X-642-68-51

PREPRINT

NASA TM X- 63119

STELLAR OPACITY PROGRAM MANUAL "STOP"

PRELIMINARY REPORT

GPO PRICE $ ____

CFSTI PRICE(S) $ ____

Hard copy (HC) 3.00

Microfiche (MF) .65

ff 653 July 65

THOMAS E. MICHELS

IRA KASKEL

SHEILA MEYER

FEBRUARY 1968

GSFC

GODDARD SPACE FLIGHT CENTER

GREENBELT, MARYLAND

X-642-68-51

STELLAR OPACITY PROGRAM MANUAL

"STOP"

Thomas E. Michels
Ira Kaskel
Sheila Meyer

February 1968

GODDARD SPACE FLIGHT CENTER
Greenbelt, Maryland

STELLAR OPACITY PROGRAM MANUAL

"STOP"

Thomas E. Michels
Goddard Space Flight Center
Greenbelt, Maryland

Ira Kaskel
Sheila Meyer
Computer Applications, Inc.
New York, New York

ABSTRACT

The new Stellar Opacity program, "STOP" is described. "STOP" is the FORTRAN version of the IBM 7090 FAP, "OPACITY" and "IONIC" programs developed by Dr. Arthur N. Cox at the Los Alamos Scientific Laboratory. A Rosseland Mean Continuous Opacity is computed and the following processes are included: Bound-free and free-free absorptions including those of the H^- ion, Compton electron scattering, H_2 and H+H molecular absorptions, and Electron conduction. Equations used for these processes as well as the "Mayer Independent Electron" and "Ionic" methods of computing occupation numbers and other equation of state data are discussed. "STOP" is available for general usage.

PRECEDING PAGE BLANK NOT FILMED.

TABLE OF CONTENTS

PRECEDING PAGE BLANK NOT FILMED.

LIST OF SYMBOLS

a_0	Bohr Radius
A	quantity used in D_i (u) calculation (cm^{-1})
A_i	Atomic weights
A_{H+H}	Absorption coefficient for H+H molecular absorption
b, b′	Quantities used in pressure equations
B_{ijk}	Partition function of ion i j, state β
B_{ij}	Partition function of ion i j, $= \sum_k B_{ijk}$
$B\nu(T)$	Planck function
C	Speed of light
D_i (u)	Mayer D for process i of absorption or scattering
D_{bf} (u)	Mayer D for Bound-free absorptions
D_{ff} (u)	Mayer D for free-free absorptions
D_s (u)	Mayer D for electron scattering
DH^-_{ff} (u)	Mayer D for H^- free free absorptions
DH^-_{bf} (u)	Mayer D for H^- bound free absorptions
D_m (u)	Mayer D for molecular absorptions of H_2^+ and H+H molecules
DP	Dominant potential described by Chandrasekhar
E_0	Potential energy of the free electrons averaged over all ion spheres
E_{ik}, E_{ijk}	Electron energy for atom i, or ion i j in state k
E_{ijk}	Electron energy relative to ground state of ion i j in state k
E'_{ik}, E'_{ijk}	Print electron energy

EP	Epsilon
E_{ion}	Total energy associated with all ions in mixture
E_i	Energy associated with atom i
$E_{(ion+exc)}$	Total energy associated with ion and all excited levels
e^2	Square of the electron charge
F_c	Energy flux for conduction
g_{ff}	Free-free Gaunt factors
g_{ijk}, g_{ik}	Statistical weight of state k, ion ij or atom i
g_{bf}	Bound-free Gaunt factors
g_{FD}	Karzas and Latter free-free Gaunt factors
g_{SD}	Green's Gaunt factors including screening
G(u), G(u, T′)	Ratio of effective scattering cross-section to Thomson
G(T)	Cross-section due to Sampson
h	Planck's constant
i	Subscript denoting particular element
I_1	Partial integral for opacity at edge e
j	Subscript denoting number of electrons missing
k	Subscript denoting state k for either ion ij or element i
k	Boltzmann constant
l	Orbital quantum number used for n = 1, 2, 3
m	Electron mass
N	Number of unit atoms per unit volume

N_e	Electron density
N_0	Avogadras Number
N_t	Total atom density
$N_{i,j+1}/N_{i,j}$	Relative abundance of ion i, j + 1 to ion i, j
NH^-/NH°	Relative abundance of the H^- ion to neutral H
nl_{max}	Maximum principal quantum number for partition function sum
nl_{ijk}	Principal quantum numbers. State k
P_i	Polynomial used in Saha equation calculation
P_e	Electron pressure
P_g	Gas pressure
P_n	Number of integrals computed between edge for integration
Q_i	Polynomial used in Saha equation calculation
RD	Debye radius
R	Gas constant
Rhc	Conversion factor 1.35977×10^{-2} kv/Ryd.
r	Average atomic radius in mixture
r_i	Average radius of sphere which contains enough electronic charge to neutralize the ionic charge of atom i
U	Photon energy scaled by (kT) = hv/kT
Ue	U value at particular edge
V	Volume per average atom
W(u)	Weighting function in opacity integral

X_i	Number fraction for element i
X_{ijk}, X_{ij}	Electron occupation in state k, ion i j or atom i
X_{ij}	Abundance of ion i j (used in ionic occupation wo.)
X_{H°	Abundance of neutral hydrogen
XB	Total number of bound electrons
XB_i	Number of bound electrons in element i
y_i	Number of free electrons off element i
y	Total number of free electrons per average atom in mixture
Y(H)	Number of free electrons from hydrogen
Z_i	Nuclear charge of atom i
Z^*_{ijk}, Z^*_{ik}	Effective nuclear charge seen by an electron in state k, ion i j or atom i

STELLAR OPACITY PROGRAM MANUAL
"STOP"

INTRODUCTION

The FORTRAN IV version of the stellar opacity program, herewith described and referred to as the "STOP" program, is essentially a duplication of the IBM 7090 FAP versions of the "IONIC" and "OPACITY" programs developed at the Los Alamos Scientific Laboratory by Dr. Arthur N. Cox. Other than the programming techniques employed, the only difference that exists in the present STOP version is that the "IONIC" and "OPACITY" codes have been combined into one program. In using the Los Alamos program to compute opacities below 10^6°K, the "IONIC" and "OPACITY" codes were run consecutively because the ionic method of computing occupation numbers was necessary for this low temperature region. After making a run with the ionic code to compute all equations of state data, the opacity code was entered to compute the absorption coefficients and opacities. For temperatures above 10^6°K, only a single run was necessary with the "OPACITY" code, as this code employed another method of computing occupation numbers called the "Mayer Independent Electron" method which was applicable for high temperatures above 10^6°K.

In the present STOP version, the user has an input option to determine which method to employ to compute occupation numbers. The two methods give the same values of opacity at temperatures near 10^6°K and this is normally the criterion for the user when making his runs. That is, for temperatures above 10^6°K, the straight opacity option would be used and for temperatures of 10^6°K or lower, one would use the ionic option.

The STOP program was designed primarily for use on the IBM 360/95 computer at the Goddard Institute for Space Studies, however, it may be used on any IBM 360 computer having a memory of 500 K bytes or larger, having a compiler which will accept the FORTRAN IV language. One should consult the USAGE section of this manual for further details on specifications.

This manual has been written for the purpose of describing the methods used in the program and of showing the prospective user how to use the program. For those already acquainted with Cox's works, accomplishing this is an easy task, however in attempting to write a manual which can be used by anyone wishing to compute stellar opacities, it was decided the following sections should be included in as clear and precise a manner as possible.

a) General Description of STOP

This section gives a brief description of Cox's method of computing opacities and describes the general flow and usage of the program. It was designed for the person who is not acquainted with Cox's work and who wishes to find out what processes and techniques are employed.

b) Users' Section

This section describes in detail how to set up input to the program and how to interpret the results printed. The various options for intermediate output are described also.

c) Cox's Continuous Opacity

This section contains a detailed description of the methods used by Cox to compute opacity. Contained in this section is a description of the "Ionic" and "Mayer Independent Electron" methods for computing occupation numbers and other equations of state data. This includes the method of dominant potential and the equations used to compute the various scattering and absorption processes used in calculating the radiative opacity. A brief description of the conductive opacity and the procedure for adding this to the radiative opacity to give the continuous opacity is also shown here.

It should be noted that Cox's chapter in "Stellar Structures" was relied upon heavily in this manual and the notations used are the same as in the article.

This project was begun at the suggestion of Dr. Albert Arking at the Goddard Institute for Space Studies, and it was under his guidance and direction that the present FORTRAN version of the program has been completed. Without his help in absorption coefficient and stellar opacity theory, understanding of the problem and ultimately completing the program would certainly not have come about. The invaluable help of John Stewart (1963) at the Los Alamos Scientific Laboratory cannot go without mention here also. His list of equations and flow charts of the Los Alamos FAP version of the program gave us much insite into many of the physical interpretations employed, and through his willingness to help and many phone conversations, we were able to complete this project.

CHAPTER I

GENERAL DESCRIPTION OF "STOP"

PRECEDING PAGE BLANK NOT FILMED.

CHAPTER I

GENERAL DESCRIPTION OF STOP

The present "STOP" program is a duplication of the IBM 7090 FAP, "OPACITY" and "IONIC" programs developed by Dr. Arthur N. Cox at the Los Alamos Scientific Laboratories. Its reason for existence is that it has been programmed entirely in FORTRAN. In describing the contents of "STOP," this section has been included to give the user a general idea of the processes used by Cox in his program and to also acquaint him with the general usage of "STOP," In a later section, a much more detailed description has included Cox's methods.

Cox's method for computing stellar opacity employs the work of many men researching in the field of absorption coefficient theory. A list of references are given at the end of his chapter "Stellar Absorption Coefficients and Opacities" in Stellar Structures, however the basis for his method stems primarily from Harris Mayer in an unpublished Los Alamos Report, LA-647, (1947) entitled "Methods of Opacity Calculations."

In this report, at the request of Edward Teller, Mayer studied the effect of line absorption on opacity for materials of extremely high temperature. He devised a method of computing the occupation of electrons in various energy states needed for calculating equation of state quantities for a one electron atom model, and calls this the "Mayer Independent Electron" method. He also describes another method of computing occupation numbers when temperatures are lower and a state of complete ionization does not necessarily exist and has referred to this as the "Ionic" method.

