KPS AMPD Winter school

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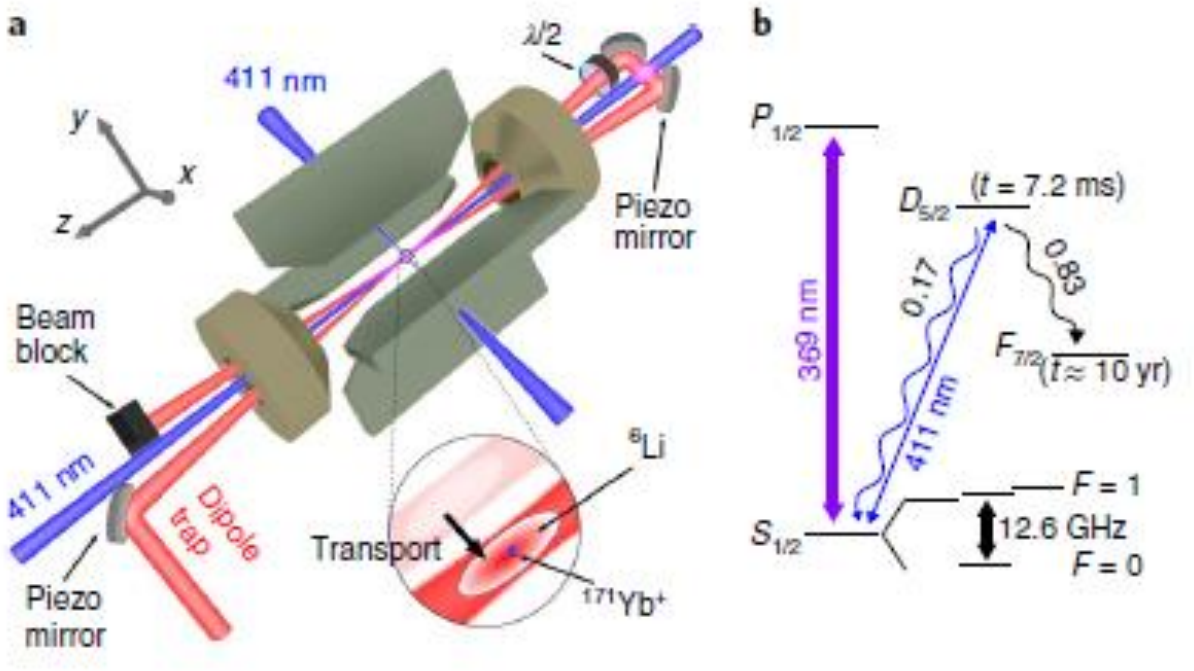
Spectroscopy and atomic structure

Atomic ion trap



Energy level symbol

Transition energy(wavelength)

Transition probability

Life time

Selection rules

⋮

?

Buffer gas (^{6}Li) cooling of a trapped ion ($^{171}Yb^+$) to the quantum regime

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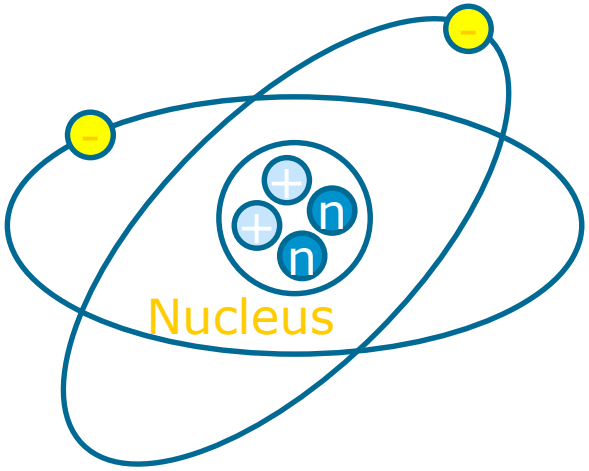
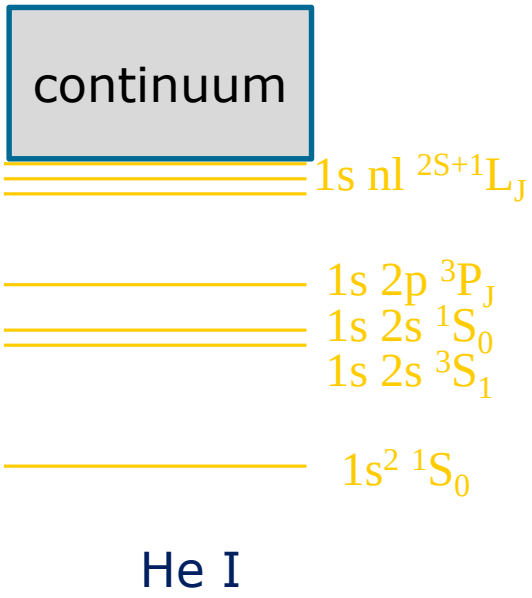
Spectroscopy and atomic structure

Primary data source	Query NIST Bibliographic Database for **Yb II** (new window)
Martin et al. 1978	Literature on Yb II Energy Levels

Configuration	Term	J	Level (eV)	Uncertainty (eV)	Landé-g	Leading percentages			Reference
$4f^{14}6s$	^2S	$^1/_2$	0.000000		1.998				L3974
$4f^{13}(^2F°)6s^2$	$^2F°$	$^7/_2$	*2.655587*		1.145	*98*	*1*	$(^2F°_{7/2})5d^2(^1S)$ $^1[^7/_2]°$	
		$^5/_2$	*3.913943*		0.862	*90*	*7*	$(^2F°_{7/2})5d6s(^3D)$ $^3[^7/_2]°$	
$4f^{14}5d$	^2D	$^3/_2$	2.846776		1.802				
		$^5/_2$	3.016869		1.202				
$4f^{13}(^2F°_{7/2})5d6s(^3D)$	$^3[^3/_2]°$	$^5/_2$	*3.317898*		1.570	*95*	*2*	$(^2F°_{7/2})(^3D)$ $^3[^5/_2]°$	
		$^3/_2$	*3.585535*		1.440	*82*	*27*	$(^2F°_{7/2})(^1D)$ $^1[^3/_2]°$	
		$^1/_2$	*4.172547*		1.320	*77*	*13*	$(^2F°_{5/2})(^3D)$ $^3[^1/_2]°$	
$4f^{14}6p$	$^2P°$	$^1/_2$	*3.355238*		0.667				
		$^3/_2$	*3.788158*		1.333				
$4f^{13}(^2F°_{7/2})5d6s(^3D)$	$^3[^{11}/_2]°$	$^9/_2$	*3.747339*		0.935	*98*	*2*	$(^2F°_{7/2})(^3D)$ $^3[^9/_2]°$	
		$^{11}/_2$	*3.789303*		1.112	*92*	*4*	$(^2F°_{7/2})(^1D)$ $^1[^{11}/_2]°$	
		$^{13}/_2$	*3.921817*		1.230	*100*			

Energy levels





Hamiltonian

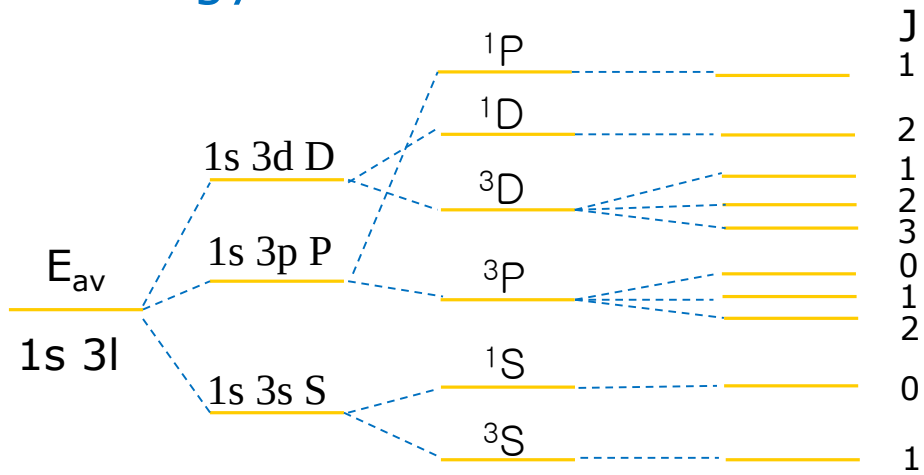
$$H = H_{kin} + H_{elec-nucl} + H_{elec-elec} + H_{S-O}$$

$$= -\sum_i \nabla_i^2 - \sum_i \frac{2Z}{r_i} + \sum\sum_{i>j} \frac{2}{r_{ij}} + \sum_i \xi_i(r_i)(\ell_i \cdot s_i)$$

Schrödinger equation

$$H\psi^k = E^k\psi^k$$

Energy-level fine structure



Sph. ave. + Coulomb direct + Coulomb exchange + S-O

Wavefunction

One-electron wavefunction

$$\boldsymbol{\varphi_i}(\boldsymbol{r_i}) = \frac{1}{r} P_{n_i l_i}(r_i) \cdot Y_{l_i m_{l_i}}(\theta_i, \emptyset_i) \cdot \sigma_{m_{s_i}}(s_{i_z})$$

Radial wavefunction

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2Z}{r}\right] P_{nl}(r) = \mathrm{E} P_{nl}(r)$$

$$P_{nl}(r) = -\left[\frac{Z(n-l-1)!}{n^2[(n+l)!]^3}\right]^{\frac{1}{2}} \rho^{l+1} e^{-\frac{\rho}{2}} L_{n+l}^{2l+1}(\rho), \qquad \rho = \frac{2Zr}{n}$$

$$L_{n+l}^{2l+1}(\rho) = -[(n+l)!]^2 \sum_{k=0}^{n-l-1} \frac{(-\rho)^k}{k!\,(n-l-1-k)!\,(2l+1+k)!} \qquad : associated\ Laguerre\ polynomial$$

Angular momentum operators and eigenvalues/angular wavefunctions

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = -\boldsymbol{i}\hbar \boldsymbol{r} \times \nabla$$

$$\boldsymbol{L^2}\Psi = l(l+1)\hbar^2\Psi$$

$$\boldsymbol{L_z}\Psi = m_l\hbar\Psi$$

$$\Psi = Y_{lm}(\theta, \emptyset) = (-1)^{(m+|m|)/2} \left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)\, e^{im\emptyset}$$

associated Legendre polynomial

$$\langle Y_{lm} | Y_{l'm'} \rangle \equiv \int_0^{2\pi} \int_0^{\pi} Y_{lm}^* Y_{l'm'} \sin\theta \, d\theta d\emptyset = \delta_{ll'}\delta_{mm'}$$

Wavefunction

Electron spin

$$\sigma_{m_s}(s_z) = \delta_{m_s s_z} \ (m_s = -1/2 \ or \ 1/2) \ , \qquad \langle \sigma_{m_s}(s_z) | \sigma_{m_s'}(s_z) \rangle = \delta_{m_s m_s'}$$

Orthonormalization $\langle Y_{lm_l}\sigma_{m_s} | Y_{l'm_l'}\sigma_{m_s'} \rangle = \delta_{ll'}\delta_{m_l m_l'}\delta_{m_s m_s'}$

$$\int_0^\infty P_{nl}(r) P_{n'l'}(r) dr = \delta_{nn'}$$

$$\langle \varphi_{nlm_l m_s} | \varphi_{n'l'm_l'm_s'} \rangle = \delta_{nn'}\delta_{ll'}\delta_{m_l m_l'}\delta_{m_s m_s'}$$

Product wavefunctions for *N*–electrons

$$\Phi = \boldsymbol{\varphi_1(r_1)\varphi_2(r_2)\varphi_3(r_3)\cdots\varphi_N(r_N)}$$

$$\Phi_c = \boldsymbol{\varphi_1(r_1)\varphi_2(r_2)\varphi_3(r_3)\cdots\varphi_N(r_N)} \quad \Phi_d = \boldsymbol{\varphi_1(r_2)\varphi_2(r_1)\varphi_3(r_3)\cdots\varphi_N(r_N)}$$

When two electrons are interchanged the probability should be unchanged.

$$|\Phi_d|^2 = |\Phi_c|^2 \quad \Phi_d = k\Phi_c, \ |k|^2 = 1, \Phi_c = k\Phi_d = k^2\Phi_c, and \ k = \pm 1$$

It is a ***fundamental postulate of quantum mechanics*** *that* Φ *be* ***antisymmetric*** *upon interchange of two electrons so that* $\Phi_d = -\Phi_c$

$$\Phi = N!^{-1/2} \sum_p (-1)^p \boldsymbol{\varphi_1(r_1)\varphi_2(r_2)\varphi_3(r_3)\cdots\varphi_N(r_N)}$$

Wavefunction

Properties of the antisymetrized wavefunction

$$\Phi = \frac{1}{N!^{1/2}} \begin{vmatrix} \boldsymbol{\varphi_1(r_1)} & \boldsymbol{\varphi_1(r_2)} & \boldsymbol{\varphi_1(r_3)} \cdots \\ \boldsymbol{\varphi_2(r_1)} & \boldsymbol{\varphi_2(r_2)} & \boldsymbol{\varphi_2(r_3)} \cdots \\ \boldsymbol{\varphi_3(r_1)} & \boldsymbol{\varphi_3(r_2)} & \boldsymbol{\varphi_3(r_2)} \cdots \\ & \vdots & \end{vmatrix}$$

Referred to as a determinantial function or Slater determinant (simpler for actual calculation)

(1) Interchanging the coordinates of two electrons is equivalent to interchanging two columns of the determinant; changes its sign.
(2) If two orbitals have the same quantum numbers, then two rows are identical; the determinant is zero. → Pauli exclusion principle
(3) If two electrons have the same coordinates, then two columns are identical; the determinant is zero

$$\langle \Phi | \Phi' \rangle = (N!)^{-1} \sum_p \sum_{p'} (-1)^{p+p'} \langle \boldsymbol{\varphi_1(r_1)\varphi_2(r_2)} \cdots | \boldsymbol{\varphi'_1(r'_1)\varphi'_2(r'_2)} \cdots \rangle$$
$$= (N!)^{-1} \textstyle\sum_p (-1)^{2p} \delta_{\Phi\Phi'} = \delta_{\Phi\Phi'}$$

Angular momentum properties

Orbital angular momentum :

$\boldsymbol{L^2}\Psi = l(l+1)\hbar^2\Psi, \qquad l = 0,1,2,3,\cdots$

$\boldsymbol{L_z}\Psi = m_l\hbar\Psi \;\; m_l = -l,-(l-1),\cdots,(l-1),l$

Orbital quantum number

Magnetic quantum number

Spin angular momentum :

$\boldsymbol{S^2}\Psi = s(s+1)\hbar^2\Psi, \qquad s = 0,\ 1/2\ ,1,3/2\cdots$

$\boldsymbol{S_z}\Psi = m_s\hbar\Psi \;\; m_s = -s,-(s-1),\cdots,(s-1),s$

Spin quantum number

Spin projection quantum number

Total angular momentum :

$\boldsymbol{J^2}\Psi = j(j+1)\hbar^2\Psi, \qquad j = 0,\ 1/2\ ,1,3/2\cdots$

$\boldsymbol{J_z}\Psi = m_j\hbar\Psi \qquad m_j = -j,-(j-1),\cdots,(j-1),j$

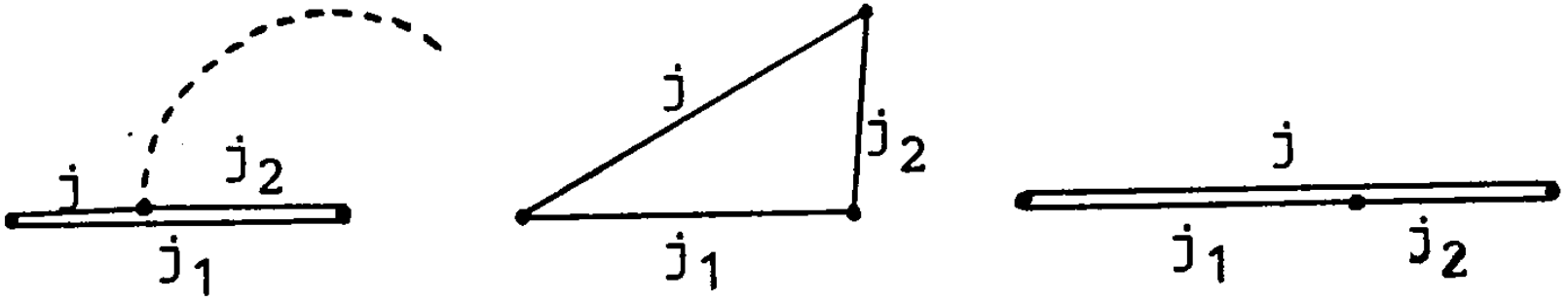
Total angular momentum quantum number

Total angular momentum projection quantum number

Angular momentum properties

Addition of two general angular momenta :

$\boldsymbol{J} = \boldsymbol{J_1} + \boldsymbol{J_2}$ $\quad |j_1 - j_2| \leq j \leq j_1 + j_2$ Triangular inequality



Clebsch-Gordon coefficients

$$\Psi_{j_1 j_2 jm} = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C(j_1 j_2 m_1 m_2; jm) \Psi_{j_1 m_1} \Psi_{j_2 m_2}$$

$$= \sum_{m_1} C(j_1 j_2 m_1 m - m_1; jm) \Psi_{j_1 m_1} \Psi_{j_2 m - m_1}$$

$$(\boldsymbol{J_{1z}} + \boldsymbol{J_{2z}}) \Psi_{j_1 m_1} \Psi_{j_2 m_2} = (m_1 + m_2) \hbar \Psi_{j_1 m_1} \Psi_{j_2 m_2}$$

Angular momentum properties

Notation of angular momentum states for *N* electrons system

$$\boldsymbol{J} = \sum_{i=1}^{N} (\boldsymbol{l_i} + \boldsymbol{s_i})$$

$\boldsymbol{L} = \sum_{i=1}^{N} \boldsymbol{l_i}$, $\boldsymbol{S} = \sum_{i=1}^{N} \boldsymbol{s_i}$ $\rightarrow$ $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$

LS or Russell–Saunders coupling scheme

LS **term** state , 2s+1 multiplicity and J **level** symbol $^{2S+1}L_J$

Parity

$$H(\boldsymbol{r_i}, \boldsymbol{p_i}, \boldsymbol{l_i}, \boldsymbol{s_i})\Psi(\boldsymbol{r_i}, \boldsymbol{s_i}) = E\Psi(\boldsymbol{r_i}, \boldsymbol{s_i})$$

$\boldsymbol{r_i} \rightarrow -\boldsymbol{r_i}$, $\boldsymbol{p_i} = -\boldsymbol{i}\hbar\boldsymbol{\nabla} = -\boldsymbol{p_i}$ $\qquad \boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = -\boldsymbol{i}\hbar\boldsymbol{r} \times \nabla$

$$H(-\boldsymbol{r_i}, -\boldsymbol{p_i}, \boldsymbol{l_i}, \boldsymbol{s_i})\Psi(-\boldsymbol{r_i}, \boldsymbol{s_i}) = E\Psi(-\boldsymbol{r_i}, \boldsymbol{s_i})$$

$$\Psi(-\boldsymbol{r_i}, \boldsymbol{s_i}) = c\Psi(\boldsymbol{r_i}, \boldsymbol{s_i})$$

$$\Psi(\boldsymbol{r_i}, \boldsymbol{s_i}) = c\Psi(-\boldsymbol{r_i}, \boldsymbol{s_i}) = c^2\Psi(\boldsymbol{r_i}, \boldsymbol{s_i}) \rightarrow c = \pm 1$$ +1=even, −1=odd

$$\prod_{i=1}^{N} R(r_i) \cdot Y_{l_i m_i}(\pi - \theta_i, \pi + \emptyset_i) \cdot \sigma_{m_{s_i}}(s_{iz}) = (-1)^{\sum l_i} \prod_{i=1}^{N} R(r_i) \cdot Y_{l_i m_i}(\theta_i, \emptyset_i) \cdot \sigma_{m_{s_i}}(s_{iz})$$

$p = (-1)^{\sum l_i}$ $\qquad {}^{2S+1}L_J^{\circ}$ for $p = -1$ odd terms

Angular momentum properties

Parity and angular momentum selection rules

$$T = \langle \Psi | \mathrm{O} | \Psi' \rangle \equiv \iiint_{-\infty}^{\infty} \Psi^*(\boldsymbol{r}_i)\mathrm{O}(\boldsymbol{r}_i)\Psi'(\boldsymbol{r}_i)dx_i dy_i dz_i \neq 0$$

$$\boldsymbol{r_i} \rightarrow -\boldsymbol{r_i} \quad = \iiint_{-\infty}^{\infty} \Psi^*(-\boldsymbol{r}_i)\mathrm{O}(-\boldsymbol{r}_i)\Psi'(-\boldsymbol{r}_i)(-dx_i)(-dy_i)(-dz_i)$$

$$= (-1)^{p+p_o+p'} \iiint_{-\infty}^{\infty} \Psi^*(\boldsymbol{r}_i)\mathrm{O}(\boldsymbol{r}_i)\Psi'(\boldsymbol{r}_i)dx_i dy_i dz_i$$

$p + p_o + p'$ must be even!

