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

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ABSTRACT: Plasma consists of particles having different velocities and therefore they may undergo collisions and the collisions intern may give rise to several processes like ionization, recombination, excitation etc. All possible processes of ionization have been discussed. In particular, theories proposed by Wilson & White, Lotz and Arnaud & Raymond have considered in brief. The ionization rate coefficients of various ionization species of Molybdenum have been computed as a function of electron temperature using the formulation proposed by Lotz by considering contribution of last three subshell for a wide range of the electron temperature and typical results are presented graphically.

KEYWORDS: *Plasma, Collisions, Ionizations, Ionization Rate Coefficients, Electron Temperature.*

1. INTRODUCTION

When matter is heated to high temperature the number of collisions made by the particles in matter are increased. In the process of collisions electrons are detached and the particles of matter gets ionized, such a ionized matter is called as plasma. The electrostatic forces between the charged particles are such that any large scale separation of charge is resisted and plasma neutrality is generally maintained. The plasma may be characterised by the values of its electron temperature, electron density, ion temperature and ion density. The plasma is also characterised by the type of particles which are ionized. The range of plasma parameters is very wide. Astrophysical plasma parameters also have large range from the cold plasma of interstellar space to that at the centres of massive stars. Laboratory plasma parameters and plasmas have more restricted ranges. An important difference between astronomical and laboratory plasmas is in their sizes and sometimes in their durations. Under the conditions of corona model valid for low density plasmas, the ionization equilibrium is determined by the balance between the process of ionization and the process of radiative and dielectronic recombinations. In this work different ionization processes and ionization cross sections and ionization rate coefficients are studied.

2. THE PROCESSES RESPONSIBLE FOR IONIZATION

2.1 ELECTRON IMPACT IONIZATION

The ionization may take place by electron impact if the incident electron has sufficient energy to detach the electron from the ion of charge z. The electron impact ionization process is represented by a reaction,

$$E^{+z} + e^{-} \rightarrow E^{+(z+1)} + e^{-} + e^{-} \qquad (1)$$

2.2 PHOTOIONIZATION

The ionization may takes place due to the absorption of photon by an ion having charge z. The photons emitted in the process of radiative recombination have sufficient energy to reionize the ions. The process of photoionization may be represented by the following reaction,

$$E^{+z} + h\nu \rightarrow E^{+(z+1)} + e^{-} \qquad (2)$$

2.3 AUTOIONIZATION

The autoionization process is most important for the ions in which there are more number of electrons in the first inner subshell compared with the number of electrons in the outer subshell [1]. It has been realised that autoionization is particularly significant for the sodium sequence ($1s^2\ 2s^2\ 2p^6\ 3s$), where eight L-shell electrons can contribute to autoionization (e.g. 2p-3p and 2p-3d transitions), while there is a single 3s valance electron that contribute readily to direct ionization [1,2].

This mechanism can be illustrated using the following steps of general reaction.

$$E^{+z} + e^{-} \rightarrow \left(E^{+z}\right)^{*} + e^{-} \rightarrow e^{-} + E^{+(z+1)} + e^{-} \qquad (3)$$

In addition to above mentioned processes of ionization, the following three mechanisms may also ionize the atoms.

3. THE PENNING REACTION

There is an important class of inelastic collisions between heavy atoms or ions and helium atoms in excited states where potential energy of helium atom is transferred to atom and therefore the atom may get excited to upper state or may get ionized. The cross section for this process is generally larger than that of other inelastic collisions between atoms or ions. Here excitation energy gets exchanged between neutral atoms. In particular, an excited atom can be 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 helium atom is in a metastable state and has longer lifetime within which it undergoes effective collision [3]. The process is then known as penning effect. This process of transfer of energy is called as Penning transfer. The process may be expressed as,

$$He^{*}I + MoI \rightarrow HeI + Mo^{*}II + e^{-} \qquad (4)$$

The Mo II ions produced during this process may be in the ground state or in excited state.

