

## Saha's ionization equation for high $Z$ elements

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**Abstract.** Saha's ionization equation has been solved for high  $Z$  elements with the aim of providing input for opacity calculations. Results are presented for two elements, tungsten and uranium. The ionization potentials have been evaluated using the simple Bohr's formula with suitable effective charges for ions. The reliability of the free electron density, ion concentrations, etc., obtained from the Saha's equation solutions has been checked by comparing the  $P_T$  and  $Z_T'$  computed from them with those given by the Thomas-Fermi-Dirac equation of state. The agreement between the two is good from temperatures above 0.2 keV.

**Keywords.** Opacity; equations of state: Saha's and TFD.

### 1. Introduction

In high  $Z$  plasmas, for temperatures in the keV range, the dominant mechanism of energy transport is by radiation through the interaction between photons and electrons. To compute this by radiative transfer equations, one needs the opacities or the absorption cross-sections for the various photon-electron processes. The chief radiative processes to be taken into account from low to high temperatures are

(i) bound-bound (line) absorption\*; (ii) bound-free (photoelectric) absorption; (iii) free-free (inverse bremsstrahlung) absorption; and (iv) various scattering process like the Thomson or Compton type.

The calculation of these cross-sections requires a complete knowledge of the energy levels and their occupation numbers at a given temperature, density and atomic composition of the plasma under consideration. This is a very difficult problem and so far solved only for the hydrogen atom or for a hydrogen-like atom. The relevant formulae, in the hydrogenic approximation are discussed in many books (*e.g.*, Pomraning 1973). The quantities needed for evaluation of these are (1) the free electron density, (2) the populations of the various ionic species and (3) the populations of the various energy states for a given ion. The method followed by various authors (*see, e.g.*, Carson 1971 for a review of this problem) is to use the Saha's equation to obtain (1) and (2). Rouse (1971) has made a detailed investigation of the applicability of the Saha's equation for different

\* Here the term 'absorption' means both absorption as well as its inverse, the emission.

temperature and density domains and proposed a modification which is valid for both low and high densities at high temperatures. He has shown that his "Screened-Coulomb modified Saha or ionization" equation gives results for iron ( $Z = 26$ ,  $\rho_0 = 7.86$  gm/cc) in agreement with the Thomas-Fermi-Dirac (TFD) equation of state.

We have extended the above type of calculations for higher  $Z$  elements. These are of relevance in laser-induced fusion studies where to reduce the expansion of hot DT plasma balls, it has been suggested that the target be surrounded by heavy high atomic number material like uranium (Winterberg 1971). In this paper, we report the results of the solution of Saha's equation for two typical high  $Z$  elements, tungsten ( $Z = 74$ ,  $\rho_0 = 19.2$  gm/cc) and uranium ( $Z = 92$ ,  $\rho_0 = 18.9$  gm/cc).

## 2. Saha's equation

The form of the Saha's equation used is

$$\frac{C_i}{C_{i+1}} = \frac{N_e h^3}{2(2\pi m_e kT)^{3/2}} \frac{U_i}{U_{i+1}} \exp(I_i/kT) \phi_i(D) \quad (1)$$

$$C = \sum_{i=1}^Z iC_i \quad (2)$$

$$C + \sum_{i=1}^R C_i = 1. \quad (3)$$

Here  $N_e$  = free electrons/cc;  $C_i$  = concentration of ion  $i = N_i/N$ , where  $N_i$  is the number/cc of ion  $i$  and  $N$ , total number of free particles/cc =  $N_e + N_a$  and  $N_a = N_i$ ;  $C = N_e/N$ ;  $I_i$  = ionization potential of the ion  $i$ ;  $U_i$  = electronic partition function of ion  $i$ ;  $D$  = screening radius =  $(3/4\pi N_e)^{1/3}$ .  $\phi_i(D)$  is the "pressure ionization" term for ion  $i$ . This takes into account the increased mobility of the electrons occupying the outer orbitals, which overlap significantly with each other at high compressions (Rouse 1971). Roughly, this term works to lower the isolated ion ionization potentials.

