Relativistic atomic structure calculations with application in fusion plasma

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OVERVIEW OF THE PRESNATION

- Atomic Structure Calculations using Configuration Interaction technique and correlation effects (CIV3), Multiconfiguration Dirac-Fock (MCDF) Method and Flexible Atomic Code (FAC)

- Application I Characterization of hot dense plasma (HDP) with its parameters temperature, electron density, skin depth, plasma frequency in LTE condition

- Application II L-shell spectroscopy of neon and fluorine like copper ions from laser produced plasma

Relativistic Atomic Structure Calculations

We calculate

- Level Energies
- Transition energy/Wavelength
- Oscillator strength
- Transition probability or radiation rates
- Life time of excited states

Theoretical Methods

- Configuration Interaction method using non relativistic hamiltonian with relativistic corrections are added using perturbation theory in Breit-Pauli approximation. For light atoms, correlation effects dominate while relativistic corrections can be added using a perturbation theory as implemented in CIV3(configuration interaction version 3)[1]

- MCDF Multi-configuration Dirac-Fock and MCDHF Multi-configuration Dirac Hartree-Fock uses a fully relativistic atomic theory and variational principal for atomic structure caculations implemented in the GRASP(General Purpose Relativistic Atomic structure Package) [2]and GRASP2K[3]

- FAC[4] Flexible Atomic code fully relativistic code used for the calculation of energy levels , radiative data and scattering data.

1. A. Hibbert, Comput. Phys. Commun. 9,141 (1975)
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Configuration Interaction method

The configuration interaction wave function can be written in the form

$$\Psi(LS) = \sum_{i=1}^{M} a_i \phi_i(\alpha_i, LS)$$

where each of the single configuration functions ϕ_i are constructed from one electron orbitals (or spin -orbitals), whose angular momenta are coupled as specified by α_i (called the seniority number) to form states of given total L, S common to all M configurations.

The orbitals used for constructing (ϕ_i) is a product of radial function, a spherical harmonics and a spin function:

$$u_{nlm}(r, m_s) = \frac{1}{r} P_{nl}(r) Y_l^m(\theta, \phi) \chi(m_s)$$

The radial part of each orbital is written as a linear combination of normalized Slater -type orbitals (STO).

$$P_{nl}(r) = \sum_{j=1}^{k} C_{jnl}\, \chi_{jnl}(r) \qquad \text{where} \qquad \chi_{jnl}(r) = \sum_{j=1}^{k} \frac{(2\xi_{jnl})^{I_{jnl}+1/2}}{[(2I_{jnl})!]^{1/2}} r^{I_{jnl}} \exp(-\xi_{jnl}\, r)$$

In obtaining the final wave function the radial function are determined, together with the coefficients (a_i) variationally.

The N- electron Hamiltonian given by

$$H_{NR} = \sum_{i=1}^{N} \left(\frac{-\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{r_i}\right) + \sum\sum_{i<j} \frac{e^2}{r_{ij}}$$

where subscript i indicates the coordinates of electron i, and $r_{ij} = |r_i - r_j|$ the double summation is over all pairs of electrons.

The Hamiltonian in the Breit-Pauli approximation becomes

$$H^N_{BP} = H^N_{NR} + H^N_{mass} + H^N_{D1} + H^N_{SO}$$

The optimum value of the wave function are: Choice of configurations; Radial functions; The expansion coefficients a_i

Types of Correlation

Hartree-Fock (HF) sea is defined as a set of orbitals occupied in the HF configuration including the orbitals that have same or smaller n values.

a) Internal – Correlation

This is described by configurations built entirely from orbitals in the HF sea (this includes near-degeneracy).

C (^{3}P) :$1s^2\ 2s^2\ 2p^2$, $1s^2\ 2p^4$, $2s^2\ 2p^4$

In terms of the first two configurations, the CI wave function of ground state of C can be written as

$$\Psi(^3P) = a_1\Phi_1\left(1s^2 2s^2 2p^{2\ 3}P\right) + a_2\Phi_2\left(1s^2 2p^{4\ 3}P\right)$$

where $a_1 = 0.94$ and $a_2 = 0.34$ with $(a_1^2 + a_2^2 = 1)$

These are very important to include due to being quite big in size and due to 2p function being in the same region of space as 2s

b) Semi internal correlation

This is described by the configurations constructed from the (N-1) orbitals of HF sea plus one electron outside the HF sea

C: $1s^2\ 2s^2\ 2p^2\ \ ^3P$ H. F.

$1s^2\ 2p^4\ \ ^3P$ Internal (same n value)

$1s^2\ 2p^3\ 3p\ \ ^3P$

$1s^2\ 2p^3\ 4f\ \ ^3P$ Semi – internal {one $\bar{e}$ has n = 3 or n = 4}

coefficients $\simeq$ 0.05 – 0.01

c) External Correlation

Out of n electrons, (N – 2) electrons are described by function in H.F. sea

2 electrons are described by functions outside H.F. sea.

C: $1s^2\ 2s^2\ 3p^2\ \ ^3P$ all external

$1s^2$ (2s 2p) 3s 3p ^{3}P (two $\bar{e}$ have n = 3)

Expansion co – efficients $\simeq$ 0.01-0.001

Choice of configurations

In general , effects (i) and (ii) involve finite C. I. and are unique to open shells. In addition these effects are strongly Z, N and symmetry dependent. The third effect i. e. external correlation involve infinite CI, therefore for practical calculations one should include HF, internal and semi-internal and some of external correlations.

Optimal choice of radial functions:

There are two possibilities for the radial functions when further configurations to HF are included. One can either fix the HF radial functions as is done in the superposition of configuration method (SOC) or allow the HF functions to vary again as is done in multi configuration Hatree-Fock (MCHF). The CIV3 code developed by Hibbert is an SOC base program, i.e. in it the HF functions are augmented by further functions

There are two ways of treating the variational principle:

(a)An initial choice of the radial function is made. The Hamiltonian matrix H is set up and diagonalised to yield eigenvalues E^j and a_i^j . Next the radial functions are changed according to some prescription and the process is repeated until there is no significant improvement in the final E^j. This scheme is particularly useful if P_{nl} depends on variable parameters and is basis of SOC method, employed in the configuration code CIV3.

(b) Indirectly the eigen value E^j may be used , together with appropriate constraints, as a variational function of the radial function (P_{nl}). From this the variation equation (or intgro-differential equations HF type) for the (P_{nl}) can be derived. Here initial choice of the (P_{nl}) and the (a_i) is made giving a new set of radial function after solving the HF type of equations. From this , the Hamiltonian matrix H may be set up and diagonalised to yield (a_i). This process is repeated until self -consistency is reached. It is the basis of the multi-configurational Hartree-Fock (MCHF) scheme also used in Froese-Fischer's code which yields numerical radial functions.

Atomic Structure Parameters

- Atomic oscillator strengths and transition probabilities are the basic parameters which characterize the strength of radiative transition between two levels of atom or ion.

- Oscillator strength is a dimensionless quantity that expresses the probability of absorption or emission of electromagnetic radiation in transitions between energy levels of an atom/ion .

- Oscillator Strength between initial and final states ψ_i and ψ_j in length and velocity form is defined as follows:

$$f_{ij}^{l} = \frac{2}{3}\frac{\Delta E}{g_i}\left| \left\langle \psi_j \right| \sum_{p=1}^{N} \vec{r_p} \left| \Psi_i \right\rangle \right|^2 \qquad \Delta E = E_f - E_i \qquad f_{ij}^{v} = \frac{2}{3}\frac{1}{\Delta E g_i}\left| \left\langle \psi_j \right| \sum_{p=1}^{N} \vec{\nabla}_p \left| \Psi_i \right\rangle \right|^2$$

Length form *Velocity form*

- Transition probability of a particular transition is the probability of the occurrence of that transition from one state to another state.

$$A_{fi} = \frac{6.6702 \times 10^{15}}{\lambda^2}\frac{g_i}{g_f} f,$$

- Lifetime for a level j is reciprocal of sum of transition probability and is given by

$$\tau_j = \frac{1}{\sum_i A_{ji}}$$

$$S = \left| \left\langle \psi_f \left| \sum_{j=1}^{N+1} r_j \right| \psi_i \right\rangle \right|^2$$

- Generalised Line strength is given by :

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Breit-Pauli energy levels and radiative lifetimes in neutral chlorine*

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Abstract. Breit-Pauli Energy levels, oscillator strengths and transition probabilities for all the transitions in Cl I between the fine structure levels of $3s^2 3p^5$, $3s^2 3p^4 3d$, $3s^2 3p^4 4s$ and $3s^2 3p^4 4p$ states are calculated using extensive configuration interaction (CI) wave functions. We have also determined the lifetimes of $3s^2 3p^4 3d$, $3s^2 3p^4 4s$ and $3s^2 3p^4 4p$ levels. The relativistic effects are included through Breit-Pauli approximation via spin-orbit, Darwin and mass correction terms. Prior to the calculations of the oscillator strengths and transition probabilities, we fine-tune the CI coefficient using experimental energies. Our results are compared with experimental and other available theoretical data. The calculated energy levels are in close agreement with most of the NIST compiled data. We predict new lifetime data for several levels where no other theoretical and/or experimental results are available, which will form the basis for the future experimental work.

PACS. 32.70.Cs Oscillator strengths, lifetimes, transition moments – 32.10.Fn Fine and hyperfine structure – 31.15.Pf Variational techniques

Table 1. Method of determining the radial functions.

Orbital	Process of optimization	
$1s$, $2s$, $2p$, $3s$	Hartree-Fock of $3p^4\,{}^3\mathrm{P}$ of Cl II (Clementi and Roetti, 1974)	
$3p$	Exponents taken from the Hartree-Fock orbital of $3p^4$ of Cl II coefficient reoptimized	
	On $3p^4 4s$ of Cl I	
	Eigen value minimized	Configurations
$3d$	$3p^4 3d\,{}^4\mathrm{D}$	$3p^4 3d$
$4s$	$3p^4 4s\,{}^4\mathrm{P}$	$3p^4 4s$
$4p$	$3p^4 4p\,{}^4\mathrm{D}^\mathrm{o}$	$3p^4 4p$
$4d$	$3p^4 3d\,{}^4\mathrm{D}$	$3p^4 3d$, $3p^4 4d$
$4f$	$3p^4 3d\,{}^4\mathrm{P}$	$3p^4 4s$, $3p^4 3d$, $3p^4 4d$, $3p^3 3d 4f$
$5s$	$3p^4 4p\,{}^4\mathrm{D}^\mathrm{o}$	$3p^4 4p$, $3p^3 4s 5s$
$5p$	$3p^4 4p\,{}^4\mathrm{P}^\mathrm{o}$	$3p^4 4p$, $3p^4 5p$
$5d$	$3p^4 3d\,{}^4\mathrm{F}$	$3p^4 3d$, $3p^4 4d$, $3p^4 5d$
$5f$	$3p^4 4p\,{}^4\mathrm{D}^\mathrm{o}$	$3p^4 4p$, $3p^4 4f$, $3p^4 5f$
$6s$	$3p^4 4s\,{}^4\mathrm{P}$	$3p^4 4s$, $3p^4 5s$, $3p^4 6s$, $3p^4 3d$, $3p^4 4d$, $3p^4 5d$, $3s 3p^5 4p$
$6d$	$3p^4 4s\,{}^4\mathrm{P}$	$3p^4 4s$, $3p^4 5s$, $3p^4 6s$, $3p^4 3d$, $3p^4 4d$, $3p^4 5d$, $3p^4 6d$