4. DUFFENDUCK REACTION

An ion in ground state collides with another ion or atom and transfers its energy to the colliding partner. In the process of collision energy as well as the charge is transferred from one ion to another ion or atom. This process is called as Duffenduck reaction. Following are few examples of Duffenduck reactions

$$\mathrm{HeII} + \mathrm{MoI} \rightarrow \mathrm{HeI} + \mathrm{Mo^{*}II} \qquad (5)$$

$$\mathrm{HeII} + \mathrm{MoI} \rightarrow \mathrm{HeI} + \mathrm{Mo^{*}III} + e^{-} \qquad (6)$$

The rate of production of ions by Duffenduck reaction depends upon the atom density, helium or hydrogen ion density and rate coefficient D of Duffenduck process. Rate of ionization of Duffenduck process is expressed as

$$\frac{dN_{E\,II}}{dt} = N_{E\,I} \times N_{He\,II} \times D \qquad (7)$$

5. CHARGE EXCHANGE REACTION

The charge exchange between highly ionized species may also be possible. In such a case the reaction may be written as,

$$A^{+n} + B^{+m} \rightarrow A^{+(n-1)} + B^{+(m+1)} \qquad (8)$$

In the above reaction the species A is transferring the positive charge to species B. As a result of this the charge on species A is decreased by 1 and charge on species B is increased by 1. In fact for studying the plasma properties the transfer of charge is not important but the energy transfer during collision is important. In the collisions leading to charge transfer, an ion transferring a positive charge gives out energy equal to its ionization energy to its colliding partner.

It should be remembered that charge transfer process is important when ions are moving through the plasma under the influence of an electric field [4].

6. Ionization Rates and Rate Coefficients of Molybdenum

The rate of production of Molybdenum ions with charge (z+1) from the ions of charge z by various processes may be expressed as,

$$\frac{dN_{Mo}{}^{z+1}}{dt} = N_{Mo}{}^{z} N_e S_{z\,Mo} + N_{Mo^{2*}} A_z + N_{Mo^z} H_{He^*} P + N_{Mo^z} N_p PH + N_{Mo^z} N_i D \qquad (9)$$

where $N_{Mo}{}^{z+1}$, the density of Molybdenum

with charge (z+1). $N_{Mo}{}^{z}$ is the density of Molybdenum atoms with charge z. P is the Penning ionization rate coefficient and D is the Duffenduck ionization rate coefficient. A_z is the Autoionization rate coefficient of the Molybdenum ions of charge z. N_P is the photon density. PH is the photoionization rate coefficient.

The first term in above equation is rate of electron impact Ionization, second term is the rate of Autoionization, third term is rate of Penning ionization, fourth term is rate of Photoionization and last term is rate of Duffenduck ionization.

The rate of photoionization process can be neglected in comparison with the other processes because the external radiation field is usually sufficiently weak in the relevant spectral region and the plasmas are in most cases optically thin to the radiation emitted during collisions between electrons and high charged impurity ions such as Molybdenum ions [5].

The contribution of autoionization process to the ionization is most important for ions in which there are large number of electrons in the first inner sub shell compared with the number in the outer shell [1]. In fact it has been realized for some times that autoionization is particularly significant for the sodium sequence ($1s^2\ 2s^2\ 2p^6\ 3s$), where eight L-shell electrons can contribute to the autoionization (e.g. 2p-3s and 2p-3d transitions); while there is only a single 3s valance electron that contributes readily to direct ionization (DI) [1,2].

O.Belly etal [1] and D.H. Sampson [2] have shown by theoretical computations that the process of autoionization is dominant over wide range of energy. The collisional excitation of an inner shell electron leads to a bound state above the first ionization limit. Two subsequent processes may occur, either the bound state interacts with the adjacent continuum to give a free electron (autoionization probability A^a) or it decays radiatively (probability A^r) to another bound state lying below the threshold.

Kowan and Mann [6] have calculated the autoionization rate for sodium like ions and found that the Autoionization rate increased the ionization rate by a factor of 2.5 [6] and they have drawn the conclusion that the autoionization is important process in Cu- like and Zn- like ions.

6.1 The Electron Impact Ionization

The Electron impact ionization rate coefficient S_z is a function of electron velocity distribution, electron energies and the electron impact ionization cross section σ_z. The relation between these parameters is often expressed as,

$$Sz = < \sigma_z\ Ve > \qquad (10)$$

If the velocity distribution and the ionization cross section σ_z as a function of electron energy are known,the ionuization rate coefficient may be obtained.