Later, Cox, at the Los Alamos Scientific Laboratory studied the problem of calculating accurate monochromatic absorption coefficients and opacities over the whole range of temperatures and densities encountered in problems of stellar structure. He extended much of Mayer's work and developed a computer program which computes a Rosseland Mean Continuous Opacity given by

$$\frac{1}{\kappa_R} = \frac{\displaystyle\int_0^\infty \frac{1}{(\kappa_\nu + \sigma_\nu)} \frac{\partial B_\nu(T)}{\partial T}\, d\nu}{\displaystyle\int_0^\infty \frac{\partial B_\nu(T)}{\partial T}\, d\nu} . \tag{1}$$

Employing both the "Mayer Independent Electron" method and the "Ionic" method to compute equation of state data, Cox's program, written in IBM 7090 FAP language can be applied for stellar temperatures from 5×10^{3}°K to well over 10^{7}°K. The "STOP" program can be used in this region as well.

Strömgren (1932) transformed equation (1) in the form which has also been described by Chandrasekhar (1939) as

$$I = \int_0^\infty \frac{\omega(u)}{\sum_i X_i^5 D_i(u)} du$$

where

$$X_i^5 D_i(u) = \frac{\rho_i}{\rho} k_i(u) u^3 = \frac{N_i \sigma_i(u) u^3}{\rho}$$

and

$$u = \frac{h\nu}{kT}$$

$\sigma_i(u)$ is the cross section for N_i particles of matter density ρ_i and mass fraction X_i and is summed over all absorption and scattering processes.

Mayer (1947) defined D in a different manner which is

$$D_i(u) = \frac{k_i(u) \rho_i u^3}{A} = \frac{N_i \sigma_i(u) u^3}{A} .$$

$K_i(u)$ is the absorption coefficient per gram per nucleus for process, i, and A has inverse length units and is

$$A = \frac{2^4}{3\sqrt{3}} \frac{he^2}{mc} \frac{N}{kT} .$$

N is the number of atoms per unit volume. The Strömgren D_i (u) has the units of cm^2/gm where the Mayer definition of D_i (u) is dimensionless.

The Mayer definition of D_i (u) is the one used by Cox in his opacity calculations and he has included the following processes in the computer program.

a) Bound free absorption, D_{bf} (u)

b) Free Free absorption, D_{ff} (u)

c) Compton Electron Scattering, Ds(u)

d) H^- bound free and free-free absorptions, DH_{bf}^- (u) and DH_{ff}^- (u)

e) H_2^+ and $H+H^*$ molecular absorption, D_m (u).

The induced emission factor is included in the definition of the weighting function w(u) and is given by

$$w(u) = \frac{15}{4\pi^4} \frac{u^7 e^{2u}}{\left(e^u - 1\right)^3}$$

w(u) has been tabulated by Mayer (1947) however the program computes w(u) for a given u value. Below the plasma frequency cut off, Up, defined by

$$Up = \frac{4\pi^{1/2}}{(kT)} \left(\frac{y}{V}\right)^{1/2} ,$$

w(u) is defined to be zero and is limited in the program to fall in the limits

$$Up \leq u \leq 30 .$$

When u > 30, w(u) is so small and the D_i (u)'s are so large that the value of the integral past this point can be neglected. The equations for the various D_i (u) processes are described in Chapter III of this manual and are also described by Cox (1965).

Once the integral, I, is computed, then the radiative opacity can be computed from

$$\kappa_R = \frac{A}{I\rho} .$$

The units of κ_R using this definition is cm^2/gm.

In actual usage, the integration for I rarely needs to be computed beyond the maximum of the weighting functions at $u \approx 7$. An estimate of the remaining integral can be made by assuming the D_i (u)'s will be no smaller at larger u values than at the edge where $u = u_e$ and $D = D_e$, then

$$\Delta I_n \leq \frac{1}{D_e} \int_{u_e}^{\infty} w(u)\, du = \frac{1}{D_e} \left[S(\infty) - S(u_e) \right]$$

If this remainder is sufficiently small compared to the value of the integral at this point, it can be neglected. S(u) is the Strömgren Function and is tabulated as a function of u for use in the opacity code.

$$S(u) = \int_{u}^{\infty} w(u)\, du$$

In order to calculate several w(u) and D_i (u) needed in the opacity integral, all the equation of state data including occupation numbers must be calculated from the users input of temperature, density, and composition mixture. Two methods are employed which were referred to earlier as the "Ionic" and "Mayer Independent Electron" methods.

The "Ionic" method is the more accurate of the two and must be used for temperatures below 10^6°K, where ion formation is possible. For temperatures above 10^6°K, the "Mayer Independent Electron" method can be used with good accuracy and is the much faster of the two methods. Both of these methods are described in detail in Chapter III of this manual and by Mayer in (LA-647).

Dr. Cox also described these two in great detail and has written some advantages and shortcomings in his article in "Stellar Structures" (1965).

An important feature which Cox has included in the "Ionic" method gives the user of the program the ability to begin the calculation by specifying the temperature, composition, and either density, or electron pressure, or degeneracy of the gas. This is done using the method of "Dominant Potential" described by Chandrasekhar (1951). Since the method depends upon the degree of ionization of the mixture, it cannot be applied when very high temperatures are encountered. Therefore, when the "Mayer Independent Electron" method is employed, these options are not available and the only input is temperature, composition, and density.

The calculation is much simpler in the temperature region 10^8°K up to above $T = mc^2$. Compton's scattering by electrons is the most important process in determining the opacity in this region and Cox uses a method due to Sampson (1959). The opacity is given by

$$\kappa_R = \frac{N_{(e+p)}\sigma_0}{\rho}\bar{G}(T)$$

where $N_{(e+p)}$ is the density of electrons and positrons, and $\bar{G}(T)$ is the Rosseland mean of the ratio of the effective Compton cross-section to σ_0, the Thomson cross section for scattering of radiation by electrons.

At very high densities where electron degeneracy becomes important the conductive opacity must be considered. Cox uses the methods of Mestel (1950) for the conductive opacity.

$$\kappa_c = \frac{4ac}{3}\left(\frac{T^3}{\rho\nu_c}\right).$$

The conductive opacity is then added to the radiative opacity to give a total continuous opacity by

$$\frac{1}{\kappa_T} = \frac{1}{\kappa_c} + \frac{1}{\kappa_R}$$

In using the program, firstly, a decision must be made as to which method of computing occupation numbers, etc. should be used. Since this can be based primarily upon the temperature, a general rule can be made.

a. For temperatures below 10^6°K use the "Ionic" method.

b. For temperatures above 10^6°K use the "Mayer Independent Electron" method.

However, one should consult Cox's article (1965) for advantages and shortcomings of this rule.

For the "Mayer" method, one inputs:

a. Temperature (°K, $\log_{10}$°K, kilovolts).

b. Composition (number fractions, mass fractions).

c. Density (gm/cm^3)

and for the "Ionic" method, one has the following options:

a. Temperature (°K, $\log_{10}$°K, kilovolts),

b. Composition (number fractions, mass fractions) and one of the following

c. Density (gm/cm^3)

or

c. electron density (electrons/cm^3)

or

c. degeneracy parameter, η.

Output options from the program give the user a wide range of flexibility. With no output options specified by the user, only the users input and final value of opacity is printed. These are given in table form if more than one case is run at one time.

Various forms of intermediate output can be obtained through the output options and these include tables of energies, ionic abundances, pressures and the like. The "Users' Section" contains these options in detail.

CHAPTER II

USERS SECTION

CHAPTER II

USERS SECTION

The "STOP" program, which is the FORTRAN version of the Los Alamos Scientific Laboratories' "OPACITY" and "IONIC" programs, was written primarily for use on the IBM 360 computer although it is compatible with any FORTRAN system. It has been written completely in the FORTRAN IV language with the standard version in double precision. It has been written such that it is compatible with any IBM 360 system having memory size of 500 K or more bytes.

The "STOP" program has combined the "OPACITY" and "IONIC" codes into one program which employs an input option to determine which mode to run under. That is, the user supplies an input option specifying either an "OPACITY" run or an "IONIC" run. The section, General Description of STOP, should be consulted for the calculations performed under each option. It suffices here to say that the "IONIC" option uses the "Ionic" method for computing occupation numbers and the "OPACITY" option uses the "Mayer independent electron method".

A complete package of the program consists of the source program (on punched cards) followed by the users input, and a data tape read by the program.

The data tape consists of two files. Contained on the first file are the Moore element data tables and on the second file are the necessary tables for screening constants, gaunt factors, etc. Complete listings of these can be obtained from the authors. In running the program, the user would include his data set behind the source program and place the data tape on logical unit 5.

Included as input are various output options which are explained below. If no output options are specified, standard output consisting of the users input and tables of opacity, temperature, and density are given.

A case is defined as one set of temperature, density, eta, or electron pressure, and composition mixture. The composition mixture can be further defined by the standard mixture ratios X, Y, Z if desired. Only X and Z are specified, however, as Y can be derived.

As shown below, one data set can consist of several cases. That is, one temperature and several densities could be input and output would be a table of opacity versus temperature and density. Any combinations of temperature, density, electron pressure, or eta, and composition mixture can be run.

Input consist of three categories:

a) Mixture cards - contained on these cards are the output options.
b) Temperature cards.
c) Density, eta, or electron pressure cards.

INPUT

These are described as follows.

