CONTRIBUTION FUNCTION OF MOLYBDENUM ATOM AND IONS IN ASTROPHYSICAL AND LABORATORY PLASMA AS A FUNCTION OF ELECTRON TEMPERATURE

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ABSTRACT:

Ionization and Recombination rate coefficients of Molybdenum atom and ions are fully determined by electron temperature. The excitation Rate Coefficient, the fractional Abundance, electron density decides the intensity of spectral line and the spectral line intensity is proportional to the contribution function. The Contribution function of Ion can be defined as the product of fractional ion abundance and its excitation rate coefficient of upper state of transition emitting the spectral line in consideration. In present work the fractional abundance, excitation rate coefficient and the Contribution function of Molybdenum ions as a function of Electron Temperature are computed and presented graphically.

KEYWORDS: Collisions, The excitation Rate Coefficient, fractional Abundance, contribution function, Electron Temperature,

1. INTRODUCTION

It is well known that energy states of atoms and ions in the plasma are populated by electron collisions and depopulated by collisions of ions with slow electrons. Besides the collisional processes the atomic and ionic states are populated and depopulated due to some radiative processes also.

Electrons passing through the plasma transfer their energy to the plasma particles by two types of collisions, i) Elastic collisions ii) Inelastic collisions.

In elastic collisions the transfer of kinetic energy of electron in to the kinetic energy of the plasma particles (atoms or ions) takes place. In this process the kinetic energy of the colliding particles is conserved. This type of collisional process is responsible to the heating of the plasma particles to some extent. In fact the second type of collision i.e. inelastic collisions are mainly responsible for the excitation of atoms and ions in the plasma. Any collision in which the internal energy of excitation of a particle is changed is referred to as inelastic collision. In this type of collision the kinetic energy of electron is converted into potential energy of colliding plasma particles and the plasma particles get excited. These particles in excited states either transfer their energy back to the electron or they undergo a transition giving radiative emission. If N_g is number of gas particles. C_e is coefficient of elastic collision. E_c is energy

transferred in elastic collisions. C_{in} is rate coefficient of inelastic collisions. E_j is energy of the jth state excited by elastic collision. C_{dex} is de-excitation rate coefficient. E_i is energy of excited particles which transfers its energy to the electrons. The rate of transfer of energy from the electrons to the plasma particles may be written as,

$$\frac{dE}{dt} = N_g C_e N_e E_c + \sum_j N_{gi} N_e C_{in} E_j - \sum_j N_{gi} N_e C_{dex} E_i \quad (1)$$

The sum runs over all possible energy states of the plasma particles.

All the processes which can populate or depopulate the states of plasma particles are listed below.

2. ELECTRON IMPACT EXCITATION (EIE)

In this case the energy from the high energy electrons is transferred to the colliding atoms or ions in the plasma. When an electron having energy more than the excitation energy of an electron rotating around nucleus of an atom / ion collides with the atom / ion may transfer its energy to the system and this may result in excitation of the rotating electron to a higher orbit. The probability of excitation depends upon energy of exciting electron and cross section of excitation at that particular energy. The excitation rate depends upon the excitation cross section and the number of effective collisions made by the electron. The number of effective collisions is function of electron velocity, which intern is a function of electron temperature (T_e).

As we know that the plasmas consists of atoms, ions and electrons, there can be two types of electron impact excitation processes depending upon whether the colliding particles are atoms in ground state or ion in ground state. And accordingly these electron impact excitation (EIE) rate coefficients are defined as direct excitation and stepwise excitation respectively. The EIE rate coefficient is expressed interms of excitation cross section σ and electron velocity V_e as $< \sigma V_e >$. Now for the two types of electron impact excitations we can write,

$$R = < \sigma_s V_e > \quad (2)$$

and

$$D = < \sigma_d V_e > \quad (3)$$

where,

R is EIE rate coefficient due to stepwise excitation.

D is EIE rate coefficient due to direct excitation.

σ_s is EIE cross section for states from ground state of ions.

σ_d is EIE cross section for the states from ground state of neutral atom.