$\mathrm{O}(\boldsymbol{r}_i) = \boldsymbol{D_e} \equiv \sum(-e)\boldsymbol{r_i}$: *Electric dipole operator* involved in the calculation of radiative transitions

$J' = J + 1, J, or\ J' = J - 1 \quad (J' = J = 0\ not\ allowed)$

For LS−coupled functions

$S' = S$

$L' = L + 1, L, or\ L' = L - 1\ (L' = L = 0\ not\ allowed)$

due to the properties of spherical harmonics in the calculation of radiative transitions and orthonormality conditions

$$\langle Y_{lm_l}\sigma_{m_s} | Y_{l'm_{l'}}\sigma_{m_{s'}} \rangle = \delta_{ll'}\delta_{m_l m_{l'}}\delta_{m_s m_{s'}}$$

Complex atoms

Electron configurations

$$(n_1 l_1)^{w_1}(n_2 l_2)^{w_2}\cdots(n_q l_q)^{w_q},\quad \sum_{j=1}^{q} w_q = N$$

A set of equivalent electrons with same $\boldsymbol{nl}$ values : a subshell $(nl)^w$

A shell of all possible subshells with given $\boldsymbol{n}$: $\mathbf{K}(\boldsymbol{n}=\mathbf{1}), \mathbf{L}\,(\boldsymbol{n}=\mathbf{2}), \mathbf{M}(\boldsymbol{n}=\mathbf{3}), \mathbf{N}(\boldsymbol{n}=\mathbf{4})$

A subshell occupied by the maximum number of electrons: ***filled*** or ***closed subshell***

$$\sum_{m_{l=-l}}^{l} 2 = 2(2l+1) = 4l+2 \quad \leftarrow m_s = +1/2\,, or\ -1/2 \quad by\ \textbf{\textit{Pauli exclusion principle}}$$

$\boldsymbol{l}$	**0**	**1**	**2**	**3**	**4**
Half-filled subshell	s^1	p^3	d^5	f^7	g^9
Closed subshell	s^2	p^6	d^{10}	f^{14}	g^{18}

For any ***filled*** or ***closed subshell*** k $\boldsymbol{L_k} = \boldsymbol{S_k} = \boldsymbol{J_k} = 0$, and commonly omitted from the configuration notation for example

Ne I $\quad 1s^2 2s^2 2p^5 3s \rightarrow 2p^5 3s$

Complex atoms

Several open subshells eg. C I : $1s^2 2s^2 2p^3$

$\boldsymbol{L} = [(\boldsymbol{L_1} + \boldsymbol{L_2}) + \boldsymbol{L_3}] + \cdots$

$\boldsymbol{S} = [(\boldsymbol{S_1} + \boldsymbol{S_2}) + \boldsymbol{S_3}] + \cdots$

$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$

Parent, daughter, granddaughter terms of final term

LS coupling cases : The electrostatic interactions between electrons are much stronger than the interaction between the spin of an electron and its own orbital motion

jj coupling cases : With increasing Z, the spin–orbit interactions become much stronger than the Coulomb terms

$\boldsymbol{l}_i + \boldsymbol{s}_i = \boldsymbol{j}_i$

$\boldsymbol{j}_1 + \boldsymbol{j}_2 = \boldsymbol{J}_2$

$\boldsymbol{J}_2 + \boldsymbol{j}_3 = \boldsymbol{J}_3$

$\vdots$

$\boldsymbol{J}_{N-1} + \boldsymbol{j}_N = \boldsymbol{J}_N$

notation $(j_1, j_2)_J$ *vs.* LS coupling notation $^{2S+1}L_J$

Intermediate coupling cases : When neither the Coulomb nor the spin–orbit Interaction is small compared with the other, the Hamiltonian matrix is not even approximately diagonal in either the jj– or LS coupling representation.

Complex atoms

Problem : List the allowed terms and levels for p^2 equivalent electrons in LS and jj coupling schemes

LS

$m_{l_1}^{m_{s_1}}$	$m_{l_2}^{m_{s_2}}$	M_L	M_S	$M = M_L + M_S$
-1^-	-1^+	−2	0	−2
	0^-	−1	−1	−2
	0^+	−1	0	−1
	1^-	0	−1	−1
	1^+	0	0	0
-1^+	0^-	−1	0	−1
	0^+	−1	1	0
	1^-	0	0	0
	1^+	0	1	1
0^-	0^+	0	0	0
	1^-	1	−1	0
	1^+	1	0	1
0^+	1^-	1	0	1
	1^+	1	1	2
1^-	1^+	2	0	2

jj

j_1	m_1	j_2	m_2	M	J

^1S, ^3S,^1P, ^3P,^1D,$^3D \rightarrow$ ^1S, ^3P, ^1D by Pauli exclusion principal

Complex atoms

Pair coupling conditions : Energy levels tend to appear in pairs and the energy depends only slightly on the spin s of the excited electron;

jK coupling	notation	LK (or Ls) coupling	notation
$\boldsymbol{l}_1 + \boldsymbol{s}_1 = \boldsymbol{j_1}$ $\boldsymbol{j}_1 + \boldsymbol{l}_2 = \boldsymbol{K}$ $K + \boldsymbol{s}_2 = \boldsymbol{J}$	$j_1[K]_J$	$\boldsymbol{l}_1 + \boldsymbol{l}_2 = \boldsymbol{L}$ $\boldsymbol{L} + s_1 = \boldsymbol{K}$ $\boldsymbol{K} + s_2 = \boldsymbol{J}$	$L[K]_J$

Statistical weight : The atom must be considered to exist in any given stationary quantum state with the same a priori probability as for any other quantum state.

For any given energy level, the number of quantum states is equal to the number of possible values of $M(= -J, -J+1, \cdots, J-1, J)$. Thus the statistical weight of a level

$$g = 2J + 1$$

The total statistical weight of any group of closely-spaced levels :

$$g = \sum_{J=|j_1-j_2|}^{j_1+j_2} (2J+1) = (2j_1+1)(2j_2+1)$$

For LS coupling, $j_1 \rightarrow L, j_2 \rightarrow S$

and jK coupling, $j_1 \rightarrow K, j_2 \rightarrow$s=2

The 3n-j symbols

The Wigner 3n–j symbols, or their close relatives the **Clebsch–Gordon** and **Racah coefficients** are practically indispensable for quantitative calculations of atomic structure and spectra.

The 3-*j* symbols are given in terms of the Clebsch–Gordan coefficients by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \equiv \frac{(-1)^{j_1-j_2-m_3}}{\sqrt{2j_3+1}} \langle j_1\, m_1\, j_2\, m_2 | j_3\, (-m_3) \rangle.$$

$$\langle j_1\, m_1\, j_2\, m_2 | j_3\, m_3 \rangle = (-1)^{-j_1+j_2-m_3} \sqrt{2j_3+1} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}.$$

$$|j_3\, m_3\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle j_1\, m_1\, j_2\, m_2 | j_3\, m_3 \rangle |j_1\, m_1\, j_2\, m_2\rangle.$$

$$C(j_1 j_2 m_1 m_2;\, j_3 m_3)$$

The 3n-j symbols

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \equiv \delta_{m_1+m_2+m_3,0}(-1)^{j_1-j_2-m_3}$$
$$\times \sqrt{\Delta(j_1 j_2 j_3)}\sqrt{(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!\,(j_3+m_3)!\,(j_3-m_3)!}$$
$$\times \sum_k \frac{(-1)^k}{x}$$

$$triangle\ coeff. \qquad \Delta(j_1 j_2 j_3) = \frac{(j_1+j_2-j_3)!\,(j_1-j_2+j_3)!\,(-j_1+j_2+j_3)!}{(j_1+j_2+j_3+1)!}$$

$$x = k!\,(j_3-j_2+k+m_1)!\,(j_3-j_1+k-m_2)!\,(j_1+j_2-j_3-k)!$$
$$\times (j_1-k-m_1)!\,(j_2-k+m_2)!$$

The Wigner 3j symbols is zero unless all these conditions are satisfied

$$j_i \geq |m_i| \geq 0\ (each\ i)$$

$j_1+j_2+j_3$ (even) and $j_1-j_2-m_3$ must be integer

$$|j_1-j_2| \leq j_3 \leq j_1+j_2 \ : triangle\ relations$$

$$max(0, j_2-j_3-m_1, j_1-j_3+m_2) \leq k \leq min(j_1+j_2-j_3, j_1-m_1, j_2+m_2)$$

The 3n-j symbols

The **Wigner 6–j** symbols

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \sum_{m_1,\ldots,m_6} (-1)^{\sum_{k=1}^{6}(j_k - m_k)} \times$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_5 & j_6 \\ m_1 & -m_5 & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ m_4 & m_2 & -m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_3 \\ -m_4 & m_5 & m_3 \end{pmatrix}.$$

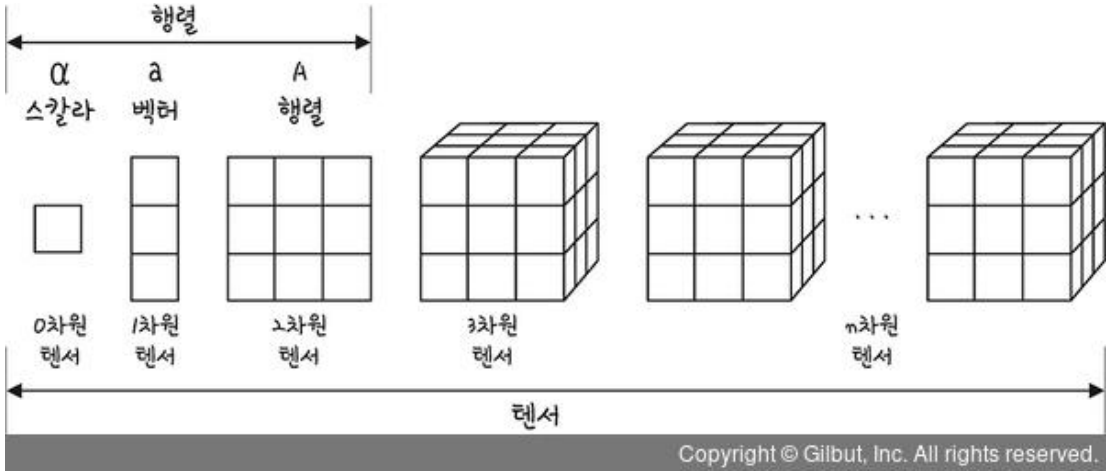
The **Wigner 9–j** symbols

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \\ j_7 & j_8 & j_9 \end{Bmatrix} = \sum_x (-1)^{2x}(2x+1) \begin{Bmatrix} j_1 & j_4 & j_7 \\ j_8 & j_9 & x \end{Bmatrix} \begin{Bmatrix} j_2 & j_5 & j_8 \\ j_4 & x & j_6 \end{Bmatrix} \begin{Bmatrix} j_3 & j_6 & j_9 \\ x & j_1 & j_2 \end{Bmatrix}.$$

The tensor operator

What is tensor?

A tensor of type (p, q) is an assignment of a multidimensional array



Wigner–Eckart Theorem

$$\langle j\,m|T_q^{(k)}|j'\,m'\rangle = \langle j'\,m'\,k\,q|j\,m\rangle\langle j\|T^{(k)}\|j'\rangle,$$

where

$$T_q^{(k)} = Y_{l=k}^{m=q}(\boldsymbol{r}), \qquad \mathrm{q} = -k, -k+1, \cdots, k-1, k$$

- $T_q^{(k)}$ is the q-th component of the spherical tensor operator $T^{(k)}$ of rank k,[2]
- $|jm\rangle$ denotes an eigenstate of total angular momentum J^2 and its z component J_z,
- $\langle j'm'kq|jm\rangle$ is the Clebsch–Gordan coefficient for coupling j' with k to get j,
- $\langle j\|T^{(k)}\|j'\rangle$ denotes[3] some value that does not depend on m, m', nor q and is referred to as the reduced matrix element.

$T^{(k)}$: irreducible tensor operator, $T_q^{(k)} = A_k(r)Y_{kq}(\theta, \emptyset)$,

Normalized spherical harmonic $C_q^{(k)}(\theta, \emptyset) \equiv (4\pi/2k+1)^{1/2}Y_{kq}(\theta, \emptyset)$

The tensor operator

$$\left\langle jm\left|T_q^{(k)}\right|j'm'\right\rangle = [j]^{-1/2} C(j'km'q;jm)\left\langle j\left\|T^{(k)}\right\|j'\right\rangle = (-1)^{-j'+k-m}\begin{pmatrix} j' & k & j \\ m' & q & -m \end{pmatrix}\left\langle j\left\|T^{(k)}\right\|j'\right\rangle$$

$$= (-1)^{j-m}\begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix}\left\langle j\left\|T^{(k)}\right\|j'\right\rangle$$

$$C(j_1 j_2 m_1 m_2; jm) = (-1)^{j_1 - j_2 + m}[j]^{1/2}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

$$[j] \equiv 2j + 1$$

For example of $C_0^{(0)} = 1$ $\quad \left\langle jm\left|C_0^{(0)}\right|j'm'\right\rangle = \langle jm|j'm'\rangle = \delta_{jm,j'm'}$

$$(-1)^{j-m}\begin{pmatrix} j & 0 & j \\ -m & 0 & m' \end{pmatrix} = \delta_{mm'}[j]^{-1/2}$$

and thus $\left\langle j\left\|C^{(0)}\right\|j'\right\rangle = \delta_{jj'}[j]^{1/2}$

Problem : Show that $\sum_{mm'}\left\langle jm\left|T_0^{(k)}\right|jm'\right\rangle$ is zero if k is nonzero, with the aid of

$$\sum_m (-1)^{j-m}\begin{pmatrix} j & j & j_3 \\ m & -m & 0 \end{pmatrix} = \delta_{j_3 0}[j]^{1/2}$$

Radial wave equations

Hartree–Fock method : Self-consistent-field (SCF) iterative method for the electron potentials and the electronic wavefunctions

$$H = \sum_{i=1}^{N}\left[-\nabla^2 - \frac{2Z}{r_i}\right] + \sum_{j\neq i}\frac{2}{r_{ij}} \qquad \langle\Psi|H_0|\Psi\rangle = \sum_k \langle\psi_k(i)|H_0|\psi_k(i)\rangle = \sum_k I_k$$

H_0 $\quad$ H_1

$\langle\Psi|H_1|\Psi\rangle$

J_{kl} : *direct term* $\qquad$ K_{kl} : *exchange term*

$$= \sum_{k,l\neq k}\left[\left\langle\psi_k(i)\psi_l(j)\left|\frac{2}{r_{ij}}\right|\psi_k(i)\psi_l(j)\right\rangle - \left\langle\psi_k(i)\psi_l(j)\left|\frac{2}{r_{ij}}\right|\psi_k(i)\psi_l(j)\right\rangle\right]$$

$$E[\Psi] = \langle\Psi|H|\Psi\rangle = \sum_i I_i + \frac{1}{2}\sum_i\sum_j [J_{ij} - K_{ij}] \qquad \delta E - \sum_k E_k\,\delta\langle\psi_k|\psi_l\rangle = 0 :$$

variational principal

$$\left[-\nabla^2 - \frac{2Z}{r_i}\right]\psi_k(i) + \left[\sum_l \int \psi_l^*(j)\frac{2}{r_{ij}}\psi_l(j)dj\right]\psi_k(i) - \left[\sum_l \int \psi_l^*(j)\frac{2}{r_{ij}}\psi_k(j)dj\right]\psi_l(i) = E_k\psi_k$$

$$\langle ab|\,1/r_{ij}\,|cd\rangle \propto \sum_{k=0}^{\infty} R^k(abcd)$$

$$R^k(abcd) = \int_0^\infty dr \int_0^\infty ds P_a(r)P_b(s)\frac{r_<^k}{r_>^{k+1}}P_c(r)P_d(s)$$: Slater integral

Configuration interaction

In general, all **configurational *states*** Φ of the same total L and S or J and the **parity** interact with one another. They are eigenvectors of the same Hamiltonian. Therefore an accurate representation of the wavefunction of a given state must generally consider the configuration interaction (CI) in atomic structure calculations. So $\Psi = \sum_v b_v \Phi_v$ where b_v is the **configuration mixing** coefficients.