Configurations for even parity states: $3s3p^6$, $3s^23p^43d$, $3s^23p^44d$, $3s^23p^44s$, $3s^23p^45s$, $3s^23p^46s$, $3s^23p^46d$, $3p^63d$, $3p^64d$, $3s^65d$, $3s3p^43d^2$, $3s3p^44d^2$, $3s3p^45d^2$, $3s^23p^23d^3$, $3s^23p^24d^3$, $3s^23p^23d^24s$, $3p^43d^24d$, $3s3p^43d4d$, $3s3p^43d5d$, $3s3p^44d5d$, $3s3p^44d6d$, $3s3p^45d6d$, $3s3p^43d4s$, $3s3p^43d5s$, $3s3p^44d5s$, $3s^23p^33d4p$, $3s^23p^33d5p$, $3s^23p^33d4f$, $3s^23p^33d5f$, $3s^23p^34d4f$, $3s^23p^34d5f$, $3p^64s$, $3p^65s$, $3p^66s$, $3s3p^44s^2$, $3s3p^45s^2$, $3s3p^46s^2$, $3p^44s^25s$, $3s3p^44s5s$, $3s3p^44s6s$, $3s3p^45s6s$, $3s^23p^34s4p$, $3s^23p^34s4f$, $3s^23p^34s5p$, $3s^23p^34s5f$, $3s3p^54p$, $3s3p^55p$, $3s3p^54f$, $3s3p^55f$, $3s3p^44p5p$, $3s3p^44f5f$.

Configurations for odd parity states: $3s^23p^5$, $3s^23p^44p$, $3s^23p^45p$, $3s^23p^44f$, $3s^23p^45f$, $3s3p^53d$, $3s3p^54d$, $3s3p^55d$, $3s3p^56d$, $3p^53d^2$, $3p^54d^2$, $3p^55d^2$, $3s^23p^33d^2$, $3s^23p^34d^2$, $3s^23p^35d^2$, $3s^23p^33d4d$, $3s^23p^33d5d$, $3s^23p^34d5d$, $3s^23p^34d6d$, $3s^23p^35d6d$, $3s^23p^33d4s$, $3s^23p^33d5s$, $3s^23p^34d5s$, $3p^64p$, $3p^65p$, $3p^54p^2$, $3p^55p^2$, $3s^23p^34p^2$, $3s^23p^35p^2$, $3s^23p^34p5p$, $3p^54p5p$, $3s^23p^34p4f$, $3p^65f$, $3s^23p^34f^2$, $3s^23p^35f^2$, $3s3p^54s$, $3s3p^55s$, $3s3p^56s$, $3s^23p^34s^2$, $3s^23p^35s^2$, $3s^23p^34s5s$, $3s^23p^34s6s$, $3s^23p^35s6s$, $3s^23p^34s4d$, $3s^23p^34s5d$.

Table 3. Excitation energies (in cm^{-1}) relative to the ground state $3s^2 3p^5$ ($^2P^o_{3/2}$) and lifetimes (ns).

Level	Term	J	Present (this work)	NIST (expt.)	LP present	LP NIST	Lifetimes (ns)
$3s^2 3p^5$	$^2P^o$	3/2	00	00	92	95	
		1/2	882	882	92	95	
$3s^2 3p^4(^3P)4s$	^4P	5/2	71959	71958	98	100	3133
		3/2	72315	72489	98	98	70.0
		1/2	72828	72827	97	99	289
	^2P	3/2	74421	74226	98	98	1.37
		1/2	74866	74866	98	99	1.34
$3s^2 3p^4(^3P)4p$	$^4P^o$	5/2	82897	82919	95	96	31.3
		3/2	83107	83131	93	94	31.4
		1/2	83345	83365	95	97	31.2
	$^4D^o$	7/2	83885	83894	99	100	25.9
		5/2	84128	84132	68	66	30.0
		3/2	84465	84485	78	82	28.6
		1/2	84637	84689	75	96	28.9
$3s^2 3p^4(^1D)4s$	^2D	5/2	84180	84120	97	100	4.52
		3/2	84161	84122	97	100	4.54
$3s^2 3p^4(^3P)4p$	$^2D^o$	5/2	84639	84648	69	68	35.5
		3/2	84932	84988	57	57	34.2
	$^2P^o$	1/2	84892	85244	65	60	9.39
		3/2	85350	85442	59	64	33.0
$3s^2 3p^4(^3P)4p$	$^4S^o$	3/2	85814	85735	94	88	46.6
	$^2S^o$	1/2	86226	85918	65	65	30.4
$3s^2 3p^4(^3P)3d$	^4D	7/2	87965	87979	98	97	249
		5/2	88087	88080	97	96	185
		3/2	88168	88189	99	97	162
		1/2	88251	88273	98	99	188
	^4F	9/2	90180	90194	99	100	8681
		7/2	90444	90488	89	53	106
		5/2	90688	90749	82	66	4.80
		3/2	90523	90949	98	90	5.89
	^4P	1/2	91035	91069	94	99	60.1
		3/2	91610	91539	98	84	0.939
		5/2	91691	91661	89	59	14.7
	^2F	7/2	91112	91089	89	53	95.4
		5/2	92006	91907	87	53	6.21
	^2D	5/2	91067	91127	71	52	0.849
		3/2	91411	91174	94	76	5.76
	^2P	1/2	91661	91564	88		2.47
		3/2	92026	92194	92		1.75
$3s^2 3p^4(^1D)3d$	^2S	1/2	93095		66		64.4
$3s^2 3p^4(^1D)4p$	$^2P^o$	3/2	94528	94314	92	97	30.9
		1/2	94698	94469	90	96	30.3
	$^2F^o$	5/2	94854	95145	99	100	34.6
		3/2	95199	95180	99	100	
	$^2D^o$	5/2	96500	96483	99	100	15.4
		3/2	96509	96486	99	100	31.2
$3s^2 3p^4(^1S)4s$	^2S	1/2	99566	99534	92	91	1.06

Table 4. Oscillator strengths and transition probabilities (s^{-1}) (see the *Supplementary Online Material* for the complete version of the table).

Upper Level	Lower Level	f_l	f_v	A_l	A_v	Others (f_l)		
						Ojha [16]	RQDO [14]	Expt[a,c,d] /SST[b]
$3s^23p^4(^3P)4s\ ^4P_{1/2}$	$3s^23p^5\ ^2P_{1/2}$	0.0009	0.0007	0.3123(7)	0.2294(7)	0.0006		
	$3s^23p^5\ ^2P_{3/2}$	0.0000	0.0000	0.3335(6)	0.3018(6)	0.0000		
$3s^23p^4(^3P)4s\ ^4P_{3/2}$	$3s^23p^5\ ^2P_{1/2}$	0.0009	0.0007	0.1549(7)	0.1199(7)	0.0006		
	$3s^23p^5\ ^2P_{3/2}$	0.0004	0.0003	0.1273(8)	0.0979(8)	0.0026		
$3s^23p^4(^3P)4s\ ^4P_{5/2}$	$3s^23p^5\ ^2P_{3/2}$	0.0001	0.0001	0.3192(6)	0.2228(6)	0.0001		
$3s^23p^4(^3P)4s\ ^2P_{3/2}$	$3s^23p^5\ ^2P_{1/2}$	0.0605	0.0505	0.1086(9)	0.0843(9)	0.0474	0.0561	0.055[a]
								0.038[c]
								0.0530[b]
	$3s^23p^5\ ^2P_{3/2}$	0.1685	0.1322	0.6194(9)	0.4860(9)	0.1324	0.1368	0.153[a]
								0.147[b]
$3s^23p^4(^3P)4s\ ^2P_{1/2}$	$3s^23p^5\ ^2P_{1/2}$	0.1326	0.1034	0.4843(9)	0.3775(9)	0.1051	0.1017	0.093[a]
								0.116[b]
	$3s^23p^5\ ^2P_{3/2}$	0.0350	0.0275	0.2616(9)	0.2060(9)	0.0264	0.0249	0.028[a]
								0.0299[b]
								0.100[c]
								0.109[d]
$3s^23p^4(^1D)4s\ ^2D_{5/2}$	$3s^23p^5\ ^2P_{3/2}$	0.0701	0.0535	0.2210(9)	0.1685(9)	0.0677		
	$3s^23p^4(^3P)4p\ ^4P_{3/2}$	0.0001	0.0012	0.4454(2)	0.6644(3)			
	$3s^23p^4(^3P)4p\ ^4P_{5/2}$	0.0000	0.0000	0.1014(2)	0.1445(3)			
	$3s^23p^4(^3P)4p\ ^4D_{5/2}$	0.0000	0.0076	0.6517(2)	0.1335(2)			
	$3s^23p^4(^3P)4p\ ^4D_{7/2}$	0.0001	0.0000	0.4898(3)	0.2606(3)			
$3s^23p^4(^1D)4s\ ^2D_{3/2}$	$3s^23p^5\ ^2P_{1/2}$	0.0850	0.0646	0.1967(9)	0.1495(9)	0.0806		
	$3s^23p^4(^3P)4p\ ^4P_{1/2}$	0.0001	0.0019	0.1862(2)	0.4388(3)			
	$3s^23p^5\ ^2P_{3/2}$	0.0050	0.0036	0.2348(8)	0.1719(8)	0.0052		
	$3s^23p^4(^3P)4p\ ^4P_{3/2}$	0.0000	0.0004	0.2046(2)	0.2707(3)			
	$3s^23p^4(^3P)4p\ ^4P_{5/2}$	0.0000	0.0000	0.1731(1)	0.1825(2)			
	$3s^23p^4(^3P)4p\ ^4D_{5/2}$	0.0000	0.0000	0.7584(-3)	0.1254(0)			
$3s^23p^4(^1S)4s\ ^2S_{1/2}$	$3s^23p^5\ ^2P_{1/2}$	0.0499	0.0428	0.3243(9)	0.2778(9)			
	$3s^23p^4(^3P)4p\ ^4P_{1/2}$	0.0000	0.0000	0.5843(4)	0.2196(4)			
	$3s^23p^4(^3P)4p\ ^4D_{1/2}$	0.0002	0.0002	0.2908(5)	0.3082(5)			
	$3s^23p^4(^3P)4p\ ^2P_{1/2}$	0.0008	0.0007	0.1196(6)	0.1044(6)			
	$3s^23p^4(^3P)4p\ ^2S_{1/2}$	0.0000	0.0000	0.3108(4)	0.3715(4)			
	$3s^23p^4(^1D)4p\ ^2P_{1/2}$	0.0006	0.0034	0.9404(4)	0.5469(5)			
	$3s^23p^5\ ^2P_{3/2}$	0.0469	0.0399	0.6200(9)	0.5272(9)			
	$3s^23p^4(^3P)4p\ ^4P_{3/2}$	0.0000	0.0000	0.1470(5)	0.3337(4)			
	$3s^23p^4(^3P)4p\ ^4D_{3/2}$	0.0000	0.0000	0.5304(4)	0.1002(5)			
	$3s^23p^4(^3P)4p\ ^2D_{3/2}$	0.0002	0.0002	0.6123(5)	0.6334(5)			
	$3s^23p^4(^3P)4p\ ^2P_{3/2}$	0.0817	0.0721	0.2206(6)	0.1946(6)			
	$3s^23p^4(^3P)4p\ ^4S_{3/2}$	0.0000	0.0000	0.1326(5)	0.1107(5)			
	$3s^23p^4(^1D)4p\ ^2P_{3/2}$	0.0007	0.0029	0.2394(5)	0.9978(5)			
	$3s^23p^4(^1D)4p\ ^2D_{3/2}$	0.0000	0.0000	0.1960(0)	0.7557(2)			
$3s^23p^4(^3P)3d\ ^4D_{7/2}$	$3s^23p^4(^3P)4p\ ^4P_{5/2}$	0.2520	0.5934	0.3238(7)	0.7624(7)	0.4120		
	$3s^23p^4(^3P)4p\ ^4D_{5/2}$	0.0124	0.0311	0.9119(5)	0.2292(6)	0.0187		