Several workers in the field have proposed various formulae for the calculation of ionization rate coefficients. Seaton has proposed the expression for the calculation of the ionization rate coefficients in terms of ionization energy and electron temperature near threshold energies. The corresponding ionization rate S_z ($cm^3 sec^{-1}$) is given by the equation,

$$S_z(T_e) = 2.2\times10^{-6}(T_e)^{1/2}\sum_{i=1}^{m}\left(\xi_i \div (\chi_z^i)^2\right)e - (\chi_z{}^i / T_e) \quad (11)$$

where ξ_i the number of electrons in i^{th} subshell (n,l) having ionization energy χ_z^i (all energies being in eV). The sum is over the subshells of the ground configuration.

A similar expression proposed by Lotz gives approximately the same value near threshold. For energies much higher than threshold it gives, however, a better representation of the true cross section in terms of ionization rates.

It is believed that the Seatons formula gives spurious results and hence may not be used for the calculation of the ionization rates. The Lotz formula gives good results and mainly used for calculations of the ionization rate coefficients [7]. The Wilson and White formula gives the rates coefficients whose values are very near to those obtained by the Lotz formula. Moreover, Wilson and White formula is easier and takes very less time for giving the results. But this formula can be used only for Maxwellian velocity distribution and it cannot be used for non - Maxwellian and mixed Maxwellian velocity distributions. That is why, we have not used this formula for further computation and only it is used for comparison.

The Empirical formula developed by Wilson and
White (unpublished) is,

$$S = \varsigma \times \frac{0.90\times10^{-6}}{\chi^{3/2}} \times \frac{(KT_e/\chi)^{1/2}}{4.88 + (KT_e/\chi)} e^{(\chi/KT_e)} cm^3 \sec^{-1} \quad (12)$$

where, χ is the ionization potential in eV. T_e is electron temperature in degrees Kelvin. ς is total number of outer electrons having the same principal quantum number.

We have computed the ionization rate coefficients S_z of Molybdenum, a major impurity in laboratory fusion plasmas by modifying Lotz formula
[8][9].

$$S_z(T_e) = 6.7\times10^{7}\sum_{i=1}^{N}\frac{a_i\xi_i}{(T_e)^{3/2}}\left\{\frac{E_1(X)}{(I_{zi}/T_e)} - \frac{b_i EXP(c_i)}{(I_{zi}/T_e)+c_i}E1(Y)\right\} \quad (13)$$

where, S_z is the ionization rate coefficient in cm^3 / Sec. T_e the electron temperature in eV. I_{zi} is the ionization energy in eV of the electrons in i^{th} subshell of the ions of charge z. ξ_i is the number of equivalent electrons in the i^{th} subshell. a_i, b_i and c_i are constants for highly ionized ions, Lotz proposed $a_i = 4.5\times10^{-14}\ cm^2\ eV^2$, $b_i = c_i = 0$. The terms $E_1(X)$ and $E1(Y)$ are exponential integral functions.

Where
$X = (I_{zi}/T_e)$,
$Y = (I_{zi}/T_e) + c_i$,

$$E_1(X) = \int_X^{\infty} X^{-1}e^{-X}dX \quad and \quad E_1(Y) = \int_x^{\infty} Y^{-1}e^{-Y}dY \quad (14)$$

where N the number of subshells contributing to the ionization.

Lotz proposed that N = 1 for H and He - like ions, N = 2 for isoelectronic sequences from Li to Ne and N = 3 for isoelectronic sequences from Na to Zn and onwards. All ionization rate coefficients Sz for all elements up to Zn have been tabulated by Lotz [10][11].

The subshell binding energies upto Zn have also been calculated by Lotz [12]. For inner subshells, we have taken ionization potentials of respective electrons instead of ionization potential of first electron of the inner subshell according to the Lotz.

7. EXCITATION AUTOIONIZATION

The Lotz formulation of the ionization rate coefficients (used by the most authors) only agrees well with low atomic number (z) ions because of the effects of excitation followed by autoionization, which increases the total measured ionization rates [13]. However, autoionization is not included in Lotz formulation and therefore we expect the

Lotz expression to be an over estimate for high z ions, because radiative stabilization reduces the importance of autoionization for the heavier ions [14].