The velocity of an electron is function of its energy and related to its energy E by the relation,

$$V_e = 5.9 \times 10^7 \, (E)^{1/2} \quad (4)$$

The number dN of the electrons having energy between E and E+dE is given for Maxwellian distribution by equation,

$$dN = N \times (2/KT_e) \times [E/(\pi KT_e)]^{1/2} \times EXP(-E/KT_e)dE \quad (5)$$

Thus the rate of excitation of energy levels by stepwise and direct excitation are respectively expressed as,

$$dR = N \times (2/KT_e) \times [E/(\pi KT_e)]^{1/2} \times (\sigma_s V_e) \times EXP(-E/KT_e) dE \quad (6)$$

and

$$dD = N \times (2/KT_e) \times [E/(\pi KT_e)]^{1/2} \times (\sigma_d V_e) \times EXP(-E/KT_e) dE \quad (7)$$

The total excitation rate coefficient can be obtained by integrating above equation within the limits from 0 to ∞.

As the excitation process does not occur if the energy of incident electron is less than the threshold energy E_s, the excitation cross section is zero for energy less than E_s. Therefore the lower limit of integration is taken as E_s instead of zero.

Further it is convenient to express the electron temperature and electron energy in eV. If T_e, E and dE are all in eV and cross section values are in cm^2, the equation (6) and equation (7) be written as,

$$R = \frac{6.7 \times 10^7}{(T_e)^{3/2}} \int_{E_s}^{\infty} \sigma_s E \; EXP(-E/KT_e) dE \;\; cm^3 \sec^{-1} \quad (8)$$

and

$$D = \frac{6.7 \times 10^7}{(T_e)^{3/2}} \int_{E_s}^{\infty} \sigma_d E \; EXP(-E/KT_e) dE \;\; cm^3 \sec^{-1} \quad (9)$$

respectively.

These equations clearly show that if the values of the excitation cross section are known at different values of the electron energy, the excitation rate coefficients may be obtained at different electron temperatures.

3. PENNING EXCITATION

Excitation energy can be exchanged between neutral atoms. In particular, an excited atom can get ionized by virtue of its excitation energy, if the later is larger than the required ionization energy. Such a process is made more probable if the excited atom is in metastable state and has thus longer lifetime in which the particle may undergo an effective collision. When one of the colliding atoms is in metastable state and the other one is in ground state, there is a probability of ionizing second atom and getting excited to the excited state depending upon the energy of the metastable atom. Such a process is referred to as penning excitation.

4. DUFFENDUCK EXCITATION

The process in which an ion having charge z in a ground state, when collide with the other ion having charge z' in ground state, transfers its energy to the colliding partner and the other ion gets ionized. This process of ionization and excitation of one ion and recombination of other ion is known as duffenduck excitation or charge transfer.

For computation of excitation rate coefficients, we have used the formula proposed by Breton [1] which is useful for computation of excitation rate coefficient of heavy atoms like molybdenum as a function of electron temperature. The formula proposed by Breton is based on the Bethe-Born approximation for optically allowed transitions [2] which is given below.

$$Q = 1.6 \times 10^{-5} e^{-\beta} \times \frac{f \overline{g}(\beta)(\beta)^{1/2}}{(\Delta E)^{3/2}} \quad (10)$$

where Q is in $cm^3 \sec^{-1}$, ΔE is the excitation energy in eV. $B = (\Delta E / T_e)$ where, T_e is in eV

f is the absorption oscillator strength.

$\overline{g}(\beta)$ is the average effective Ground factor.

The expression for $\overline{g}(\beta)$ which is proposed by Mewe [3] is given below.

$$\overline{g}(\beta) = A + (B\beta - C\beta^2 + D)e^{\beta} \; E_1(\beta) + C\beta. \quad (11)$$

where A, B, C and D are adjustable parameters. This formula may also include optically forbidden monopole or quadrapole transitions (for example H - like ions, the 1s $\rightarrow$ ns or 1s $\rightarrow$ nd transitions respectively) and spin exchange transitions (for example singlet-triplet transitions in He like ions). In these cases, f in equation (1) assumes the f values of the allowed transitions to the level with the same principle quantum number. For example, for the transition 1s $\rightarrow$ ns and 1s $\rightarrow$ nd in the H - like sequence the f value of 1s $\rightarrow$ np is chosen: for 1s2 $^1S \rightarrow$ 1s 2s^3S in the He like sequence, that of 1s2 $^1S \rightarrow$ 1s 2p ^1P is used.

The molybdenum transition that are included in excitation rate coefficient computations together with wavelengths λ, the excitation energies ΔE and the f values, we used the values in C. Breton et al [1]. The isoelectronic sequences and transitions considered are the same as for

Iron; the wavelength λ were either taken from calculations [6] or elsewhere obtained by extrapolation. The absorption oscillator strength f were taken from [4 to 7] otherwise, we used the systematic trends of f in isoelectronic sequences [4] as a function of nuclear charge Z_n, starting from the values for Iron. Thus for $\Delta n = 0$ transitions, we used $f \sim (f_1/Z)$: for $\Delta n \neq 0$ transitions $f \sim (f_0 + f_1/Z)$. In this second case we have assumed that $f_1/Z < f_0$ and have taken for Mo the same values as for Fe (this is justified by the fact that, in all cases considered in [5], the variations of f between Fe and Mo are smaller than 5%).