Multi-Configuration Dirac-Fock (MCDF) method

- Fully relativistic method.
- Mainly used for highly charged ions and based on jj coupling scheme
- There is a choice of optimization procedures in MCDF method
- In optimal level (OL), each atomic energy level is determined in its self-consistent calculation
- In Extended average level (EAL) method, which is used in present calculation, the weighted sum of trace of the Hamiltonian is minimized.
- It includes all relativistic corrections. In MCDF Breit correction and leading quantum electrodynamics (QED) are taken into account.
- Breit interaction is a correction to the coulomb repulsion between two electrons due to the exchange of a virtual (transverse) photon.
- Quantum electrodynamics (QED) predicts additional two- body interaction and results in splitting of some of the degenerate levels coming by solving Dirac equations.
- The first significant QED correction come due to finite size of the nucleus, while the second is due to a bound electron emitting a virtual photon and absorbing it again in the field of the nucleus. The third most significant QED correction is called the vacuum polarization and it is due to the creation and annihilation of virtual electron-positron pairs in the field of the nucleus.

Flexible Atomic Code (FAC)

- FAC also employs a fully relativistic approach based on the Dirac equation, which allows its application to ions with large values of nuclear charge.
- FAC is based on the relativistic configuration interaction with independent particle basis wavefunctions.
- The energy levels of an atomic ion having N electrons are obtained by diagonalizing the Relativistic Hamiltonian H defined earlier.
- In Flexible Atomic Code (FAC), the orbitals are optimized self consistently and the average energy of a fictitious mean configuration with orbital occupation numbers is minimized.

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REVIEW

Multiconfigurational Dirac–Fock atomic structure calculations for Cl-like tungsten

Man Mohan, Sunny Aggarwal, and Narendra Singh

Abstract: Energy levels, lifetimes, and wavefunction compositions have been calculated for all levels of odd parity $3s^23p^3$ ground configuration as well as $3s3p^6$ and $3s^23p^43d$ even parity excited configurations in highly charged Cl-like tungsten ion. Transition probabilities, oscillator strengths, and line strengths for E1, E2, M1, and M2 transitions have been obtained using the fully relativistic multiconfiguration Dirac–Fock (MCDF) approach including the correlations within the $n = 3$ complex, some $n = 3 \rightarrow n = 4$ single and double excitations and Breit and quantum electrodynamics effects. For comparison from our calculated energy levels, we have also calculated the energy levels by using the fully relativistic flexible atomic code (FAC). The validity of the method is assessed by comparison with previously published experimental and theoretical data. The excellent agreement observed between our calculated results and those obtained using different approaches confirm the accuracy of our results. Additionally, we have predicted some new atomic data for W^{37+} that are not available so far and may be important for plasma diagnostic analysis in fusion plasma.

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Résumé : Nous avons calculé les niveaux d'énergie les temps de vie et la composition des fonctions d'onde pour tous les niveaux de parité impaire pour la configuration du fondamental $3s^23p^3$, aussi bien que pour des configurations excitées paires $3s3p^6$ et $3s^23p^43d$ dans les ions de tungstène de type Cl hautement chargés. Nous avons obtenu les probabilités de transition, les forces d'oscillateur et les intensités de raie pour les transitions E1, E2, M1 et M2, en utilisant l'approche à configurations multiples de Dirac-Fock complètement relativiste (MCDF), qui inclut les corrélations à l'intérieur du complexe $n = 3$, quelques excitations simples et doubles $n = 3 \rightarrow n = 4$ et les effets d'électrodynamique quantique et de Breit. Pour comparer avec nos résultats, nous

e only.'

Table 2. MCDF Dirac–Coulomb (DC), Breit, and quantum electrodynamics (QED) contributions to the energy (Ryd) as a function of the orbital set.

		MCDF							
Label	J	DC	Breit	QED	Total	NIST	FAC	%diff1	%diff2
$3s^23p^2\ ^2P^o$	3/2	0	—	—	0	0	0	0	0
$3s^23p^4(^2_2P)3d\ ^4D$	3/2	17.5346	−0.0433	−0.0379	17.4534	17.344	17.3021	−0.63	0.87
$3s^23p^4(^2_2P)3d\ ^4D$	5/2	18.0469	−0.095	−0.0378	17.9141	17.7943	17.7589	−0.67	0.87
$3s^23p^4(^2_2P)3d\ ^4P$	1/2	18.0674	−0.0536	−0.0386	17.9752	17.87	17.8204	−0.59	0.86
$3s^23p^4(^2_2P)3d\ ^4F$	7/2	18.3485	−0.12	−0.0377	18.1905	18.0508	18.0288	−0.77	0.89
$3s^23p^4(^1_0S)3d\ ^2D$	3/2	19.7029	−0.0473	−0.038	19.6176	19.46	19.4633	−0.81	0.79
$3s^23p^4(^1_2D)3d\ ^2F$	7/2	23.6667	−0.258	−0.0377	23.3713	23.2796	23.2269	−0.39	0.62
$3s^23p^4(^2_2P)3d\ ^4F$	9/2	23.8571	−0.279	−0.0376	23.5406	23.4394	23.3937	−0.43	0.62
$3s^23p^4(^2_2P)3d\ ^2P$	1/2	24.2836	−0.213	−0.0407	24.0296	24.02	23.8864	−0.04	0.60
$3s^23p^2\ ^2P^o$	1/2	25.8148	−0.31	0.0297	25.5348	25.5	25.5375	−0.14	−0.01
$3s^23p^4(^2_0P)3d\ ^4P$	5/2	25.9218	−0.198	−0.0379	25.6854	25.5	25.5710	−0.73	0.45
$3s^23p^4(^2_2P)3d\ ^4P$	3/2	26.4267	−0.213	−0.0374	26.1767	26.13	26.0159	−0.18	0.61
$3s^23p^4(^2_2P)3d\ ^2D$	5/2	26.7541	−0.233	−0.0376	26.4839	26.60	26.3286	0.43	0.59
$3s3p^6\ ^2S$	1/2	40.2029	−0.108	−0.201	39.8947	41.2	39.8073	3.16	0.22
$3s^23p^4(^2_2P)3d\ ^4D$	1/2	42.5049	−0.366	−0.0135	42.1254	42.2	42.0211	0.17	0.25
$3s^23p^4(^2_2P)3d\ ^4F$	3/2	43.3303	−0.402	−0.0078	42.9204	42.9	42.8086	−0.05	0.26
$3s^23p^4(^2_2P)3d\ ^4F$	5/2	43.9474	−0.416	−0.0076	43.5241	43.5	43.4053	−0.06	0.27
$3s^23p^4(^1_2D)3d\ ^2G$	7/2	44.1046	−0.469	−0.0076	43.6284	43.67	43.5075	0.09	0.28
$3s^23p^4(^1_2D)3d\ ^2F$	5/2	46.3972	−0.408	−0.0086	45.9809	45.78	45.8331	−0.44	0.27
$3s^23p^4(^1_2D)3d\ ^2P$	3/2	46.5579	−0.383	−0.0084	46.1664	45.99	46.0378	−0.38	0.28
$3s^23p^4(^1_2D)3d\ ^2S$	1/2	47.0529	−0.307	−0.0579	46.6876	46.45	46.5654	−0.51	0.26
$3s^23p^4(^2_2P)3d\ ^4D$	7/2	48.9118	−0.547	−0.0078	48.3574	—	48.2587	—	0.20
$3s^23p^4(^2_2P)3d\ ^2P$	3/2	49.5835	−0.519	−0.008	49.0564	—	48.9523	—	0.21
$3s^23p^4(^2_2P)3d\ ^2F$	5/2	49.9225	−0.552	−0.0078	49.3626	—	49.2349	—	0.26
$3s^23p^4(^1_2D)3d\ ^2G$	9/2	49.977	−0.627	−0.0077	49.3420	—	49.2573	—	0.17
$3s^23p^4(^1_2D)3d\ ^2D$	5/2	50.4083	−0.523	−0.0081	49.8777	—	49.7674	—	0.22
$3s^23p^4(^2_2P)3d\ ^2F$	7/2	51.0874	−0.572	−0.008	50.5070	—	50.3918	—	0.23
$3s^23p^4(^1_2D)3d\ ^2D$	3/2	52.81	−0.546	−0.008	52.2359	—	52.1382	—	0.23
$3s^23p^4(^1_2D)3d\ ^2P$	1/2	53.4982	−0.504	−0.0173	52.9774	—	52.8527	—	0.24
$3s^23p^4(^2_2P)3d\ ^2D$	3/2	71.7371	−0.704	0.0186	71.0520	—	70.9735	—	0.11
$3s^23p^4(^1_0S)3d\ ^2D$	5/2	76.2701	−0.836	0.016	75.4505	—	75.3921	—	0.08

Note: The total is compared with observed and FAC. All energies are relative to the ground state.
%diff1 = (NIST − MCDF)/NIST * 100.
%diff2 = (MCDF − FAC)/MCDF * 100.

Table 4. Transition data for E1 transitions from $3s^2 3p^3\ ^2P_{3/2}$: levels and $2J$ for lower level, i; upper level, k; wavelength, λ (Å); line strength, S (length form); oscillator strength, f (length form); and transition rate, A_{ji} (length form).

Levels		$2J$							
i	k	i	k	λ (Å)	A_{ji} (s^{-1}) (MCDF)	A_{ji} (s^{-1}) (FAC)	f_{ij}	S_{ij} (au)	Vel/len
$3s^2 3p^3\ ^2P^o$ – $3s3p^6\ ^2S$		1	1	6.35×10^{1}	3.24×10^{10}	6.75×10^{9}	1.96×10^{-2}	8.18×10^{-3}	0.84
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4D$		1	1	5.49×10^{1}	6.28×10^{9}	4.74×10^{9}	2.84×10^{-3}	1.03×10^{-3}	0.96
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4F$		1	3	5.24×10^{1}	3.42×10^{9}	1.27×10^{9}	2.82×10^{-3}	9.73×10^{-4}	1.1
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^1_2D)3d\ ^2P$		1	3	4.42×10^{1}	3.97×10^{8}	4.20×10^{9}	2.32×10^{-4}	6.76×10^{-5}	1.4
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^1_2D)3d\ ^2S$		1	1	4.31×10^{1}	3.22×10^{9}	4.74×10^{9}	8.96×10^{-4}	2.54×10^{-4}	0.75
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^2P$		1	3	3.87×10^{1}	2.73×10^{9}	7.08×10^{8}	1.23×10^{-3}	3.13×10^{-4}	1.1
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^1_2D)3d\ ^2D$		1	3	3.41×10^{1}	8.10×10^{11}	9.44×10^{11}	2.82×10^{-1}	6.34×10^{-2}	1.1
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^1_2D)3d\ ^2P$		1	1	3.32×10^{1}	1.31×10^{12}	1.52×10^{12}	2.16×10^{-1}	4.72×10^{-2}	1.0
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^2D$		1	3	2.00×10^{1}	2.49×10^{12}	2.91×10^{12}	2.99×10^{-1}	3.94×10^{-2}	1.0

Note: Last column represents ratio of vel. and len. form of oscillator strength.

