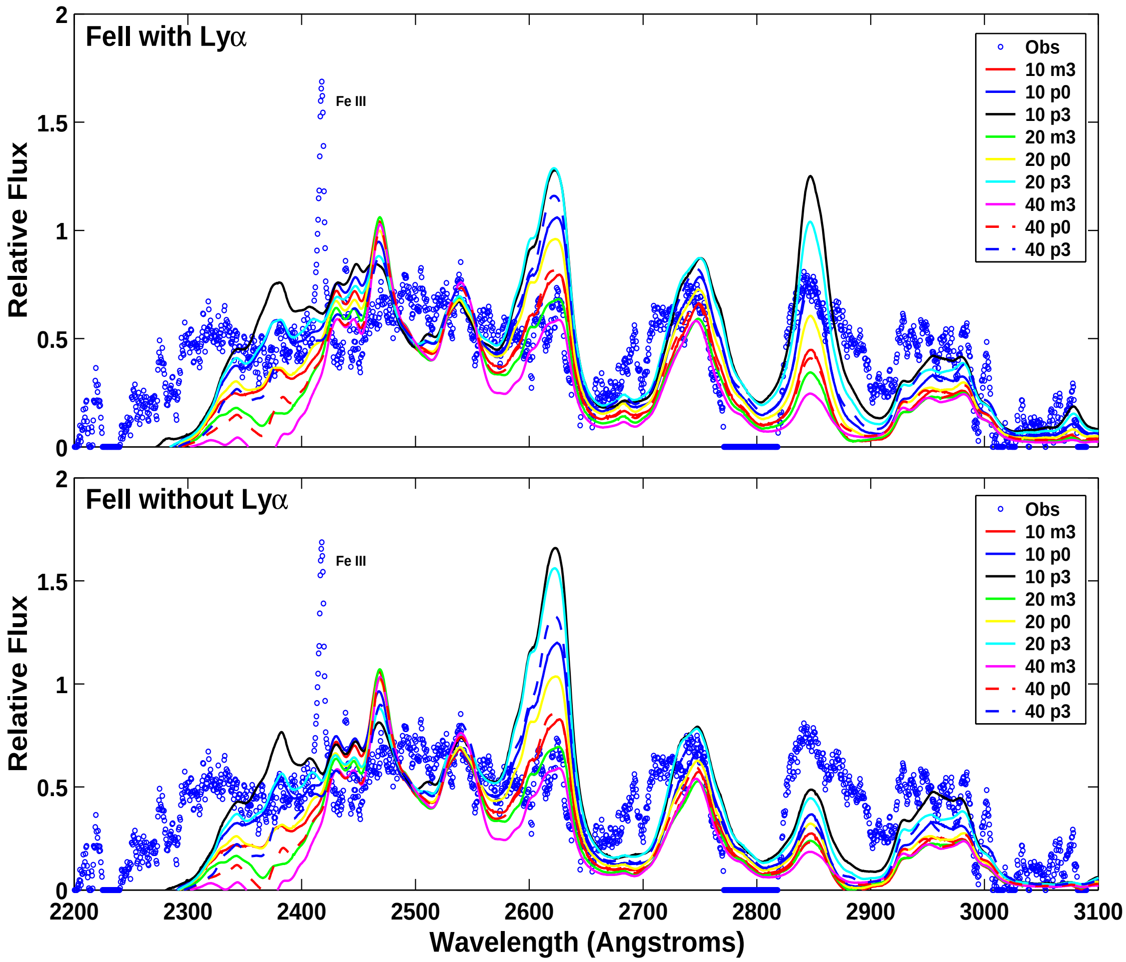
• Atomic & Opacity Databases (from OP & IP)

• TOPbase (OP) at CDS:
http://vizier.u-strasbg.fr/topbase/topbase.html
• TIPbase (IP) at CDS:
http://cdsweb.u-strasbg.fr/tipbase/home.html
• OPserver for opacities at the OSC: http://opacities.osc.edu/
• Latest radiative data at NORAD-Atomic-Data at OSU:
http://www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/index.html