For the ground state of Be, $\Psi(\mathrm{Be}) = b_1\Phi(1s^2 2s^2) + b_2\Phi(1s^2 2p^2) + \cdots$

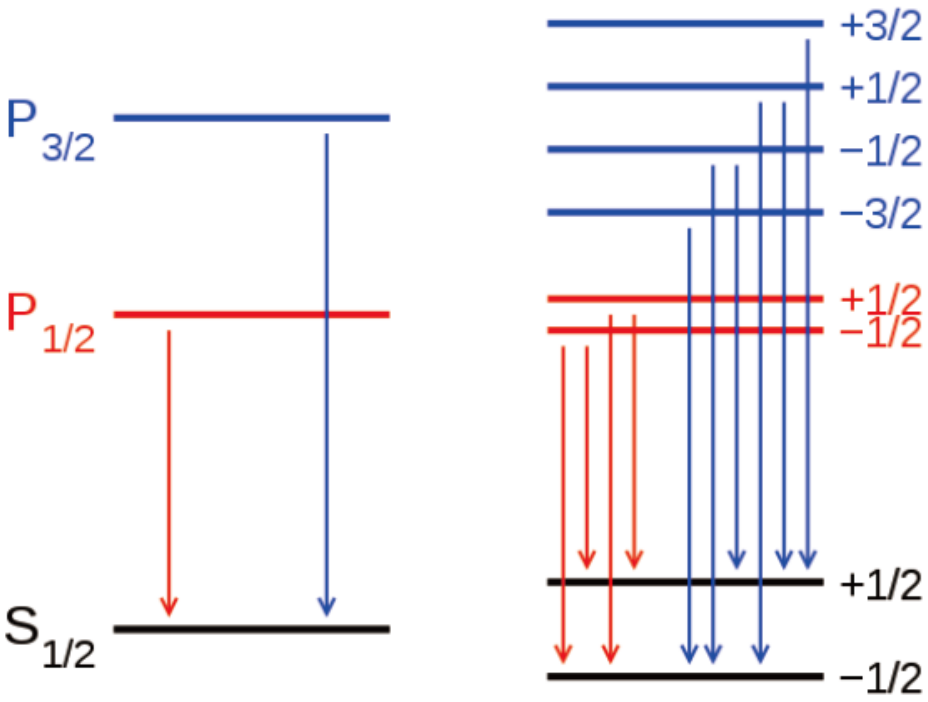
In solving Hartree–Fock equations, **CI wavefunctions**: the mixing coefficients are obtained by the variational principle while keeping the radial functions frozen. **MCHF wavefunctions**: the variational procedure determines both the mixing coefficients and the radial functions.

External fields and nuclear effects

$$H = H_0 + V_{\mathrm{M}} \quad V_{\mathrm{M}} = -\vec{\mu} \cdot \vec{B} \qquad \vec{\mu} \approx -\frac{\mu_{\mathrm{B}} g \vec{J}}{\hbar}$$

$$E_{\mathrm{Z}}^{(1)} = \langle nljm_j | H_{\mathrm{Z}}' | nljm_j \rangle = \langle V_M \rangle_\Psi = \mu_{\mathrm{B}} g_J B_{\mathrm{ext}} m_j$$

Landé g–factor



Zeeman effect

Isotope shift : Nuclear *mass* & *size* effect

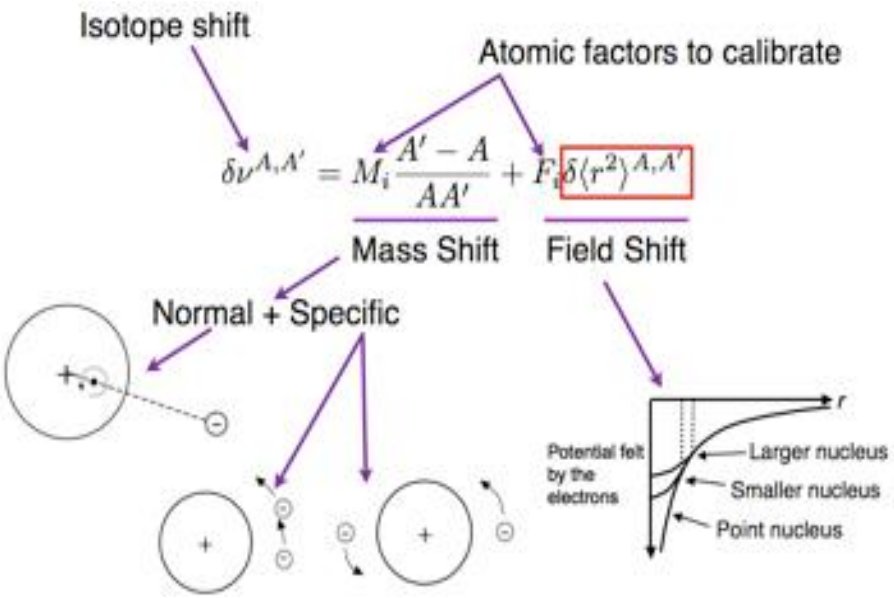
Isotope shift (IS)=Mass shift (MS)+Field shift (FS)

MS=Normal Mass shift (NMS)+Specific Mass (shift)

$$\frac{P^2}{2M} = \frac{m}{M}\left\{\frac{\sum_i p_i^2}{2m} + \frac{\sum_{i\neq j} p_i p_j}{2m}\right\},$$

$$NMS \equiv \delta E_h - \delta E_l = -\frac{m}{M_h}E + \frac{m}{M_l}E = \frac{M_h - M_l}{M_h M_l}mE$$

$$SMS = \left(\frac{m}{M_h} - \frac{m}{M_l}\right)\Delta k = -\frac{M_h - M_l}{M_h M_l}m\Delta k,\ k \equiv \frac{1}{m}\left\langle \sum_{i>j} p_i \cdot p_j \right\rangle$$

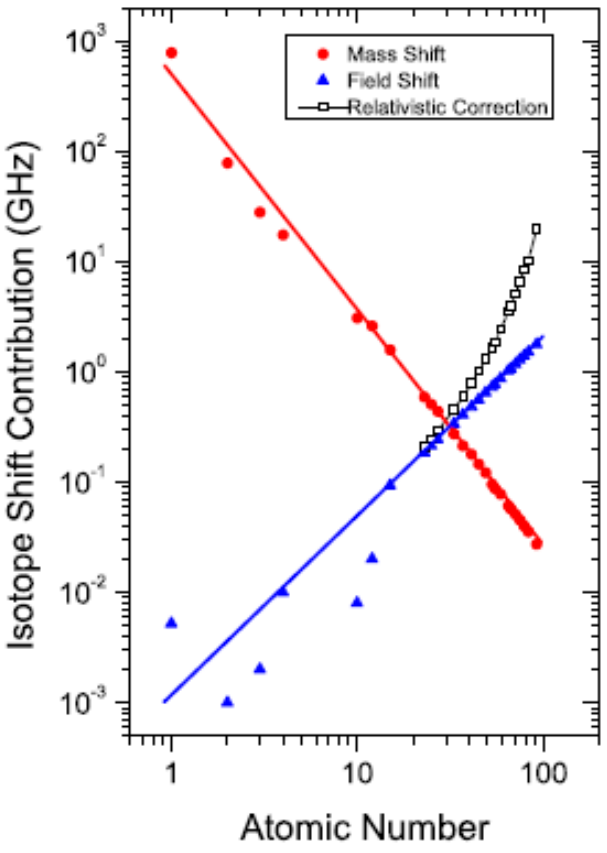


FS(Field Shift)

$$\delta E = \int_0^{r_0} V(r)\cdot\left(\phi_1^2 + \phi_2^2\right)dr$$

$$\delta E_h - \delta E_l = \pi\left|\Psi(0)\right|^2 a_0^3 / Z \cdot f(Z).\delta\left\langle r^2\right\rangle$$

Isotope shift : Nuclear *mass* & *size* effect



$$\nabla_i^2 = \frac{p_e^2}{2m_e} + \frac{p_N^2}{2m_N} = p^2\left(\frac{1}{2m_e} + \frac{1}{2m_N}\right) = \frac{p^2}{2\mu^2}$$

$$\mu = \frac{m_e m_N}{m_e + m_N} = m_e\left(\frac{1}{1 + m_e/m_N}\right)$$

Reduced mass in center of mass frame

$$E_n = -\frac{1}{n^2}\frac{\mu e^4}{2\hbar^2} = -\frac{1}{2n^2}\alpha^2\mu c^2 = h\nu_n = h\frac{c}{\lambda_n}$$

$$m_p/m_D = 0.5003,\ m_p/m_e \cong 1836.15 >> 1$$

$$\frac{\mu_p}{\mu_D} = \frac{1 + m_e/m_D}{1 + m_e/m_p} \approx 1 + \frac{m_e}{m_D} - \frac{m_e}{m_p} = 1 - \frac{m_e}{m_p}\left(1 - \frac{m_p}{m_D}\right) \approx 1 - 0.500\frac{m_e}{m_p}$$

$$\frac{\lambda_D}{\lambda_H} = \frac{\mu_p}{\mu_D} \approx 1 - \frac{m_e}{2m_p}, \quad \frac{\lambda_D - \lambda_H}{\lambda_H} = \frac{\Delta\lambda}{\lambda_H} = -\frac{m_e}{2m_p}$$

		λ_H	λ_D	$\Delta\lambda$
red	(3rd order)	655.69(11)nm	655.40(15)nm	–0.29(19)nm
red	(4th order)	655.74(11)nm	655.50(11)nm	–0.24(15)nm
green	(4th order)	485.68(11)nm	485.46(11)nm	–0.22(16)nm
green	(5th order)	485.73(8)nm	485.54(8)nm	–0.19(12)nm

Hyperfine structure : Nuclear *spin* & *shape* effect

Magnetic dipole interaction

$$\mu_I = g_i \mu_N I \qquad H_\mu = -\vec{\mu}_N . \vec{B} \qquad \hat{H}_\mu = A \vec{I} . \vec{J} \qquad \vec{F} = \vec{I} + \vec{J}$$

$$F^2 = I^2 + J^2 + 2 \vec{I} . \vec{J}$$

$$E_\mu = (\frac{A}{2})[F(F+1) - I(I+1) - J(J-1)]$$

$$\vec{I} . \vec{J} = \frac{(F^2 - I^2 - J^2)}{2}$$

$$E_\mu = AC/2$$

$$C = F(F+1) - I(I+1) - J(J-1)$$

Electric quadrapole interaction

$$Q = < I, I | r^2 (3cos^2\theta - 1) | I, I > \qquad V_Q = (\frac{1}{e}) < J, J | \frac{\partial^2 \phi}{\partial z^2} | J, J >$$

$$\phi\left(\vec{r}\right) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho\left(\vec{r'}\right)}{\left|\vec{r} - \vec{r'}\right|} d^3 r'$$

$$E_Q = (\frac{eQ}{4}) < \partial^2\phi/\partial z^2 > [\frac{\frac{3}{2}C(C+1) - 2I(I+1)J(J+1)}{IJ(2J-1)(2I-1)}]$$

Total hyperfine splitting

$$\Delta E = \frac{AC}{2} + \frac{B}{4}[\frac{\frac{3}{2}C(C+1) - 2I(I+1)J(J+1)}{IJ(2I-1)(2J-1)}]$$

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)]^{1/2}} \langle \Psi(PJ) \| T^{(1)} \| \Psi(PJ) \rangle$$

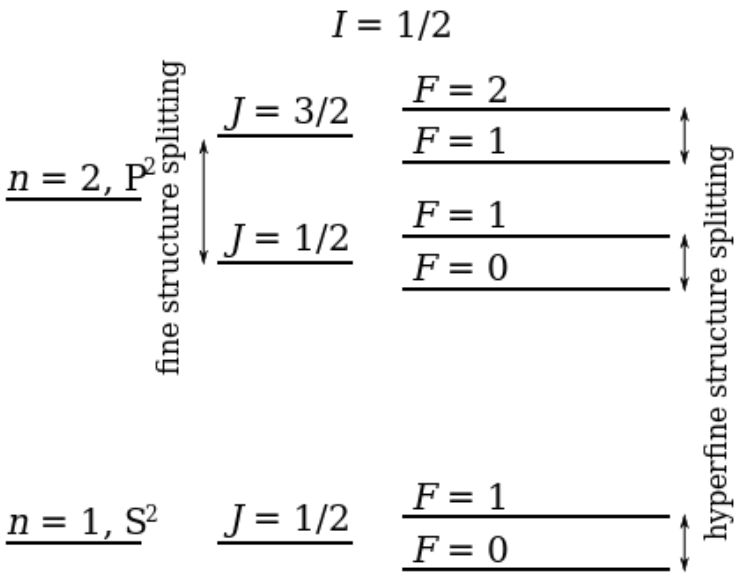
$$B_J = 2Q \left[\frac{J(2J-1)}{(J+1)(2J+3)} \right]^{1/2} \langle \Psi(PJ) \| T^{(2)} \| \Psi(PJ) \rangle$$

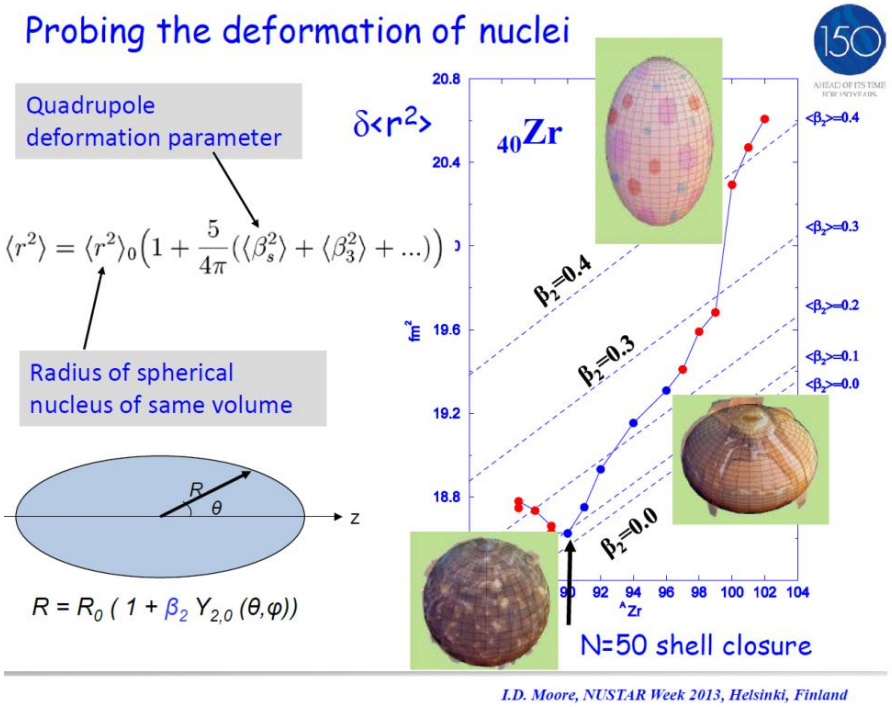
Hyperfine structure : Nuclear *spin* & *shape* effect

The quadrupole moment Q of a nucleus is a measure of the departure of the mean distribution of the nuclear charge from spherical symmetry.

$Q = 0$, spherically symmetric distribution (e.g. a sphere)
$Q > 0$, prolongated ellipsoidal distribution (e.g. a football)
$Q < 0$, Oblate distribution (e.g. door knob)

Hydrogen hyperfine splitting





Selection rules of radiative transitions

$$T = \langle \Psi | \mathrm{O} | \Psi' \rangle \equiv \iiint_{-\infty}^{\infty} \Psi^*(\boldsymbol{r}_i)\mathrm{O}(\boldsymbol{r}_i)\Psi'(\boldsymbol{r}_i)dx_i dy_i dz_i \neq 0$$

Allowed transitions		Electric dipole (E1)	Magnetic dipole (M1)	Electric quadrupole (E2)	Magnetic quadrupole (M2)	Electric octupole (E3)	Magnetic octupole (M3)
Rigorous rules	(1)	$\Delta J = 0, \pm 1$ $(J = 0 \nleftrightarrow 0)$		$\Delta J = 0, \pm 1, \pm 2$ $(J = 0 \nleftrightarrow 0, 1;\ \frac{1}{2} \nleftrightarrow \frac{1}{2})$		$\Delta J = 0, \pm 1, \pm 2, \pm 3$ $(0 \nleftrightarrow 0, 1, 2;\ \frac{1}{2} \nleftrightarrow \frac{1}{2}, \frac{3}{2};\ 1 \nleftrightarrow 1)$	
	(2)	$\Delta M_J = 0, \pm 1$		$\Delta M_J = 0, \pm 1, \pm 2$		$\Delta M_J = 0, \pm 1, \pm 2, \pm 3$	
	(3)	$\pi_\mathrm{f} = -\pi_\mathrm{i}$	$\pi_\mathrm{f} = \pi_\mathrm{i}$		$\pi_\mathrm{f} = -\pi_\mathrm{i}$		$\pi_\mathrm{f} = \pi_\mathrm{i}$
LS coupling	(4)	One electron jump $\Delta L = \pm 1$	No electron jump $\Delta L = 0,$ $\Delta n = 0$	None or one electron jump $\Delta L = 0, \pm 2$	One electron jump $\Delta L = \pm 1$	One electron jump $\Delta L = \pm 1, \pm 3$	One electron jump $\Delta L = 0, \pm 2$
	(5)	If $\Delta S = 0$ $\Delta L = 0, \pm 1$ $(L = 0 \nleftrightarrow 0)$	If $\Delta S = 0$ $\Delta L = 0$	If $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2$ $(L = 0 \nleftrightarrow 0, 1)$		If $\Delta S = 0$ $\Delta L = 0, \pm 1, \pm 2, \pm 3$ $(L = 0 \nleftrightarrow 0, 1, 2;\ 1 \nleftrightarrow 1)$	
Intermediate coupling	(6)	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1, \pm 2$		If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ $\pm 2, \pm 3$ $(L = 0 \nleftrightarrow 0)$	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1$ $(L = 0 \nleftrightarrow 0)$	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ $\pm 2, \pm 3, \pm 4$ $(L = 0 \nleftrightarrow 0, 1)$	If $\Delta S = \pm 1$ $\Delta L = 0, \pm 1,$ ± 2 $(L = 0 \nleftrightarrow 0)$