Table 5. Transition data for M2 transitions from $4s^2 4p^3\ ^2P$ levels and $2J$ for lower level, i; upper level, k; wavelength, λ (Å); line strength, S (length form); oscillator strength, f (length form); transition rate; and A_{ji} (length form).

Levels		$2J$						
i	K	i	k	λ (Å)	A_{ji} (s^{-1}) (MCDF)	A_{ji} (s^{-1}) (FAC)	f_{ij}	S_{ij} (au)
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4D$		3	3	5.22×10^{1}	3.41×10^{0}	3.48×10^{0}	1.39×10^{-12}	3.54×10^{-4}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4D$		3	5	5.09×10^{1}	1.52×10^{1}	1.35×10^{1}	8.84×10^{-12}	2.08×10^{-3}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4P$		3	1	5.07×10^{1}	3.68×10^{1}	3.76×10^{1}	7.08×10^{-12}	1.65×10^{-3}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4F$		3	7	5.01×10^{1}	3.78×10^{1}	2.79×10^{1}	2.84×10^{-11}	6.40×10^{-3}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^1_0S)3d\ ^2D$		3	3	4.65×10^{1}	1.52×10^{2}	1.40×10^{2}	4.93×10^{-11}	8.84×10^{-3}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^1_2D)3d\ ^2F$		3	7	3.90×10^{1}	3.65×10^{4}	3.24×10^{4}	1.66×10^{-8}	1.77×10^{0}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^2P$		3	1	3.79×10^{1}	9.94×10^{4}	9.09×10^{4}	1.07×10^{-8}	1.05×10^{0}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4P$		3	5	3.55×10^{1}	2.59×10^{4}	2.40×10^{4}	7.33×10^{-9}	5.86×10^{-1}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^4P$		3	3	3.48×10^{1}	3.26×10^{4}	3.19×10^{4}	5.93×10^{-9}	4.48×10^{-1}
$3s^2 3p^3\ ^2P^o$ – $3s^2 3p^4(^3_2P)3d\ ^2D$		3	5	3.44×10^{1}	2.28×10^{3}	3.34×10^{3}	6.06×10^{-10}	4.42×10^{-2}
$3s^2 3p^3\ ^2P^o$ – $3s3p^6\ ^2S$		3	1	2.28×10^{1}	5.74×10^{3}	1.01×10^{3}	2.25×10^{-8}	4.79×10^{-1}

Table 6. Comparison of computed wavelengths (Å) from different theories with observed wavelengths for transitions from $3s^23p^3\ ^2P$ to selected upper levels.

Upper	$2J_i$	$2J_k$	This work MCDF	ASD	Other theory
$3s^23p^3(^1D_2)3d\ ^2S$	3	1	19.52	19.62[a]	19.537[†], 19.442[‡]
$3s^23p^3(^1D_2)3d\ ^2P$	3	3	19.74	19.81[a]	19.786[†], 19.726[‡]
$3s^23p^3(^1D_2)3d\ ^2F$	3	5	19.82	19.90[a]	19.867[†], 19.789[‡]
$3s^23p^3(^3P_2)3d\ ^4D$	3	5	50.87	51.21[§]	52.558[§]
$3s^23p^3(^3P_2)3d\ ^4D$	3	3	52.21	52.54[§]	51.209[§]

[a]Ref. 11.

[†]Calculation of ref. 11 using FAC.

[‡]Calculation of ref. 11 using GRASP.

[§]Ref. 9.

Table 7. Comparison of radiative transition probability A (in S^{-1}) and transition wavelengths (Å) for other available M1 and E2 lines in W^{37+}.

Transition	λ^a	$\lambda^†$	A^a	$A^†$	$A^‡$	Type
$3s^23p^3\ ^2P_{3/2} - 3s^23p^3\ ^2P_{1/2}$	35.63	35.68	3.95×10^8	3.91×10^8	3.94×10^8	M1+E2

[a]From ref. 41.

[†]This work.

[‡]From ref. 40.

Atomic structure calculations for Ni 24+

- We present accurate 165 fine-structure energy levels related to the configurations $1s^2 2s^2$, $1s^2 2p^2$, $1s^2 nln'l'$ (n=2, n'=2,3,4,5, l=s,p l'=s,p,d,f,g) of Ni 24+ which may be useful ion for astrophysical and fusion plasma.

- For the calculations of energy levels and radiative rates, we have used the multiconfiguration Dirac-Hartree-Fock (MCDHF) method employed in GRASP2K code.

- The calculations are carried out in the active space approximation with the inclusion of the Breit interaction, the finite nuclear size effect, and quantum electrodynamic corrections.

- The transition wavelengths, transition probabilities, line strengths, and absorption oscillator strengths are reported for electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1), magnetic quadrupole (M2) transitions from the ground state.

- We have compared our calculated results with available theoretical and experimental data and good agreement is achieved.

- The present complete set of results should be of great help in line identification and the interpretation of spectra, as well as in the modelling and diagnostics of astrophysical and fusion plasmas.

Ref. : *N. Singh and S. Aggarwal.* Radiat. Phys. Chem. 144, 426 (2018).

Computational methodology

Systematic Calculations using MCDHF method have many option in GRASP2K which can be used for different atomic system and requirements

- Configurations that define the CSFs in the expansion.
- Types of correlation, valence-valence correlation, core-valence correlation and core-core correlation
- How radial function of one-electron orbitals that define CSFs are determined.
- Set of orbitals and the method by which they are derived.

C. F. Fischer. Atoms 2, 1-14 (2014)

Selection of Configurations that define the CSFs in the expansion

Method 1

- In our calculations, to construct atomic state functions, we have used the active space approach. We have performed our calculations using two different ways. In first approach, the initial estimate for the radial orbital is generated by solving the Dirac equation in Thomas-Fermi potential for a single reference configuration ($2s^2$ for even level and 2s2p for odd levels).

- We have allowed the single, double, triple and quadrupole excitations from the active set with n=2,3,4,5. Orbits are increased in a methodical way in order to control the convergence of our calculations. This procedure is performed for every J-value separately.

- In quadrupole excitation, wave-function expansions increase rapidly in size by increasing nl which has increased number of CSF, as shown in Table 1(a). We have achieved the convergence of our calculated results in n=3,4,5. We would like to state that our calculations become unmanageable for n>5 due to degree of complexity in this approach. Therefore, we have used another approach in our calculation.

Method 2

In Second approach, we have performed SD excitation from the multi-reference set (for $1s^2 2s^2,\ 1s^2 2p^2,\ 1s^2 2s3s,\ 1s^2 2s3d$ even level and $1s^2 2s2p,\ 1s^2 2s3p$ for odd level) to generate configuration state functions. The effect of different type of correlations has been included in a proper way. We have increased the orbitals in a systematic way in order to handle the convergence of our computations and enhance the active set layer by layer. To reduce processing time as a result of the large number of orbitals, we optimized set of orbitals for even and odd parity states separately. Thus, we enhanced the size of the active set as shown below

AS1 = {n=3, l=0-2}

AS2 = AS1 + {n=4, l=0-3}

AS3 = AS2 + {n=5, l=0-4}

AS4 = AS3 + {n=6, l=0-4}

AS5 = AS4 + {n=7, l=0-4}

The numbers of CSFs which are generated are shown in Table 1 (b).

Set of orbitals and the method by which they are derived.

EAL and EOL Schemes

- In extended optimal level (EOL) calculation, the energy functional may be a linear combination of total energies for a set of ASFs.
- A simpler strategy is to compute the radial functions from an energy functional that is defined in terms of the average energy of all CSFs in the wave function expansion of all ASFs. This method is referred to as the (EAL) method.
- The difference is that the EAL omits the interaction between CSFs in the orbital optimization phase of the calculation and there is no large distinction between orbitals that are part of the MR set and other orbitals.
- In the EOL calculation, correlation orbitals are more contracted and total energies lower than in a similar EAL calculation.
- GRASP uses EAL method while GRASP2K uses EOL method.
- So in all CI methods, difference is configurations that define CSFs in expansion and determination of radial wave functions of orbitals included in CSFs.

Table 1(a) Number of configuration state functions (CSFs) used in the atomic state function expansion for the given angular momentum and parity (JP) considering only quadruple excitations (Cal[a])

J+	3l	4l	5l	J-	3l	4l	5l
0	211	2149	13592	0	180	2040	13302
1	436	5384	36634	1	460	5476	36894
2	534	7250	52481	2	516	7168	52238
3	380	6930	57161	3	392	6988	57354
4	228	5588	53512	4	222	5540	53342
5	89	3650	43358	5	90	3672	43466

Table 1(b) Number of configuration state functions (CSFs) used in the atomic state function expansion for the given angular momentum and parity (JP) considering SD excitations (Cal[b])

J+	3l	4l	5l	6l	7l	J-	3l	4l	5l	6l	7l
0	147	629	1637	3180	5258	0	102	442	1156	2252	3730
1	297	1478	4094	8160	13676	1	258	1144	3080	6064	10096
2	351	1886	5513	11190	18917	2	276	1372	3998	8088	13642
3	237	1640	5386	11372	19598	3	102	1168	3872	8154	14014
4	128	1165	4406	9705	17062	4	98	766	3046	6750	11878
5	44	642	2975	6942	6942	5	34	388	1992	4696	8500

Table 2. Total energies (Cal[a] & Cal[b]) (in cm^{-1}) of Be-like Ni. We provide the energies from NIST database [23], the observed and calculated energies by Landi [20] and other available energies [15,28,29]

S.No	Configuration	Term	J	Parity	Cal[a]	Cal[b]	NIST	Observed	Landi	other
1	$1s^22s^2$	^1S	0		0	0	0	0	0	0
2	$1s^22s2p$	^3P	0	-	374086.2	378761	378190	378687	378720	378198[a] 378961.8[c]
3	$1s^22s2p$	^3P	1	-	414982.8	418504.8	418720	418653	419.315	418729.9[a]
4	$1s^22s2p$	^3P	2	-	545271.6	548114.8	549500	549599	551636	549512[a] 549579[b]
5	$1s^22s2p$	^1P	1	-	849052.1	850157	847558	847894	854374	
6	$1s^22p^2$	^3P	0	+	1105520	1049805	1048300	1049246	1052805	
7	$1s^22p^2$	^3P	1	+	1210624	1156471	1154300	1155102	1159043	
8	$1s^22p^2$	^3P	2	+	1261352	1206111	1207800	1208115	1213918	
9	$1s^22p^2$	^1D	2	+	1432932	1378517	1379100	1380464	1389093	
10	$1s^22p^2$	^1S	0	+	1665814	1614168	1611000	1611675	1623950	

Table 3. Comparison between the present calculations of transition wavelength (λ in nm) and other references.