ACHIEVEMENTS OF THE OP & THE IP

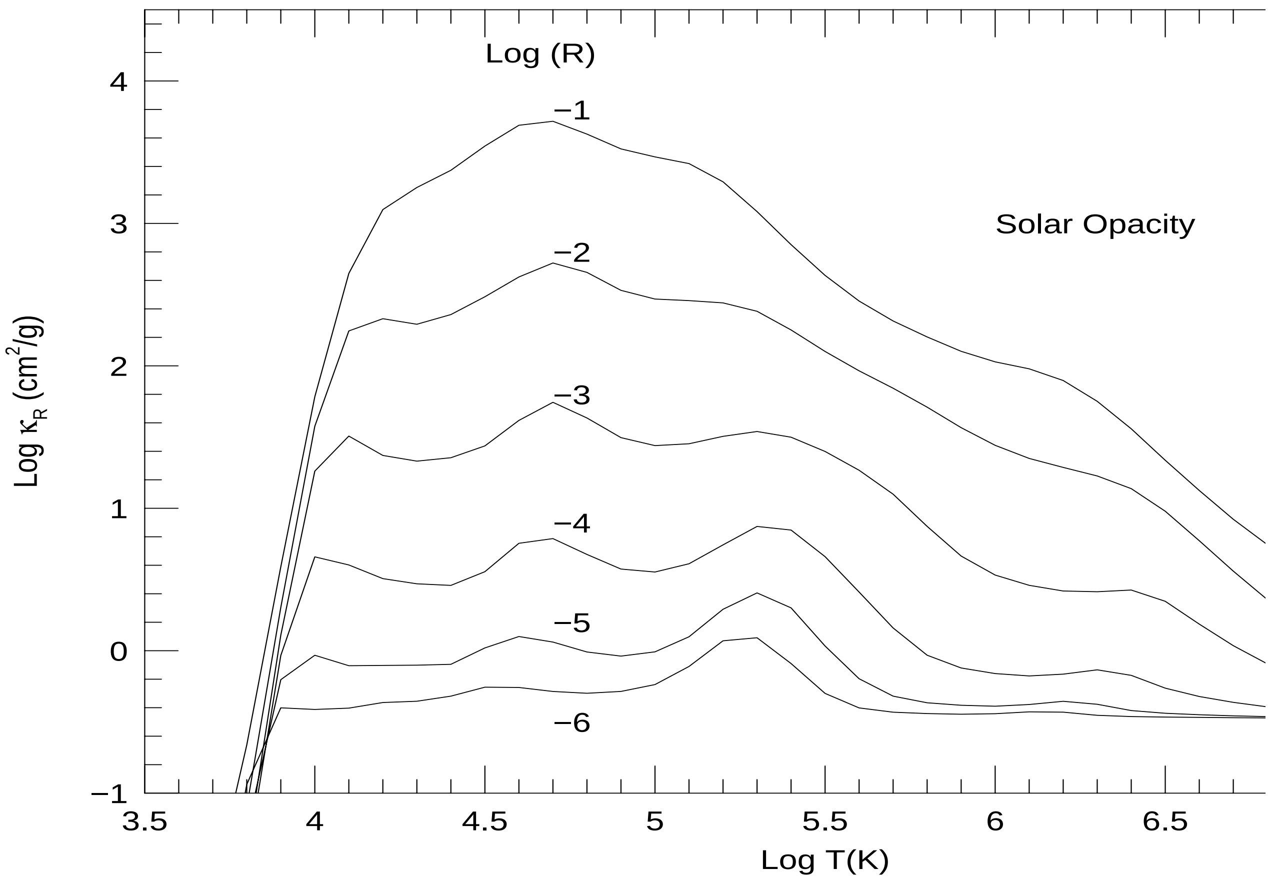
- The first detailed study of the atomic processes for most of the atoms and ions
- Found new features in photoionization cross sections
- OP opacities agreed with those computed under the OPAL, and both solved the outstanding problem on pulsations of cepheids
- Results from the OP and the IP continue to solve many outstanding problems, e.g., spectral analysis of blackhole environment, abundances of elements, opacities in astrophysical plasmas, dark matter
- HOWEVER, these are not complete and sufficiently accurate enough to solve all astrophysical problems

Observation & Modeling: Emission spectra of Fe I - III in active galaxy 1 Zwicky 1
(Sigut, Pradhan, Nahar 2004)



- Blue - Observation; Curves - Various Models with 1000 energy levels, millions of transitions
- With (top) and without (bottom) Lyman-alpha fluorescent excitation of Fe II by recombining H-atoms. The models reproduce many of the observed features, but discrepancies indicate need for more accurate calculations.

SOLAR OPACITY
(Seaton et al 1993)