8. Results and Discussion

Ionization rate coefficients of all the Molybdenum ions have been computed using Lotz formula. While obtaining the ionization rate coefficients using Lotz formula, contribution of last three subshells have been taken into consideration. The ionization process of highly ionized species starts at relatively higher electron temperature.

The results obtained for the ionization of Molybdenum ions using Lotz formula by considering contribution of last three subshells as a function of electron temperature are plotted in figure (1), figure (2) and figure (3). The nature of all the curves is almost similar. The ionization process of highly ionized species starts at relatively higher electron temperature. Initially as the electron temperature is increased, the ionization rate coefficient increases. The rate of increase is high at low electron temperature. As electron temperature is increased further, the rate of increase of rate coefficient for all ionization species decreases. The curves show that the ionization rate coefficients get saturated at certain values of electron temperature.

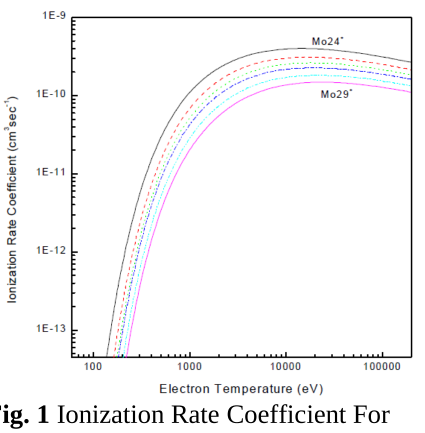

Fig. 1 Ionization Rate Coefficient For Molybdenum Ions As A Function Of Electron Temperature Using Lotz formula *by considering contribution of last three subshells.*

Note: i) Dashed Curve Represents For Mo XXVI Ion. ii) Dotted Curve Represents For MoXXVII Ion. iii)Dash and Dot Curve Represents For Mo XXVIII Ion. iv) Dash Dot Dot Curve Represents For Mo XXIX Ion.

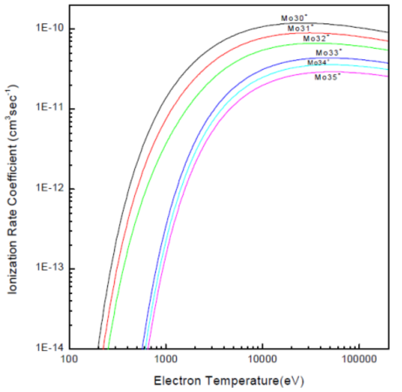

Fig. 2

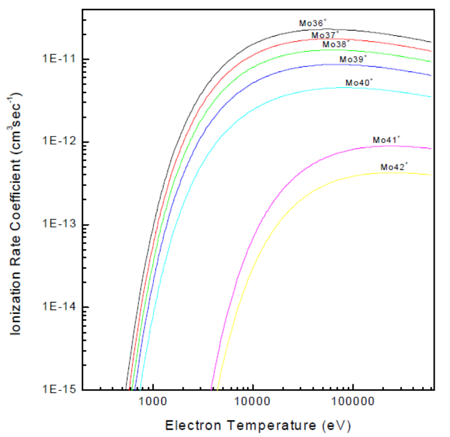

Fig. 3

Fig. 2 and Fig. 3 *Electron Impact Ionization Rate Coeffiecinet Of Molybdenum ions As A Function Of Electron Temperature Using Lotz formula by considering contribution of last three subshells .*

9. Conclusion

1. Wilson and White formula (unpublished) gives quick electron impact ionization rate coefficient compared to Lotz formula. Moreover, if we consider the contribution of last three subshell to the electron impact ionization, values of electron impact ionization rate coefficients using Wilson and White formula gives values very close to the values obtained using Lotz modified formula.

2. Excitation autoionization contribution to ionization should be considered when the number of electrons in the outer subshell are less than the first inner subshell of ion.

3. As the electron temperature of Molybdenum ions is increased, the ionization rate coefficient increases. The rate of increase is high at low electron temperature. As electron temperature is increased further, the rate of increase of rate coefficient for all ionization species decreases. The curves show that the ionization rate coefficients get saturated at certain values of electron temperature.

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