Transition number	i	J	Calculated Wavelength	Available result
1	$1s^22s^2\ ^1S_0$	$1s^22s2p\ ^3P_1$	23.894	23.889[a]
2	$1s^22s^2\ ^1S_0$	$1s^22s2p\ ^3P_2$	18.244	18.197[a]
3	$1s^22s^2\ ^1S_0$	$1s^22s2p\ ^1P_1$	11.762	11.803[a]
4	$1s^22s^2\ ^1S_0$	$1s^22s3p\ ^1P_1$	0.93469	0.93400[b]
5	$1s^22s^2\ ^1S_0$	$1s^22s3p\ ^3P_1$	0.93861	0.93900[b]

Ref. [a]: Safronova U I 2000 *Mol. Phys.* **98** 1213
Ref. [b]: Dere K P, Landi E, Young P R and DelZanna G 2001 *Astrophys. J. Suppl. Ser* **134** 331

Table 4. Comparison between the present calculations of oscillator strength(gf) and other references.

i	j	Calculated value	Available result
$1s^2 2s^2\ {}^1S_0$	$1s^2 2s2p\ {}^3P_1$	2.173D-03	2.165E-03[c]
$1s^2 2s^2\ {}^1S_0$	$1s^2 2s2p\ {}^1P_1$	1.476E-01	1.486E-01[c] 1.450E-01[a]

Table 5. Comparison between the present calculations of transition probabilities (A in s^{-1}) and other references.

i	j	Calculated A_{ij}	Available result
$1s^2 2s^2\ {}^1S_0$	$1s^2 2s2p\ {}^3P_1$	8.462E+07	8.629E+07[d], 7.62E+07[a], 8.438E+07[c]
$1s^2 2s^2\ {}^1S_0$	$1s^2 2s2p\ {}^3P_2$	1.370E+01	1.388E+01[d], 1.38E+01[a]
$1s^2 2s^2\ {}^1S_0$	$1s^2 2s2p\ {}^1P_1$	2.373E+10	2.352E+10[d], 2.407E+10[c]

Ref. [a]: Safronova U I 2000 *Mol. Phys.* **98** 1213
Ref. [c]: Landi E and Bhatia A K 2009 *Atomic data nucl. Data tables* **95** 547
Ref. [d]: Cheng K T, Chen M H and Johnson W R 2008 *Phys. Rev. A* **77** 0525a04

Theoretical study of energy levels and radiative properties of Be-like W^{70+}

- We report an extensive theoretical study of the Be-like W^{70+} spectrum in a wide energy range. We present accurate calculated 215 fine-structure energy levels related to the configurations $1s^22s^2$, $1s^22p^2$, $1s^2nl n'l'$ (n=2, n'=2-7 l=s, p l'=s, p, d, f, g), which may be useful ion for fusion plasma research.

- We have identified wavelengths of extreme ultraviolet (EUV) and X-ray transitions using the multiconfiguration Dirac-Hartree-Fock (MCDHF) method implemented in the GRASP2K code.

- The calculations are carried out in the active space approximation with the inclusion of the Breit interaction, the finite nuclear size effect, and quantum electrodynamic corrections. Transition data are reported for multipole transitions from the ground state. We have discussed discrepancy graphically with available results. We have also graphically explained the convergence in excitation energies with active sets.

- The present complete set of results should be of help in line identification and the interpretation of spectra, as well as in modeling and diagnostics of fusion plasmas.

N. Singh, S. Aggarwal and M. Mohan, *J. Electron Spectrosc. Relat. Phenom.* **229**, 124 (2018).

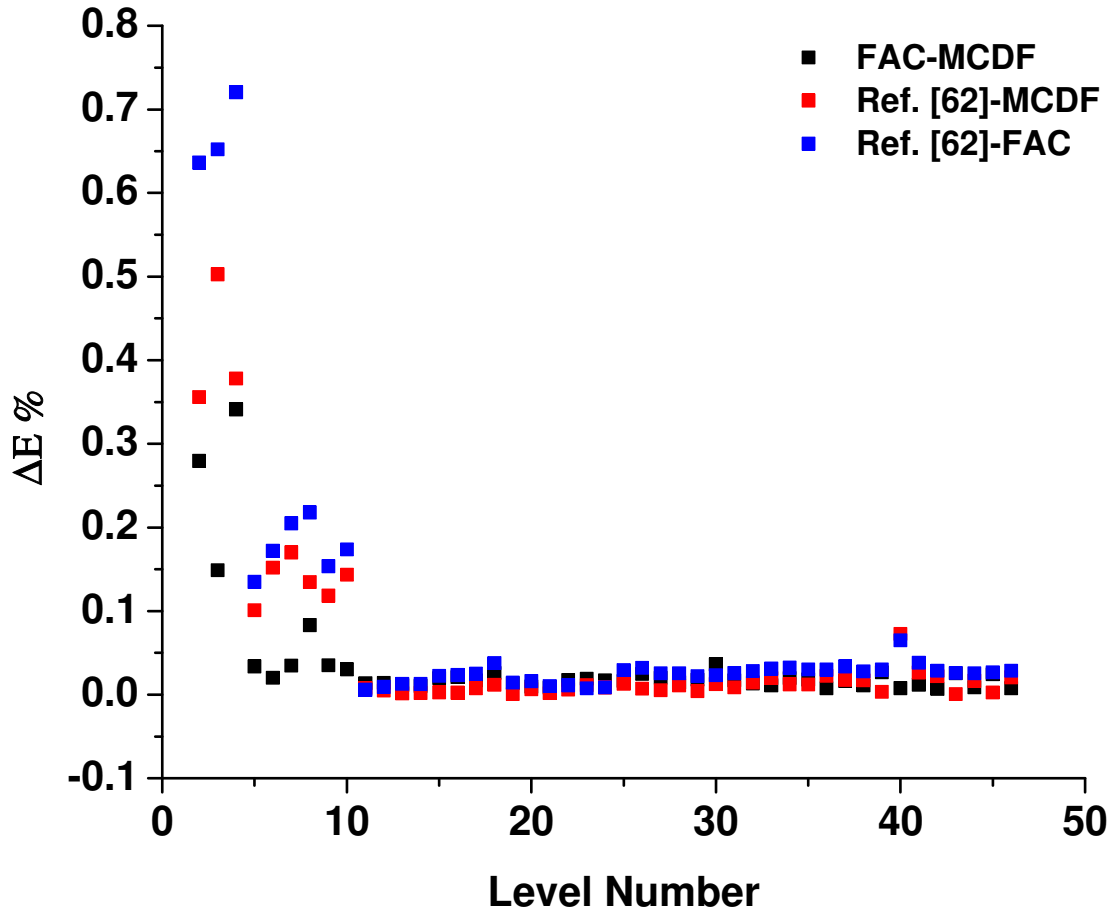

Figure 1. Percentage difference in excitation energies of MCDF, FAC and Ref. [62] for lowest 46 levels

Ref. Safronova U I and Safronova A S 2010 J. Phys. B. 43 074026

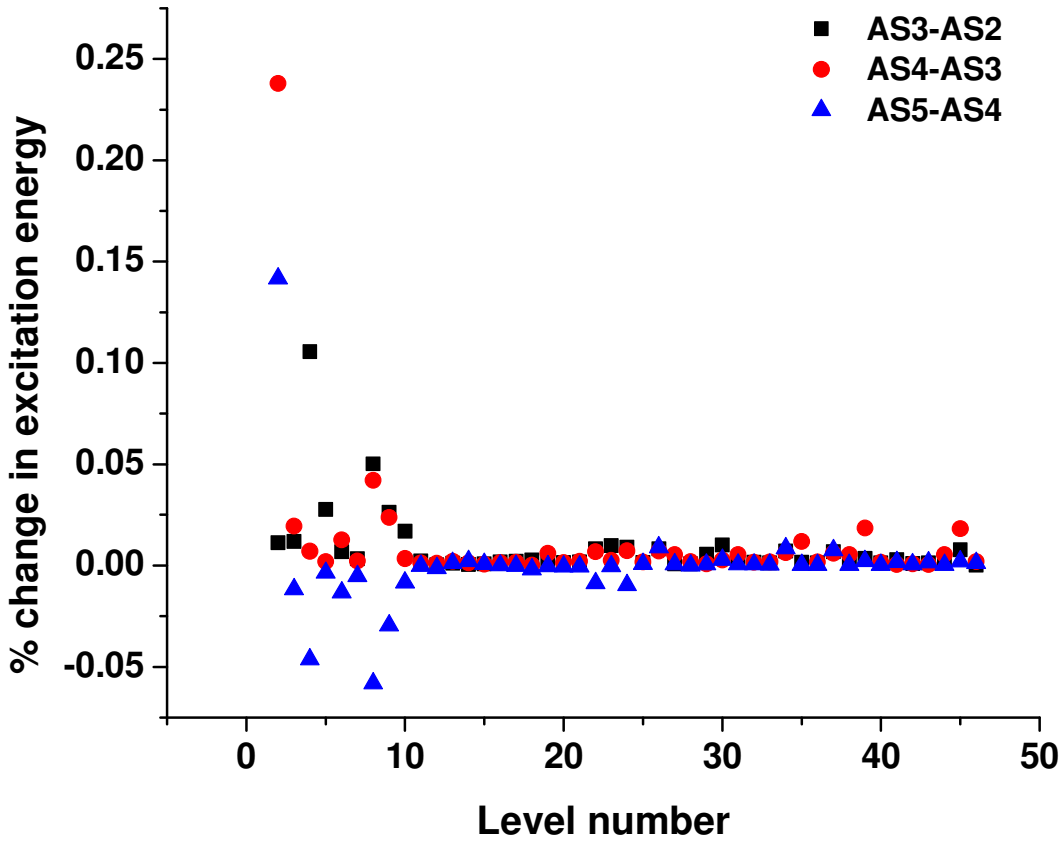

Figure 2. Percentage change in excitation energies in consecutive sets for lowest 46 levels

TABLE 1: No. of Configuration State Function (CSF) for n=4 to 7 for Be-like W^{70+}

J+	AS2	AS3	AS4	AS5	J-	AS2	AS3	AS4	AS5
0	1274	3631	7296	12269	0	1100	3348	6954	3730
1	3076	9292	19124	32572	1	2907	9070	18997	32688
2	4040	12777	26654	45671	2	3686	12232	26132	45386
3	3640	12766	27552	47998	3	3426	12498	27476	48360
4	2745	10824	24163	42762	4	2539	10540	24043	43048
5	1614	7580	17790	32244	5	1535	7556	18031	32960

TABLE 2: Total energies (GRASP2K and FAC) (in cm^{-1}) with J values and Parity of Be-like W^{70+}

S.No	Level	J	Parity	GRASP2K	FAC	ΔE
1	$1s^2 2s^2\ ^1S$	0	+	0	0	-----
2	$1s^2 2s2p\ ^3P$	0	-	1384107.71	1387973.978	-0.27933
3	$1s^2 2s2p\ ^3P$	1	-	1658484.28	1660951.403	-0.14876
4	$1s^2 2p^2\ ^3P$	0	+	3905964.21	3919287.222	-0.34109
5	$1s^2 2s2p\ ^3P$	2	-	13325340.21	13329853.07	-0.03387
6	$1s^2 2s2p\ ^1P$	1	-	14059678.12	14062517.09	-0.02019
7	$1s^2 2p^2\ ^3P$	1	+	15501254.35	15506638.73	-0.03474
8	$1s^2 2p^2\ ^1D$	2	+	15639799.74	15652794.66	-0.08309
9	$1s^2 2p^2\ ^3P$	2	+	27541607.57	27551249.16	-0.03501
10	$1s^2 2p^2\ ^1S$	0	+	28099697.35	28108200.7	-0.03026

TABLE 3: Energy levels (in cm^{-1}) for Be-like W^{70+} for lowest 46 fine structure levels. Results of Safronova also presented for comparison.