출처 Wikipedia

Hyperfine splitting and selection rules : $\mathrm{F} = \mathrm{I} + \mathrm{J}$ has similar mathematical form with $\mathrm{J} = \mathrm{L} + \mathrm{S}$, and obeys similar selection rules as above table

Electric and magnetic multipole transitions

Einstein's *A* coefficient, the radiative transition rate from level *j* to *i*

$$A_{ji} = \frac{g_i}{g_j}\frac{8\pi\nu_{ji}^2}{c^3} h\nu_{ji} B_{ij}, \quad B_{ij} = \frac{2\pi}{3}\frac{c^2 e^2}{h^2\nu_{ji}^2}\left|\left\langle j\left|\frac{p}{m_e c} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\right|i\right\rangle\right|^2$$

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = 1 + i\boldsymbol{k}\cdot\boldsymbol{r} + \frac{(i\boldsymbol{k}\cdot\boldsymbol{r})^2}{2!} + \cdots = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

Dipole E1 Higher order M1, E2, ...

$$\frac{e}{m_e c}\langle j|\boldsymbol{p}|i\rangle = \frac{\omega}{c} i\langle j|\boldsymbol{D}|i\rangle, \boldsymbol{D} = e\boldsymbol{r}$$

$$A_{ji} = \frac{g_i}{g_j}\frac{4e^2\omega_{ji}^3}{3\hbar c^3}\langle j|\boldsymbol{r}|i\rangle^2 \ (1/s)$$

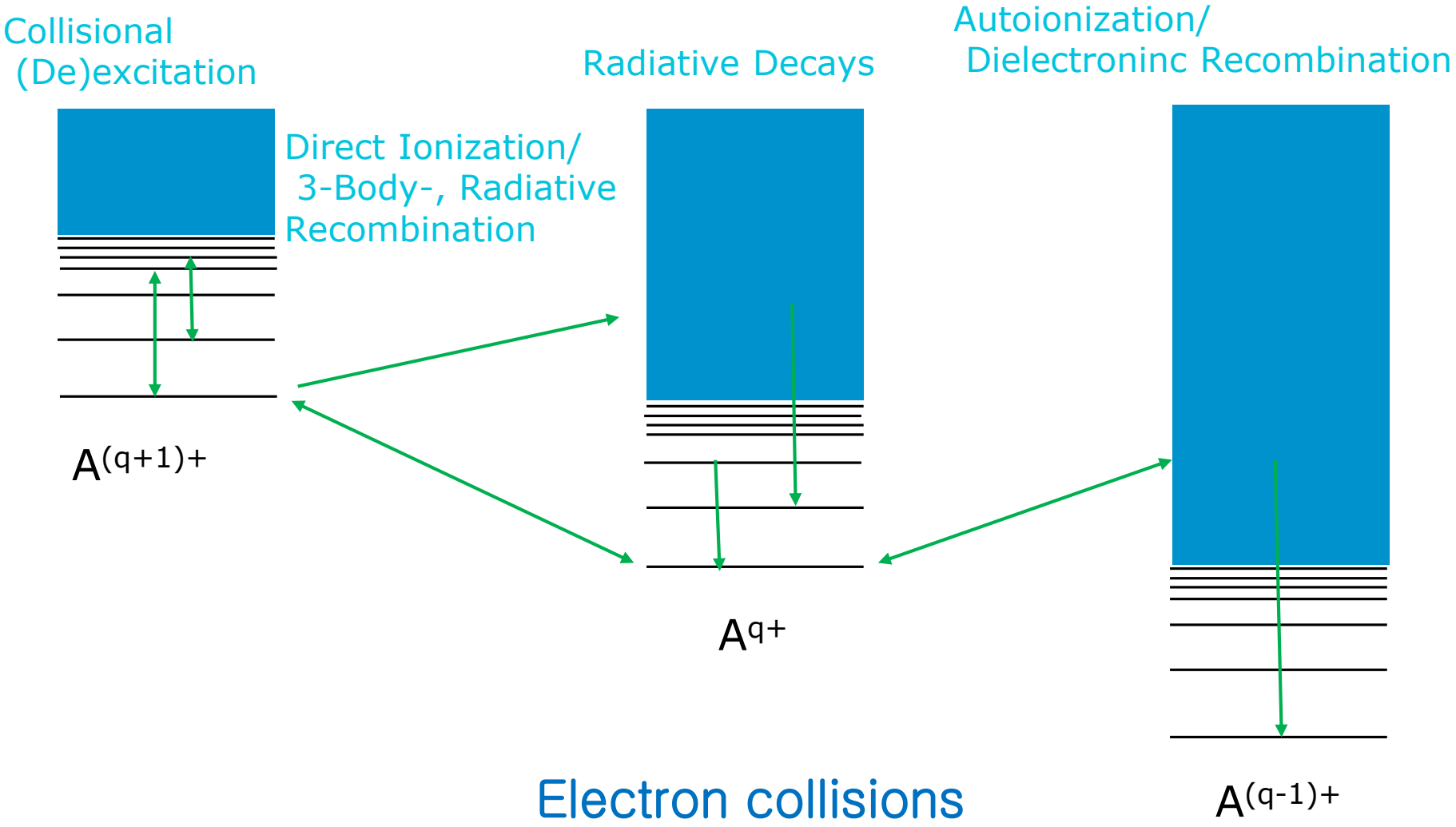
Dimensionless oscillator strength $f_{ij} = \frac{g_j}{g_i}\frac{m_e c^3}{2e^2\omega^2} A_{ji}$, $f_{ji} = \frac{g_i}{g_j} f_{ij}$

Lifetime τ of a level *i*

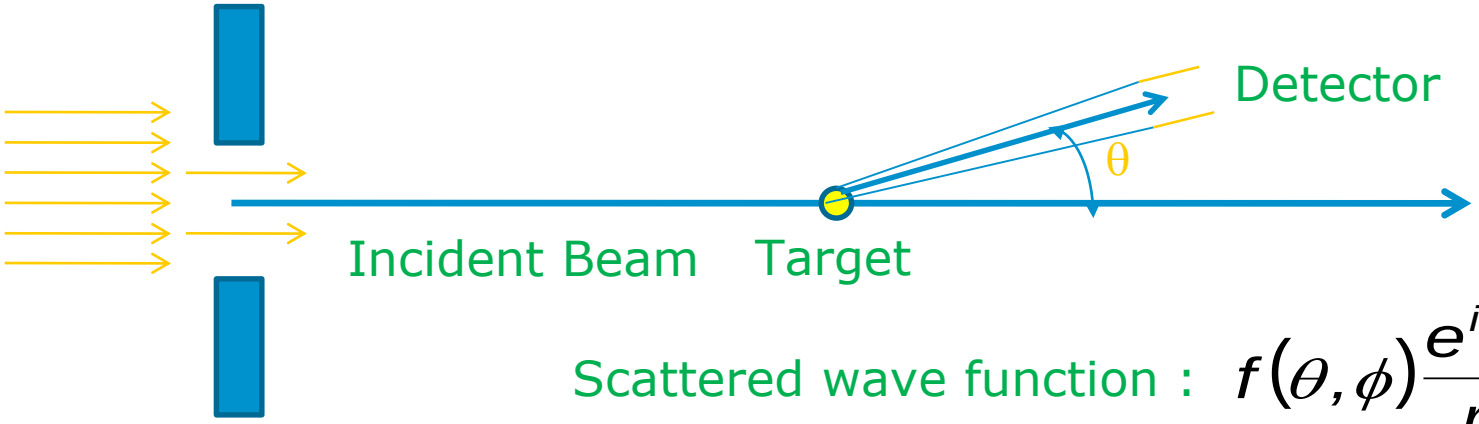
$$\frac{1}{\tau_i} = \sum_k A_{ik}$$

Collision

Atomic processes in plasma



Cross section and rate coefficient



Scattered wave function : $f(\theta,\phi)\frac{e^{ikr}}{r}$

Differential Cross Section : $\frac{d\sigma(\theta)}{d\Omega} = |f(\theta,\phi)|^2$

Total Cross Section : $\sigma = \int_{4\pi} (\frac{d\sigma}{d\Omega}) d\Omega$

Rate Coefficient : $\alpha(v_0) = \langle \sigma v \rangle = \int \sigma(v)\, v\, f(v_0, \mathbf{v})\, d^3v$

Close coupling *vs*. DW approximations

e+atom/ion process, (N+1)−electron system

Close coupling approximation

$$\Psi = \sum_i^{n_f} \Phi_i\,(x_1, \cdots, x_N)\frac{1}{r}F_i(r) + \sum_j^{n_b} \chi_j(x_1, \cdots, x_{N+1})c_j \qquad H_{N+1}\Psi_E = E\Psi_E$$

$$H_{N+1} = \sum_{i=1}^{N+1}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1}\frac{2}{r_{ij}}\right\} \qquad E = E_i + \epsilon_i$$

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + k_i^2\right]F_i(r)$$

$$= 2\sum_j\left[V_{ij}(r)F_j(r) + \int_0^\infty dr' W_{ij}(r,r')F_j(r')\right] + \sum_{nl}\lambda_{i,nl}P_{nl}(r)\delta_{l,l_i}$$

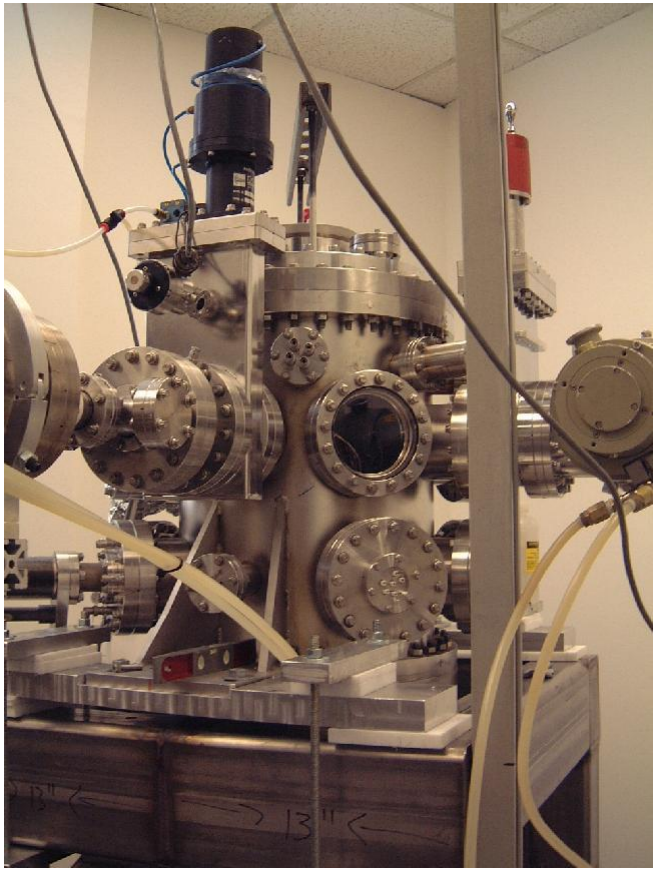
Distorted wave approximation

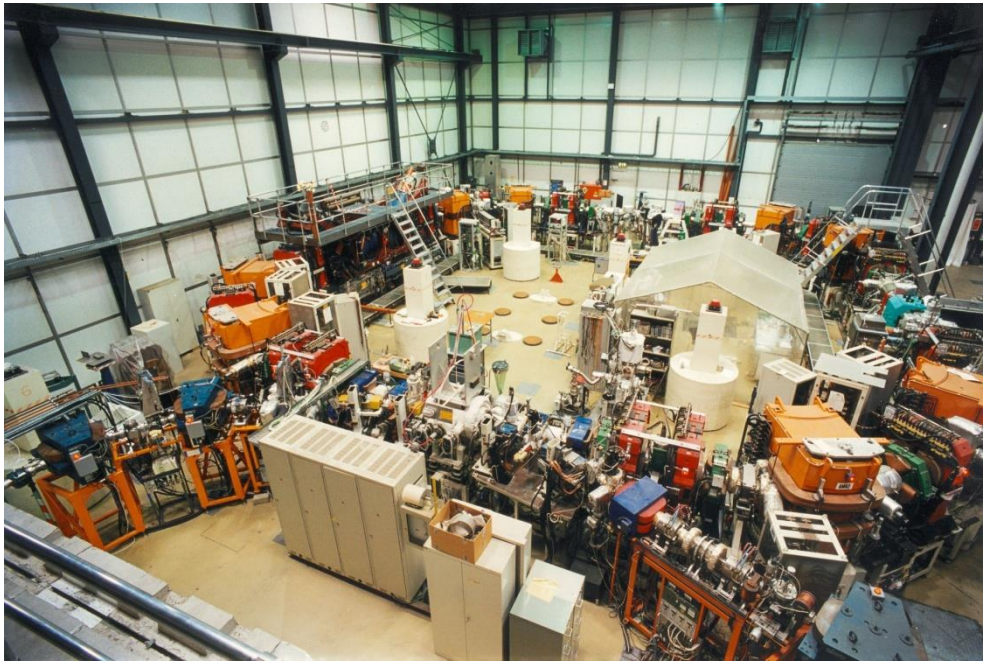
$$\Psi = \Phi_i(x_1, \cdots, x_N)\frac{1}{r}F_i(r) \text{ : no channel coupling}$$

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2Z}{r} + k_i^2\right]F_i(r) = 0$$

Collision

Cross section measurement





Max Flank Institute for Nuclear Physics, Germany (**TSR**, test storage ring)

Lawrence Livermore National Laboratory, USA (**EBIT**, electron beam ion trap)

Korea : Homemade UNIST EBIT, IBS EBIT(S) …

Atomic codes

Dirac Equation

$$\psi_{n\kappa m} = \frac{1}{r}\begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa m}(\theta,\phi,\sigma) \\ iQ_{n\kappa}(r)\chi_{-\kappa m}(\theta,\phi,\sigma) \end{pmatrix}$$

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)P_{n\kappa} = \alpha\left(\epsilon_{n\kappa} - V + \frac{2}{\alpha^2}\right)Q_{n\kappa}$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)Q_{n\kappa} = \alpha\left(-\epsilon_{n\kappa} + V\right)P_{n\kappa}$$

Relativistic angular quantum number

$$\kappa = (l-j)(2j+1)$$

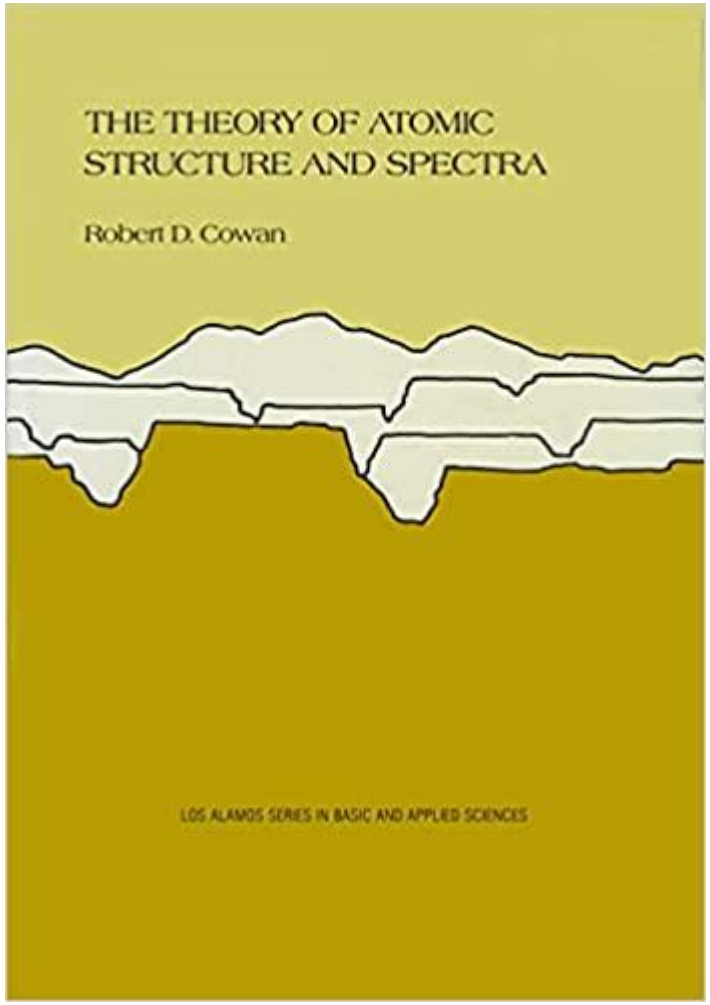
Nonrelativistic Hamiltonian :
MCHF (multi-configuration Hartree-Fock)
SUPERSTRUCTURE/AUTOSTRUCTURE
CIV3

HFR…

Relativistic Hamiltonian :
MCDF(multi-configuration Dirac-Fock),
GRASP/GRASP92
HULLAC, **FAC** codes…

R-MATRIX/BPRM/DARC …

FAC (Flexible Atomic Code) : *M. F. Gu, Can. J. Phys* **86** *675 (2008)*



atoms

MDPI

Article

Cowan Code: 50 Years of Growing Impact on Atomic Physics

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check for updates

Abstract: The famous Cowan's book, "The Theory of Atomic Structure and Spectra", published in 1981, and his suite of computer codes based on it, continue to be highly influential in atomic physics and many other research areas. As of September 2018, there have been more than 5000 citations to Cowan's book and codes, and each year adds about 150 citations to this list. The present work briefly describes what these codes do and why they are responsible for most of the current progress in the analyses of atomic spectra. Various modifications of these codes, including my own, will also be described.

Keywords: Cowan code; atomic structure; energy levels; transition probabilities; semiempirical parametric calculations

1. Introduction

Although Cowan's classic book [1] was published in 1981, the early versions of his computer codes that are generally referred to this book were fully developed as early as in 1968 [2], which accounts for the 50-year period mentioned in the title of the present paper. The program package usually called "the Cowan code" consists of four separate codes. Some parts of this package were developed even earlier [3,4].

When I received an invitation to make a talk at the 11th International Conference on Atomic and Molecular Data and their Applications (ICAMDATA-2018), Robert Duane Cowan was still alive (see Figure 1). He died on 26 July 2018 in a hospice in Albuquerque at an age of 98. The main facts of his biography can be found in an obituary available online [5]. The present article is a transcript of my talk given on 13 November 2018 at Cambridge, Massachusetts.