All numbers should be right adjusted:

	columns	variable
CARD 1	1 - 7	MIXTURE
	19 - 20	NZ = no. of elements in mixture
	31	If non-zero, intermediate print-out for data tables
	32	If non-zero, intermediate print-out for opacity tables
	33	If non-zero, print-out of initial conditions
	34	If non-zero, print-out of intermediate iterations for ionic code
	35	If non-zero, print-out of converged values and data passed to opacity code
	42	If zero: Mayer Independent electron method If non-zero: ionic method
	50	IFRAC = 1 - number fractions IFRAC = 2 - mass fractions IFRAC = 3 - basic set of mass fractions, X,Z IFRAC = 4 - basic set of number fractions, X,Z

The format for this card is: (A6, 4X, I10, 10X, 12I1, I8)

Example:

```
    MIXTURE        11          11111        1       4
```

	columns	variable
CARD 2	9 - 10	atomic number
	11 - 30	fractional amount as specified by IFRAC

The format for this card is: (I10, E20.8)

Example:
6 4.45E-4

CARD 3	same as card 2	
CARD NZ + 1	same as card 2	

Note: one card per element

The following card is omitted if IFRAC = 1 or 2:

CARD NZ + 2	1 - 16	X
	17 - 32	Z

The format for this card is (2E16.8)

Example:
.5994 .0048

CARD NZ + 3	1 - 5	TEMP
	19 - 20	number of temperatures
	29 - 30	= 0 : temperature in kv = 1 : temperature as log 10 (temperature in degrees K) = 2 : temperature in degrees K

The format for this card is (A6, 4X, 2I10)

Example:
TEMP 1 1

CARD NZ + 4	1 - 16	TEMP (1)
	17 - 32	TEMP (2)
	33 - 48	TEMP (3)
	49 - 64	TEMP (4)
	65 - 80	TEMP (5)

The format for this card is (5E16.8). Use as many cards as required, with at most five temperatures per card.

Example:
    5.8

	columns	variable
CARD NZ + 5	This card has to be one of the following three:	
option 1:	1 - 7	DENSITY
	19 - 20	number of densities
	30	= 1 : density as gm/cm^3 = 2 : density as log 10 (density) gm/cm^3
option 2:	1 - 3	ETA
	19 - 20	number of etas
	30	= 3
option 3:	1 - 10	ELEC PRESS
	19 - 20	number of el. pressures (J/CM^3)
	30	= 4

The format for this card is (A6, 4X, 2I10)

Example:

```
      DENSITY          2               2
```

CARD NZ + 6 This card has the same format as card NZ + 4, depending on which option is selected.

The above comprises a complete data set. Multiple runs may be submitted by repeating the above. At end of last set of data, there must be a card containing END in columns 1 - 3.

Example:

```
MIXTURE              1          11111     1        1
          2           1.000
TEMP                 1          1
          5.2
DENSITY              1          1
        1.E2
END
```

OUTPUT

Example:

Normal Output

```
                                                  CONTINUOUS STELLAR OPACITY
                                                         NEW MIXTURE
                                                         THETA(KV)
   0.13657671D-01
                                                        RHO (GM/CM3)

   0.10000000D-02
            ATOMIC WEIGHTS (A SUB I)               NO. FRACTIONS (N SUB I)          ATOMIC NOS. (Z SUB I)
               0.40030000D 01                         0.10000000D 01                   0.20000000D 01

INPUT OPTION SPECIFIES IONIZATION  RUN



                                                        MIXTURE COMPOSITION



OCCUPATION NOS. FROM IONIZATION PROGRAM

X=     0.0          Y=     1.0000      Z=     0.0

AT. NOS.      AT. WTS.      NO. FRACTS.   MASS FRACTS.
   2           4.003        1.00000D 00   1.00000D 00


                            1.00000D 00   1.00000D 00


                          RHO             1.00000D-03
                          LOG RHO             -3.000

T(K)=        1.58500D 05 K(R)             9.89546D 02
LOG T(K)=          5.200 K(T)             9.89858D 02
THETA(KV)= 1.36577D-02 LOG K(T)                2.996
```

Output Option 1

TABLE 1-

NL(K)	K	G(K)	N(K)	DEL(K)	L(K)	NU(K)
1S	1	2.0	1.	3.0	0	2.
2S	2	2.0	2.	42.0	0	2.
2P	3	6.0	2.	30.0	1	6.
3S	4	2.0	3.	207.0	0	2.
3P	5	6.0	3.	180.0	1	6.
3D	6	10.0	3.	126.0	2	10.
4	7	32.0	4.	528.0		32.
5	8	50.0	5.	1275.0		50.
6	9	72.0	6.	2628.0		72.
7	10	98.0	7.	4851.0		98.
8	11	128.0	8.	8255.9		128.
9	12	162.0	9.	13203.0		162.
10	13	200.0	10.	20100.0		200.

TABLE 2- SIGMA SUB NL,NL

0.62500	0.83950	0.97120	0.89540	0.97950	0.99920	0.98700	0.99400	0.99700	0.99900	1.00000	1.00000	1.00000
0.20990	0.60160	0.64840	0.75700	0.81010	0.93220	0.94000	0.97000	0.98400	0.99000	0.99300	0.99500	1.00000
0.24280	0.64840	0.72660	0.78080	0.84550	0.95700	0.94000	0.97000	0.98400	0.99000	0.99300	0.99500	1.00000
0.09950	0.33650	0.34700	0.59770	0.61910	0.65820	0.85000	0.92000	0.95500	0.97000	0.98000	0.99000	1.00000
0.10880	0.36000	0.37580	0.61910	0.64640	0.69240	0.85000	0.92000	0.95500	0.97000	0.98000	0.99000	1.00000
0.11100	0.41430	0.42530	0.65820	0.69240	0.77440	0.85000	0.92000	0.95500	0.97000	0.98000	0.99000	1.00000
0.06169	0.23500	0.23500	0.47810	0.47810	0.47810	0.70500	0.83000	0.90000	0.95000	0.97000	0.98000	0.99000
0.03976	0.15520	0.15520	0.33120	0.33120	0.33120	0.53100	0.72000	0.83000	0.90000	0.95000	0.97000	0.98000
0.02769	0.10930	0.10930	0.23880	0.23880	0.23880	0.40000	0.57400	0.73500	0.83000	0.90000	0.95000	0.97000
0.02039	0.08082	0.08082	0.17820	0.17820	0.17820	0.31020	0.45900	0.61000	0.74500	0.83000	0.90000	0.95000
0.01563	0.06250	0.06250	0.13780	0.13780	0.13780	0.24250	0.37100	0.50600	0.63500	0.75000	0.83000	0.90000
0.01234	0.04938	0.04938	0.10980	0.10980	0.10980	0.19360	0.29900	0.42200	0.54400	0.65600	0.76000	0.83000
0.01000	0.04000	0.04000	0.09000	0.09000	0.09000	0.15840	0.24500	0.34900	0.46600	0.57600	0.67000	0.76500

TABLE 3 - FERMI-DIRAC INTEGRALS- MAYER INDEPENDENT ELECTRUN METHOD, TABLES 3,4

ETA	F1/2(ETA)
30.	0.10969484D 03
25.	0.83498094D 02
20.	0.59812795D 02
10.	0.21344466D 02
4.	0.57707624D 01
2.	0.25024528D 01
0.0	0.67809100D 00
-2.	0.11458783D 00
-4.	0.16127738D-01
-2.	-0.21664138D 01
-4.	-0.41272416D 01
-6.	-0.61216580D 01
-8.	-0.81209008D 01
-10.	-0.10120798D 02
-12.	-0.12120784D 02
-14.	-0.14120782D 02
-16.	-0.16120782D 02
-18.	-0.18120782D 02
-20.	-0.20120782D 02
-22.	-0.22120782D 02
-24.	-0.24120782D 02
-26.	-0.26120782D 02
-28.	-0.28120782D 02
-30.	-0.30120782D 02