S.No	Level	J	Parity	AS2	AS3	AS4	AS5	Safronova
1	$1s^2 2s^2\ ^1S$	0	+	0	0	0	0	0
2	$1s^2 2s2p\ ^3P$	0	-	1385280.74	1385435.4	1382145.9	1384107.7	1379200
3	$1s^2 2s2p\ ^3P$	1	-	1658802.27	1658999.7	1658678	1658484.3	1650190
4	$1s^2 2p^2\ ^3P$	0	+	3912176.51	3908050.5	3907773.2	3905964.2	3891250
5	$1s^2 2s2p\ ^3P$	2	-	13329762.7	13326086	13325819	13325340	13311900
6	$1s^2 2s2p\ ^1P$	1	-	14062380.6	14063327	14061549	14059678	14038380
7	$1s^2 2p^2\ ^3P$	1	+	15502919.2	15502404	15502057	15501254	15474930
8	$1s^2 2p^2\ ^1D$	2	+	15650162.6	15642312	15648899	15639800	15618770
9	$1s^2 2p^2\ ^3P$	2	+	27550430	27543207	27549758	27541608	27509020
10	$1s^2 2p^2\ ^1S$	0	+	28105879.2	28101098	28102045	28099697	28059470

➢The reliability of calculated line strengths and fine structure energies can be checked from the uncertainty from following relations:

$$\Delta S = \frac{S(length) - S(velocity)}{Max(S(Length, Velocity)}$$

$$\Delta E = \frac{E(Exp.) - E(Cal.)}{E(Exp.)}$$

➢While uncertainty in transition probability can be calculated using below relation:

$$\Delta A = (\Delta S + \Delta E) A$$

TABLE 4: Weighted oscillator strengths gf, wavelengths (in Å), transition probabilities A (in s^{-1}) and line strengths S (in a.u.) for the electric dipole (E1) transitions from ground state in Be-like W^{70+}. C and B indicate Coulomb and Babushkin gauge.

I	J	λ(Å)	Gauge	A (s^{-1})	gf	S	ΔS	ΔE	ΔA
1	3	60.296	C	5.5040E+09	8.9998E-03	1.7865E-03	0.0347	0.14876	1.009E+09
			B	5.3128E+09	8.6872E-03	1.7244E-03			0.974E+09
1	6	7.1125	C	1.1691E+13	2.6600E-01	6.2285E-03	0.0147	0.02019	0.0407E+13
			B	1.1519E+13	2.6210E-01	6.1370E-03			0.0401E+13
1	13	1.1205	C	4.7250E+14	2.6681E-01	9.8424E-04	0.0085	0.01143	0.0941E+14
			B	4.6846E+14	2.6454E-01	9.7583E-04			0.0933E+14

C. F. Fischer. Phys. Scr. T134, 014019 (2009)

Theoretical study of Extreme Ultraviolet and Soft X-ray transitions of In^{45+} and Sn^{46+} with plasma parameters

- In the present work, the spectroscopic study of atomic parameters of In^{45+} and Sn^{46+} are examined and diagnosed in an extensive and detailed manner by adopting GRASP2K package based on fully relativistic Multi-Configuration Dirac-Hartree-Fock (MCDHF) wave-functions.
- We have presented energy levels of lowest 40 levels and radiative data for electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1) and magnetic quadrupole (M2) transitions within Extreme Ultraviolet (EUV) and Soft X-ray (SXR) range for In^{45+} and Sn^{46+} from ground state within lowest 40 levels.
- We have matched our results with theoretical results available only for few lowest levels and found good agreement with them. We have also discussed discrepancies with them. Further, due to insufficiency of atomic data for higher excited states, we have carried out similar parallel calculation by employing fully relativistic flexible atomic code (FAC) to check the reliability and authenticity of higher excited states. Our calculated energy levels match well with our FAC results.
- Characterization of hot dense plasma (HDP) with its parameters temperature, electron density, skin depth, plasma frequency is demonstrated in this work. We believe that our presented data may be beneficial in future for comparisons and identification of spectral lines, in plasma modelling and in fusion and astrophysical plasma research.

N. Singh, A. Goyal and M. Mohan, J. Electron Spectrosc. Relat. Phenom. **227**, 23 (2018).

Line intensity ratio and plasma parameters

The change in radiative parameters such as transition wavelength, transition probability, etc. leads to a change in plasma parameters. The consideration of plasma as optically thin under LTE makes the characterization and analysis of HDP simple and straightforward. The ratio of intensity of any two spectral lines in hot dense plasma in terms of plasma temperature and radiative data is given by

$$R = \frac{I_1}{I_2} = \frac{\lambda_2}{\lambda_1}\frac{A_1}{A_2}\frac{g_1}{g_2}\exp\left(-\frac{E_1 - E_2}{kT}\right)$$

The minimum value of electron density for HDP plasma of Be-like ions given by

$$n_e \geq 1.6 \times 10^{12} T^{1/2} (\Delta E)^3$$

n_e is the electron density, T is the plasma temperature in K and $\Delta E = E_1 - E_2$ in eV.

The relations of other parameter with electron density and plasma temperature is given below

$$n_e = 0.124 \times 10^{-9} \omega_e^2$$

$$n_e = 28.1961 \times 10^{10} \delta^{-2}$$

$$\Gamma = 0.225593 \times 10^{-2} \times n_e^{\frac{1}{3}} T^{-1}$$

In above expressions, ω_e, δ, Λ and Γ are plasma frequency, skin depth, plasma parameter and coupling parameter resp. For the calculation of line intensity ratio and electron density of HDP, spectral lines $1s^2 2s^2 {}^1S_0$-$1s^2 2s2p\ {}^3P_1^o$ and $1s^2 2s^2 {}^1S_0$-$1s^2 2s2p\ {}^1P_1^o$ are opted.

Table1: Energy levels (in cm^{-1}) for Be-like In for lowest 40 fine structure levels for different active sets.

S.No	Configuration	Term	J	Parity	GRASP2K				FAC	Others
					n=4	n=5	n=6	n=7		
1	$2s^2$	^1S	0	+	0.00	0.00	0.00	0.00	0.00	0.00
2	2s2p	^3P	0	-	737879.95	731799.19	738147.01	738315.28	739291.48	738369.41[b] 738404.28[c]
3	2s2p	^3P	1	-	897394.97	897280.90	897443.00	897326.22	898381.56	896424.65[b] 896385.69[c]
4	$2p^2$	^3P	0	+	2140531.47	2140096.38	2136835.89	2136646.22	2140066.26	2136750.43[b]
5	2s2p	^3P	2	-	2667272.06	2664779.51	2665121.74	2665093.27	2668721.04	2669011.78[b] 2667362.86[c]
6	2s2p	^1P	1	-	3139318.07	3138802.67	3138524.84	3138196.35	3140075.24	3135424.88[b] 3133615.38[c]
7	$2p^2$	^3P	1	+	3865474.89	3864596.52	3864755.90	3864597.20	3866743.15	3865846.90[b]
8	$2p^2$	^1D	2	+	3983231.98	3978530.63	3977606.35	3977768.81	3983570.90	3980767.72[b]
9	$2p^2$	^3P	2	+	5863828.05	5859344.66	5858517.26	5858760.04	5864444.32	5863808.74[b]
10	$2p^2$	^1S	0	+	6224793.12	6224061.94	6219565.44	6219393.11	6224977.40	6219959.40[b]

[b]C. Nazé, S. Verdebout, P. Rynkun, G. Gaigalas, M. Godefroid, and P. Jönsson, At. Data Nucl. Data Tables 100, 1197–1249 (2014)

[c]K. T. Cheng, M. H. Chen, and W. R. Johnson, Phys. Rev. A 77, 052504 (2008).

Table2: Energy levels (in cm^{-1}) for Be-like Sn for lowest 40 fine structure levels for different active sets.

S.No	Configuration	Term	J	Parity	GRASP2K				FAC	Others
					n=4	n=5	n=6	n=7		
1	$2s^2$	^1S	0	+	0.00	0.00	0.00	0.00	0.00	0.00
2	2s2p	^3P	0	-	757904.20	751723.45	758188.76	758160.16	759437.84	758327.78[b] 757374.33[c] 758506.26[d]
3	2s2p	^3P	1	-	922794.98	922676.04	922841.48	921801.14	923890.26	921716.41[b] 921801.52[c] 921672.46[d]
4	$2p^2$	^3P	0	+	2198644.99	2198199.83	2194892.65	2194816.18	2198385.51	2187481.70[a] 2194881.33[b] 2193721.93[d]
5	2s2p	^3P	2	-	2864245.15	2861700.55	2862024.62	2862004.32	2865816.02	2865998.16[b] 2864285.09[c] 2863914.05[d]
6	2s2p	^1P	1	-	3345063.17	3344551.63	3344290.22	3344180.13	3345959.44	3341208.82[b] 3339361.76[c] 3338603.56[d]
7	$2p^2$	^3P	1	+	4094539.46	4093654.32	4093819.25	4093765.33	4096042.33	4124367.27[a] 4095087.95[b] 4092004.07[d]
8	$2p^2$	^1D	2	+	4214385.99	4209584.89	4208720.75	4208634.17	4214942.97	4212080.51[b] 4208670.48[d]
9	$2p^2$	^3P	2	+	6271143.16	6266197.62	6265437.22	6265367.12	6271622.32	6271020.26[b] 6265561.12[d]
10	$2p^2$	^1S	0	+	6638195.75	6637466.05	6632978.13	6632830.46	6638628.28	6689806.23[a] 6633603.90[b] 6627867.68[d]

[a]C. C. Sang, Y. Sun, and F. Hu, J. Quant. Spectrosc. Radiat. Transfer 179, 177–186 (2016).

[b]C. Nazé, S. Verdebout, P. Rynkun, G. Gaigalas, M. Godefroid, and P. Jönsson, At. Data Nucl. Data Tables 100, 1197–1249 (2014)

[c]K. T. Cheng, M. H. Chen, and W. R. Johnson, Phys. Rev. A 77, 052504 (2008).

[d]M. S. Safronova, W. R. Johnson, and U. I. Safronova, Phys. Rev. A 53, 4036–4053 (1996).