The excitation rate of an energy level of an ion is given by,

$$\frac{dN_u}{dt} = N_e N_z R_{zu} \qquad (12)$$

where, N_e is the electron density. N_z is the fractional density of the ion of charge z. R_{zu} is the electron impact excitation rate coefficient of the state of ion of charge z.

The excited states in the plasma are dexcited by ratdiative transitions. Therefore we may write,

$$\frac{dN_u}{dt} = \frac{-N_u}{\tau} \qquad (13)$$

where τ is the radiative life time of the state.

When the plasma is in steady state the excitation rate of a state would be equal to dexcitation rate. Therefore,

Rate of excitation = Rate of dexcitation.

The energy states of the ions dexcite only because of the radiative decay and therefore we may write,

Rate of excitation = Rate of dexcitation by radiative decay.

In other words,

Rate of excitation α Rate of photon emission.

Rate of excitation α Intensity of radiation.

Therefore, Intensity of radiation α Rate of photon emission and Rate of excitation of the energy states.

5. THE EXCITATION RATE COEFFICIENTS

The excitation rate coefficient is very useful function in computing the contribution functions of various spectral lines. In present work, we have computed excitation rate coefficients of Mo XXV through Mo XLII using Bretons formula [1] and results for Mo XXV to Mo XXVIII and Mo XXXV to Mo XXXVIII are displayed in figure (1) and figure (2) respectively as a function of electron temperature.

In all figures it is observed that the general behavior of the curves is almost similar for all the iron and molybdenum ions. From the nature of the graph, it is seen that, initially, as the electron temperature is increased from lower value, the excitation rate coefficient increases linearly. But as the electron temperature approaches to a value at which the excitation rate coefficient becomes maximum, the excitation rate coefficient increases non-linearly. The non linearity in the curve increases as excitation rate coefficient approaches towards saturation. Further; the electron temperature increases, the value of electron temperature at which excitation rate coefficient saturates, the excitation rate coefficient decreases but rate of decrease in excitation rate coefficient will be very slow. From graphs in figure (1) through figure (2), it shows that the excitation rate coefficient (ERC) is very sensitive function of the electron temperature before it reaches its peak value but the variation of the function becomes very slow varying function of electron temperature near its saturation value.
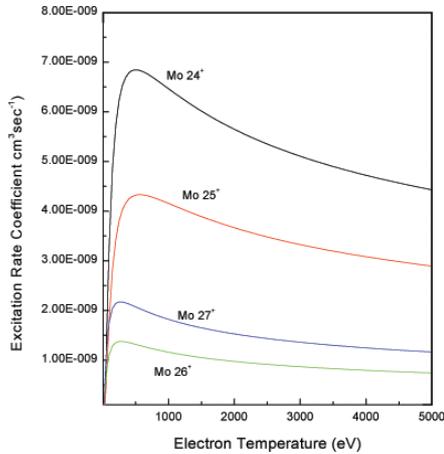
Fig. 1
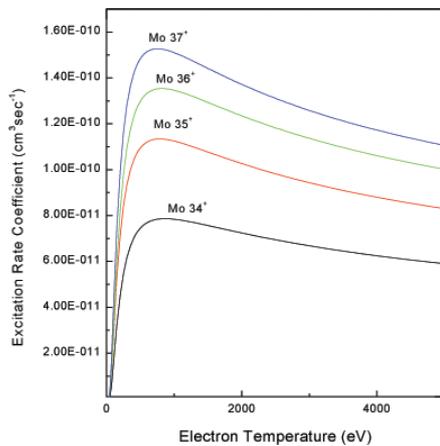
Fig. 2

Fig. 1 and Fig. 2: *Excitation Rate Coefficient As A Function Of Electron Temperature.*

6. FRACTIONAL ABUNDANCE

Plasma consists of the electrons and the ions with different charges. The collision between the atoms, ions of different charges and electrons results in ionization. At the same time the ions may capture the electrons and results in formation of ions of lower charge. The ionization and Recombination processes compete each other so that the ionization rate and recombination rate reach, each to a certain value and equilibrium is attained. As long as the electron temperature is not changed the equilibrium remains in a particular state. A change in electron temperature results in changing the densities of ions and electrons. Thus densities of ions and electrons are completely dictated by the electron temperature. The plasma emission depends upon the fraction of total density of species remaining in a particular ionized state, the electron density and the electron temperature.