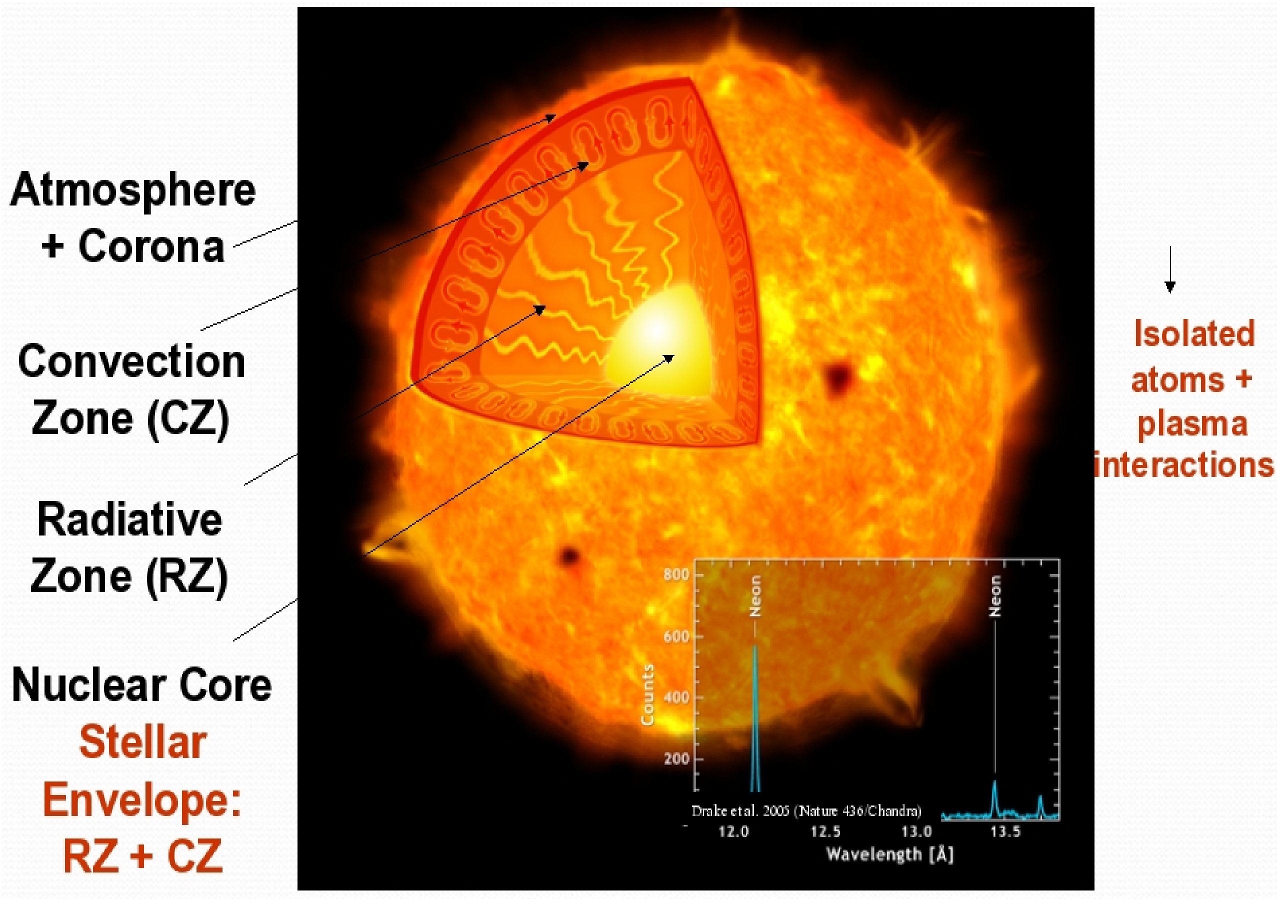


• The Rosseland mean opacity κ_R in several temeprature-density regimes throughout the solar interior characterized by the parameter
$\mathbf{R = \rho(g/cc)/T_6^3,\ \ T_6 = T * 10^{-6}}$

• For the sun, **-6 $\leq$ R $\leq$ -1**

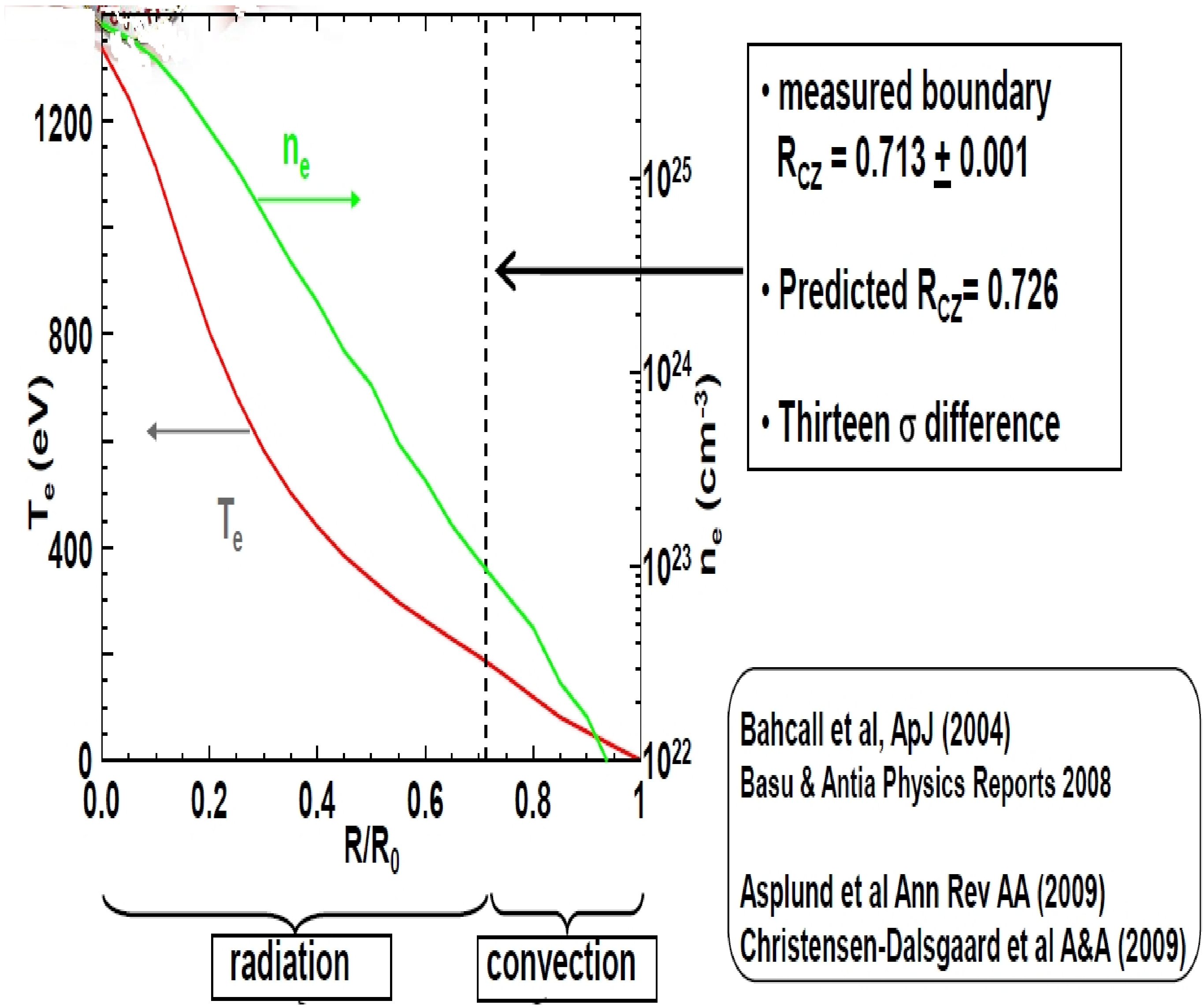
• The bumps and kinks in the curves represent higher opacities due to excitation/ionization of different atomic species at those temperatures (H-, He-, Z-, and inner-shell bumps)