## 3. Calculation of ionization potentials

We treat each ion as a hydrogen-like atom, with the outermost electron in the field of charge  $Z_i$  such that

$$Z_i = Z - S. \quad (4)$$

Here  $Z$  is the nuclear charge and  $S$ , the screening constant, due to the inner core electrons. The ionization potentials were then evaluated as

$$I_i = \frac{RZ_i'^2}{n_i^2} \quad (5)$$

where  $R$  is the Rydberg's constant ( $= 13.58$  eV) and  $n_i$  the principal quantum number. Of the many different prescriptions available in literature for the evaluation of  $S$ , we have preferred to use the values given by Burns (1964). He has estimated these for hydrogen-like atoms, by matching the analytic hydrogen-

like wave functions with the ones computed by the Hartree-Fock method, under the assumption that the effective quantum number  $n^* = n$  for any orbital. This ensures self-consistency in the use of formula (5). The relative energy levels of the different atomic orbitals for  $W$  and  $U$ , have been taken as

$$1s < 2s < 2p < 3p < 4s < 4p < 4d < 4f < 5s < 5p < 5d < 6s^\dagger.$$

As stated by Kastner (1969), formula (3) should give accurate values for high  $Z$  elements, (error for  $W \sim 3\%$ ) as the screening constants are strictly valid for  $Z \rightarrow \infty$  case. However, the first few ionization potentials for  $W$  are of higher values (e.g., 150 eV for  $6s$  compared to the experimental value 8 eV). This does not very much effect the solution of Saha's equation as the pressure ionization terms take care of this. The very low values of  $\Phi_i(D)$  for the outer electrons, make the contributions of their  $C_i$ 's negligible. In other words, these electrons can be treated as ionized at a given temperature, irrespective of the value of their ionization potentials.

#### 4. Results

Equations (1-3) were solved by iteration by a computer program run on BESM-6 at Trombay.  $\phi_i(D)$ 's and  $U_i$ 's were evaluated by using the expressions and constants given by Rouse (1971). The ground state degeneracy for each ion was found by Hund's rule. The free electron densities at different temperatures for  $\rho/\rho_0 = 1.0$  are given in table 1. Also shown is ratio  $Ne/Ne_T$  (at full ionization). The ion densities for  $W$  and  $U$  are illustrated in figures 1 and 2. These show that for  $U$  even at a temperature of 10 keV, the  $K$  shell is substantially intact and that for  $W$  it is almost ionized. The ratio  $I_p/T$ , where  $I_p$  is the ionization potential at the peak  $C_i$  at a given  $T$ , varies with temperature from 5 to 2.7, compared to the value 2.8 expected for an ideal Planck's distribution. The high value at low temperatures is again a reflection of the effect of the pressure ionization term. This is similar

Table 1. Free electron densities for  $\rho/\rho_0 = 1.0$

Temperatures	$W$		$U$	
	$Ne$	$Ne/Ne_T^*$	$Ne$	$Ne/Ne_T$
0.2 keV	$1.38 \times 10^{24}$	0.30	$1.17 \times 10^{24}$	0.27
0.5	2.83	0.61	2.33	0.53
0.7	3.00	0.64	2.96	0.67
1.0	3.93	0.84	3.10	0.70
3.0	4.51	0.969	4.12	0.94
5.0	4.52	0.971	4.30	0.977
8.0	4.651	0.999	4.303	0.977
10.0	4.652	0.9995	4.34	0.986
$Ne_T$	4.654	—	4.40	—

\*  $Ne_T$  = free electron density at full ionization.

† These are not independent of atomic number. Their variation with  $Z$  is given by Evans (1966).