TABLE 4 -

ETA	F PRIME
-4.0	0.99361300
-3.0	0.98301700
-2.0	0.95643500
-1.0	0.89698600
-0.2	0.81580900

0.56893672D 00	0.71785274D 00	0.91741777D 00	0.10837759D 01	0.11516132D 01	0.11195757D 01	0.11195757D 01	0.11195757D 01
0.35247191D 00	0.36582216D 00	0.36840210D 00	0.38243496D 00	0.38615344D 00	0.40995919D 00	0.42715817D 00	0.46180363D 00
0.55602510D 00	0.70380873D 00	0.90497601D 00	0.10751741D 01	0.11489508D 01	0.11202845D 01	0.11202845D 01	0.11202845D 01
0.34301762D 00	0.35613941D 00	0.35574614D 00	0.37231930D 00	0.37302270D 00	0.39956185D 00	0.41299505D 00	0.45045034D 00
0.54379416D 00	0.69034063D 00	0.89280555D 00	0.10664465D 01	0.11458872D 01	0.11204661D 01	0.11204661D 01	0.11204661D 01
0.33417389D 00	0.34707285D 00	0.34386182D 00	0.36283123D 00	0.36067994D 00	0.38979470D 00	0.39964464D 00	0.43974059D 00
0.53218737D 00	0.67741848D 00	0.88091992D 00	0.10576537D 01	0.11424990D 01	0.11202029D 01	0.11202029D 01	0.11202029D 01
0.32587710D 00	0.33855920D 00	0.33268208D 00	0.35390814D 00	0.34905829D 00	0.38059598D 00	0.38704254D 00	0.42961606D 00
0.52115440D 00	0.66501280D 00	0.86932563D 00	0.10488422D 01	0.11388481D 01	0.11195626D 01	0.11195626D 01	0.11195626D 01
0.31807266D 00	0.33054395D 00	0.32214717D 00	0.34549599D 00	0.33809774D 00	0.37191215D 00	0.37513044D 00	0.42002569D 00
0.51065012D 00	0.65309488D 00	0.85802432D 00	0.10400479D 01	0.11349846D 01	0.11186013D 01	0.11186013D 01	0.11186013D 01
0.31071345D 00	0.32298007D 00	0.31220359D 00	0.33754775D 00	0.32774455D 00	0.36369665D 00	0.36385524D 00	0.41092426D 00
0.50063417D 00	0.64163738D 00	0.84701418D 00	0.10312983D 01	0.11309497D 01	0.11173656D 01	0.11173656D 01	0.11173656D 01
0.30375854D 00	0.31582646D 00	0.30280355D 00	0.33002236D 00	0.31795045D 00	0.35590858D 00	0.35316895D 00	0.40227193D 00
0.49107030D 00	0.63061450D 00	0.83629111D 00	0.10226149D 01	0.11267776D 01	0.11158947D 01	0.11158947D 01	0.11158947D 01
0.29717207D 00	0.30904723D 00	0.29390411D 00	0.32288367D 00	0.30867199D 00	0.34851210D 00	0.34302790D 00	0.39403319D 00
0.48192590D 00	0.62000179D 00	0.82584919D 00	0.10140141D 01	0.11224963D 01	0.11142219D 01	0.11142219D 01	0.11142219D 01
0.29092258D 00	0.30261076D 00	0.28546673D 00	0.31609979D 00	0.29987002D 00	0.34147534D 00	0.33339248D 00	0.38617634D 00
0.47317145D 00	0.60977643D 00	0.81568150D 00	0.10055082D 01	0.11181294D 01	0.11123753D 01	0.11123753D 01	0.11123753D 01
0.28498232D 00	0.29648912D 00	0.27745663D 00	0.30964241D 00	0.29150920D 00	0.33477003D 00	0.32422671D 00	0.37867309D 00
0.46478031D 00	0.59991707D 00	0.80578032D 00	0.99710675D 00	0.11136965D 01	0.11103789D 01	0.11103789D 01	0.11103789D 01
0.27932562D 00	0.29055747D 00	0.26984246D 00	0.30348634D 00	0.28355760D 00	0.32837100D 00	0.31549785D 00	0.37149790D 00
0.45672833D 00	0.59040378D 00	0.79613766D 00	0.98881671D 00	0.11092141D 01	0.11082535D 01	0.11082535D 01	0.11082535D 01
0.27393353D 00	0.28509367D 00	0.26255962D 00	0.29760904D 00	0.27598620D 00	0.32225566D 00	0.30717604D 00	0.36462790D 00
0.44899347D 00	0.58121788D 00	0.78674518D 00	0.98064312D 00	0.11046961D 01	0.11060168D 01	0.11060168D 01	0.11060168D 01
0.26878343D 00	0.27977792D 00	0.25569094D 00	0.29199026D 00	0.26876870D 00	0.31640374D 00	0.29923401D 00	0.35804219D 00
0.44155569D 00	0.57234210D 00	0.77759455D 00	0.97258949D 00	0.11001543D 01	0.11036842D 01	0.11036842D 01	0.11036842D 01
0.26385868D 00	0.27469240D 00	0.24910442D 00	0.28661180D 00	0.26188110D 00	0.31079692D 00	0.29164687D 00	0.35172205D 00
0.43439661D 00	0.56376016D 00	0.76867740D 00	0.96465801D 00	0.10955986D 01	0.11012690D 01	0.11012690D 01	0.11012690D 01
0.26385868D 00	0.27469240D 00	0.24910442D 00	0.28661180D 00	0.26188110D 00	0.31079692D 00	0.29164687D 00	0.35172205D 00
0.43439661D 00	0.56376016D 00	0.76867740D 00	0.96465801D 00	0.10955986D 01	0.11012690D 01	0.11012690D 01	0.11012690D 01
0.26385868D 00	0.27469240D 00	0.24910442D 00	0.28661180D 00	0.26188110D 00	0.31079692D 00	0.29164687D 00	0.35172205D 00
0.43439661D 00	0.56376016D 00	0.76367740D 00	0.96465801D 00	0.10955986D 01	0.11012690D 01	0.11012690D 01	0.11012690D 01

TABLE 14 FERMI-DIRAC INTEGRALS, IONIC METHOD

ETA	F(1/2)(ETA)	2/3 F(3/2)
-4.0	1.61277000D-02	1.61790000D-02
-3.0	4.33664000D-02	4.37410000D-02
-2.0	1.14587800D-01	1.17201000D-01
-1.0	2.90509000D-01	3.07233000D-01
-0.2	5.77470000D-01	6.43197000D-01
0.4	9.20505000D-01	1.08635800D 00
1.0	1.39637530D 00	1.77445500D 00
1.6	2.01349600D 00	2.79033400D 00
2.2	2.76934400D 00	4.21843800D 00
2.8	3.65490500D 00	6.13950300D 00
3.4	4.65897700D 00	8.62802300D 00
4.0	5.77072650D 00	1.17518010D 01
5.0	7.83796100D 00	1.85349640D 01
6.0	1.01442850D 01	2.75073350D 01
7.0	1.26646380D 01	3.38948110D 01
8.0	1.53804860D 01	5.29017290D 01
9.0	1.82775600D 01	6.97161610D 01
10.0	2.13444720D 01	8.95134400D 01
12.0	2.79517770D 01	1.38707970D 02
14.0	3.51429710D 01	2.01709500D 02
16.0	4.28730050D 01	2.79638680D 02
18.0	5.11060780D 01	3.73536740D 02
22.0	6.89680000D 01	6.13087120D 02
26.0	8.85440000D 01	9.27557000D 02
30.0	1.09690000D 02	1.32353000D 03

Output Option 2

```
EDGE      UU          D SUB BF      D SUB FF     D SUB S      D SUB H-,M   SUM D,S      W(U)         PARTIAL I(N)  LAMBDA        K (LAMBDA)
  1 0.0               0.0           0.46027D-02  0.0          0.0          0.46027D-02  0.0                        0.0           0.0
  1 0.21095D-01       0.0           0.53409D-02  0.72977D-10  0.0          0.53409D-02  0.0                        0.43022D 05   0.14078D 08
  1 0.42190D-01       0.0           0.54270D-02  0.29499D-09  0.0          0.54270D-02  0.0                        0.21511D 05   0.35389D 07
                                                                                                     0.0
                                                                                                     SIGMA I(N)
                                                                                                     0.0

EDGE      UU          D SUB BF      D SUB FF     D SUB S      D SUB H-,M   SUM D,S      W(U)         PARTIAL I(N)  LAMBDA        K (LAMBDA)
  2 0.42190D-01   0.39082D-06   0.54270D-02  0.29499D-09  0.0          0.54274D-02  0.0                        0.21511D 05   0.35391D 07
  2 0.76651D-01   0.51210D-06   0.52238D-02  0.99042D-09  0.0          0.52243D-02  0.13798D-05                0.11840D 05   0.10146D 07
  2 0.11111D 00   0.60605D-06   0.50637D-02  0.21168D-08  0.0          0.50644D-02  0.61934D-05                0.81680D 04   0.46021D 06
                                                                                                     0.26183D-04
                                                                                                     SIGMA I(N)
                                                                                                     0.26183D-04

EDGE      UU          D SUB BF      D SUB FF     D SUB S      D SUB H-,M   SUM D,S      W(U)         PARTIAL I(N)  LAMBDA        K (LAMBDA)
  3 0.11111D 00   0.95391D-06   0.50637D-02  0.21168D-08  0.0          0.50647D-02  0.61934D-05                0.81680D 04   0.46024D 06
  3 0.12262D 00   0.98355D-06   0.50126D-02  0.25924D-08  0.0          0.50136D-02  0.92354D-05                0.74015D 04   0.37200D 06
  3 0.13412D 00   0.10136D-05   0.49671D-02  0.31193D-08  0.0          0.49681D-02  0.13292D-04                0.67666D 04   0.30636D 06
                                                                                                     0.43211D-04
                                                                                                     SIGMA I(N)
                                                                                                     0.69394D-04

EDGE      UU          D SUB BF      D SUB FF     D SUB S      D SUB H-,M   SUM D,S      W(U)         PARTIAL I(N)  LAMBDA        K (LAMBDA)
  4 0.13412D 00   0.71171D-04   0.49671D-02  0.31193D-08  0.0          0.50383D-02  0.13292D-04                0.67666D 04   0.31069D 06
  4 0.13533D 00   0.71174D-04   0.49626D-02  0.31777D-08  0.0          0.50338D-02  0.13786D-04                0.67061D 04   0.30471D 06
  4 0.13654D 00   0.70785D-04   0.49581D-02  0.32367D-08  0.0          0.50289D-02  0.14294D-04                0.66466D 04   0.29886D 06
                                                                                                     0.66295D-05
                                                                                                     SIGMA I(N)
                                                                                                     0.76024D-04

EDGE      UU          D SUB BF      D SUB FF     D SUB S      D SUB H-,M   SUM D,S      W(U)         PARTIAL I(N)  LAMBDA        K (LAMBDA)
  5 0.13654D 00   0.13311D-03   0.49581D-02  0.32367D-08  0.0          0.50912D-02  0.14294D-04                0.66466D 04   0.30257D 06
  5 0.13715D 00   0.13301D-03   0.49559D-02  0.32664D-08  0.0          0.50889D-02  0.14553D-04                0.66173D 04   0.29968D 06
  5 0.13775D 00   0.13291D-03   0.49537D-02  0.32963D-08  0.0          0.50866D-02  0.14816D-04                0.65882D 04   0.29683D 06
                                                                                                     0.34607D-05
                                                                                                     SIGMA I(N)
                                                                                                     0.79485D-04

EDGE      UU          D SUB BF      D SUB FF     D SUB S      D SUB H-,M   SUM D,S      W(U)         PARTIAL I(N)  LAMBDA        K (LAMBDA)
  6 0.13775D 00   0.15329D-03   0.49537D-02  0.32963D-08  0.0          0.51070D-02  0.14816D-04                0.65882D 04   0.29802D 06
  6 0.19249D 00   0.15938D-03   0.47933D-02  0.66098D-08  0.0          0.49527D-02  0.57922D-04                0.47148D 04   0.14413D 06
  6 0.24722D 00   0.16345D-03   0.46819D-02  0.11194D-07  0.0          0.48453D-02  0.16150D-03                0.36710D 04   0.83256D 05
  6 0.30196D 00   0.16668D-03   0.45981D-02  0.17142D-07  0.0          0.47648D-02  0.36800D-03                0.30055D 04   0.53467D 05
  6 0.35670D 00   0.16924D-03   0.45315D-02  0.24546D-07  0.0          0.47008D-02  0.73312D-03                0.25443D 04   0.36836D 05
  6 0.41143D 00   0.17138D-03   0.44774D-02  0.33505D-07  0.0          0.46488D-02  0.13267D-02                0.22059D 04   0.26688D 05
  6 0.46617D 00   0.17311D-03   0.44323D-02  0.44118D-07  0.0          0.46054D-02  0.22338D-02                0.19465D 04   0.20079D 05
  6 0.52090D 00   0.17455D-03   0.43939D-02  0.56488D-07  0.0          0.45685D-02  0.35552D-02                0.17423D 04   0.15556D 05
  6 0.57564D 00   0.17578D-03   0.43607D-02  0.70721D-07  0.0          0.45366D-02  0.54086D-02                0.15766D 04   0.12339D 05
  6 0.63037D 00   0.17684D-03   0.43318D-02  0.86924D-07  0.0          0.45087D-02  0.79287D-02                0.14397D 04   0.99770D 04
  6 0.68511D 00   0.17777D-03   0.43062D-02  0.10521D-06  0.0          0.44841D-02  0.11268D-01                0.13247D 04   0.81980D 04
                                                                                                     0.32646D 00
                                                                                                     SIGMA I(N)
```