SOLAR OPACITY & ABUNDANCES

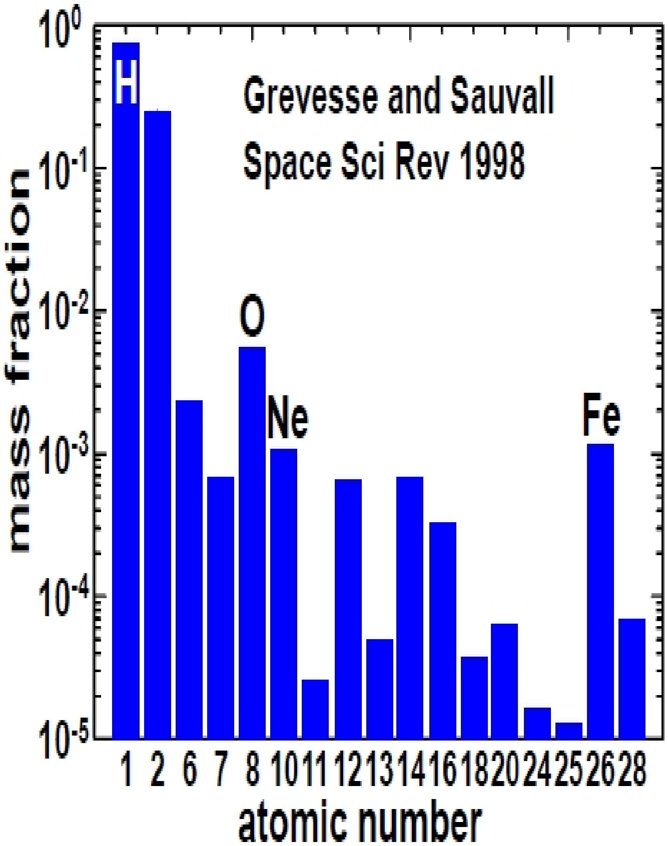


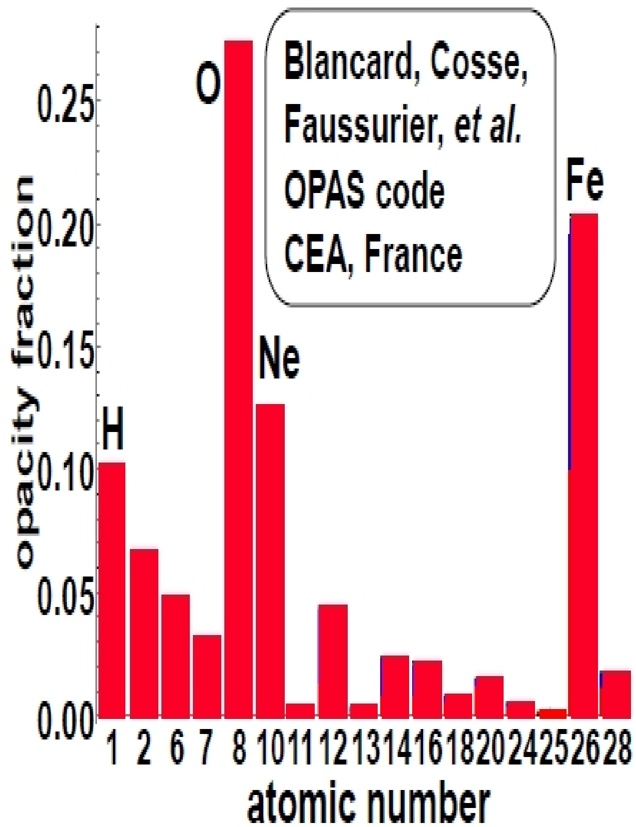
- At the convection zone boundary, R_{CZ}, the temperature T_e ~193 eV (2 MK), density $n_e \sim 10^{23}/cm^3$ (HED - High Energy Density)
- HED condition → important elements: O, Ne, especially Fe (Fe XVII-XIX)
- Recent determination from measurements and 3D hydro NLTE models: 30-40% lower abundances of C, N, O, Ne, Ar than the standard abundances
- Optical depth in the sun depends on the interior opacity (κ) through elemental abundances
- The opacity can determine R_{CZ}

DISCREPANCY IN SOLAR RADIAIVE AND CONVECTION ZONES BOUNDARY (R_{CZ})



- The measured boundary, from helioseismology, of R_{CZ} is 0.713
- The calculated R_{CZ} is 0.726 - large





- oxygen, neon, and iron are most important at the CZ base
- The importance of any single element is diluted by the mixture

<u>Example:</u>

Changing Fe opacity by 1.5x causes ~11% change in total mean opacity

Determination of OPACITY: RADIATIVE ATOMIC PROCESSES

1. Photoexcitation - Photon absorption for a bound-bound transition

$$\mathbf{X^{+Z} + h\nu \rightarrow X^{+Z*}}$$

- **Oscillator Strength (f_{ij})**

Monochromatic opacity (κ_ν) depends on f_{ij}

$$\kappa_\nu(\mathbf{i} \rightarrow \mathbf{j}) = \frac{\pi \mathbf{e^2}}{\mathbf{mc}} \mathbf{N_i f_{ij}} \phi_\nu \tag{32}$$