Table 11: Plasma temperature (T in K), Line intensity ratio (R), electron density (n_e in cm^{-3}), Plasma frequency (ωe) in Hz and skin depth (δ) in cm for optically thin plasma for spectral lines 1 and 2 of Be-like ions

In				
T (in K)	R	n_e	ω_e	δ
$2x10^6$	2.654E-04	4.845E+22	1.976E+16	2.412E-06
$4x10^6$	5.941E-04	6.852E+22	2.350E+16	2.028E-06
$6x10^6$	7.772E-04	8.392E+22	2.601E+16	1.833E-06
$8x10^6$	8.889E-04	9.691E+22	2.795E+16	1.706E-06
$1x10^7$	9.635E-04	1.083E+23	2.956E+16	1.613E-06
$1x10^8$	1.288E-03	3.426E+23	5.256E+16	9.072E-07
$1x10^9$	1.326E-03	1.083E+24	9.346E+16	5.101E-07
$1x10^{10}$	1.330E-03	3.426E+24	1.662E+17	2.869E-07
Sn				
T (in K)	R	n_e	ω_e	δ
$2x10^6$	1.941E-04	6.902E+22	2.359E+16	2.021E-06
$4x10^6$	4.806E-04	9.762E+22	2.805E+16	1.700E-06
$6x10^6$	6.502E-04	1.196E+23	3.105E+16	1.536E-06
$8x10^6$	7.562E-04	1.380E+23	3.336E+16	1.429E-06
$1x10^7$	8.280E-04	1.543E+23	3.528E+16	1.352E-06
$1x10^8$	1.148E-03	4.881E+23	6.273E+16	7.601E-07
$1x10^9$	1.186E-03	1.543E+24	1.116E+17	4.274E-07
$1x10^{10}$	1.190E-03	4.881E+24	1.984E+17	2.404E-07

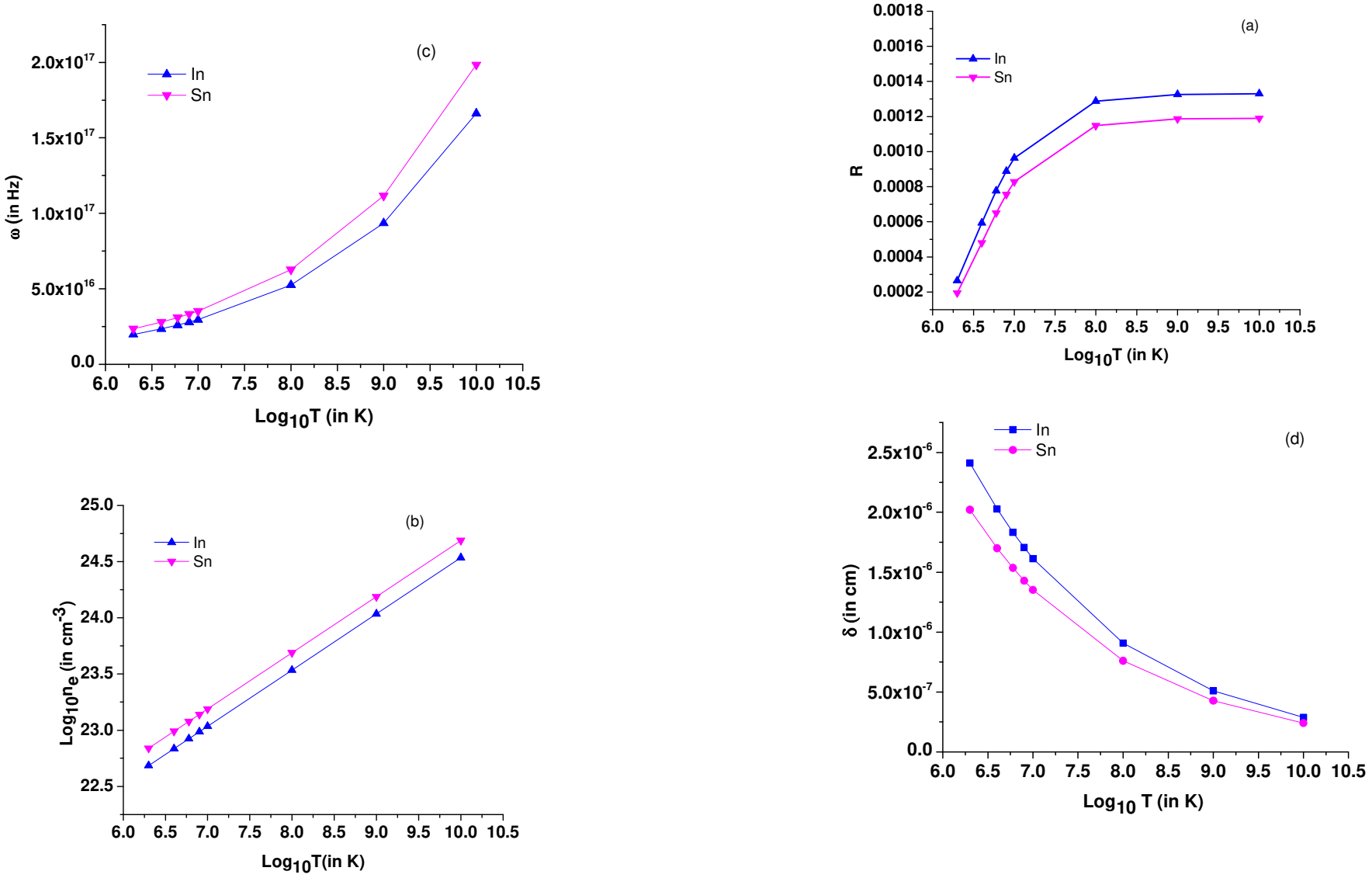

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Figure 2. (color online) (a) line intensity ratio (b) electron density (c) Plasma frequency (d) Skin depth as a function of plasma temperature for Hot dense plasma of Be-like ions for spectral lines 1 and 2

L-shell spectroscopy of neon and fluorine like copper ions from laser produced plasma

- Ne, F, and O-like Rydberg resonance lines along with some of the inner shell satellite lines of Copper plasma, in the wavelength range of 7.9–9.5A° are experimentally observed using a thallium acid phthalate crystal spectrometer.

- Transition wavelengths, transition probabilities, and oscillator strengths of these lines are calculated using the Multi-Configuration Dirac-Fock method and compared with experimental results.

- Anaylsis of distribution of various charge states of Cu ions and determination of temperature and density of plasma using FLYCHK.

- Effect of opacity on charge state distribution of ions is studied.

C. Kaur, S. Chaurasia, N. Singh, J. Pasley, S. Aggarwal and M. Mohan. Physics of Plasmas 26, 023301(2019).

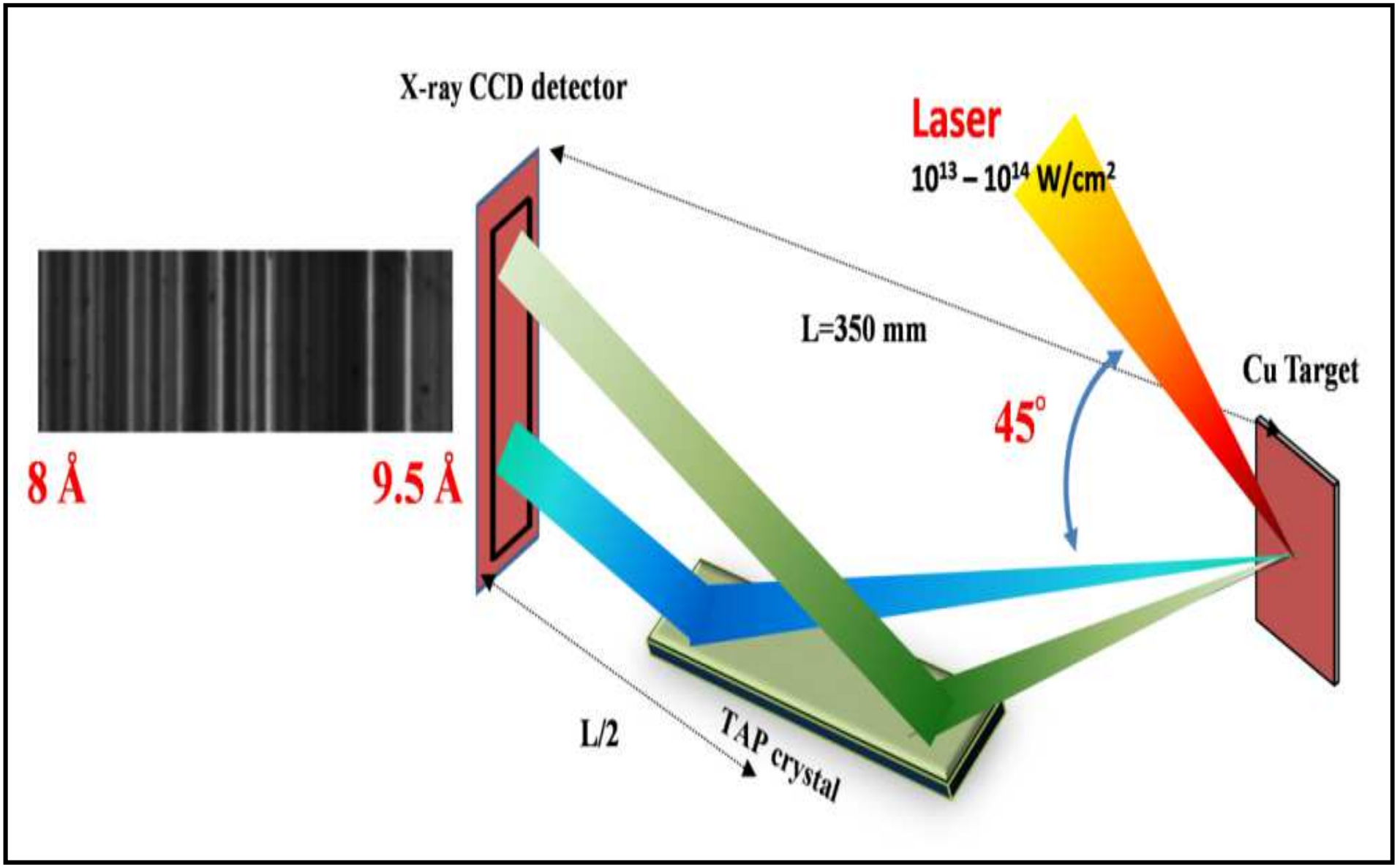


Figure 1. schematic of experimental setup

TABLE I. Calculated wavelength, transition rates, and oscillator strengths of Ne-like transitions along with the corresponding configurations.