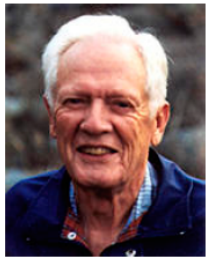


Figure 1. Robert Duane Cowan (24 November 1919–26 July 2018).

Hyperfine structure of Al

Al (Z=13) isotopes (A = 22-43)

- Natural occurrence : ^{27}Al(stable, ~100%), ^{26}Al(radioactive isotope, $t_{1/2}=7.2 \times 10^5$y, produced in the atmosphere by spallation with cosmic-ray protons)
- All other radioisotopes : $t_{1/2} < 7$ minutes
- ^{23}Al : Proton-halo structure
- $^{31\text{-}33}$Al : Neutron-rich isotopes in the vicinity of island of inversion
- ^{26}Al : Self-conjugate nucleus (N=Z)

Al atomic energy levels

Configuration	Term	J	Level (eV)
$3s^2 3p$	$^2P^\circ$	$^1/_2$	0.0000000
		$^3/_2$	0.0138938
$3s^2 4s$	^2S	$^1/_2$	3.1427212
$3s3p^2$	^4P	$^1/_2$	3.598072
		$^3/_2$	3.603844
		$^5/_2$	3.613244
$3s^2 3d$	^2D	$^3/_2$	4.0214836
		$^5/_2$	4.0216502
$3s^2 4p$	$^2P^\circ$	$^1/_2$	4.0852554
		$^3/_2$	4.0872183
$3s^2 5s$	^2S	$^1/_2$	4.6728909

Lower levels

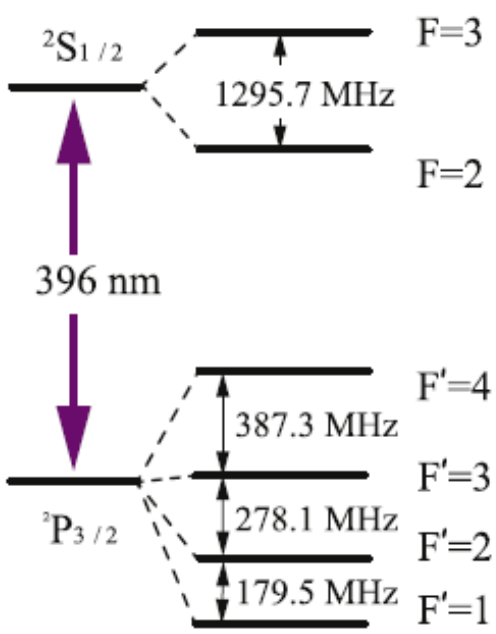
Upper level

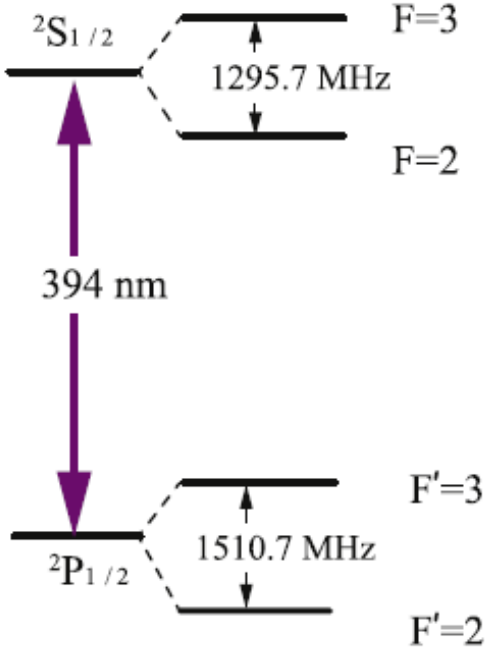
Energy units

$$E = h\nu = hc/\lambda$$

$$E(eV) = 4.1357 \times 10^{-6}\nu(GHz)$$
$$= 1.2398/\lambda(\mu m)$$

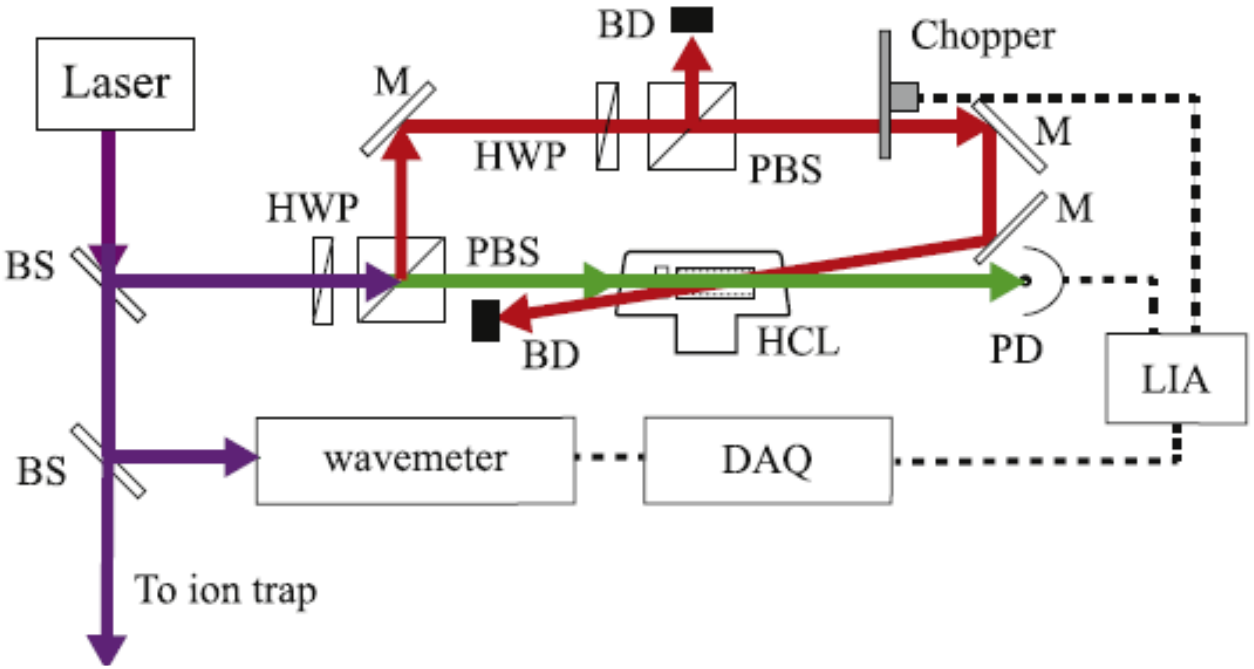
Hyperfine splittings



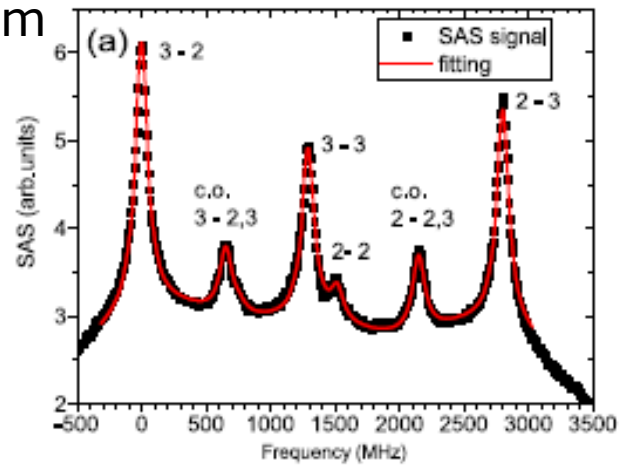


UV laser spectroscopy

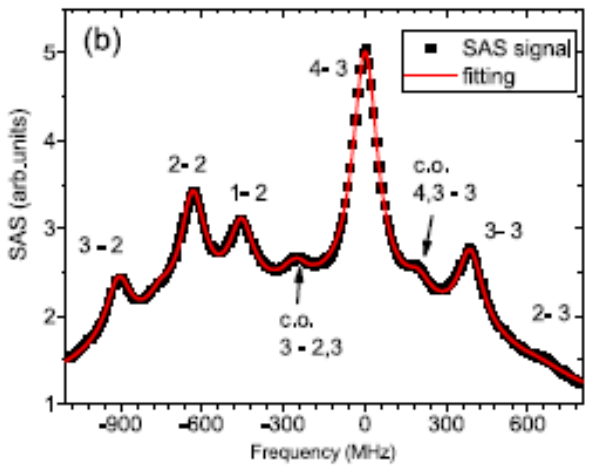
Ref. Hongli Liu et al., UV laser spectroscopy of Al atoms in hollow-cathode lamp, J. Phys. B **51** (2018) 225002



394nm



396nm



A and B hyperfine coupling constants

Table 1. The A and B hyperfine coupling constants of aluminum atoms.

$^2P_{1/2}$ A(MHz)	$^2P_{3/2}$ A(MHz)	$^2P_{3/2}$ B(MHz)	$^2S_{1/2}$ A(MHz)	Measurement method	References
503.58(27)	94.47(8)	11.75(37)	431.89(11)	saturation absorption	Present work
502.04(97)	93.76(71)	19.12(86)	431.84(91)	laser spectroscopy	Nakai(2007)[27]
502.034 6(5)[a]	94.272 26(10)[a]	9.459 49(35)[a]	—	far-infrared laser magnetic resonance	Brown(1999)[28]
—	94.1(6)	20.2(19)	—	laser spectroscopy	Levins(1997)[26]
—	93(2)	14(9)	—	2-photon laser spectroscopy	Weber(1987)[25]
—	—	—	421(15)	laser spectroscopy	Zhan-Kui(1982)[24]
502.033 6(5)	—	—	—	atomic beam magnetic resonance	Harvey(1972)[23]
—	94.277 67(10)	18.915 26(70)	—	atomic beam magnetic resonance	Martin(1968)[22]
502.05	—	—	—	atomic beam magnetic resonance	Lew(1953)[21]
—	94.25(4)	18.76(25)	—	atomic beam magnetic resonance	Lew(1949)[20]
498.33	100.98	19.59	407.18	theoretical calculation	Sur(2005)[29]

[a] The values are extrapolated from the data of Martin(1968) [22].

MCDF (Multi-configuration Dirac-Fock) calculation

Preliminary single configuration calculation with MCDF code

Level	Energy (eV) (NIST DB)	A(MHz)	B(MHz)
$3s^2 3p\ {}^2P_{1/2}$	0 (0)	406.66	
$3s^2 3p\ {}^2P_{3/2}$	0.01398 (0.01389)	80.47	14.98
$3s^2 4s\ {}^2S_{1/2}$	2.85552 (3.14272)	241.88	

- Input parameters
  Nuclear spin : I=5/2
  Magnetic dipole moment : $\mu_I = 3.6415069\mu_N$
  Electric quadrupole moment : $Q = 0.1466$b

Ref. N. J. Stone, Table of nuclear magnetic dipole and electric quadrupole moments, Atomic Data and Nuclear Data Tables **90** (2005) 75–176

- Used code
  MCDFGME by Jean-Paul DESCLAUX and Paul INDELICATO in France

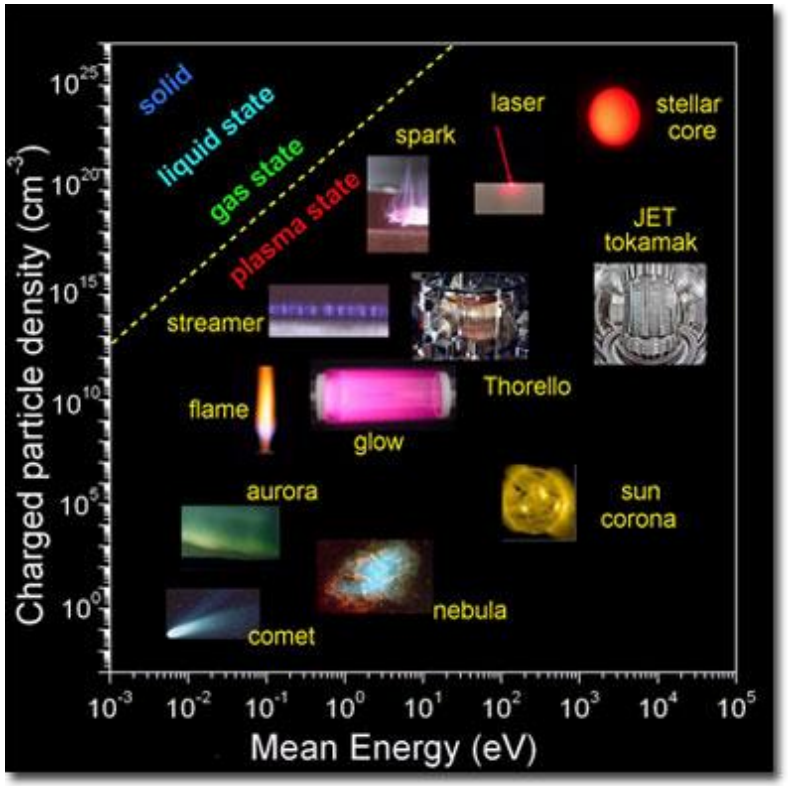
⇨ **Configuration interaction** calculation will be performed for **better accuracy.**

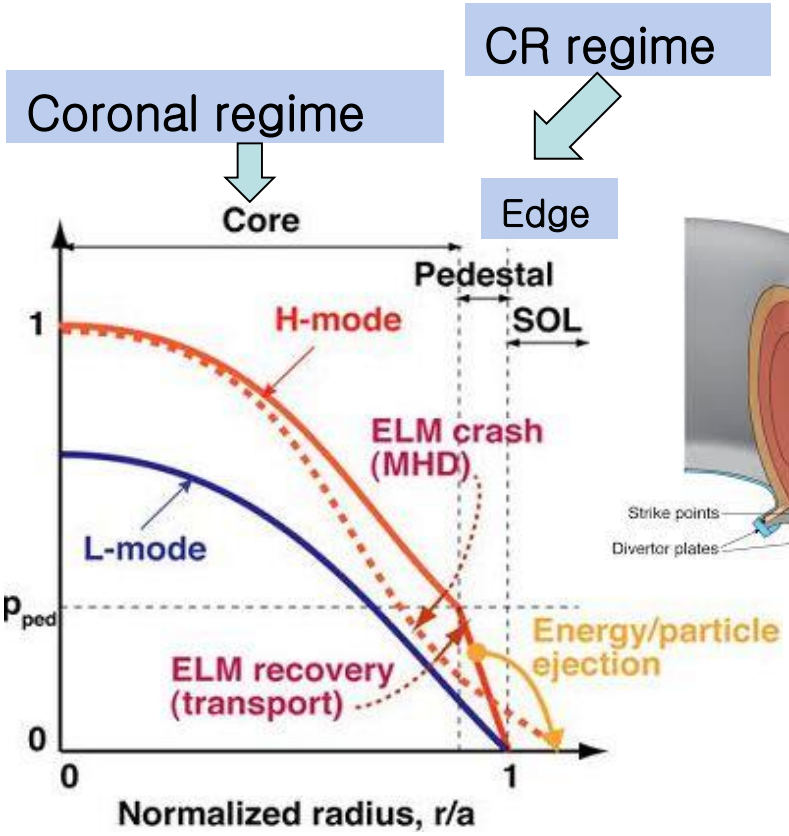
Nuclear moments data

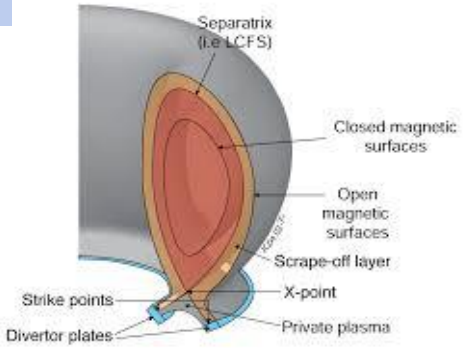
Nucleus	E (level)	$\tau_{1/2}$	I^{π}	μ (nm)*	Q (b)	Ref. Std.	Method	Reference
$^{25}_{13}$Al	0	7.18 s	$5/2^+$	3.6455(12)			β-NMR	1976Mi11
$^{26}_{13}$Al	0	7×10^5 y	5^+	+2.804(4)		$^{27}_{13}$Al	ABLS	1996Co04
					+0.27(3)	$^{27}_{13}$Al	ABLS	1997Le19
$^{27}_{13}$Al	0	Stable	$5/2^+$	+3.6415069(7)		$^{2}_{1}$H	N	1968Ep01
					+0.1466(10)		R	1999Ke07
					+0.1402(10)		R	1992Su01
					+0.150(6) a		Mu-X	1982We04
$^{28}_{13}$Al	0	2.24 m	3^+	3.242(5)			β-NMR	1981Mi14
					0.175(14)	$^{27}_{13}$Al	β-NMR	1978St31
	31	1.91 ns	2^+	+4.3(4)			IPAC	1972He22
$^{31}_{13}$Al	0	644 ms	$(5/2^+)$	(+)3.79(5)			LMR	2002Bo22