N_i = ion density in state i, ϕ_ν = profile factor

- **κ inclues ~100M transitions of mid-Z elements**

2. Photoionization - Photon absorption for a bound-free transition: Direct -

$$\mathbf{X^{+Z} + h\nu \rightarrow X^{+Z+1} + \ e}$$

3. Autoionization (AI) in photoionization process :

$$\mathbf{e + X^{+Z} \rightleftharpoons (X^{+Z-1})^{**}} \rightleftharpoons \begin{cases} e + X^{+Z} & \text{AI} \\ X^{+Z-1} + h\nu & \text{DR} \end{cases}$$

Doubly excited "autoionizing state" $\rightarrow$ resonance

- **Photoionization Cross Sections (σ_{PI})**

κ_ν **depends on** σ_{PI}

$$\kappa_\nu = \mathbf{N_i}\sigma_{\mathbf{PI}}(\nu) \tag{33}$$

<u>κ_ν **depends also on processes**</u>

- **Inverse Bremstrahlung free-free Scattering:**

$$\mathbf{h}\nu + [\mathbf{X_1^+} + \mathbf{e}(\epsilon)] \rightarrow \mathbf{X_2^+} + \mathbf{e}(\epsilon'), \tag{34}$$

Cross section - from the elastic scattering matrix elements for electron impact excitation. An approximate expression for the free-free opacity is

$$\kappa_\nu^{\mathbf{ff}}(\mathbf{1},\mathbf{2}) = \mathbf{3.7} \times \mathbf{10^8}\mathbf{N_e}\mathbf{N_i}\mathbf{g_{ff}}\frac{\mathbf{Z^2}}{\mathbf{T^{1/2}}\nu^{\mathbf{3}}} \tag{35}$$

where g_{ff} **is a Gaunt factor**

- **Photon-Electron scattering:**

a) Thomson scattering when the electron is free

$$\kappa(\mathbf{sc}) = \mathbf{N_e}\sigma_{\mathbf{Th}} = \mathbf{N_e}\frac{\mathbf{8}\pi\mathbf{e^4}}{\mathbf{3m^2c^4}} = \mathbf{6.65} \times \mathbf{10^{-25}\ cm^2/g} \tag{36}$$

b) Rayleigh scattering when the electron is bound

$$\kappa_\nu^{\mathbf{R}} = \mathbf{n_i}\sigma_\nu^{\mathbf{R}} \approx \mathbf{n_i}\mathbf{f_t}\ \sigma^{\mathbf{Th}}\left(\frac{\nu}{\nu_{\mathbf{I}}}\right)^{\mathbf{4}} \tag{37}$$

$h\nu_I$ **= binding energy,** f_t **= total oscillator strength associated with the bound electron.**

The total monochromatic opacity is then given by

$$\kappa_\nu = \kappa_\nu(\mathbf{bb}) + \kappa_\nu(\mathbf{bf}) + \kappa_\nu(\mathbf{ff}) + \kappa_\nu(\mathbf{sc}) \tag{38}$$

Mean Opacity: The equation of state (EOS)

- Requires ionization fractions and level populations of each ion of an element in levels with non-negligible occupation probability
- Saha equation - number density for ionization state $n_S(X^i)$ of excited ion X^i at thermal equilibrium as

$$\mathbf{n_S(X^i) = \frac{g_i}{2g_s} \frac{h^3}{(2\pi m_e kT)^{\frac{3}{2}}} \exp\left(-\frac{E_{gi}}{kT}\right) n_e n(X^+)} \quad (39)$$

In LTE the level populations are given by the Boltzmann equation,

$$\mathbf{\frac{N_i}{N_j} = \frac{g_i}{g_j}\ e^{-h\nu/kT}} \quad (40)$$

The combination of the Saha-Boltzmann equations specify the Equation-of-State (EOS), in LTE

$$\mathbf{N_{ij} = \frac{N_j g_{ij} e^{-E_{ij}/kT}}{U_j}} \quad (41)$$

g_{ij}= statistical factor of level i of ionization state j, the partition function is

$$\mathbf{U_j = \sum_i g_{ij} e^{(-E_{ij}/kT)}} \quad (42)$$

There are several ways to modify the Saha-Boltzmann equations to incorporate the effect of plasma interactions into the EOS. The modified density function is then

$$\mathbf{N_{ij} = \frac{N_j g_{ij} w_{ij} e^{-E_{ij}/kT}}{U_j},} \tag{43}$$

where the partition function is

$$\mathbf{U_j = \sum_i g_{ij} w_{ij} e^{(-E_{ij}/kT)}} \tag{44}$$

Rosseland mean $\kappa_R(T,\rho)$:

Harmonic mean opacity averaged over the Planck function, ρ is the mass density (g/cc),

$$\frac{\mathbf{1}}{\kappa_{\mathbf{R}}} = \frac{\int_0^\infty \frac{1}{\kappa_\nu}\mathbf{g(u)du}}{\int_0^\infty \mathbf{g(u)du}},$$

where g(u) is the Planck weighting function

$$\mathbf{g(u) = \frac{15}{4\pi^4}\frac{u^4 e^{-u}}{(1-e^{-u})^2}, \quad u = \frac{h\nu}{kT}}$$

g(u), for an astrophysical state is calculated with different chemical compositions H (X), He (Y) and metals (Z), such that

