NIST National Institute of Standards and Technology U.S. Department of Commerce

Atomic collisions

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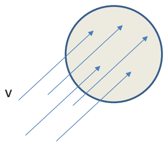
Collisions in plasmas

- More than one particle: collisions!
- Elastic, inelastic



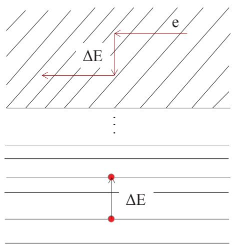
Number of collisions per unit time:

n[1/cm³]*v[cm/s]*Area[cm²] ~ [1/s]

Equilibrium plasma: $T_e = T_A$

$$\frac{v_e}{v_A} = \sqrt{\frac{M}{m_e}}$$

Collision (excitation)



Main binary quantity: cross section **σ(E)** [**cm²**]

Effective area for a particular process

$$\sigma(E) = \int \left| f(E,\theta,\varphi) \right|^2 d\Omega$$

f is the scattering amplitude

Process rate in plasmas:

$$R[s^{-1}] = N\langle\sigma v\rangle \equiv N \int_{E_{min}}^{E_{max}} \sigma(E)\cdot v \cdot f(E)\,dE$$

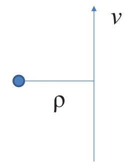
rate coefficient

Basic Parameters

- Cross sections are probabilities
  - Classically: $\sigma(\Delta E, E) = \int_0^\infty P(\Delta E, E, \rho)\cdot 2\pi\rho\, d\rho$
- Typical values for atomic cross sections
  - $a_0 \sim 5\cdot 10^{-9}$ cm $\Rightarrow \pi a_0^2 \sim 10^{-16}$ cm²
- Collision strength Ω (dimensionless, *on the order of unity*):

$$\sigma_{ij}(E) = \pi a_0^2 \frac{Ry}{g_j E}\Omega_{ij}(E)$$

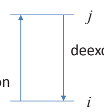
  - Ratio of cross section to the de Broglie wavelength squared
  - Symmetric w/r to initial and final states



Direct and inverse

- Quantum mechanics tells us that characteristics of direct and inverse processes are related

ΔE is the excitation threshold



$$\Omega_{ij}(E+\Delta E) = \Omega_{ji}(E)$$

Klein-Rosseland formula:

$$g_i(E+\Delta E)\sigma_{exc}(E+\Delta E) = g_j E \sigma_{dxc}(E)$$

$A(i) + e \leftrightarrow A(j) + e$

Rates: $g_i\langle\sigma v\rangle_{exc} = g_j\langle\sigma v\rangle_{dxc}\cdot e^{-\Delta E/T}$

Milne formula for photoionization/photorecombination: $\hbar\omega = E + I_Z$

$A + h\nu \leftrightarrow A^+ + e$

$$g_Z\sigma_{ph}(\hbar\omega) = \frac{2mc^2}{\hbar^2\omega^2}g_{Z+1}\sigma_{rr}(E)$$

Types of transitions for excitation

Examples in He I:

- Optically(dipole)-allowed
  - P·P' = -1 (different parity)
  - |Δ*l*| = 1
  - ΔS = 0
  - σ(E→∞) ~ ln(E)/E

$1s^2\ ^1S \rightarrow 1s2p\ ^1P$
$1s2p\ ^3P \rightarrow 1s4d\ ^3D$

- Optically(dipole)-forbidden
  - ΔS = 0
  - σ(E→∞) ~ 1/E

$1s2s\ ^1S \rightarrow 1s3s\ ^1S$
$1s2s\ ^3S \rightarrow 1s4d\ ^3D$

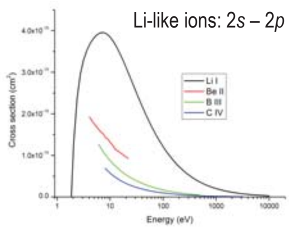
- Spin-forbidden (EXCHANGE!)
  - ΔS ≠ 0
  - σ(E→∞) ~ 1/E³