Applications : Plasma spectroscopy

Temperatures and densities for various plasmas



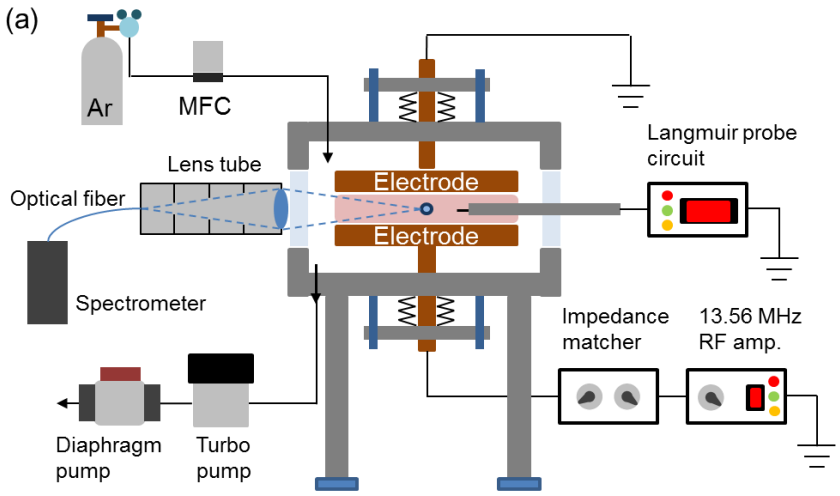


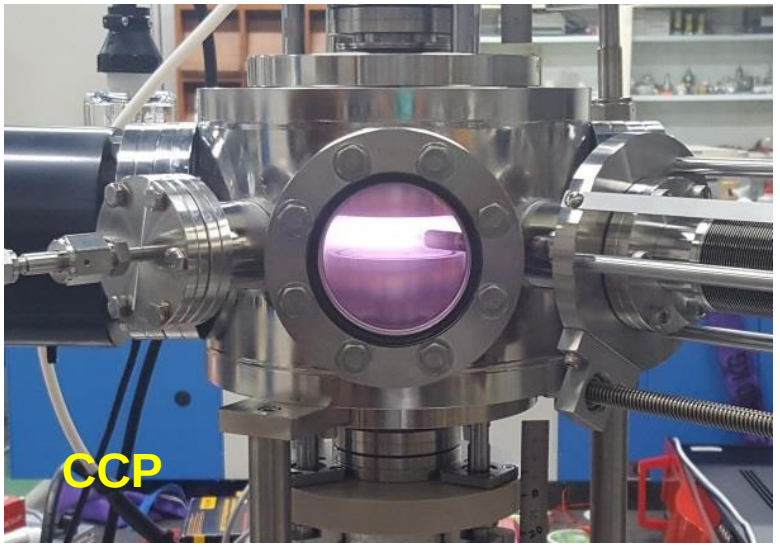


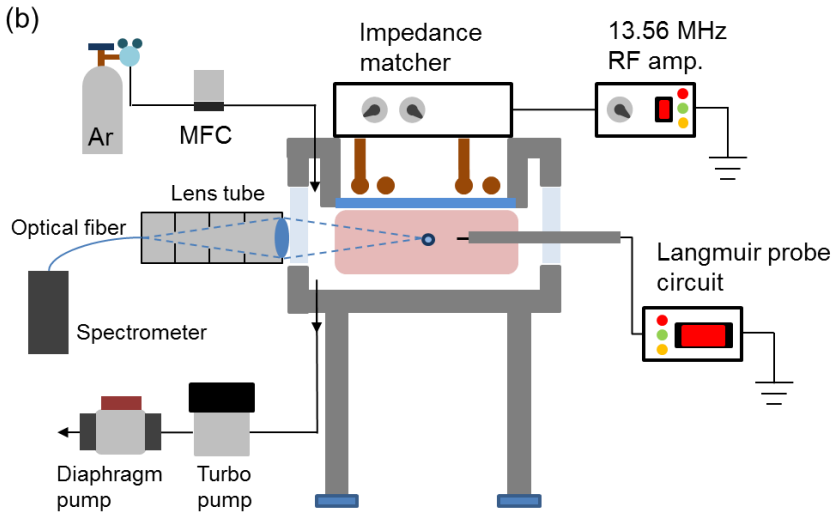
Tokamak Plasma Models

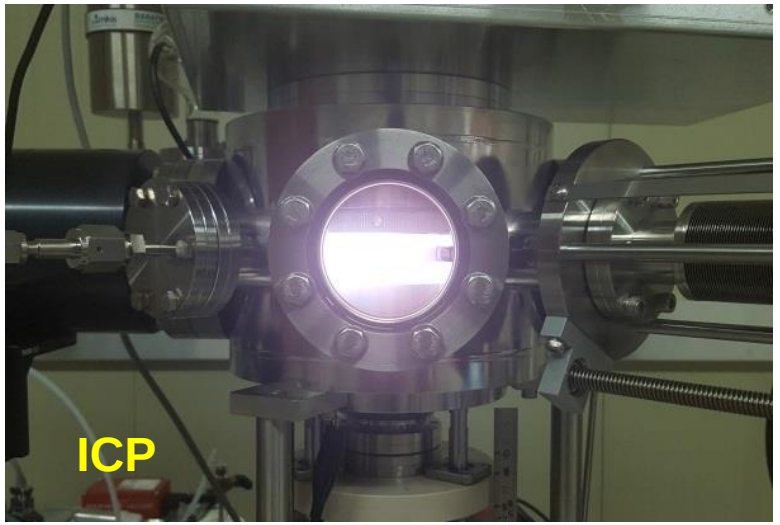
OES in low temperature & low density plasmas

Experimental setup









CRM for low temperature plasma

Steady state balance equation for excited levels

$$\frac{\partial N_i}{\partial t} + \nabla \cdot (D_a \nabla N_i) = \left(\frac{\partial N_i}{\partial t}\right)_{CR}, \quad \nabla \cdot (D_a \nabla N_i) \approx \nu_i^d N_i \;, \frac{\partial N_i}{\partial t} = 0$$

In the weakly ionizing plasma conditions $N_0 \alpha_I \gg n_+ \alpha_R$, $n_+ \approx n_e$

Populating terms **Depopulating terms**

$$\Rightarrow \sum_{j \neq i} n_e \alpha_{ji}^{ex} N_j + \sum_{j>i} \eta_{ji}(N_i) A_{ji} N_j = \sum_{j \neq i} n_e \alpha_{ij}^{ex} N_i + \sum_{j<i} \eta_{ij}(N_j) A_{ij} N_i + n_e \alpha_i^{\mathrm{I}} N_i + \sum_j \alpha_{ij}^{\mathrm{I}} N_i N_j + \nu_i^d N_i$$

Nonlinear terms

Ground level population

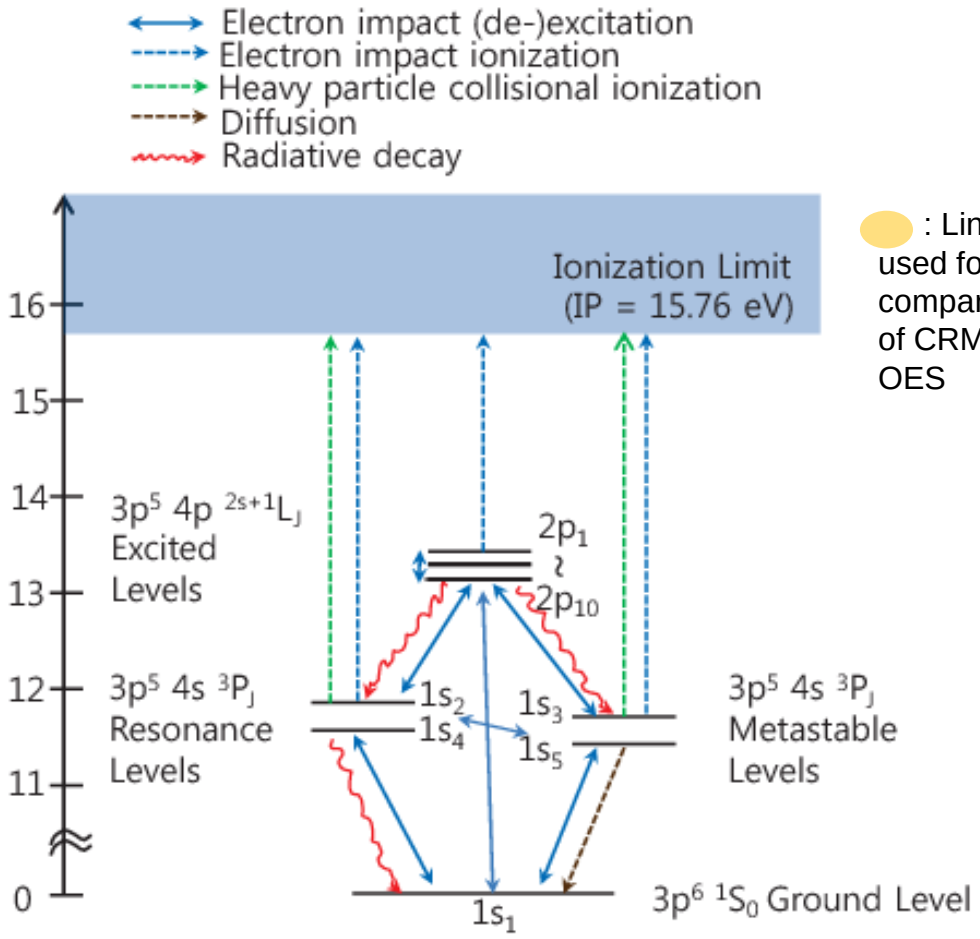
$$p_{tot} = N_0 k_B T_g + n_+ k_B T_i + n_e k_B T_e \approx N_0 k_B T_g$$

$$N_0 \cong \frac{p_{tot}}{k_B T_g} \; (constant)$$

Diagnostics for plasma parameters

Minimization of $\Delta(n_e, T_{eff}, R_{eff}, L_{eff}) = \sum \left(\frac{I_{ik}^{\mathrm{CRM}} - I_{ik}^{\mathrm{OES}}}{I_{ik}^{\mathrm{OES}}} \right)^2 \;, I_{ik}^{\mathrm{CRM}} = \frac{N_i \eta_{ik} A_{ik}}{\lambda_{ik}}$

CRM for Ar plasma

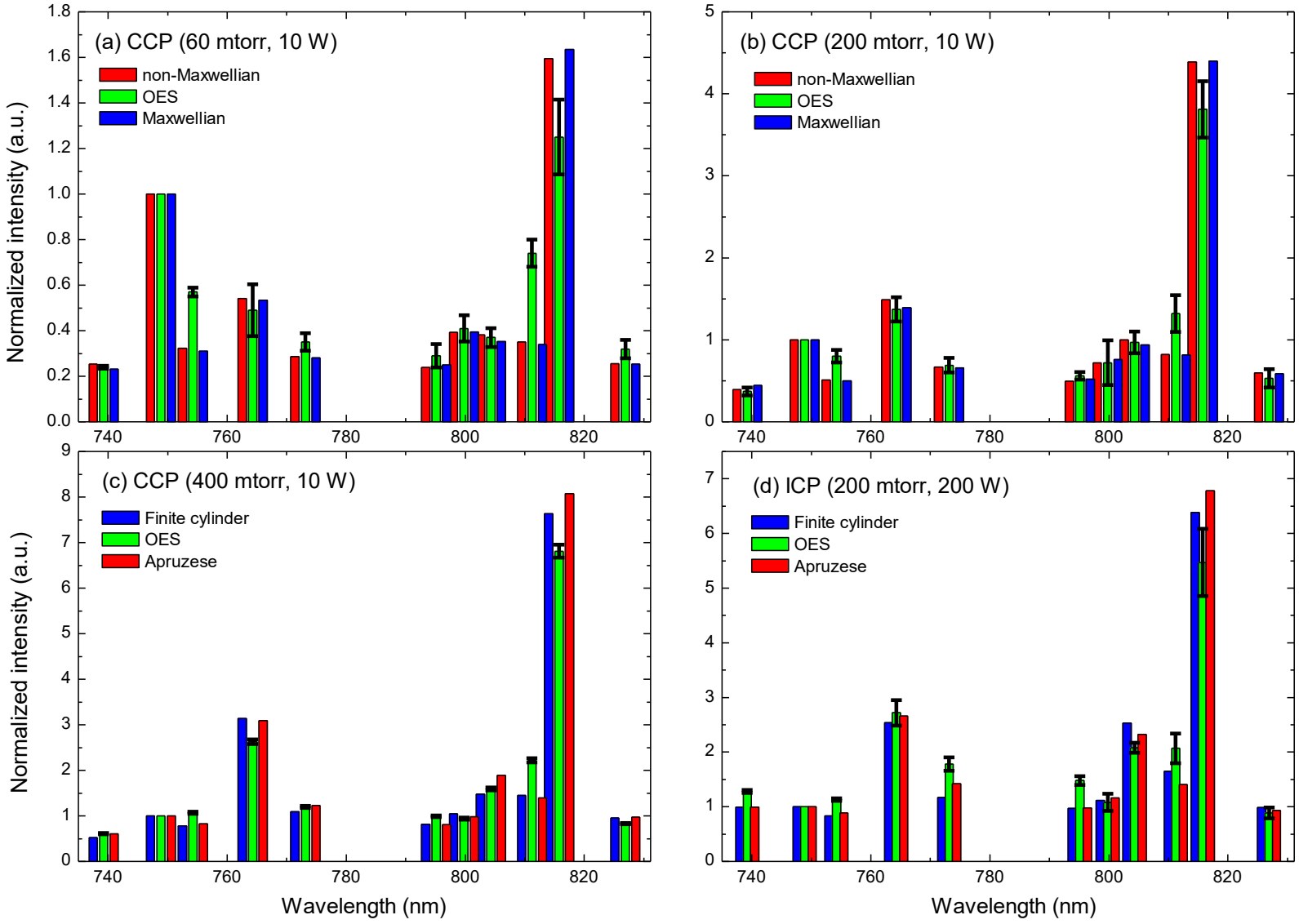


: Lines used for comparison of CRM with OES

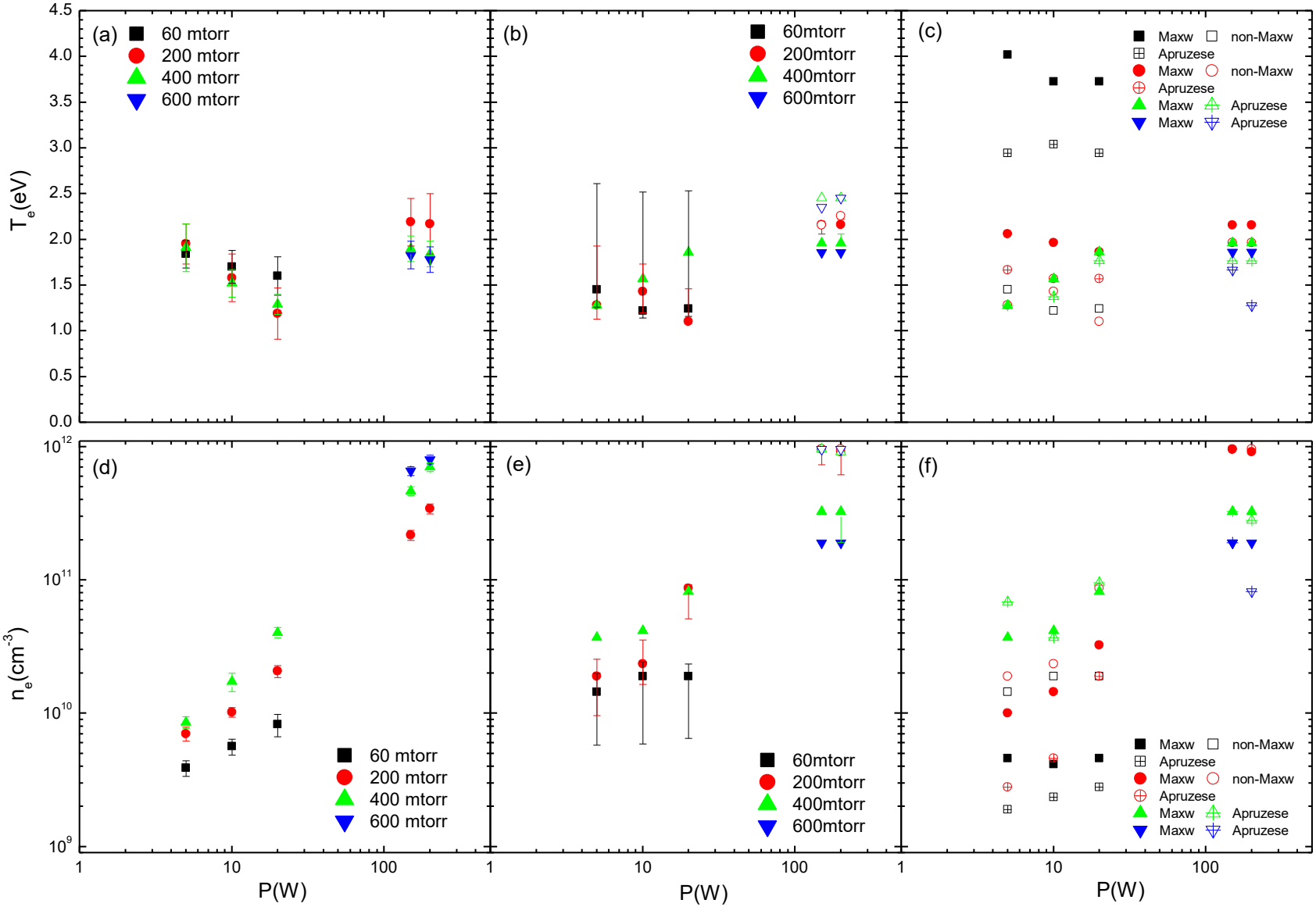
Transition wavelength (nm) and probability (10^8 1/s) in parentheses

Excited Levels	Resonance Levels		Metastable Levels	
	$1s_2$ (J=1)	$1s_4$ (J=1)	$1s_3$ (J=0)	$1s_5$ (J=2)
$2p_1$ (J=0)	750.39 (0.45)	667.73 (0.002)		
$2p_2$ (J=1)	826.45 (0.15)	727.29 (0.02)	772.42 (0.12)	696.54 (0.06)
$2p_3$ (J=2)	840.82 (0.22)	738.40 (0.08)		706.72 (0.04)
$2p_4$ (J=1)	852.14 (0.14)	747.12 (0.0003)	794.82 (0.19)	714.70 (0.006)
$2p_5$ (J=0)	858.01	751.47 (0.40)		
$2p_6$ (J=2)	922.45 (0.05)	800.62 (0.05)		763.51 (0.25)
$2p_7$ (J=1)	935.42 (0.01)	810.37 (0.25)	866.79 (0.02)	772.38 (0.05)
$2p_8$ (J=2)	978.45 (0.01)	842.46 (0.22)		801.48 (0.009)
$2p_9$ (J=3)				811.53 (0.33)
$2p_{10}$ (J=1)	1148.8 (0.002)	965.78 (0.05)	1047.0 (0.01)	912.30 (0.19)