The amount of the fraction of the total density of species remaining in a particular ionized state is called as fractional abundance of that ion.

Equation for the time rate of change of population density of ion of charge z can be written as,

$$\frac{dN_z}{dt} = n_e \left\{ -N_z S_z + N_{z-1}\ S_{z-1} - N_z\ \alpha_z + N_{z+1}\ \alpha_{z+1} \right\}$$

(14)

where z takes all values between 0 and maximum charge on the ion.

The ionization state of each element of atomic number z is controlled by electron impact ionization (including autoionization) from state $z \to z+1$ with total rate coefficient $S_{z,z}$ ($cm^3\ sec^{-1}$) and radiative plus dielectronic recombination $z+1 \to z$ with rate coefficient $\alpha_{z,z+1}$ ($cm^3\ sec^{-1}$)

In steady state, the time rate of change of population density of ion of charge z will be zero.

In steady state condition, where the time rate change of population density of ion of charge z will be zero , the equation (14) reduces to,

$$N_z\ \alpha_z = N_{z+1}\ \alpha_{z+1}$$

The population density ratio ($N_{z,z+1}/N_{z,z}$) of two adjacent ion stages $Z^{+(z+1)}$ and Z^{+z} can be derived from above steady state equation as,

$$\frac{N_{z+1}}{N_z} = \frac{S_z}{\alpha_{z+1}}$$

(15)

where $S_{(z)}$ is ionization rate coefficient of ion of charge z. α_{z+1} is recombination rate coefficient of ion of charge z+1. N_z and N_{z+1} are densities of ion with charge z and z+1 respectively.

6.1 EXPRESSION FOR FRACTIONAL ABUNDANCE

Thus, population density ratio ($N_{z, z+1}$ / $N_{z,z}$) can be evaluated in terms of S_z and α_{z+1}. As the values of S_z and α_{z+1} are fully determined by the electron temperature. Therefore the fractional abundance and population density of any ion in the plasma depends only on the electron temperature [8]. The fractional abundacne of a particular species can be evaluated by using equation (15).

By putting z = 0, 1, 2, ... in equation (15) we get,

$$A = \frac{N_1}{N_0} = \frac{S_0}{\alpha_1} \qquad (16)$$

$$B = \frac{N_2}{N_1} = \frac{S_1}{\alpha_2} \qquad (17)$$

$$C = \frac{N_3}{N_2} = \frac{S_2}{\alpha_3} \qquad (18)$$

$$D = \frac{N_4}{N_3} = \frac{S_3}{\alpha_4} \qquad (19)$$

, ……………… and so on.
Let us multiply equation (16) by equation (17) to get,

$$A \times B = \frac{N_2}{N_0} = \frac{S_0}{\alpha_1} \times \frac{S_1}{\alpha_2} \qquad (20)$$

On multiplying equation (20) by equation (18) we get,

$$A \times B \times C = \frac{N_3}{N_0} = \frac{S_0}{\alpha_1} \times \frac{S_1}{\alpha_2} \times \frac{S_2}{\alpha_3} \qquad (21)$$

Taking product of the equation (19) and equation (21) we get,

$$A \times B \times C \times D = \frac{N_4}{N_0} = \frac{S_0}{\alpha_1} \times \frac{S_1}{\alpha_2} \times \frac{S_2}{\alpha_3} \times \frac{S_3}{\alpha_4} \qquad (22)$$

…….. and so on.
On adding equations (16), (20), (21), and (22) we get,

$$F = A+(A \times B)+(A \times B \times C)+(A \times B \times C \times D) + - - - -$$

$$F = \frac{N_1}{N_0} + \frac{N_2}{N_0} + \frac{N_3}{N_0} + \frac{N_4}{N_0} + \ - - - -$$

$$F = \frac{N_1 + N_2 + N_3 + N_4 + - - - -}{N_0} \qquad (23)$$

The equation for fractional abundance can be written as,

$$\text{Fractional abundance } = \frac{1}{F+1} \qquad (24)$$

Fractional abundance

$$= \frac{1}{\dfrac{N_1 + N_2 + N_3 + N_4 + - - - -}{N_0} + 1}$$

Fractional abundance

$$= \frac{1}{\dfrac{N_0 + N_1 + N_2 + N_3 + N_4 + - - - -}{N_0}}$$

Fractional abundance

$$= \frac{N_0}{N_0 + N_1 + N_2 + N_3 + N_4 + - - - -}$$

(25)