$1s^2\ ^1S \rightarrow 1s2p\ ^3P$
$1s2p\ ^3P \rightarrow 1s4d\ ^1D$

Order of cross sections

- *General* order
  - *optically allowed > optically forbidden > spin forbidden*
- OA: long-distance, similar to E1 radiative transitions
- The larger Δ*l*, the smaller cross section

Li-like ions: 2*s* – 2*p* excitation



Excitation cross sections for ions are **NOT** zero at the threshold

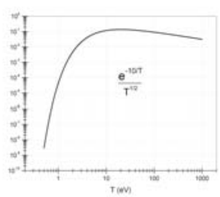
From cross sections to rates

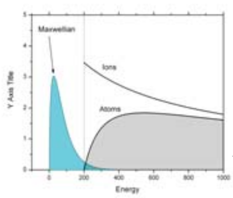
Rate coefficients for an arbitrary energy distribution function

$$\langle v\sigma\rangle = \int_{E_{min}}^{E_{max}} v\cdot\sigma(E)\cdot f(E)\,dE \xrightarrow{Maxw} \left(\frac{8}{\pi m T^3}\right)^{1/2}\int_{\Delta E}^{\infty} E\cdot\sigma(E)\cdot e^{-E/T}\,dE$$

For σ(E) = A/E: $\langle v\sigma\rangle \propto \frac{e^{-\frac{\Delta E}{T}}}{\sqrt{T}}$

Often only threshold is important:





Effective collision strength:

$$\gamma(T_e) = \frac{1}{T_e}\int \Omega(E)\exp\left(-\frac{E}{T_e}\right)dE$$

$$R_{ji}(T_e) = \left(\frac{8}{\pi m T_e}\right)^{1/2}\frac{\pi a_0^2}{g_i}Ry\cdot\gamma_{ji}(T_e)$$

van Regemorter-Seaton formula

- Optically-allowed excitations

$X \equiv E/\Delta E_{ij}$ $\quad \sigma_{ij}(E) = \pi a_0^2 \frac{8\pi}{\sqrt{3}} \left(\frac{Ry}{\Delta E_{ij}} \right)^2 \frac{g(X)}{X} f_{ij}$

Gaunt factor

oscillator strength

$$X \to \infty : g(X) \approx \frac{\sqrt{3}}{2\pi} \ln(X) \qquad \sigma(E) \approx \frac{6.51 \cdot 10^{-14}}{(\Delta E[eV])^2} \frac{\ln(X)}{X} f_{ij} \quad [cm^{-2}]$$

"*Recommended*" Gaunt factors:

Atoms:

$$g(\Delta n = 0, X) = \left(0.33 - \frac{0.3}{X} + \frac{0.08}{X^2}\right) \ln(X)$$

$$g(\Delta n \neq 0, X) = \left(\frac{\sqrt{3}}{2\pi} - \frac{0.18}{X}\right) \ln(X)$$

Ions:

$$g(\Delta n = 0, X) = \left(1 - \frac{1}{Z}\right)\left(0.7 + \frac{1}{n}\right)\left[0.6 + \frac{\sqrt{3}}{2\pi}\ln(X)\right]$$

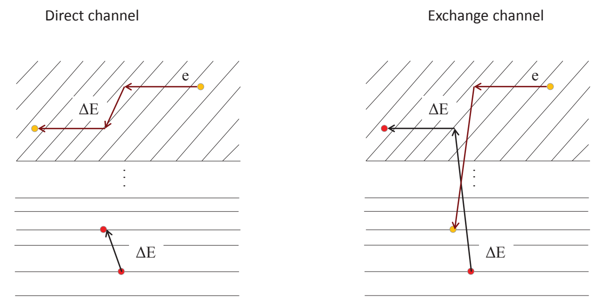
$$g(\Delta n \neq 0, X) = 0.2 (X < 2), \frac{\sqrt{3}}{2\pi} \ln(X) \ for \ X \geq 2$$