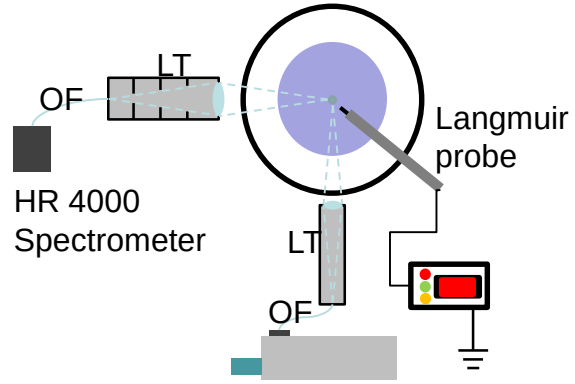
Measured and modeled spectra for Ar I



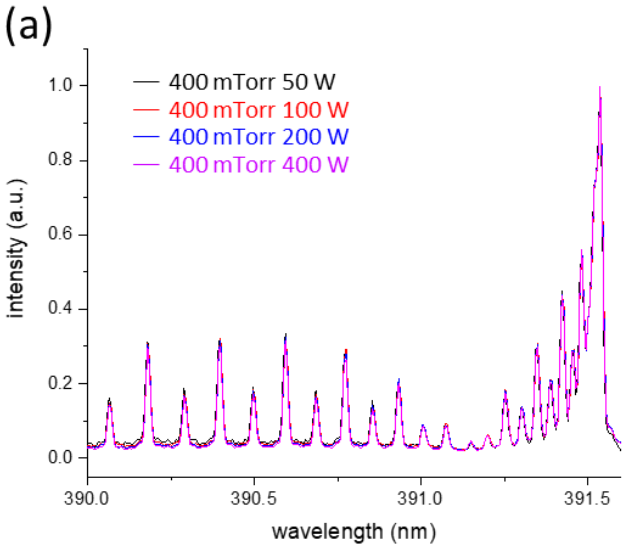
Diagnostics : OES with CRM *vs*. LP measurement

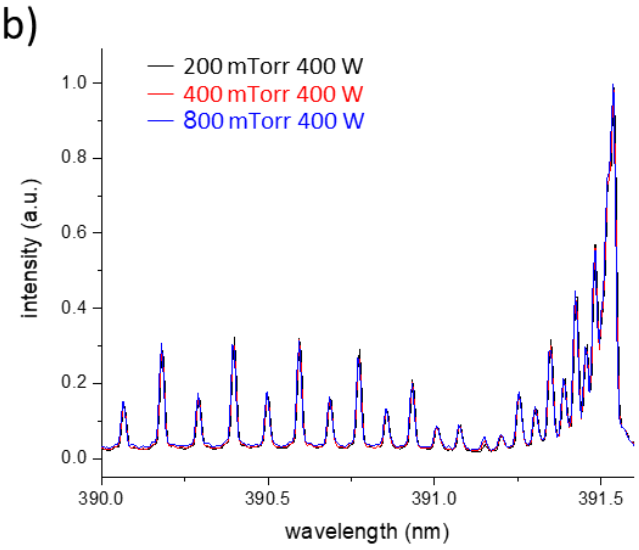


OES for low temperature He plasma



LT: lens tube
OF: optical fiber
MFC: mass flow controller



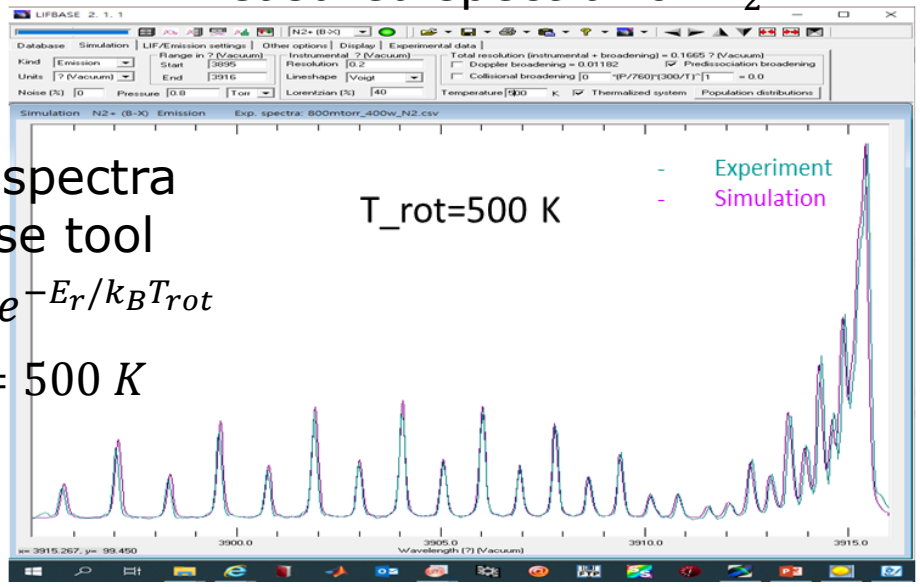


Gas temperature

T_g can be estimated with the N_2^+ rotational temperature obtained from the emission spectra of the N_2^+ transition $B^2\Sigma_u^+, v = 0 \rightarrow X^2\Sigma_g^+, v' = 0$ by inserting small amount of N_2 gas into the He plasma.

Measured spectra for N_2^+

(c)



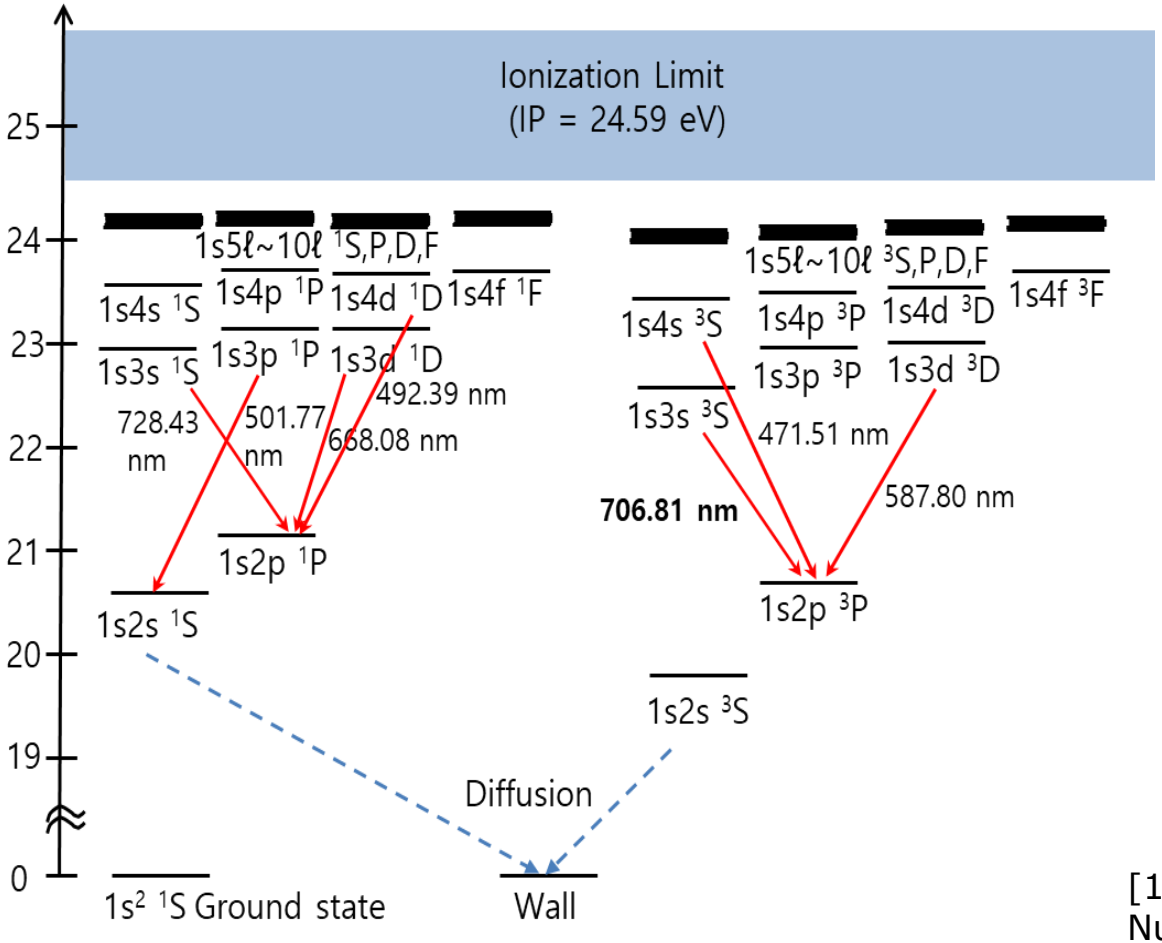
Modeled spectra by LIFbase tool

$I = D_0 k^4 S e^{-E_r/k_B T_{rot}}$

$\Rightarrow T_g \approx T_{rot} = 500\ K$

CRM for low temperature He plasma

Energy levels



$up\ to\ 1snl\ (n = 10, \ell = 3)$

Kinetic processes

1. $\mathrm{He} + \mathrm{e} \rightarrow \mathrm{He}^* + \mathrm{e}$ $\quad \alpha_{ij}^{ex}$ [1]
2. $\mathrm{He} + \mathrm{e} \rightarrow \mathrm{He}^+ + 2\mathrm{e}$ $\quad \alpha_i^{\mathrm{I}}$ [1]
3. $\mathrm{He}^* \rightarrow \mathrm{He} + h\nu$ $\quad \lambda_{ij}, A_{ij}$ [2]
4. $\mathrm{He}(1s2\ell) + \mathrm{He}(1s2\ell') \rightarrow \mathrm{He}^+ + \mathrm{He} + \mathrm{e}$ $\quad \alpha_{ij}^{\mathrm{I}}$

$$2.9 \times 10^{-9} \left(T_g/300\right)^{1/2} (cm^3/s)$$

5. $\mathrm{He}(1s2s) \rightarrow to\ wall$ $\quad \nu_i^d$

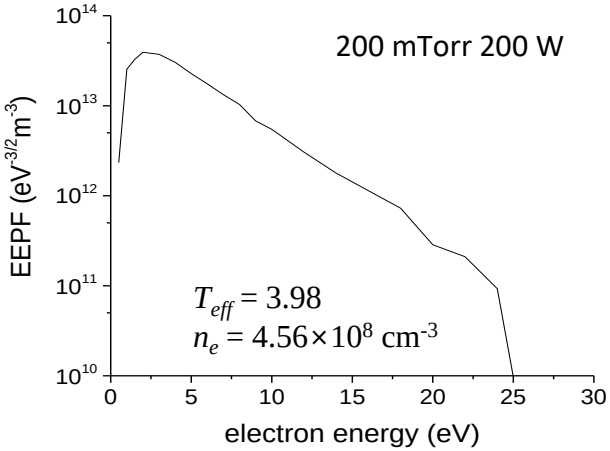
$$\nu_i^d = D_a \left(\left(\frac{2.405}{R_{eff}}\right)^2 + \left(\frac{\pi}{L_{eff}}\right)^2 \right),$$

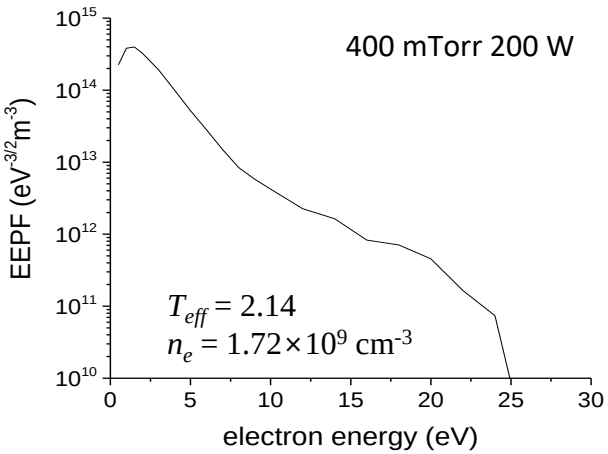
$$D_a = 8.992 \times 10^{-2} \frac{T_g^{3/2}}{p}\ (cm^3/s)$$

[1] Y. Ralchenko, et al., Atomic Data and Nuclear Data Tables 94 (2008) 603.
[2] G.W.F Drake, D.C. Morton, Astrophys. J. Suppl. Series 170 (2007) 251.

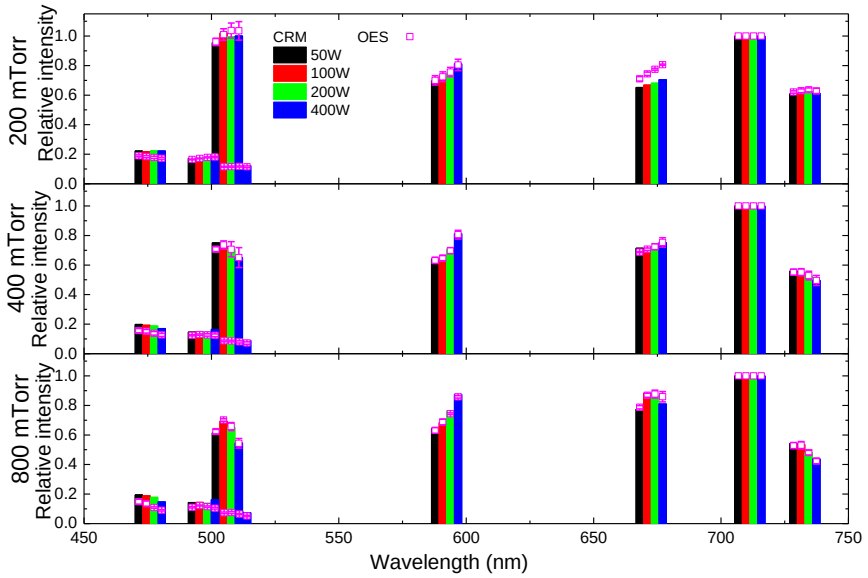
CRM for low temperature He plasma

Non-Maxwellian electron energy distribution

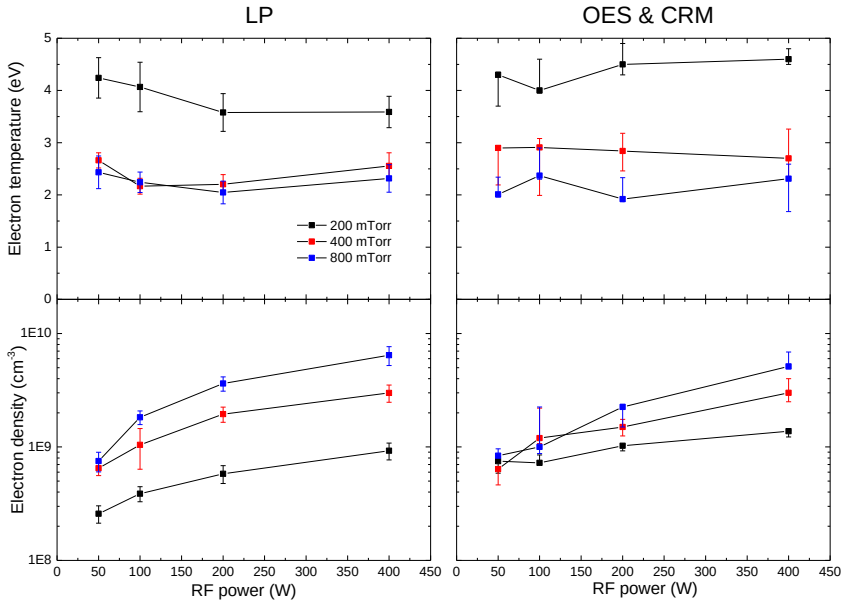




OES and CR modeling spectra



Electron temperature and density



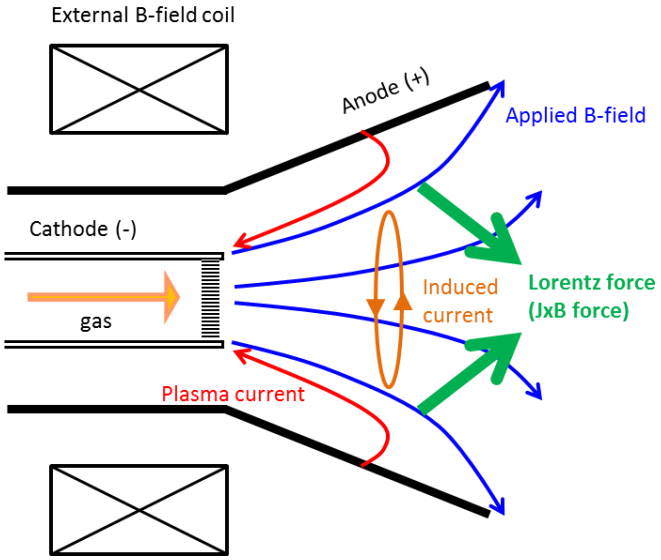
K.-B. Chai and D.-H. Kwon, Spectrochimica Acta Part B **183** 106269 (2021).