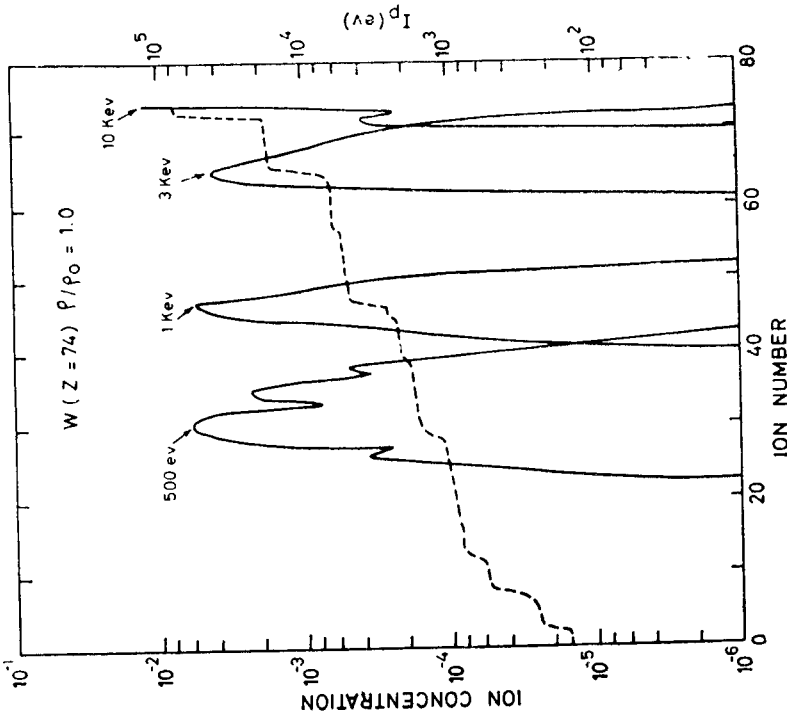


Figure 1. Ion concentrations at various temperatures for W for  $\rho/\rho_0 = 1.0$ . The ionisation potentials are shown by the dotted line.

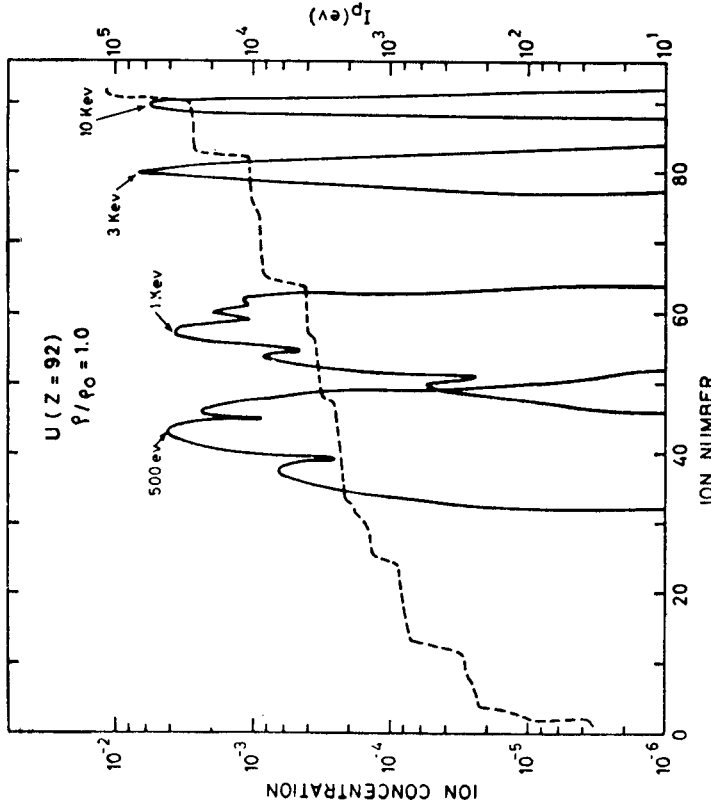


Figure 2. Ion concentrations at various temperatures for U for  $\rho/\rho_0 = 1.0$ . The ionisation potentials are shown by the dotted line.

to that found by Pritzker *et al* (1975) for uranium plasmas although their treatment of the pressure ionization term and the calculation of ionization potentials is different.

To check the reliability of the above numbers, we computed the  $P_T$  vs  $E_T$  curves and compared them with the curves obtained from TFD Kirzhnits corrected equation of state (McCarthy 1965). The various contributions to  $P_T$  and  $E_T$  are

$$E_T = E_{k.e.} + E_{ion} + E_{exc} + \bar{V}_{p.e.}$$

and

$$P_T = P_a + P_e + \bar{P}_{p.e.}$$

Here  $E_{k.e.}$  = kinetic energy of ions and electrons =  $3/2 NkT = 3/2(P_a + P_e)$ ,  $E_{ion}$  is the ionization energy,  $E_{exc}$  the excitation energy and  $\bar{V}_{p.e.}$  is one-half the potential energy of the free electrons in the fields of various ions (Coulomb correction), as formulated by Rouse (1971). Figures 3 and 4 show the above comparison for  $W$  and  $U$ . The agreement of our results with TFD EOS is good from temperatures above 0.2 keV. This close agreement shows that the model of Saha's equation and the phenomenological method of the calculation of ionization potentials are quite reasonable and, therefore, the opacities, evaluated using the inputs as given above, will be reliable and self-consistent. The use of ionization potentials\* based on the energy levels derived from x-ray wavelength data (Bearden and Burr 1967) was also investigated. The values