EDGE	UU	D SUB BF	D SUB FF	D SUB S	D SUB H-,M	SUM D,S	W(U)	PARTIAL I(N)	LAMBDA	K (LAMBDA)
11	0.36721D 01	0.61090D 00	0.39558D-02	0.82423D-05	0.0	0.61486D 00	0.95196D 01		0.24715D 03	0.14345D 05
11	0.38038D 01	0.61802D 00	0.39503D-02	0.91314D-05	0.0	0.62198D 00	0.10576D 02		0.23855D 03	0.13098D 05
11	0.39354D 01	0.62486D 00	0.39448D-02	0.10084D-04	0.0	0.62882D 00	0.11666D 02		0.23061D 03	0.11991D 05
11	0.26709D 02	0.74525D 00	0.34391D-02	0.30849D-02	0.0	0.75177D 00	0.93855D-03		0.33979D 02	0.46770D 02
11	0.26841D 02	0.74496D 00	0.34372D-02	0.31307D-02	0.0	0.75153D 00	0.85160D-03		0.33813D 02	0.46071D 02
11	0.26972D 02	0.74467D 00	0.34353D-02	0.31769D-02	0.0	0.75128D 00	0.77257D-03		0.33648D 02	0.45385D 02
11	0.27104D 02	0.74438D 00	0.34335D-02	0.32236D-02	0.0	0.75104D 00	0.70076D-03		0.33484D 02	0.44712D 02
11	0.27236D 02	0.74409D 00	0.34317D-02	0.32708D-02	0.0	0.75079D 00	0.63552D-03		0.33322D 02	0.44052D 02
11	0.27367D 02	0.74379D 00	0.34298D-02	0.33184D-02	0.0	0.75054D 00	0.57626D-03		0.33162D 02	0.43405D 02
11	0.27499D 02	0.74350D 00	0.34280D-02	0.33665D-02	0.0	0.75029D 00	0.52244D-03		0.33003D 02	0.42770D 02
11	0.27630D 02	0.74320D 00	0.34262D-02	0.34150D-02	0.0	0.75004D 00	0.47357D-03		0.32846D 02	0.42148D 02
11	0.27762D 02	0.74290D 00	0.34244D-02	0.34640D-02	0.0	0.74979D 00	0.42920D-03		0.32690D 02	0.41537D 02
11	0.27894D 02	0.74260D 00	0.34226D-02	0.35135D-02	0.0	0.74954D 00	0.38893D-03		0.32536D 02	0.40938D 02
11	0.28025D 02	0.74230D 00	0.34208D-02	0.35634D-02	0.0	0.74929D 00	0.35238D-03		0.32383D 02	0.40351D 02
11	0.28157D 02	0.74200D 00	0.34190D-02	0.36138D-02	0.0	0.74904D 00	0.31922D-03		0.32232D 02	0.39774D 02
11	0.28289D 02	0.74170D 00	0.34172D-02	0.36647D-02	0.0	0.74878D 00	0.28913D-03		0.32082D 02	0.39208D 02
11	0.28420D 02	0.74140D 00	0.34154D-02	0.37161D-02	0.0	0.74853D 00	0.26184D-03		0.31933D 02	0.38652D 02
11	0.28552D 02	0.74109D 00	0.34137D-02	0.37679D-02	0.0	0.74827D 00	0.23710D-03		0.31786D 02	0.38107D 02
11	0.28684D 02	0.74078D 00	0.34119D-02	0.38202D-02	0.0	0.74802D 00	0.21465D-03		0.31640D 02	0.37572D 02
11	0.28815D 02	0.74048D 00	0.34102D-02	0.38730D-02	0.0	0.74776D 00	0.19431D-03		0.31496D 02	0.37047D 02
11	0.28947D 02	0.74017D 00	0.34084D-02	0.39263D-02	0.0	0.74750D 00	0.17586D-03		0.31352D 02	0.36531D 02
11	0.29079D 02	0.73986D 00	0.34062D-02	0.39801D-02	0.0	0.74725D 00	0.15915D-03		0.31211D 02	0.36025D 02
11	0.29210D 02	0.73955D 00	0.34039D-02	0.40343D-02	0.0	0.74699D 00	0.14400D-03		0.31070D 02	0.35528D 02
11	0.29342D 02	0.73924D 00	0.34018D-02	0.40891D-02	0.0	0.74673D 00	0.13027D-03		0.30930D 02	0.35040D 02
11	0.29473D 02	0.73893D 00	0.33999D-02	0.41443D-02	0.0	0.74647D 00	0.11784D-03		0.30792D 02	0.34560D 02
11	0.29605D 02	0.73861D 00	0.33982D-02	0.42000D-02	0.0	0.74621D 00	0.10658D-03		0.30655D 02	0.34090D 02
11	0.29737D 02	0.73830D 00	0.33968D-02	0.42563D-02	0.0	0.74595D 00	0.96381D-04		0.30520D 02	0.33627D 02
11	0.29868D 02	0.73799D 00	0.33956D-02	0.43130D-02	0.0	0.74569D 00	0.87146D-04		0.30385D 02	0.33173D 02
11	0.30000D 02	0.73767D 00	0.33946D-02	0.43702D-02	0.0	0.74543D 00	0.78785D-04		0.30252D 02	0.32727D 02
								0.26185D 03		

SIGMA I(N)
0.11974D 04

K(R)(CM2/GM)	R(D)(BOHR R)	PLASMA FR U	MAX. E(I)S	MIN. SCR FTR	LAST U	SIGMA I(N)	R FRACTION
0.98994602D 03	0.17761522D 02	0.46192874D-01	0.17345714D 00	0.99589950D 00	0.30000000D 02	0.11974169D 04	0.20779120D-06

K(C)(CM2/GM)
0.11108315D 08

K(CM2/GM)
0.98985781D 03

THETA(KV)	THETA(RYD)	THETA(K)	LOG THETA(K)	RHO(GM/CM3)	LOG RHO	MU(GM/MOLE)	V(BOHR R3)	AV(BOHR R2)
0.136577D-01	0.100409D 01	0.158500D 06	0.520003D 01	0.100000D-02	-0.300000D 01	0.400300D 01	0.448454D 05	0.281289D 00

Output Option 3

```
                                    NEW CASE

INTIAL CONDITIONS-

NO. OF ELEMENTS(I)=  1
NO. OF ELEMENT H IN I ARRAY(IHN)=  0

    THETA(KV)     THETA(RYD)     THETA(K)    LOG THETA(K)  RHO(GM/CM3)      LOG RHC     MU(GM/MOLE)    V(BOHR R3)   AV(BOHR R2)
  0.136577D-01  0.100409D 01  0.158500D 06  0.520003D 01  0.100000D-02 -0.300000D 01  0.400300D 01  0.448454D 05  0.281289D 00



  THETA(KV)     PE(J/CM3)   RHO(GM/CM3)     V(CM3/GM)   EI(KV/ATOM)       EI(J/GM)        EPSILON  DEBYRAD(CM)     T(DEG K)        5C40/T
1.36577D-02   6.58633D-07  1.00000D-03   0.0          0.0          0.0         2.30628D-01  9.14260D-08  1.58500D 05  3.17981D-02

        ETA   Y(EL/ATOM)   NT(MOL/CM3)    NE(EL/CM3)   B(J/GM-KV)  BP(J/GM-KV)    PN(J/CM3)    PG(J/CM3)       LOG PE  ITERATE ETA
-6.92009D 00  2.00000D 00  1.50505D 20  3.01009D 20  0.0          0.0          0.0          0.0         -6.18136D 00  0.0

     EO(KV)  F(1/2)(ETA)    2/3 F(3/2)   V(BR3/AT)  LOADED DELTA  (FOP3/2)/NT
0.0          8.75365D-04  8.75365D-04  4.48454D 04  1.00000D-10  0.0
```