KAERI AF-MPD divertor simulator

Motivation of the construction of KAERI divertor plasma simulator

In order to develop divertor materials and cooling techniques resisting **high heat** and **particle fluxes** (ITER cases are 10 MW/m^2 and particle flux of 10^{24} /m^{2}s, DEMO cases are the much larger) we have constructed lab-scale divertor plasma simulator

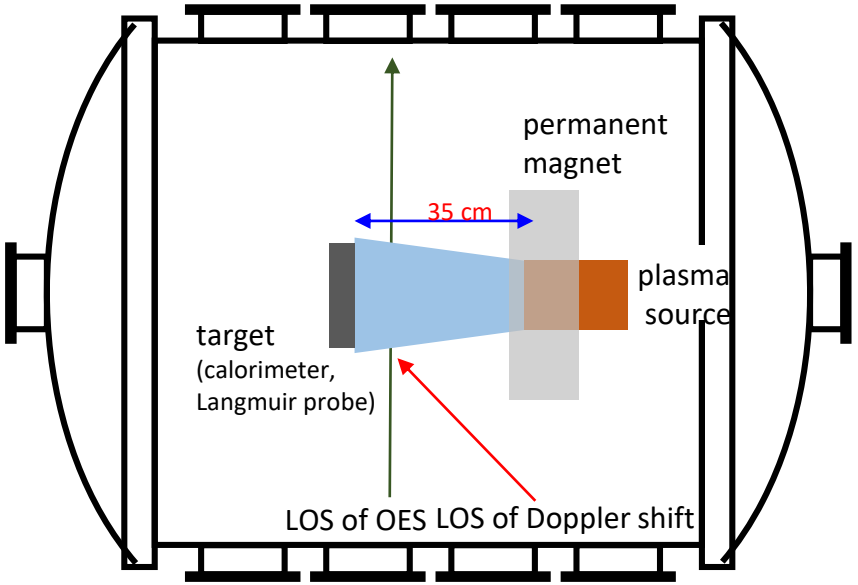
Applied-Field MagnetoPlasmaDynamic thruster (AF-MPD thruster) concept is used in KAERI divertor simulator



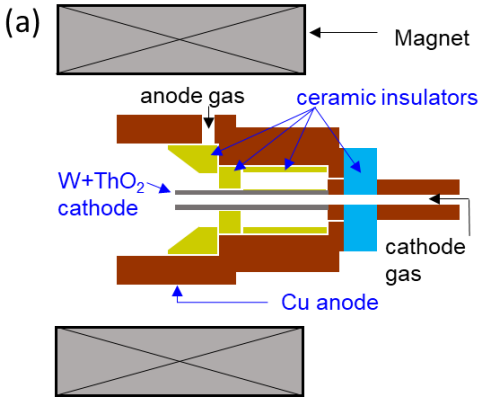
- Anode radius = 4/2 cm (type I/ type II), cathode radius = 0.6/0.4 cm (type I/ type II)
- Anode material: Cu, cathode material: W+ThO_2 (2%)
- Insulating material : ceramic (Al_2O_3)
- Sustain power supply : DC 100 kW (200 V, 500 A)
- External B-field: 0.17 T (NdFeB permanent magnet)
- Both anode & cathode can be water-cooled

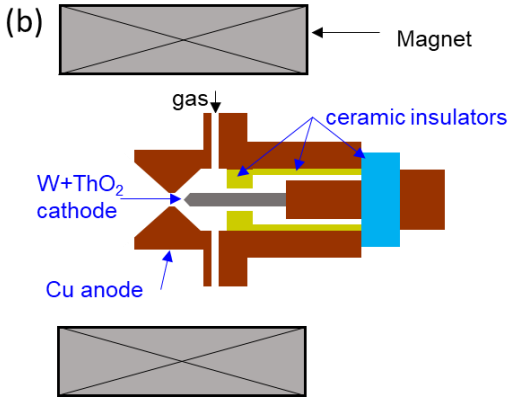
⇨ Operates at relatively low gas pressure (~1s mTorr) for PSI study and no need for separate Target chamber and additional vacuum system

KAERI AF-MPD divertor simulator



Plasma source schemes

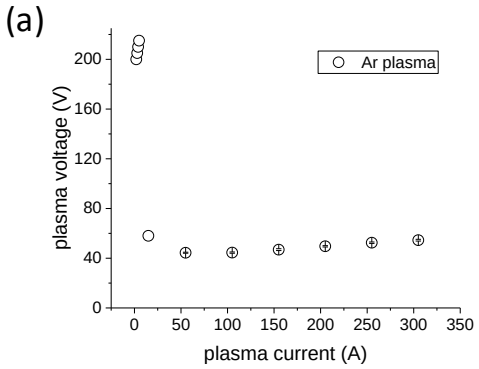


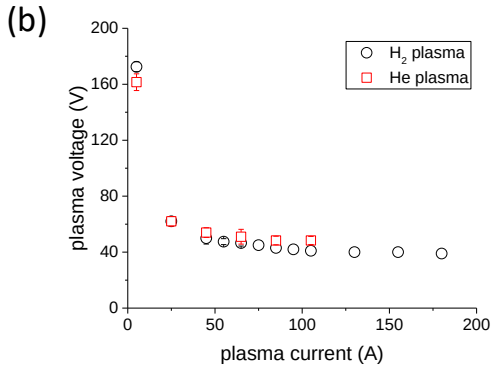


Type I for Ar

Type II for H_2, He

Arc characteristics



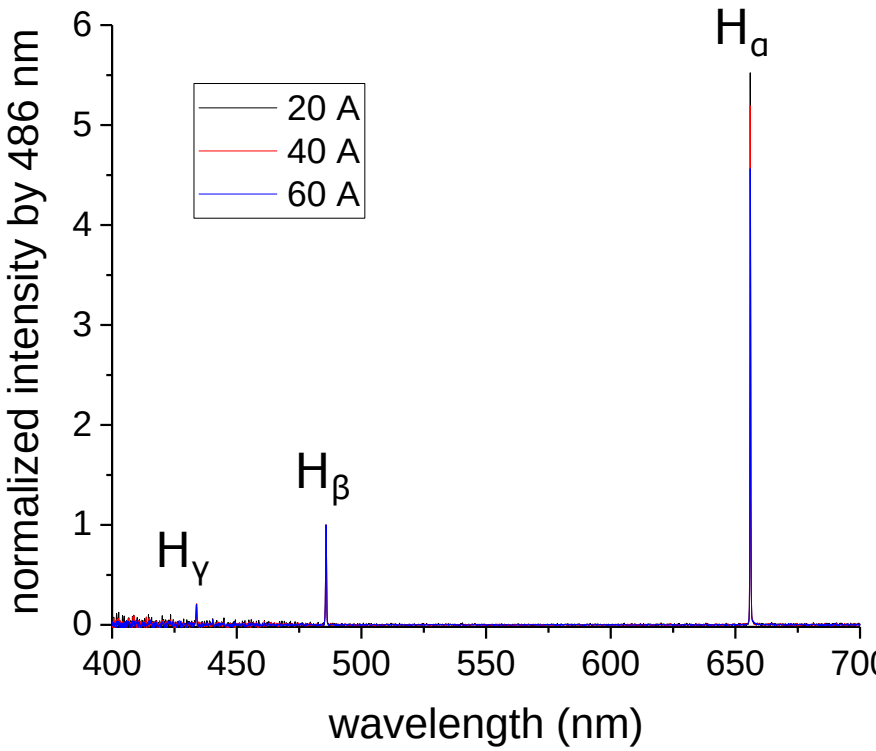


CRM for H plasma in KAERI divertor simulator

Considered processes

$H(n\geq1) + e \rightarrow H(n'\geq n) + e$ (1)
$H(n\geq1) + e \rightarrow H^+ + 2e$ (2)
$H(n\leq40) \rightarrow H(n' \leq n) + hv$ (3)
$H^+ + e \rightarrow H(n\leq40) + hv$ (4)
$H_2 + e \rightarrow H(n=1) + H(n'\leq3) + e$ (5)
$H_2 + e \rightarrow 2H(n=2) + e$ (6)
$H_2 + e \rightarrow H^+ + H(n=1) + e$ (7)
$H_2 + e \rightarrow H_2^+ + 2e$ (8)
$H_2^+ + e \rightarrow H(n=1) + H(n\geq2)$ (9)
$H_2^+ + e \rightarrow H^+ + H(n\leq2) + e$ (10)
$H_2^+ + e \rightarrow 2H^+ + e$ (11)
$H_3^+ + e \rightarrow 3H(n=1)$ (12)
$H_3^+ + e \rightarrow H_2 + H(n=2)$ (13)
$H_3^+ + e \rightarrow H^+ + 2H(n=1) + e$ (14)
$H_2^+ + H_2 \rightarrow H(n=1) + H_3^+$ (15)

Spectra for H



Cross section data from
R. K. Janev, D. Reiter, and U. Samm, Report JUEL-4105 (2003)
R. K. Janev et al., Elementary processes in Hydrogen –Helium plasmas (Berlin: Springer, 1987)

CRM for H plasma in KAERI divertor simulator

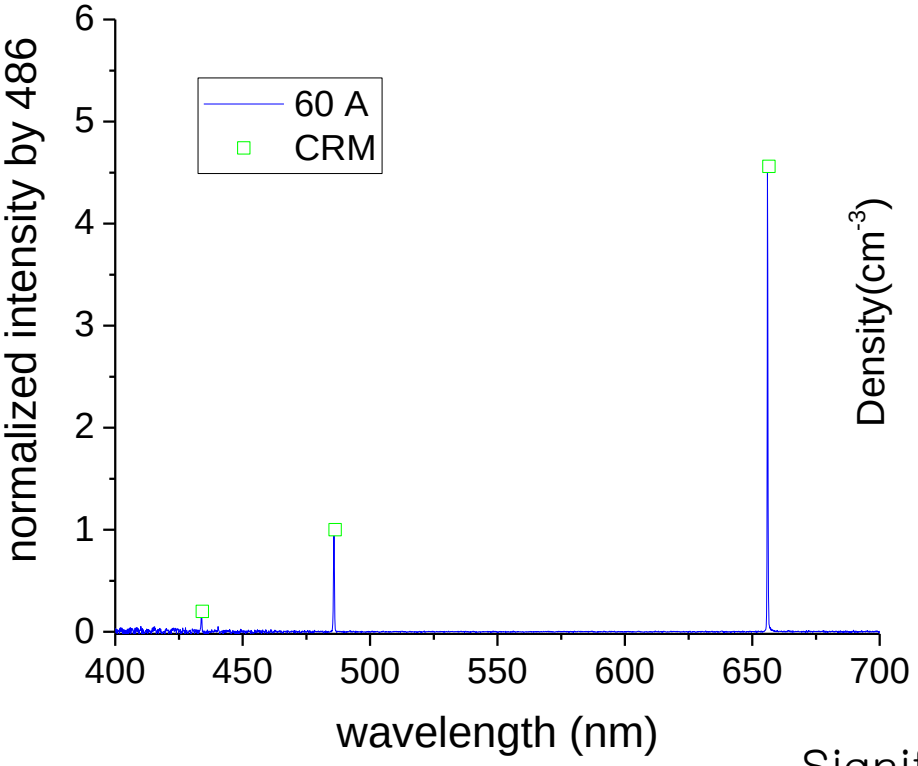
Rate balance equations for atomic levels $n_{a,j}$

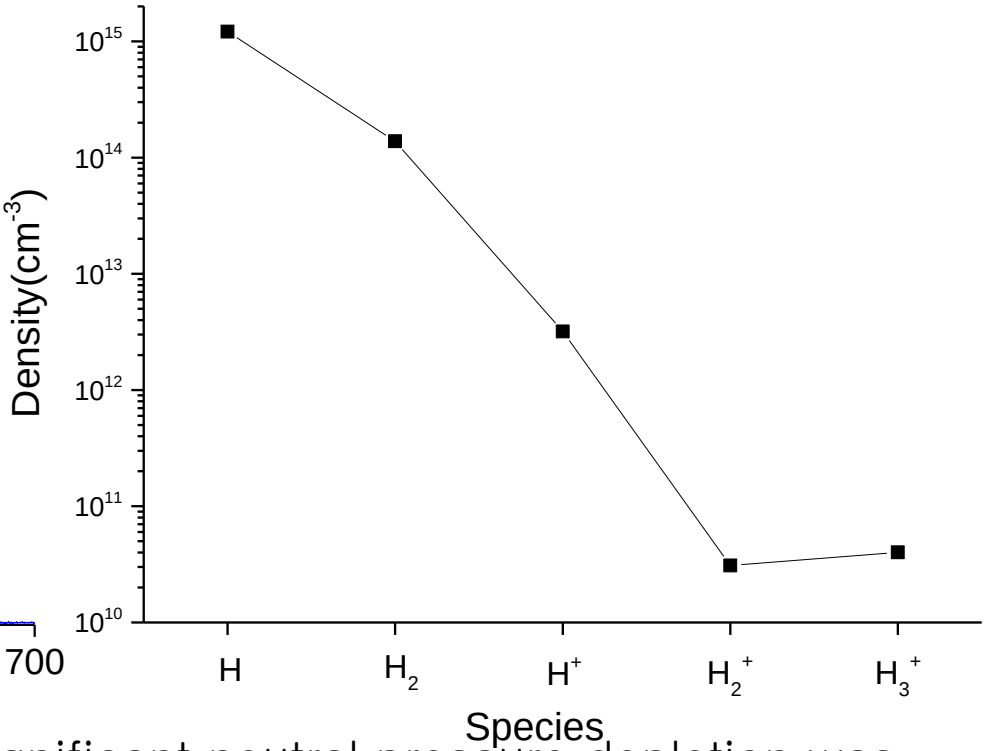
$$\frac{dn_{a,j}}{dt}=\sum_{q>j}^{40}\eta_{qj}A_{qj}n_{a,q}-\left(\sum_{q<j}\eta_{jq}A_{jq}+\frac{\gamma}{\tau}\delta_{j1}\right)n_{a,j}+$$
$$n_e\left(\sum_{q\neq j}\beta_{1,qj}n_{a,q}-\sum_{q\neq j}\beta_{1,jq}n_{a,j}-\beta_{2,j}n_{a,j}\right)+n_e\beta_{4,j}n_1$$
$$+n_e\left(\beta_{5,j}+\beta_6\delta_{j2}+\beta_7\,\delta_{j1}\right)n_m+n_e\left(\beta_{9,j}+\beta_{10,j}\right)n_2+$$
$$n_e\left(\beta_{12}\delta_{j1}+\beta_{13}\,\delta_{j2}+\beta_{14}\,\delta_{j1}\right)n_3+n_m\beta_{15}n_2+\delta_{j1}\sum_{i=1}^{3}\zeta_{ai}\left(\frac{\mu}{R}\right)^2D_{Ai}n_i$$

$$\frac{dn_i}{dt}=\delta_{i1}n_e\sum_{j=1}^{40}\left(\beta_{2,j}n_{a,j}-\beta_{4,j}n_1+2\beta_{11}n_2\right)+\delta_{i2}n_e\left(\beta_8n_m-\sum_{j=1}^{40}\beta_{9,j}\,n_2\right)$$
$$+(\delta_{i1}-\delta_{i2})n_e\sum_{j=1}^{2}\beta_{10,j}\,n_2-\delta_{i3}n_e(\beta_{12}+\beta_{13})n_3+(\delta_{i1}-\delta_{i3})n_e\beta_{14}n_3+$$
$$(\delta_{i3}-\delta_{i2})n_2\beta_{15}n_m-\left(\frac{\mu}{R}\right)^2D_{Ai}n_i$$

$$p_{tot}=n_mk_BT_m+k_BT_a\left(\sum_{j=1}^{40}n_{a,j}+n_1\right)+n_ek_BT_e+n_mk_B(n_2+n_3)$$

CRM for H plasma in KAERI divertor simulator





CRM

$T_m \approx T_a = 600K$, $P_{tot} = 100\ mtorr$

$R = 3.0$ cm (Infinate Cylinder)

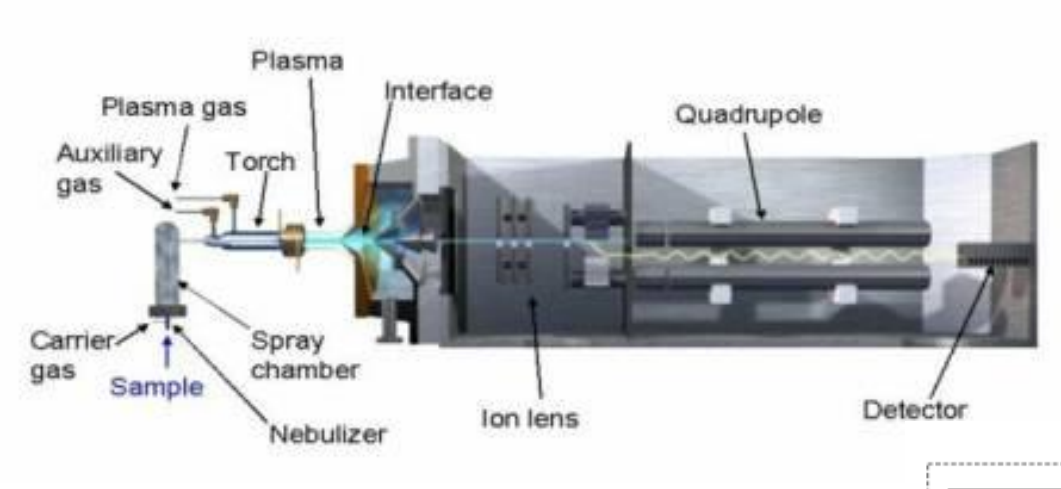
$n_e = 3.6 \times 10^{12}(cm^{-3})$, $T_e = 3.6$ eV

vs. LP measurement

$n_e = 1.7 \times 10^{12}(cm^{-3})$, $T_e = 4.0$ eV

Significant neutral pressure depletion was measured unlike CRM and the pressure balance is questionable. So rate balance equation for n_m of H_2 will be used instead of the pressure balance equation and the quasi-neutrality ($n_e \cong n_1 + n_2 + n_3$) will be used for n_3 of H_3^+ Instead of the rate balance equation.

Analytical chemistry by ICP-MS & OES



ICP-MS

Example of U

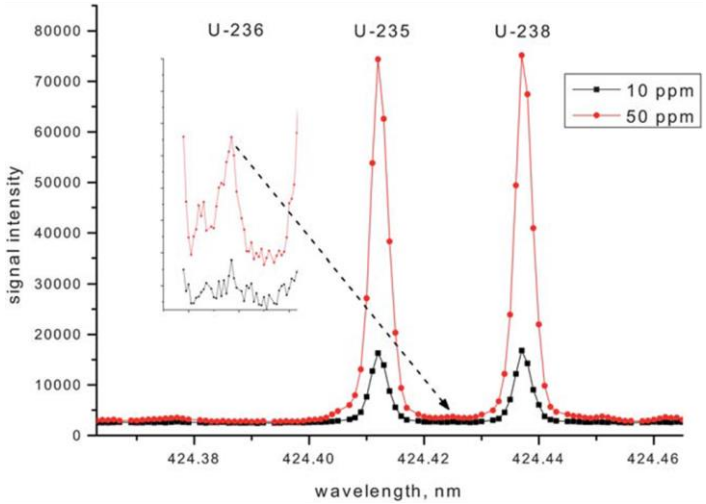
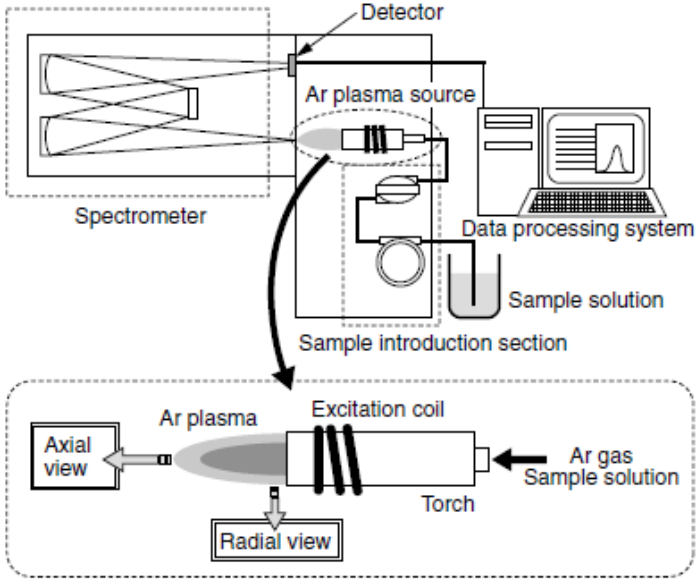


Fig. 1 highlights the spectral separation of ^{235}U and ^{238}U at ~424.4 nm, demonstrating the resolving power of the optical system of this commercially available ICP-OES instrument. This

2pm scanning!



ICP-OES

KAERI ADC (PEARL DB)

https://pearl.kaeri.re.kr