Scaling of Excitations

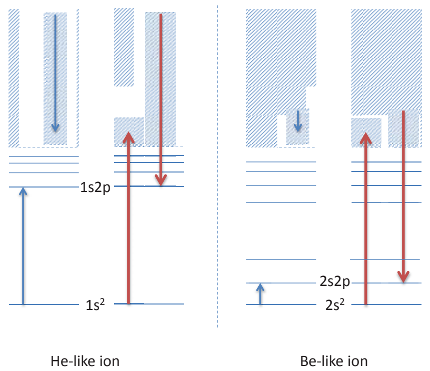
$$\sigma_{ij}(E) \propto \frac{f}{\Delta E_{ij}^2}$$

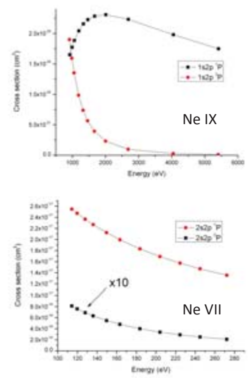
- n-scaling
  - Δn=1
    - f~n, $\Delta E \sim n^{-3}$, ~~$\sigma \sim n^7$~~, **$\sigma \sim n^4$**
  - Into high n
    - $f \sim n^{-3}$, $\Delta E \sim n^0$, **$\sigma \sim n^{-3}$**
- Z-scaling
  - Δn=0
    - $f \sim Z^{-1}$, ΔE~Z, **$\sigma \sim Z^{-3}$, $\langle v\sigma \rangle \sim Z^{-2}$**
  - Δn≠0
    - $f \sim Z^0$, $\Delta E \sim Z^2$, **$\sigma \sim Z^{-4}$, $\langle v\sigma \rangle \sim Z^{-3}$**

Direct and Exchange

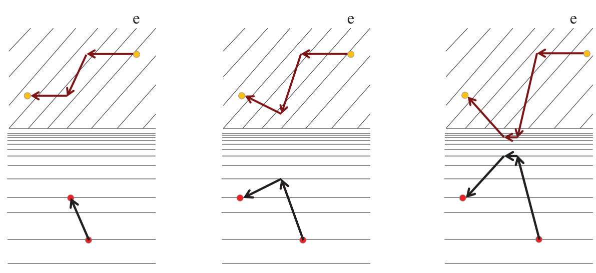


Direct and Exchange (cont'd)



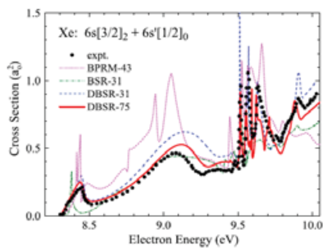


Resonances in excitation

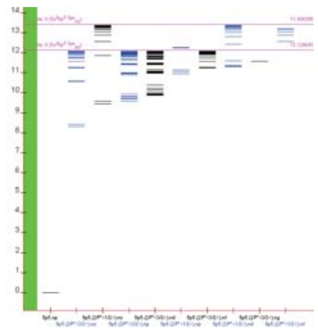


Direct excitation Intermediate states Intermediate AI states

Experiment vs theory



Zatsarinny and Bartschat, 2010

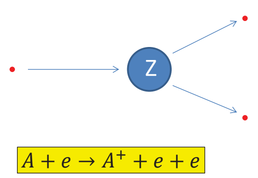


NIST ASD Grotrian Diagram

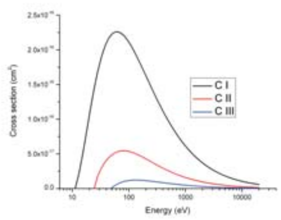
Collisional Methods and Codes

- Plane-wave Born
- Coulomb-Born (better for highly-charged ions)
- Distorted-wave method
- Close-coupling (CC) methods
  - Convergent CC (CCC)
  - R-matrix (with PS, Dirac, etc.)
  - B-splines
  - Time-Dependent CC
  - …
- Relativistic versions are available