Output Options4 & 5

```
EACH LINE = B, FIRST 13 TERMS, MAX N USED.

1.4042D 00 7.71D-01 5.45D-01 C.0       0.0      0.C      8.82D-02 0.0      0.0      C.0      0.0      0.0      C.0      0.0      2
2.2571D 00 1.54D CO 7.78D-02 2.33D-01 4.50D-02 1.35D-01 2.24D-01 0.0      0.0      C.0      0.0      0.0      0.0      0.0      3

EACH ROW = Z, N(1)/N(0), N(2)/N(1), ...., N(Z)/N(Z-1)

2   3.30291D C2 1.14655D 01

EACH ROW = Z, P, Q, Y, R(BOHR RADII)
2      .87748D 00    2.08722D 00    1.91931D 00    2.20399D 01

EACH ROW = Z, X(0), X(1), ...., X(Z)

2   2.42822D-C4 8.C2018D-02 9.19555D-01


 THETA(KV)     PE(J/CM3)  RHO(GM/CM3)    V(CM3/GM)  EI(KV/ATOM)      EI(J/GM)      EPSILON  DEBYRAD(CM)     T(CEG K)       5C40/T
1.36577D-02  6.32061D-07  1.CCCCOD-03  1.00000D C3  7.46171D-02  1.79918D-C3  2.18185D-01  9.39848D-C8  1.585CCC C5  3.17981D-C2

       ETA   Y(EL/ATCM)  NT(MCL/CM3)   NE(EL/CM3)   B(J/GM-KV)  BP(J/GM-KV)   PN(J/CM3)    PG(J/CM3)       LCG PE  ITERATE ETA
-6.96127D 00  1.91931D 00  1.50505D 20  2.88865D 20  7.03682D-02  6.78245D-C2  3.29210D-07  9.26325D-07 -6.19924D CO -6.96125D 00

    EO(KV)  F(1/2)(ETA)    2/3 F(3/2)  V(BR3/AT) LOADED DELTA  (FOP3/2)/NT
7.10718D-04  8.40050D-C4  8.40C50D-04  4.48454D 04  1.00000D-10  2.6811CD 00

E(I+EX)(KV/AT) E(I+EX)(J/GM) TOT E(J/GM)       DELTA   TOT LEVELS   TOT LEVEL DUMP
7.57658D-02  1.82688D-03  3.16395D-03  1.00000D-10        11             12

Z(I)    J   NL           NI              X(IJK)          E(IJK)(KV)        Z*(IJK)


 2      0   1S      -2.42822D-C4      3.88004D-01      -3.81842D-02      1.69127D 00

 2      0   1S       2.42822D-04      1.C9834D 00      -2.03252D-02      1.24375C OC
 2      0   2S       2.42822D-04      3.88004D-01      -5.76219D-04      6.15284D-01
 2      0   2P       2.42822D-04      1.25657D-01      -1.51753D-03      8.09615D-01
 2      0   2P       C.0              6.28286D-02      -1.51753D-03      8.09615C-01      M

 2      1   1S       8.02C18D-02      6.83179D-01      -5.01525D-02      1.93406C 00
 2      1   2S       8.02018D-02      3.44793D-02      -9.36528D-03      1.72164D 00
 2      1   2P       8.02018D-02      1.C3375D-01      -9.35697D-03      1.72093D 00
 2      1   3S       8.02018D-02      1.99334D-02      -1.88140D-03      1.30983D 00
 2      1   3P       8.02018D-02      5.97279D-02      -1.86487D-03      1.30565D 00
 2      1   3D       8.02018D-C2      9.93058D-02      -1.83182D-03      1.29724C 00
```

CHAPTER III

COX'S CONTINUOUS OPACITY

CHAPTER III

COX'S CONTINUOUS OPACITY

In describing both of the occupation number methods as well as the opacity calculation as a whole, the following subscript notation has been used. The subscript, i, refers to the particular element present in the mixture and, j, refers to the number of electrons off element i. Therefore, if equation of state quantities are being discussed, say E_{ij}, reference is to the total energy associated with ion i j implying element i, with j electrons missing. The subscript, k, refers to a particular state associated with either ion, i j, or element i.

In the "Mayer Independent Electron" method, applicable for high temperatures of 10^6°K or higher, (described by Mayer in LA 647, 1947, p. 26ff) all atoms are assumed to be completely ionized and the electron wave functions approach those of a free electron and are therefore independent of the positions of the nucleus. In this case, only the position of an electron in the field of the nearest nucleus needs to be computed.

Therefore, the electron state energy in this method need only to be referred to by E_{ik}. That is, in the "Mayer Independent Electron" method one computes equation of state quantities using only the subscripts i and k, which refer to a particular nucleus i, and state k, associated with this nucleus.

In the "Ionic" method, used primarily for temperatures below 10^6°K, the assumption is that an electron is in a state of sufficiently low energy that it will be temporarily bound to a given nucleus. For each nucleus which may have several electrons bound at the same time, the one electron wave functions will depend upon all the bound electrons for each nucleus. Therefore, one must speak of the number of ions of each type. This has the advantage of taking into account the interactions of the free electrons and ions.

Therefore in the "Ionic" method all three subscripts i, j, and k are used to denote, say the electron state energy E_{ijk}, which refers to the energy of an electron in state k of ion i j.

For example, in referring to Cox's equation (143) for bound-free absorption, in his article in Stellar Structures, the sum goes over all states of all the nuclei in the mixture with ionization energy less than $(u \cdot kT)$ and equation (143) would take the following forms for each method:

Ionic

$$D_{bf} = \sum_{i,j,k} X_i \, X_{ij} \, X_{ijk} \frac{4\pi^4 \, m^2 \, c^8}{h^4 \, (kT)^2} \frac{Z_{ijk}^{*\prime 4}}{r_k^5} q_{bf} \, g_{bf}$$

Mayer Independent Electron

$$D_{bf} = \sum_{i,k} X_i \, X_{ik} \frac{4\pi^4 \, m^2 \, e^8}{h^4 \, (kT)^2} \frac{Z_{ik}^{*\prime 4}}{n_k^5} q_{bf} \, g_{bf} \; .$$

MAYER INDEPENDENT ELECTRON METHOD

For a given composition, temperature and density, all electrons are assumed to be ionized from the atoms. The number of free electrons per average atom is then

$$y = \sum_i X_i \, Z_i \; .$$

Using the Fermi-Dirac distribution, the number of electrons in bound state k of element i is

$$X_{ik} = \frac{g_{ik}}{e^{\frac{E_{ik} - \eta}{kT}} + 1}$$

where

g_{ik} is the degeneracy of state k and

E_{ik} is the interaction energy of electron in state k with the nucleus.

For this first approximation, the total number of bound electrons per average atom in the system is

$$XB = \sum_{i,k} X_i X_{ik}$$

and a new number of free electrons is

$$y = \sum_i X_i \left(Z_i - \sum_k X_{ik} \right) .$$

These equations are repeated until successive y values differ by a predetermined amount.

The energy, E_{ik}, of the bound electrons, which includes perturbations by other bound electrons and continuum depression due to free electrons is due to Mayer (1947) and is given by

$$E_{ik_{Ryd}} = -\frac{Z_{ik}^{*2}}{n_{ik}^2} + \frac{y_i}{r_i} \left[3 - \frac{\delta_k}{r_i^2 Z_{ik}^{*2}} \right] + \frac{3}{5} \sum_i \frac{X_i y_i^2}{y r_i}$$

with the effective charge given by

$$Z_{ik}^* = Z_i - \sum_{k' \neq k} X_{ik'} \sigma_{kk'} - X_{ik} \left(1 - \frac{1}{g_{ik}} \right) \sigma_{kk}$$

where the quantity

$$\delta_k = \overline{r}_k^2 Z_k^{*2}$$

is tabulated by Mayer (1947) $\overline{r}_k$ is the average radius of state k in Bohr radii. The quantity

$$\frac{\delta_k}{r_i^2 Z_{ik}^{*2}}$$

is limit to be ≤ 1. If > 1, it should be set $= 1$, for calculation.

The quantity on the right in the energy equation,

$$\frac{3}{5} \sum_i \frac{X_i y_i^2}{y r_i}$$

is the negative of the potential energy of the free electrons averaged over all ion spheres and is usually called E_0. The screening constants σ_{kk}, are tabulated by Mayer also. r_i, the average radius of a sphere which contains enough electronic charge to neutralize the ionic charge of atom i, is

$$r_i = \left[\frac{y_i}{y} \frac{3}{4\pi} V\right]^{1/3} a^{-1} \text{ (Bohr Radii)}$$

where V, the volume per average atom is

$$V = \frac{\mu_c}{\rho N_0} = \frac{\sum X_i A_i}{\rho \nu_0}$$

and a_0 is the Bohr Radius.

This method for obtaining occupation numbers converges rapidly except when atoms are nearly neutral or for temperatures greater than approximately 10^6 °K. However, it does not work for stellar atmosphere temperatures and densities because the energies needed in the occupation number expression is very sensitive to the presence of other bound electrons in the same atom.

The degeneracy parameter, η, for free electrons is obtained in the Los Alamos code by an iteration procedure using a table of η vs. Fermi-Dirac integrals $F_{1/2}(\eta)$ depending upon the state of the degeneracy. This procedure is outlined below.

For $\eta \leq -28$, no iteration is necessary and

$$\eta = \ln\left[F_{1/2}(\eta = -28)\right] + \ln \frac{2}{\sqrt{\pi}}$$

For $\eta > -28$

A first guess is made of

$$F_{1/2}(\eta) = \frac{2\pi^2}{(kT)^{3/2} V} y$$

after which a table of η vs. $F_{1/2}(\eta)$ is entered to interpolate (quadratic) to obtain η_i. Using this value of η, a new value of $F_{1/2}(\eta)$ is computed from one of the following:

$$= \frac{2}{3}\eta^{3/2}\left(1 + \frac{1.23}{\eta^2}\right); \qquad \eta > 30$$

$$= \frac{2}{3}\eta^{3/2}\left(1 + \frac{1.23}{\eta^2} + \frac{1.25}{\eta^4}\right); \qquad 4 \leq \eta \leq 30$$

$$= \left(0.008\eta^3 + 0.187\eta^2 + 0.525\eta + 0.678\right) + \left(-0.012\eta^2 + 0.019\eta - 0.009\right)|\eta|; \qquad -2 \leq \eta \leq 4$$

$$= 0.8062e^{\eta} - 0.3133e^{2\eta} + 0.1569e^{3\eta}; \qquad -28 < \eta < -2$$

and the table is re-entered to obtain a new η_{i+1}. This process is repeated until a consistent η, or

$$\left| \frac{\eta_i - \eta_{i-1}}{\eta_i} \right| < \epsilon_\eta$$

is obtained. The program has set $\epsilon_\eta = 10$ and for the first iteration $\eta_{i-1} = 2 \times 10^4$. Also an average value for the number of bound electrons in each energy state for each iteration given by

$$X_{ik} = \frac{X_{ik_{new}} + X_{ik_{old}}}{2} .$$

At this point when a consistent number of free electrons, y, occupation numbers, X_{ik}, etc. exists the equation of state quantities can be calculated.

The matter energy equation of state is computed by adding the energy of ionization and excitation to the kinetic energy of the free electrons. If the densities are high, electrostatic corrections for interactions between all the free charged particles must be made to both the energies and pressures. The energy expression given below by Cox differs from that given previously because the interaction energy between free electrons and the nucleons as well as the potential energy of the free electron cloud are included.