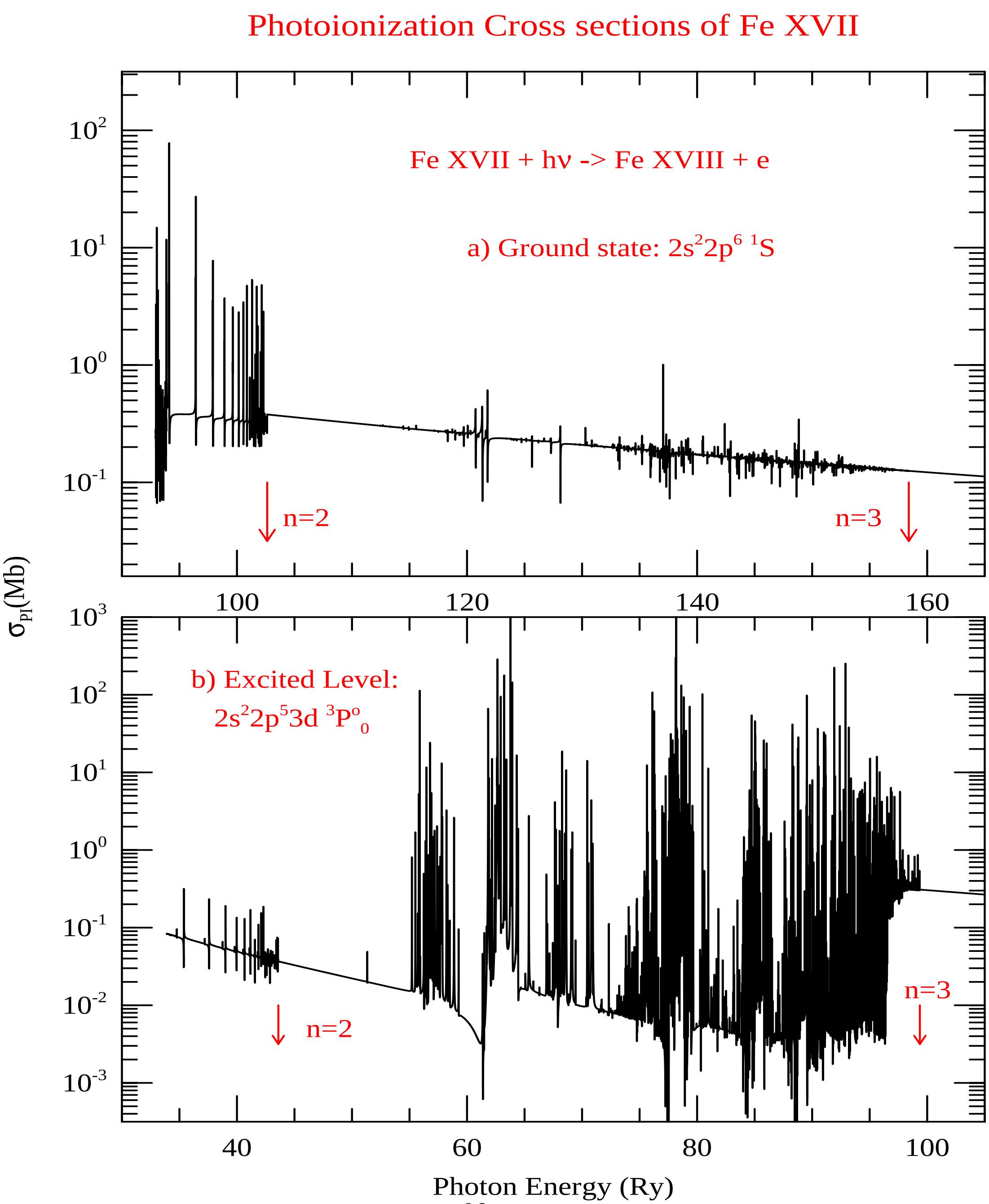
$$\mathbf{X + Y + Z = 1}$$

Solar abundaces: X=0.7, Y=0.28, Z=0.02

PHOTOIONIZATION CROSS SECTION: Fe XVII

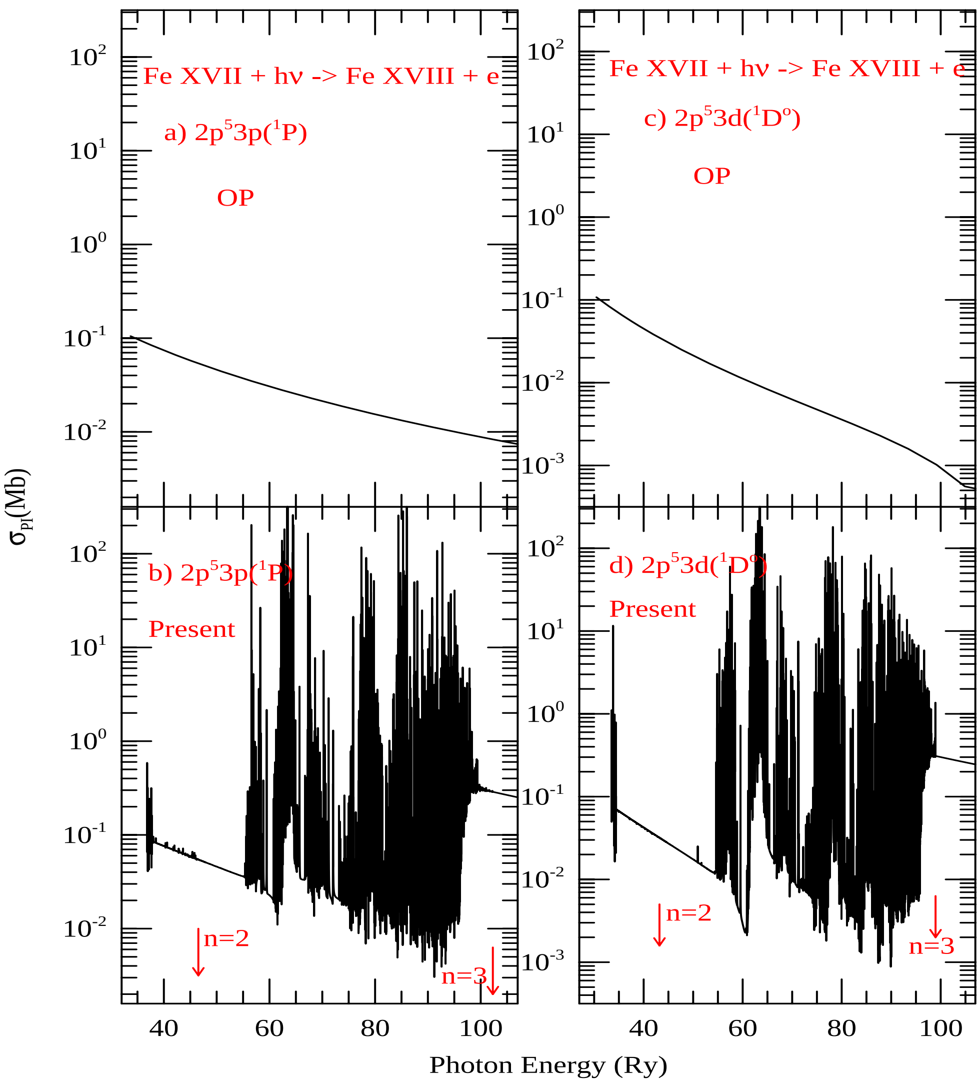
- **Top: Ground level: n=2 resonances are important**
- **Bottom: Excited level: n=3 resonances are important**