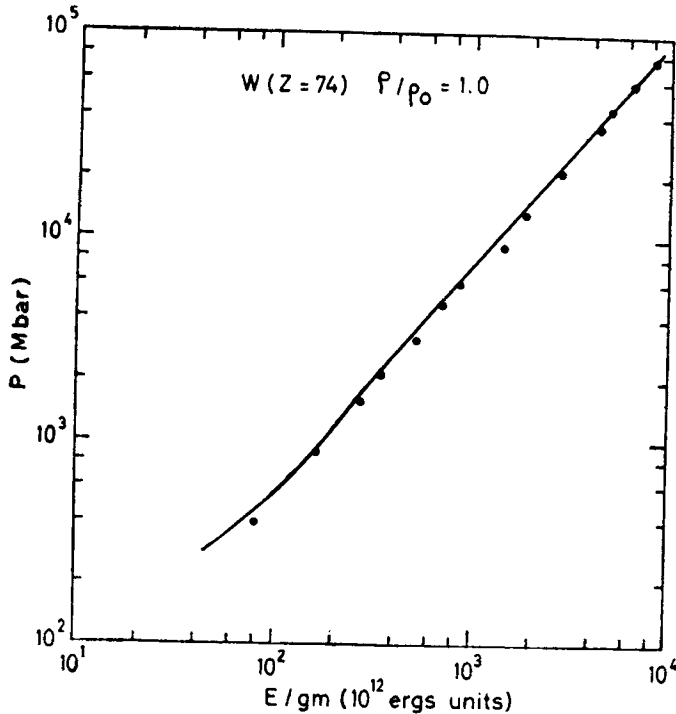


Figure 3.  $E_T$  vs.  $P_T$  diagram for  $W$ . The full curve is the TFD Kirzhnits curve. The  $\bullet$  are our calculated values.

\* These will not be for isolated ions and as expected from screening rules, were lower than given by equation (5).

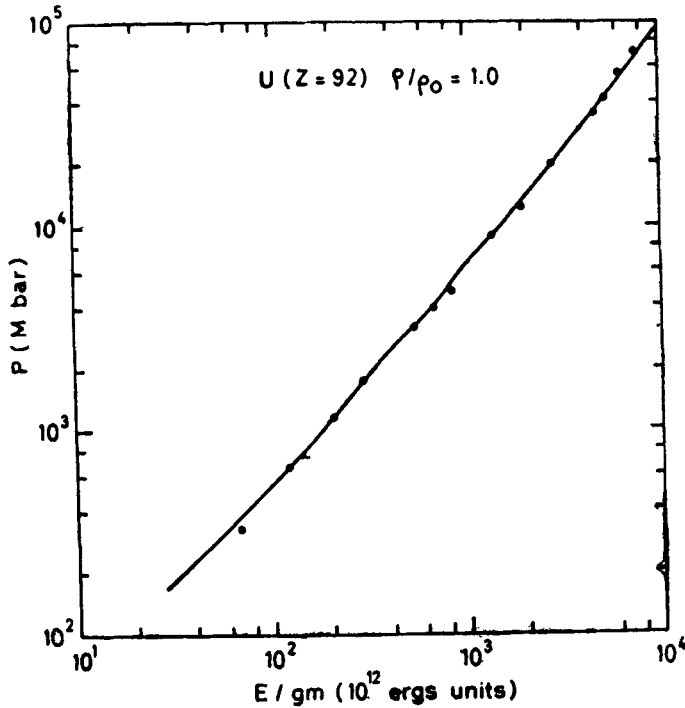


Figure 4.  $E_T$  vs.  $P_T$  diagram for  $U$ . The full curve is the TFD Kirzhnits curve. The  $\bullet$  are our calculated values.

$P_T$  at a given  $E_T$ , were always higher than the TFD EOS values, as expected. The assignment of different values for electronic partition functions, like taking them to be equal to ground state degeneracies or  $U_i = 1$  for all  $i$ , had very little effect on the  $P_T$  and  $E_T$  values. The peaks in figures 3 and 4 were, however, slightly shifted. The calculations were also made for other density ratios. The agreement between TFD EOS and Saha's was again good.

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