This energy for nucleus i is

$$E_{i_{Ryd}} = \sum_k X_{ik} \left[- \frac{Z_{ik}^{**2}}{n_k^2} - \frac{y_i \overline{r_k}}{r_i^3} \right] - \frac{9}{5} \frac{y_i^2}{r_i} + \frac{3}{2} (kT)_{Ryd}.$$

where n_k is the principal quantum number of state k. Z_{ik}^{**} is the effective charge seen by the electron in state k and is

$$Z_{ik}^{**} = Z_i - \sum_{k'<k} X_{ik'} \sigma_{kk'} - \frac{X_{ik}}{2} \left(1 - \frac{1}{g_{ik}}\right) \sigma_{kk}$$

The sum is over all states which have energy less than that in state k. σ_{kk} are the Slater screening constants and as before, are in tabular form for use in the code.

The total matter energy is given by Mayer and is

$$E_{Ryd} = \sum_i X_i E_i + \frac{V(kT)_{Ryd}^{5/2}}{2\pi^2} F_{3/2}(\eta)$$

where $F_{3/2}(\eta)$ is the Fermi-Dirac integral of order 3/2. The total pressure equation which is from Mayer also is

$$P_{(Ryd/B.Ryd^3)} = P_e + \sum_i X_i \frac{(kT)_{Ryd}}{V} ,$$

with the electron pressure given by

$$P_e = \frac{(kT)_{Ryd}}{V} \left[\frac{2}{3} V \frac{(kT)_{Ryd}^{3/2}}{2\pi^2} F_{3/2}(\eta) - \frac{3}{5} \frac{1}{(kT)_{Ryd}} \sum_c X_i \frac{y_i^2}{r_i} \right.$$

$$\left. - \frac{1}{3} \sum_{i,k} X_i X_{ik} y_i \frac{\bar{r}_k^2}{r_i^3} \right]$$

At this point, all quantities needed to complete the opacity integral

$$I = \int_0^\infty \frac{w(u)}{\sum_i D_i(u)} du$$

are tabulated and pertinent quantities are sorted on increasingly negative energy E_{ik}, and u is computed from

$$u = \frac{|E_{ik}|}{(kT)_{Ryd}} .$$

Since the integrand for I is discontinuous at each u value or edge, integration must be performed between each u value separately and then added together to form the total integral I. Integration between each edge is done using Simpson's rule.

IONIC METHOD

For temperatures in the range of 5×10^3°K to 10^6°K, Cox has developed the following method, referred to as the "Ionic" method, for calculating occupation numbers.

One starts this method by calculating the equation of state of a given mixture, temperature, T (°K) and degeneracy parameter, η. The form of the Saha Equation applicable to any degree of electron degeneracy is

$$\frac{X_{i,j+1}}{X_{i,j}} = \frac{B_{i,j+1}}{B_{i,j}} \exp\left[-\frac{\chi_{ij} - \frac{(j+1)e^2}{R_D}}{kT} - \eta - \frac{E_0}{kT}\right]$$

where

$x_{i,j}$ - no. fraction for ion $i \cdot j$, i = element, j = no. of electrons missing

$B_{i,j}$ - partition function of ion i, j

$\chi_{i,j}$ - energy needed to ionize ion i, j to $i, j+1$

$(j+1)\, e^2/R_D$ - correction to ionization energy for interaction between charged particles

η - degeneracy parameter corrected by E_0/kT

E_0 - potential energy of the free electrons-averaged over all ion spheres. Enables one to ignore interaction energy of the free electron with themselves and with other ions

R_D - Debye Radius.

The Debye Radius considering all charged particles is

$$R_D = \left[\frac{4\pi N_t e^2 \left(y + \sum_i X_i \sum_j j^2 X_{ij}\right)}{kT}\right]^{-1/2}$$

where

$$N_t = \text{atom density} = \rho N_0/\mu_c = \rho N_0 \Big/ \sum_i X_i A_i .$$

The partition function for ion ij, summed over all excited states from the ground state to principal quant. no. $n_{max} = (j+1)\, r_{B.Rad.}$

$$B_{ij} = \sum_k g_{ijk} \exp\left[- \frac{\epsilon_{ijk} + \frac{y_i}{r_i}\left(3 - \frac{\delta_{n_k}}{\left(r_i Z^*_{ijk}\right)^2}\right)_{kv}}{kT_{kv}}\right]$$

g_{ijk} statistical weight, if not tabulated, then either $2n^2$ or $2(21+1)$

ϵ_{ijk} excitation energy alone the ground state

y_i electrons off element i

r_i average radius for element $= \left(3/4\pi\ y_i/y\ V\right)^{1/3}/a_0$

V volume/average element

a_0 Bohr radius

Ryd hydrogen atom ionization energy - 136 ev.

$\delta_{n_k} = \bar{r}_k^2 \, Z^{*2}$ Bohr rad.^{2} tabulated by Mayer ion sphere model.

ϵ_{ijk} is either tabulated by Moore energy level data or computed using screening constants.

$$Z^*_{ijk} = Z_i - \sum_k \nu_k \sigma_{kk}$$

and

$$\epsilon_{ijk} = -\frac{Z^{*2}_{ijk}}{n_{ijk}} + \chi_{ij}$$

ϵ_{ijk} may include states where more than one electron is excited above the ground level and are tabulated from Moore "Atomic Energy Level Data," NBS Circ. 467, 1, 2, 1949 and 1952.

If level data does not exist for a particular state, screening constants given by Mayer and Karzas are used with the Bohr model of the atom to compute these data. Hydrogen like statistical weights are used, that is $g_{ijk} = 2n^2$, $(n > 6)$, or $2(2l + 1)$, $(n \leq 6)$.

In cases of low temperatures where most atoms are neutral, the perturbation of the energy levels is due principally to neutral atoms. Therefore, a partition function is cut off when the orbit of the excited level has a radius greater than the mean separation between nuclei.

The procedure for solving the ionization equation is as follows. Once initial values for the ionization equation is made, one solves the two polynomials

$$P_i = \frac{\text{no. of nuclei of element } i}{X_{i0}} = 1 + \frac{X_{i1}}{X_{i0}} + \frac{X_{i2}}{X_{i1}}\frac{X_{i1}}{X_{i0}} + \cdots + \frac{X_{iz}}{X_{iz-1}} \cdots \frac{X_{i1}}{X_{i0}}$$

$$Q_i = \frac{\text{no. of electrons from element i}}{X_{i0}} = \frac{X_{i1}}{X_{i0}} + 2\frac{X_{i2}}{X_{i1}}\frac{X_{i1}}{X_{i0}} + \cdots$$

$$+ Z\frac{X_{iz}}{X_{iz-1}} \cdots \frac{X_{i1}}{X_{i0}} .$$

Therefore, y_i, the number of electrons from element i, is

$$y_i = \frac{Q_i}{P_i} = \frac{\text{frec electrons from element i}}{\text{no. of nuclei of element i}}$$

and the total no. of free electrons per average element is

$$y = \sum_i X_i \, y_i$$

The electron density is then computed from

$$N_e = \frac{4\pi(2nkT)^{3/2}}{h^3} F_{1/2}(\eta)$$

and the average atom density

$$N_t = \frac{N_e}{y} = \rho \frac{N_0}{\mu_c}$$

where, ρ, the matter density is

$$\rho = N_t \frac{\mu_c}{N_0}$$

PRECEDING PAGE BLANK NOT FILMED.

If the case is non-degenerate

$$P_e = \frac{\rho N_0 y}{\mu_c} (kT)$$

and

$$b' = b = \frac{R}{\mu_c}\left(\sum_i X_i + y\right)$$

The occupation numbers can then be calculated from

$$X_{ijk} = \nu_k g_{ijk} \exp\left[* \frac{-\epsilon_{ijk} + \frac{y_i}{r_i} \quad 3 - \left(\frac{\delta_{n_k}}{\left(r_i \; z^*_{ijk}\right)^2}\right)_{kv}}{kT} \right]$$

Corresponding effective charges and energies for each level along with ionic abundances are tabulated for future use in the absorption coefficient calculation.

METHOD OF DOMINANT POTENTIAL

Cox has developed a method using the method of dominant potential described by Chandrasekhar (1951) whereby one can input either temperature and density or temperature and the state of degeneracy, η, or electron pressure, Pe for the computer program.

The method, as described by Chandrasekhar is as follows:

Letting $\chi^{(n)}$, N_e, $N^{(n)}$ and N^{n-1} be the ionization energy, the electron density, and atom density with (n) and (n - 1) electrons, then

$$\frac{N^{(n-1)}}{N^{(n)}} N_e = 2 \frac{g^{(n-1)}}{g^{(n)}} \frac{(2\pi n kT)^{3/2}}{h^3} e^{\chi^{(n)}/kT}$$

where $g^{(n-1)}$ and $g^{(n)}$ are statistical weights. Then the state of ionization can be inferred from the value of a dominant potential ψ defined by the equation

$$e^{\psi/kT} = \frac{2}{Nc}\frac{(2\pi\, n\, kT)^{3/2}}{h^3}$$

because, if $\chi^{(n)} = \psi$ then apart from the statistical weights, the number of atoms with n electrons will equal the number of atoms with $(n-1)$ electrons. In a first approximation one can say that an atom with nuclear charges, z, will be mostly $(z-n)$ fold ionized if $\chi^{(n)} \cong \psi$.

The method, as employed by Cox, is described below, and after one of the following methods are completed, the ionization equation is computed as before assuming that the temperature $\theta = kT$, degeneracy η, and the density ρ are all self consistent.

Temperature, Density Input

First the atom density, N_t, is computed from

$$N_{t\,(atom/cm^2)} = \frac{N_0\,\rho}{\mu_c} = \frac{N_e}{y}$$

where No is Avogadros number, μ_c the cold mean molecular weight $= \Sigma\, X_i\, A_i$ and y the total number of free electrons per average atom.

The dominant potential equation

$$e^{\psi/kT} = \frac{2}{Ne}\frac{(2\pi\, n\, kT)^{3/2}}{h^3}$$

is written as follows to calculate the known quantities.

$$\ln y + \frac{\psi}{kT} = \ln\left(\frac{\theta^{3/2}}{N_t}\right) + \ln\left(\frac{2(2\pi\, n)^{3/2}}{h^3}\right) = \text{DPC}$$

The unknown quantity on the left, $(\ln y + \psi/kT)$, will be referred to as the dominant potential constant DPC. This equation is iterated using the known ionization energies for each ion, ij, in the mixture to get a consistent pair of y and ψ for the given temperature and atom density.