Ionization cross sections



$A + e \to A^+ + e + e$



Lotz formula:

$$\sigma_{ion}(n,E) = 2.76 \pi a_0^2 \frac{Ry^2}{I_n} \frac{\ln(E/I_n)}{E} = 2.76 \pi a_0^2 \frac{n^4}{Z^4} \frac{\ln X}{X}$$

Same theoretical methods as for excitation: Born, Coulomb-Born, DW, CC, CCC, RMPS…

3-Body Recombination

$A + e \leftrightarrow A^{+} + e + e$

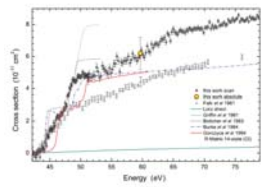
3-body rate coefficient $\alpha_{Z+1}(T_e)$ from ionization rate coefficient $S_Z(T_e)$:

$$\alpha_{Z+1}(T_e) = \frac{1}{2}\frac{g_Z}{g_{Z+1}}\left(\frac{2\pi\hbar^2}{m_e T_e}\right)^{3/2} exp\left[\frac{E_Z}{T_e}\right] S_Z(T_e)$$

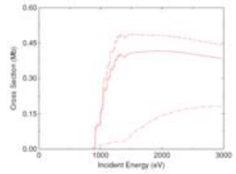
Rates from rate coefficients: $n_e S_Z(T_e)$ but $n_e^2 \alpha_{Z+1}(T_e)$

Likes high-n states; $\alpha(T_e) \sim 1/T_e^{9/2}$

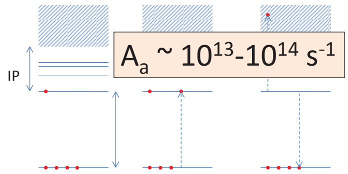
Excitation-Autoionization



$3p^6 3d$ Ti^{3+}: van Zoest et al, 2004



$3s^2 3p^6 3d^{10} 4s^2$ Xe^{24+}: Pindzola et al, 2011



When EA is important:

- few electrons on the outermost shell
- Mid-Z multielectron ions
- …but less important for higher Z (rad!)

EA in ionization cross sections is not required for detailed modeling with AI states!

Selection rules

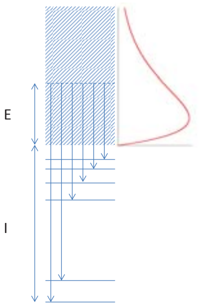
- Examples of AI states: $1s2s^2$, $1s^2 2pnl$ (high n)
- Same old rule: **before** = **after**
- $A^{**} \rightarrow A^{*} + \varepsilon l$
  - ***Exact***: $P_j = P_i$; $\Delta J = 0$
  - *Approximate* (LS coupling): $\Delta S = 0$, $\Delta L = 0$

LS selection rule violation

- $2p^2\ ^1S \rightarrow 1s + \varepsilon s$: *good*
- $2p^2\ ^1D \rightarrow 1s + \varepsilon d$: *good*

- $2p^2\ ^3P \rightarrow 1s + \varepsilon p$: *parity/L violation*!
  - BUT: $\Psi(2p^2\ ^3P_2) = \alpha\Psi(2p^2\ ^3P_2) + \beta\Psi(2p^2\ ^1D_2) + \ldots$
  - and $\Psi(2p^2\ ^3P_0) = \alpha'\Psi(2p^2\ ^3P_0) + \beta'\Psi(2p^2\ ^1S_0) + \ldots$
  - YET: $A_a(2p^2\ ^3P_1) \approx 0$

Radiative Recombination

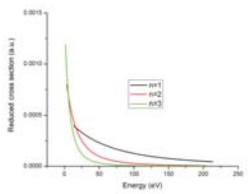


$A^{Z+} + e \rightarrow A^{(Z-1)} + h\nu$ (inverse of photoionization)