Arrows point energy limits of n=2 & 3 core states



COMPARISON OF PHOTOIONIZATION CROSS SECTIONS

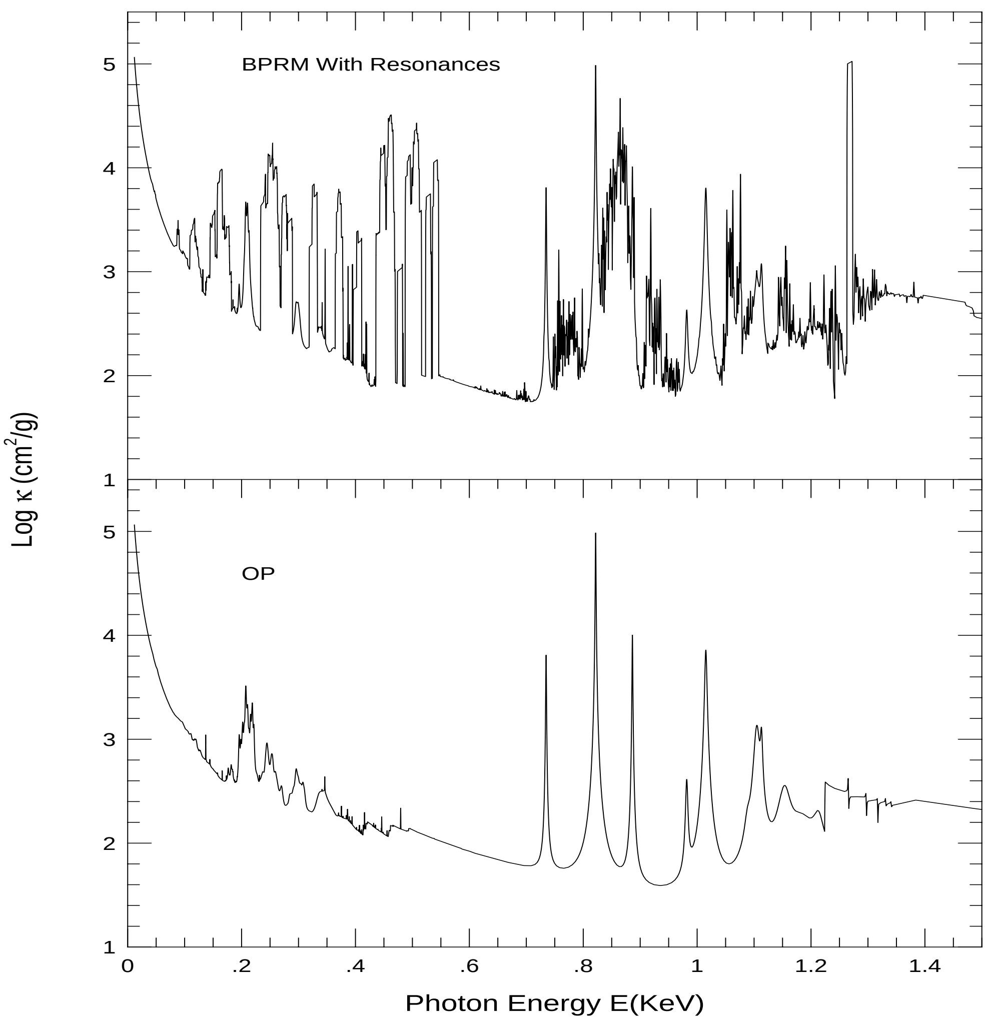
- **Photoionization cross sections of Fe XVII: (a,b) level $2p^53p^1P$ & (c,d) level $2p^53d(^1D^o)$**
- **Present σ_{PI} (Nahar et al 2010) is much more highly resolved than those given by the Opacity Project (OP). Without inclusion of n=3 core states, σ_{PI} is considerably underestimated**