The denominator term can be written as,

$$N_0 + N_1 + N_2 + N_3 + N_4 + - - - - = \sum N_{z'}$$

Therefore, the equation (25) can be written as,

Fractional abundance of neutral atoms

$$= \frac{N_0}{\sum\limits_{z'} N_{z'}} \qquad (26)$$

The sum runs over all possible ionized states.
N_0, the density of neutral atoms. The sum runs over all possible ionized states.

The equation (26) gives the fractional abundance of neutral atom.

In general, the fractional abundance of an ion of charge z can be written as,

$$F_z = \frac{N_z}{\sum\limits_{z'} N_{z'}} \qquad (27)$$

Where F_z, the fractional abundance of ion of charge z. N_z, the density of ion with

charge z. The sum runs over all possible ionized states

To study the behavior of Fractional abundance of neutral atoms and different ionic species of Molybdenum, we have computed fractional abundance of these atoms and ions using equation (27) as a function of electron temperature using equation (28). The Fractional abundance of Molybdenum ions are presented graphically as a function of electron temperature in figure (3) and figure(5)
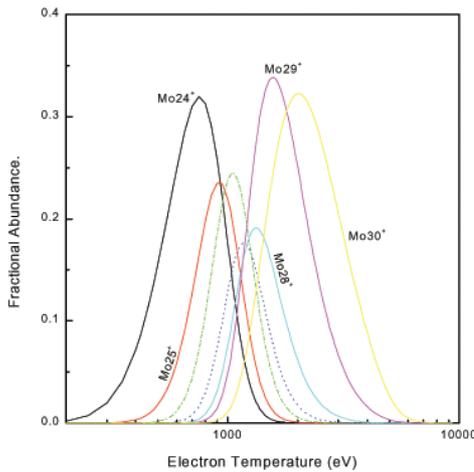
Fig. 3
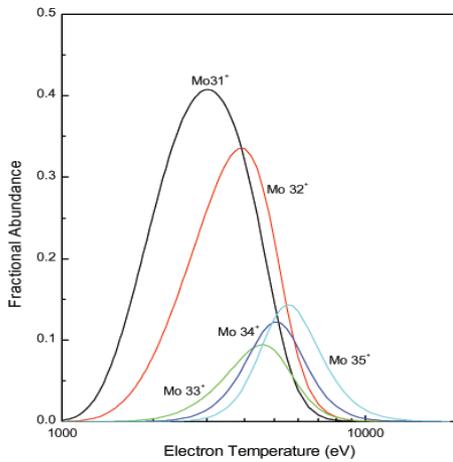
Fig. 4

Fig. 3 and fig. 4 : *Fractional Abundance Of Molybdenum Ions As A Function Of Electron Temperature.*
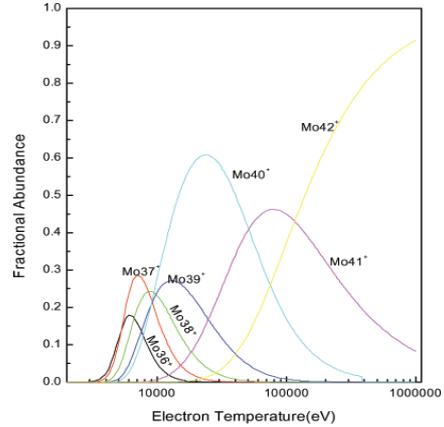
Fig. 5 : *Fractional Abundance Of Molybdenum Ions As A Function Of Electron Temperature. (The Dash Dot Curve) represents Mo XXVII and dotted curve represents Mo XXVIII*

7. THE CONTRIBUTION FUNCTION

The contribution function is an electron temperature dependent part of the flux emitted by a spectral line and it is a measure of spectral line intensity because, spectral line intensity is proportional to their contribution function. The contribution function can be defined as the product of fractional ion abundance and the excitation rate coefficient of the upper state of the transition emitting the spectral line in consideration. The equation for contribution function can be written as,

$$C(z) = N_Z R_{zu} \qquad (28)$$

Where N_Z is the fractional density of the ion of charge z and R_{zu} is the electron impact excitation rate coefficient of the state u of ion of charge z

8. RESULTS AND DISCUSSION

In present work, we have computed contribution function $C(z)$ by taking product of fractional abundance of an ion of charge z and electron impact excitation rate coefficient R_{zu} of state u of ion charge z for few spectral lines of molybdenum ions and are presented graphically in figure (6) through figure (8).