$h\nu = E + I$

Semiclassical Kramers cross section: $\sigma_{Kr}(E) = \frac{64\alpha}{3\sqrt{3}}\frac{Z^4}{n^5}\left(\frac{Ry}{E+I}\right)^3 \pi a_0^2$

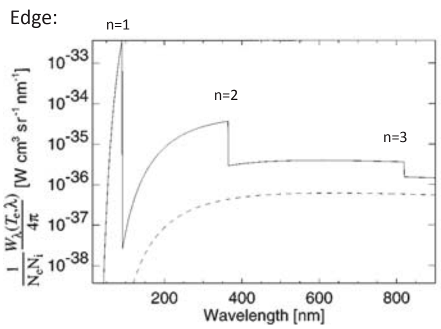
Quantummechanical cross section: $\sigma_{ph}(E) = \sigma_{Kr}(E)\cdot G_n^{bf}(E)$

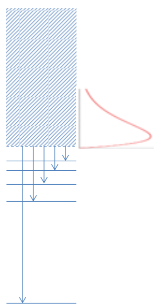


Cross section Z-scaling:

$$\sigma\left(\frac{h\nu}{Z^2}\right) \propto \frac{1}{Z^2}$$

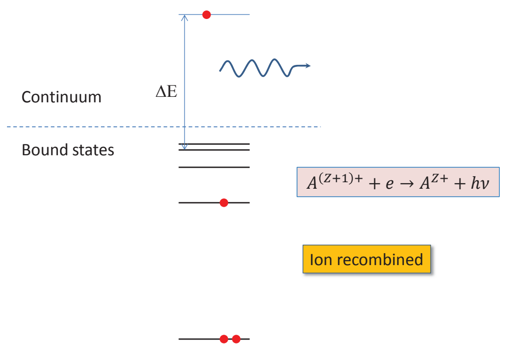
FF+BF at Alcator C-mod: 1 eV, H



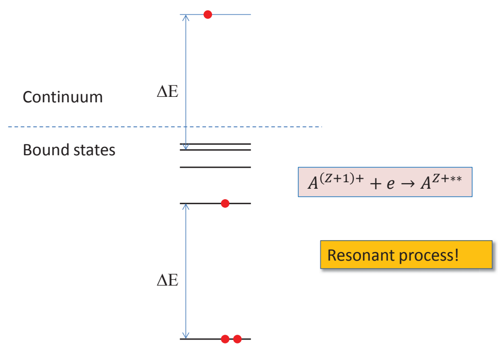


Lumma et al (1997)

Radiative recombination



DR step 1: dielectronic capture



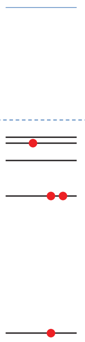
Dielectronic capture + autoionization = no recombination

DC and AI are direct and inverse

Continuum

Bound states

$A^{(Z+1)+} + e \rightarrow A^{Z+**} \rightarrow A^{(Z+1)+} + e$



DR step 2: radiative stabilization

$\Delta E(\Delta n = 0) \propto z$
$\Delta E(\Delta n \neq 0) \sim 13.6eV \cdot z^2$

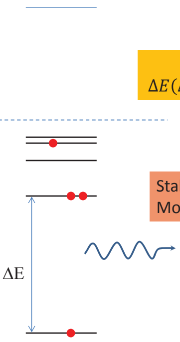
Continuum

Bound states

Stabilizing transition: Mostly x-rays

$A^{(Z+1)+} + e \rightarrow A^{Z+**} \rightarrow A^{Z+*} + h\nu$

ΔE



Dielectronic Recombination

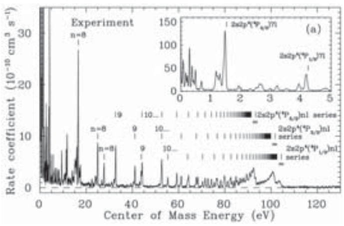
DC AI
$A^+ + e \rightarrow A^{**} \rightarrow A^+ + e$
↓ RS
$A^* + h\nu$