MONOCHROMATIC OPACITY OF Fe XVII

(Nahar et al. 2011)

- **Monochromatic opacity** κ **of Fe XVII at temperature T = 2.24** $\times 10^6$ **K and electron density** $N_e = 10^{23}$ **cm**$^{-3}$**, corresponding to the base of the solar convection zone where the ion is the largest contributor to opacity.**



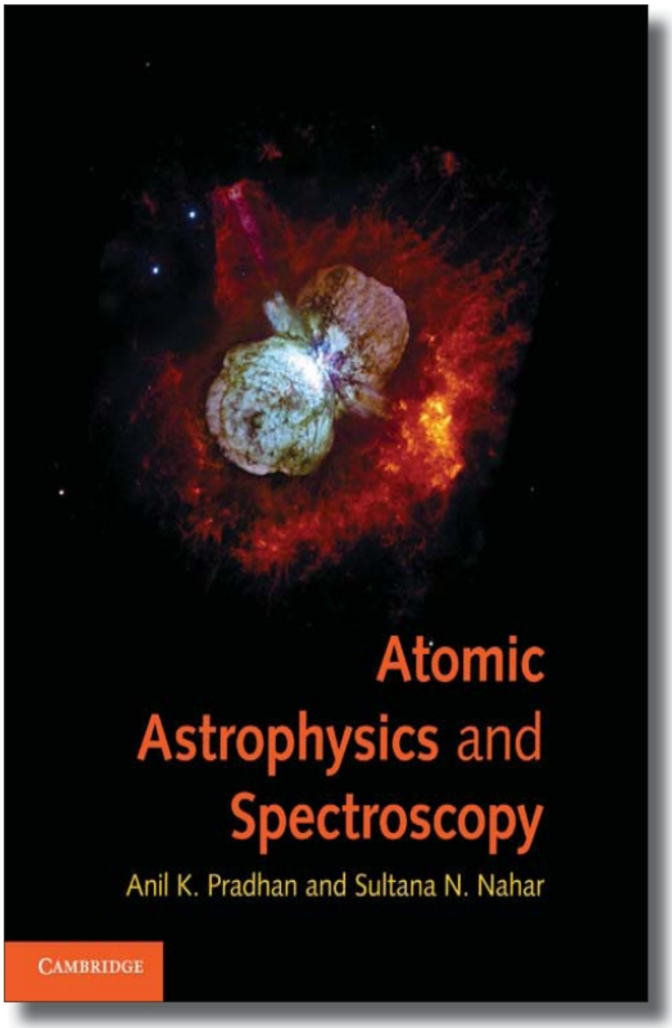
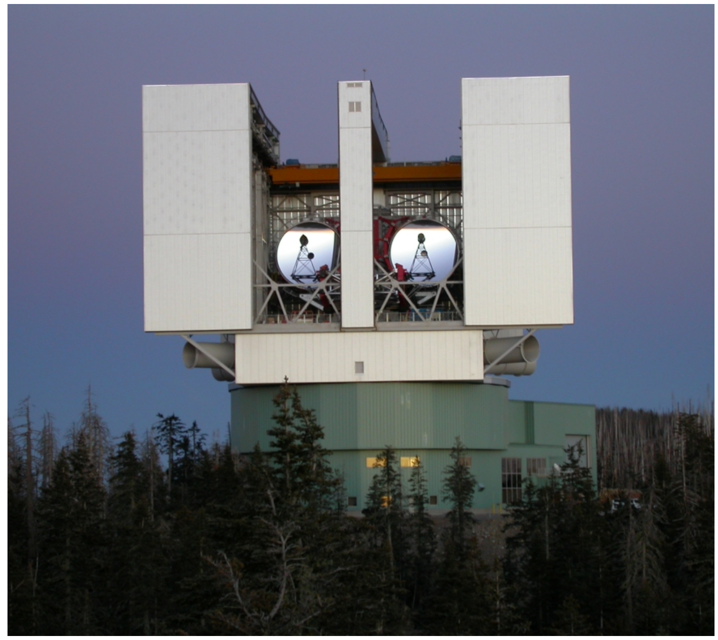


Table of Contents

T · H · E OHIO STATE UNIVERSITY

and Arizona, Germany, Italy

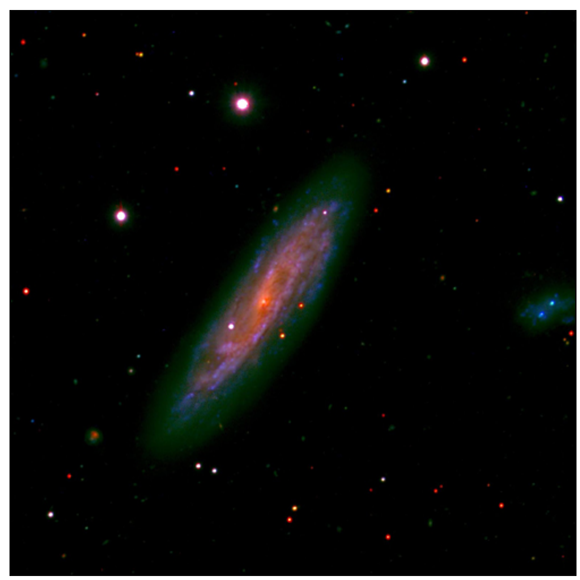


Large Binocular Telescope (LBT)

Largest Telescope: 8.4m Mirrors (11.8m), NIR-Optica

Galaxy: M101

Galaxy: M51



Galaxy: NGC 2770