The general nature of all curve is similar. The contribution function of ion in consideration rises almost linearly up to its peak value as electron temperature rises. As the electron temperature increases above the electron temperature where contribution function becomes maximum, the contribution function decreases linearly up to the electron temperature at which contribution function is about 60% of its peak value. For further increase in electron temperature the contribution function decreases non-linearly and non-linearity in curves increases as electron temperature rises for higher values.
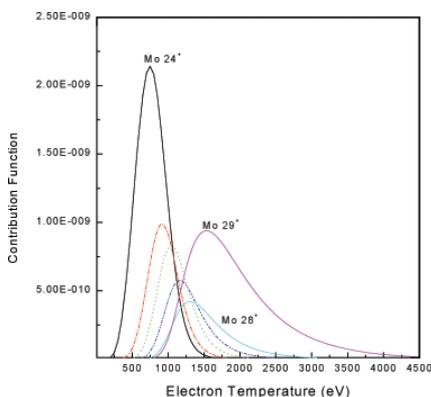
Fig. 6 *Contribution Function Of Molybdenum Ions As A Function Electron Temperature. (Dash dot curve represents Mo XXVI, Dotted curve represents Mo XXVII and dash dot curve represents Mo XXVIII)*
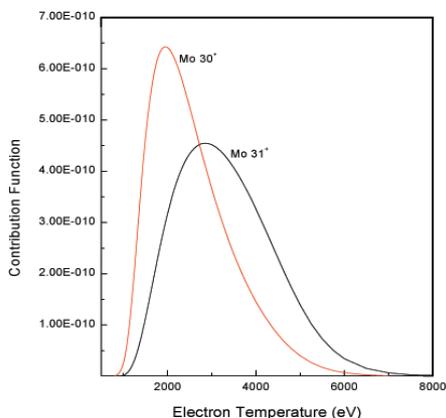
Fig. 7 *Contribution Function Of Molybdenum ions As A Function Of Electron Temperature.*
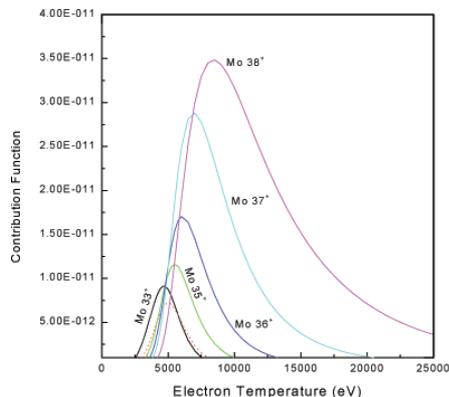
Fig. 8 *Contribution Function Of Molybdenum ions As A Function Of Electron Temperature. (Dotted curve represents Mo XXXV)*

The table 1 shows the wavelength of the Molybdenum transition and the electron temperature at which the contribution function is 100% and 30%.

Table 1

Ion	Wave length (A)	The electron Temperature(eV) At which contribution function is 100%	The range of electron temperature (eV) during which contribution is above 30%
Mo XXV	77	750	420 – 1100
Mo XXVI	69	900	600 – 1275
Mo XXVII	72	1050	750 – 1450
Mo XXVIII	76.5	1175	850 – 1650
Mo XXIX	142	1300	950 – 1950
Mo XXX	155	1525	1075 – 2600
Mo XXXI	117	1950	1250 – 3700
Mo XXXII	143	2850	1375 – 5000
Mo XXXIII	04.8	4000	2350 – 6000
Mo XXXIV	04.75	4600	3100 – 6500
Mo XXXV	45	5000	3500 – 7000
Mo XXXVI	50	5500	2950 – 11750
Mo XXXVII	47.5	6000	3400 – 9500
Mo XXXVIII	52	7000	4800 – 12000
Mo XXXIX	52	8500	5500 – 17250
Mo XL	86	11750	6500 – 32000
Mo XLI	00.71	32000	11500 – 112500
Mo XLII	00.685	85000	26500 - 480000

9. CONCLUSION

The contribution function of ion rises almost linearly up to its peak value. As the electron temperature increases above the electron temperature where contribution function becomes maximum, the contribution function decreases linearly. For further increase in electron temperature the contribution function decreases non-linearly and non-linearity in curves increases as electron temperature rises further.

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