Example: **Δn=0 for Fe XX $2s^22p^3$**

$2s^22p^3\ {}^4S_{3/2} + e \rightarrow 2s2p^4({}^4P_{5/2})nl$

$2s^22p^3\ {}^4S_{3/2} + e \rightarrow 2s2p^4({}^4P_{5/2})nl$

$2s^22p^3\ {}^4S_{3/2} + e \rightarrow 2s2p^4({}^4P_{5/2})nl$



$n \geq 7$

Savin et al, 2004

Dielectronic Recombination

DC AI
$A^+ + e \rightarrow A^{**} \rightarrow A^+ + e$
↓ RS
$A^* + h\nu$

Examples:

$1s^2 + e \rightarrow 1s2pnl \rightarrow 1s^2nl + h\nu$

$1s^22s^2 + e \rightarrow 1s^22s2pnl \rightarrow 1s^22s^2nl + h\nu$

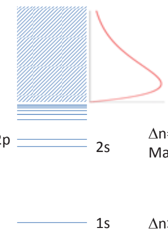
$1s^22s^2 + e \rightarrow 1s2s^22pnl \rightarrow 1s^22s^2nl + h\nu$

$1s^2 + e \rightarrow 1s2pnl \rightarrow 1s^2nl + h\nu$

$1s^22s + e \rightarrow 1s^22pnl \rightarrow 1s^22snl + h\nu$

$1s^22s + e \rightarrow 1s^23pnl \rightarrow 1s^22snl + h\nu$

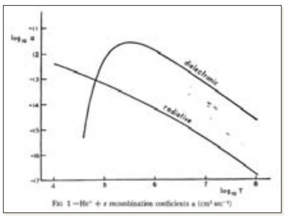
$1s^22s + e \rightarrow 1s2s2pnl \rightarrow 1s^22snl + h\nu$



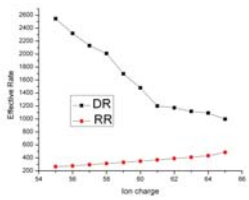
Δn=0: high n important, Major difficulty: n→∞

Δn>0: high n not as important

Is DR important?..



A. Burgess, ApJ **139**, 776 (1964)



W ions: T_e = 9000 eV, N_e = 10^{14} cm^{-3} (NLTE-7 Workshop, unpublished)

Answer: YES

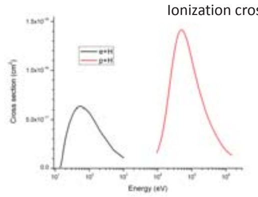
Burgess (1964) was the first to show importance of DR for solar corona ionization balance

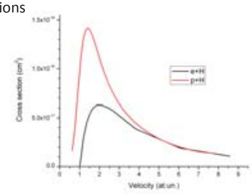
There exist a number of recommended formulas for rate coefficients of variable quality; **Z < 30** (Burgess-Merts-Magee-Cowan, Badnell et al, Mazzotta et al, Hahn, Gu,…)

$$\alpha_{DR} = \frac{1}{T_e^{3/2}} \sum_i C_i \exp\left(-\frac{E_i}{T_e}\right)$$

Heavy-particle collisions

Ionization cross sections





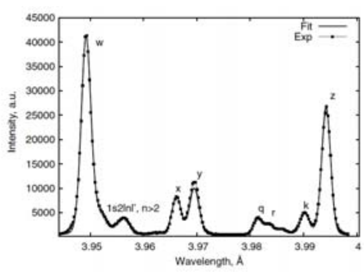
In ***thermal*** plasmas electrons are always more important for excitations than heavy particles
Exception: closely-spaced levels (e.g., 2s and 2p in H-like ions)

Neutral beams: **E ~ 100 keV** ⇒ heavy particle collisions are of highest importance