Notation	Lower level (i)	Upper level (j)	λ (in Å) (MCDF)	A_{ji} (s^{-1}) (MCDF)	f_{ij} (MCDF)	S_{ij} (a.u.) (MCDF)	Type	λ_{FLYCHK} (Å)
4D	$2s^22p^6\,^1S_0$	$2s^22p^54d\,^1P_1$	9.2443	1.12×10^{13}	4.30×10^{-1}	1.31×10^{-2}	E1	9.2673
4C	$2s^22p^6\,^1S_0$	$2s^22p^54d\,^3D_1$	9.1144	1.06×10^{13}	3.97×10^{-1}	1.19×10^{-2}	E1	9.1254
	$2s^22p^6\,^1S_0$	$2s^22p^55s\,^1P_1$	8.5723	3.89×10^{11}	1.29×10^{-2}	3.63×10^{-4}	E1	
	$2s^22p^6\,^1S_0$	$2s^22p^55d\,^3P_1$	8.4708	7.86×10^{10}	2.54×10^{-3}	7.08×10^{-5}	E1	
5D	$2s^22p^6\,^1S_0$	$2s^22p^55d\,^1P_1$	8.4562	6.14×10^{12}	1.97×10^{-1}	5.50×10^{-3}	E1	
	$2s^22p^6\,^1S_0$	$2s^22p^55s\,^3P_1$	8.4507	1.23×10^{12}	3.96×10^{-2}	1.10×10^{-3}	E1	
4A, 4B	$2s^22p^6\,^1S_0$	$2s2p^64p\,^3P_1$	8.3899	1.12×10^{12}	3.55×10^{-2}	9.80×10^{-4}	E1	8.3823
	$2s^22p^6\,^1S_0$	$2s2p^64p\,^1P_1$	8.3763	3.14×10^{12}	9.91×10^{-2}	2.73×10^{-3}	E1	
5C	$2s^22p^6\,^1S_0$	$2s^22p^55d\,^3D_1$	8.3419	3.98×10^{12}	1.24×10^{-1}	3.42×10^{-3}	E1	8.344
	$2s^22p^6\,^1S_0$	$2s^22p^56s\,^1P_1$	8.1413	2.02×10^{11}	6.03×10^{-3}	1.62×10^{-4}	E1	
	$2s^22p^6\,^1S_0$	$2s^22p^56D^3P_1$	8.0893	3.26×10^{10}	9.60×10^{-4}	2.56×10^{-5}	E1	
6D	$2s^22p^6\,^1S_0$	$2s^22p^56D^1P_1$	8.0809	4.51×10^{12}	1.32×10^{-1}	3.52×10^{-3}	E1	8.0844
6F	$2s^22p^6\,^1S_0$	$2s^22p^56S^3P_1$	8.032	6.84×10^{10}	1.99×10^{-3}	5.25×10^{-5}	E1	
6C	$2s^22p^6\,^1S_0$	$2s^22p^56D^3D_1$	7.9761	2.56×10^{12}	7.32×10^{-2}	1.92×10^{-3}	E1	7.975

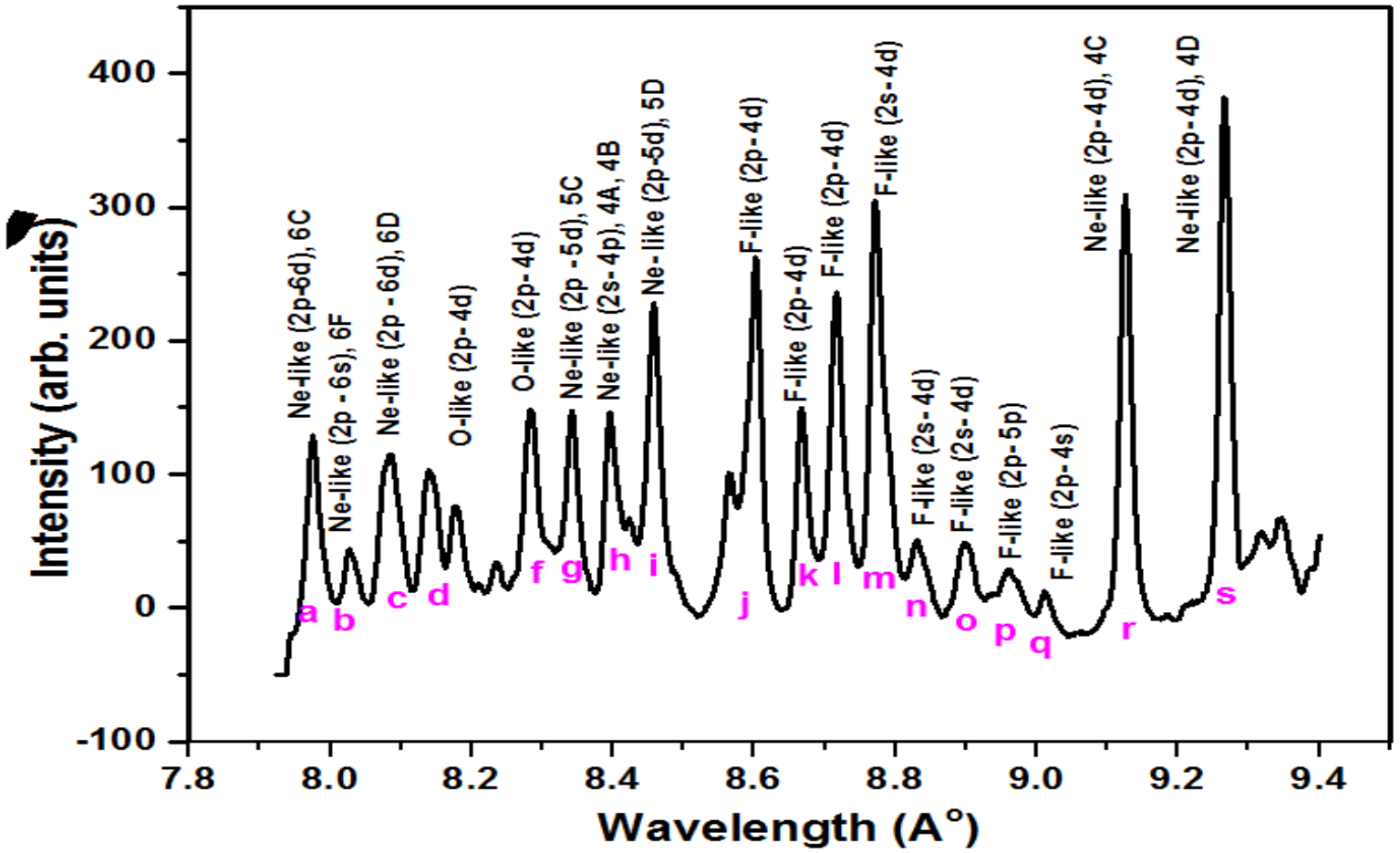


Figure 3: The experimental spectrum at intensity with the identified transitions

1st year

We plan to calculate fine structure energies, radiative data such as transition energies, transition wavelengths, line strength, oscillator strength and radiative rates (transitions/ wavelengths required)

- Tungsten ions (W10+ - W25+) using GRASP and FAC,

- Be-like ions, Fe-like ions and Al-like ions using GRASP2K and FAC

- In addition to this, we will also compute atomic data of liquid metals (Li, Sn and Ga) and their ions.

2nd year

- We will calculate fine structure energies, radiative data such as transition energies, transition wavelengths, line strength, oscillator strength and radiative rates of ions of Ar and Ne ions using CIV3 and GRASP.

- We will study atomic processes and plan to calulate electron impact excitation cross-section and photoionization cross-section using the wavefunctions from GRASP calculations

  Tungsten ions (W10+ -W25+) using DARC and FAC

  (Li, Sn and Ga) and their ions using DARC and FAC

- We will also compare the results from different codes, databases such as ADAS, CHIANTI, NIST etc. and online computing codes to check the accuracy of results.

3rd year

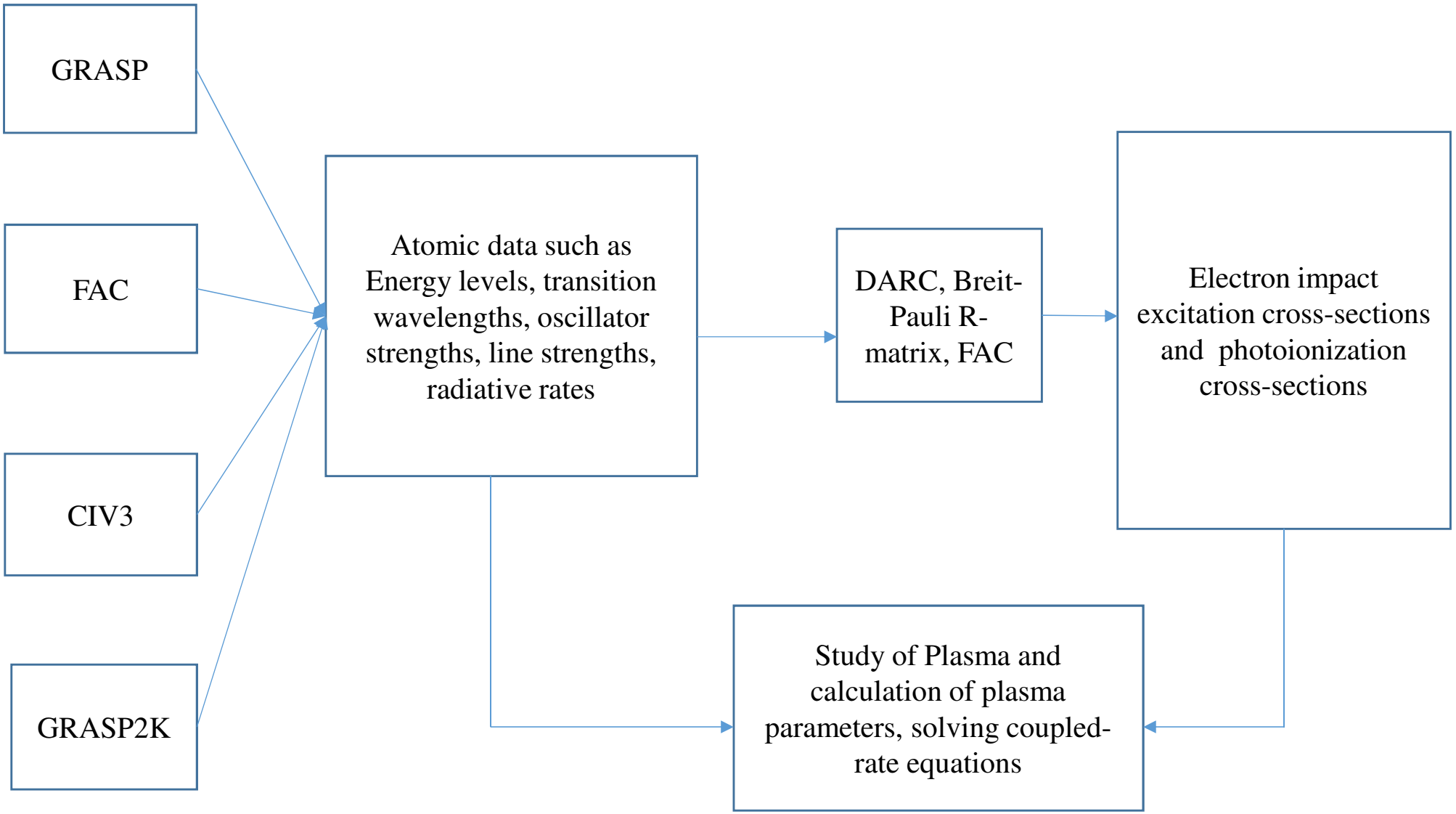
- We will study atomic processes and plan to calculate electron impact excitation cross-section and photoionization cross-section using the wave functions from GRASP and CIV3 calculations

  For ions of Ar and Ne ions using BPRM and DARC

  Be-like ions, Fe-like ions and Al-like ions

- In 3rd year, we also plan to study plasma embedded systems an calculate plasma screening effect on excitation energies and radiative properties.

Application of Relativistic Atomic Data codes in Plasma diagnostics



THANK YOU