Charge exchange H + A^{z+} ⇒ H^+ + $A^{(z-1)+}(n)$

- Very large cross sections **> 10^{-15} cm^2**; $\sigma(Z) \sim Z \cdot 10^{-15}\ cm^2$
- High excited states populated: **n ~ $Z^{0.77}$**
- Higher *l* values are preferentially populated but it depends on collision energy

He-like lines and satellites

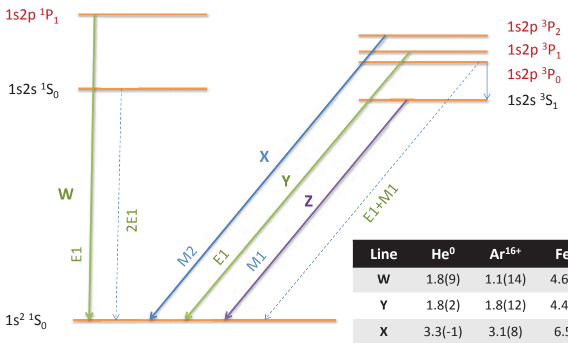


O.Marchuk et al, J Phys B 40, 4403 (2007)

Energy levels in He-like Ar

- Ground state: $1s^2\ {}^1S_0$
- Two subsystems of terms
  - Singlets **1s*nl* ¹L**, J=*l* (example $1s3d\ {}^1D_2$)
  - Triplets **1s*nl* ³L**, J=*l*-1,*l*,*l*+1 (example $1s2p\ {}^3P_{0,1,2}$)
- Radiative transitions within each subsystem are strong, between systems depend on Z

He-like Ar Levels and Lines

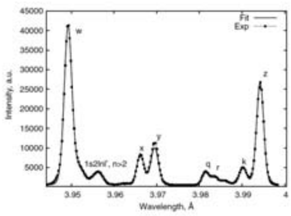


Line	He^0	Ar^{16+}	Fe^{25+}	Kr^{34+}
W	1.8(9)	1.1(14)	4.6(14)	1.5(15)
Y	1.8(2)	1.8(12)	4.4(13)	3.9(14)
X	3.3(-1)	3.1(8)	6.5(9)	9.3(10)
Z	1.3(-4)	4.8(6)	2.1(8)	5.8(9)

Z-scaling of A's

- W[E1]: $A(1s^2\ ^1S_0 - 1s2p\ ^1P_1) \propto \mathbf{Z^4}$
- Y[E1]: $A(1s^2\ ^1S_0 - 1s2p\ ^3P_1)$
  - $\propto \mathbf{Z^{10}}$ for low Z
  - $\propto \mathbf{Z^8}$ for large Z
  - $\propto \mathbf{Z^4}$ for very large Z
- X[M2]: $A(1s^2\ ^1S_0 - 1s2p\ ^3P_2) \propto \mathbf{Z^8}$
- Z[M1]: $A(1s^2\ ^1S_0 - 1s2s\ ^3S_1) \propto \mathbf{Z^{10}}$

1*s*2*lnl* satellites



- 1l2l2l'
  - $1s2s^2$: $^2S_{1/2}$
  - 1s2s2p:
    - $1s2s2p(^1P)\ ^2P_{1/2,3/2}$
    - $1s2s2p(^3P)\ ^2P_{1/2,3/2}$; $^4P_{1/2,3/2,5/2}$
  - $1s2p^2$
    - $1s2p^2(^1D)\ ^2D_{3/2,5/2}$
    - $1s2p^2(^3P)\ ^2P_{1/2,3/2}$; $^4P_{1/2,3/2,5/2}$
    - $1s2p^2(^1S)\ ^2S_{1/2}$
- 1s2lnl'
  - Closer and closer to W
  - Only 1s2l3l can be reliably resolved
  - Contribute to W line profile

Databases for Collisions

- IAEA
- NIFS
- TIPbase
- CCC Database
- CAMDB
- …

NIFS database