The procedure is as follows:

Using a starting guess of $\psi = 5 \cdot (kT)_{kv}$, compute for all elements in the mixture, a number of electrons off element i, y_i from the following

$$y_i = j + e^{\frac{\psi - \chi_{ij}}{kT_{kv}}}$$

where j is the number of electrons off element i for the ion when ψ is just less than the ionization potential, χ_{ij} to ionize the atom to ion $i, j+1$. Then compute the step y^l from

$$y^l = \sum_i X_i y_i$$

and a new value for ψ from DPC. That is

$$\psi_{new} = (kT)_{kv}\left[DPC - \ln\left(\frac{y^l + y^{l-1}}{2}\right)\right]$$

where $y = y'$. Then compute a new set of y_i's, y and ψ and keep iterating until succeeding y^l values converge to some predetermined amount ϵ. The code has $\epsilon = 0.1$.

Once y is known, then the electron density, Ne, and electron pressure, Pe, can be calculated using Fermi-Dirac statistics as follows. First compute the electron density, N_e

$$Ne = N_t \cdot y$$

and the Fermi-Dirac integral of order 1/2 in the non-relativistic case

$$F_{1/2}(\eta) = \frac{h^3 \, Ne}{4\pi(2n\,kT)^{3/2}}$$

Knowing this, existing tables of η, $F_{1/2}(\eta)$, $F_{3/2}(\eta)$ can be entered to compute the other two and compute the non-relativistic electron pressure from

$$Pe = Ne(kT)^{2/3} \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)}$$

$$= \frac{4\pi(2n)^{3/2}}{h^3} (kT)^{5/2} \left(\frac{2}{3} F_{3/2}(\eta)\right).$$

At this point, the ionization equation can be solved assuming a consistent set of Ne, y, Pe, η $F_{1/2}(\eta)$ and $F_{3/2}(\eta)$ for the given input of temperature, (kT), and density, ρ.

<u>(Temperature, degeneracy) or (Temperature, electron pressure) Input</u>

This method is started by first computing either the electron pressure, Pe, or the Fermi-Dirac integrals depending upon the input for the non-relativistic case from

$$Pe = \frac{2}{3} F_{3/2}(\eta) \frac{4\pi(2n)^{3/2}}{h^3} (kT)^{5/2}$$

$F_{3/2}(\eta)$ and $F_{1/2}(\eta)$ can be obtained in a table from the inputted, η. If Pe was input the above equation is solved for $F_{3/2}(\eta)$ obtaining η and $F_{1/2}(\eta)$ from tables vs. 2/3 $F_{3/2}(\eta)$.

Then with Pe, η, $F_{1/2}(\eta)$ and 2/3 $F_{3/2}(\eta)$ known, the electron density is computed from

$$Ne = \frac{Pe\, F_{1/2}(\eta)}{(kT)\, \frac{2}{3} F_{3/2}(\eta)} ,$$

and the dominant potential ψ from

$$e^{\psi/kT} = \frac{2}{Ne} \frac{(2\pi n kT)^{3/2}}{h^3} .$$

The number of electrons off element i, can be computed from

$$y_i = y + e^{\psi - \chi_{ij}/(kT)_{kv}}$$

where j is chosen as before.

Now the total number of free electrons from an average atom in the mixture, y, the atom density Nt, and the matter density ρ can be computed from the previous equations

$$y = \sum_i X_i y_i$$

$$Nt = \frac{Ne}{y}$$

$$\rho = \frac{Nt \mu_c}{No}$$

Now, as in the temperature, density input, one has a consistent set of all quantities needed to begin the ionization equation calculation.

After the ionization equation is solved, the same procedure is followed as in the "Mayer Independent Electron" method to solve the opacity integral, I.

First all quantities are tabulated and sorted on increasingly negative E_{ijk}. u is computed from

$$u = \frac{E_{ijk}}{(kT)_{kv}}$$

and the integration is performed between each edge using the trapezoidal rule.

THE PROCESSES

<u>Bound-free Absorption, D_{bf}</u>

Cox writes the following equation for D_{bf} (u) (equation 143)

$$D_{bf}^{(a)} = \frac{K_{bf}\,\rho u^3}{A} = \sum_{i,j,k} X_i\, X_{ij}\, X_{ijk} \frac{4\pi^4 n^2 e^8}{h^4 n_k^5 (kT)^5}\, q_{bf}\, g_{bf}$$

where K_{bf} is the absorption coeff/gm for ion ij and is summed over all energy states, K per ion, that is

$$K_{ff} = \sum_{i,j,k} X_i\, X_{ij}\, X_{ijk}\, \sigma_{bf_{ijk}} \frac{N}{\rho} .$$

The cross section for bound free absorptions σ_{bf} given by Cox (equation 23) is

$$\sigma_{bf} = \frac{2^6\,\pi^4}{3\sqrt{3}} \frac{Z_h^{t*4}\, me^{10}}{ch^6\, n^5\, \nu^3}\, q_{bf}\, g_{bf}$$

X_i is the number fraction of element i, X_{ij} is the abundance of ion ij (element i, ionized j times) such that $X_i\, X_{ij}$ is the number fraction of ion ij, and X_{ijk} is the occupation no. or probability that an electron exists in state k of ion ij.

$Z_k^{*'}$ is the effective nuclear charge seen by an electron in state k considering screening to both bound and free electrons, n is the principal quantum number, ν the frequency (sec^{-1}) and the other atomic constants have their usual meaning.

q_{bf} is the correction to the cross section for the availability of the final state, and is

$$q_{bf} = \left[e^{\eta - u - (E_{ijk}/kT)} + 1\right]^{-1}$$

η defines the matter state of degeneracy and will be referred to as the degeneracy parameter from here on,

$$u = \frac{h\nu}{kT}$$

and according to Mayer's A definition

$$A = \frac{2^4 \, hc^2}{3\sqrt{3}\, mc} \, \frac{N}{kT} \; .$$

q_u is the gaunt factor making σ_{bf} the non-classical cross section. In comparing Cox's published equation with that in the code, or

$$D_{bf}^{1} = \sum_{1'=1}^{1} \frac{Z_{1'}^{*'4}}{(kT)_{Ryd}^{2}} \, \frac{X_{1'} \, X_{i1'}}{n_{1'}^{5}} \, q_{bf_{1'}} \, g_{bf_{1'}} \; ,$$

a discrepancy of the factor

$$\frac{4\pi^4 m^2 e^8}{h^4},$$

is discovered, however this is exactly the energy of one Rydberg squared and cancels when using the temperature in Rydbergs.

The "STOP" uses a set of tables of computed bound-free gaunt factors obtained from John Stewart at the Los Alamos Scientific Laboratory which uses a polynomial fit approximation developed there of the Karzas and Latter (1958a, b, 1961) bound-free gaunt factors.

Cox states, "The bound-free gaunt factors depend on the initial state quantum numbers and photon energy in excess of the ionization energy. All extensive opacity calculations assume that bound-free transitions occur in hydrogen-like atoms where the electric fields are Coulomb, and in this case, the free electron energy parameter on which g_{bf} depends can be scaled by the effective nuclear charge $Z^{*'}$."

The most recent and most accurate hydrogen-like gaunt factors are those by Karzas and Latter (1958a, 1961, 1958b). These are functions of

$$\frac{\gamma_i^2}{(u-u_e)}$$

where

u_e = u at the present edge.

The effective charge $Z_{l'}^{*'}$ is defined by

$$Z_{l'}^{*'} = -\left(E_{l'} - E_0\right)^{1/2} n_{l'}$$

where $E_{1'}$ represents the electron energy in state $1'$ and E_0 is the potential energy of the free electrons averaged over all ion spheres. This shift in the energy zero point enables one to ignore the interaction energy of the free electrons with themselves and with the ions which are assumed to have bound electrons with orbits small compared to $\bar{r}_i$ · $\bar{r}_i$ is the average radius of a sphere which contains enough electronic charge to neutralize the ionic charge of atom i. E_0 is defined by

$$E_0 = -\frac{3}{5}\frac{1}{y}\sum_i \frac{X_i y_i^2}{\bar{r}_i} .$$

y_i is the number of free electrons off element i, (and is taken as an approximate effective nuclear charge seen in state k in later calculation)

$$y = \sum_i X_i y_i$$

and

$$r_i = \left(\frac{y_i}{y}\frac{3}{4\pi} V\right)^{1/3} \Big/ a_0$$

whose V is the volume per average atom

$$V = \frac{\mu_c}{\rho N_0} = \frac{\sum_i X_i \mu_{ci}}{\rho N_0}$$

a_0 is the Bohr radius, N_0 is Avogadros number and μ_c is the mean molecular weight. ρ, is the density in gm/cm^3.

The summation is over all edges which have ionization energy less than $u_e \cdot (kT)$.

Free-Free Absorption D_{ff}

Cox has derived the following definition for $D_{ff}(u)$ which is used in the code.

$$D_{ff}(u) = \frac{K_{ff}\,\rho u^3}{A} = \sum_i X_i \frac{2\pi^2 mc^4}{h^2} \frac{y_i}{kT} \ln\left(1 + e^{\eta}\right) g_{ff}$$

with K_{ff} the absorption coeff/gm and may be summed overall particles in the mixture.

$$K_{ff} = \sum_{i,j} X_i \, X_{ij} \, \sigma_{ffij} \frac{N}{\rho}$$

where the sum goes over all ionization stages, j, for each element i, N is the particle density and ρ the matter density: The cross section σ_{ij} is given by Cox as

$$\sigma_{ij} = \frac{2^5 \pi^2 Z^{*2} e^6 kT}{3\sqrt{3}\,h^4 c\nu^3} \ln \; 1 + e^{\eta} \; \bar{g}_{ff}$$

The free-free gaunt factors $\bar{g}_{ff}$ are those by Karzas and Latter (1958a, b, 1961) and have been averaged over the Fermi-Dirac distribution and corrected by Green (1958, 1960) for screening of the nuclear charge and availability of a final state. The Karzas and Latter data is in tabular form and the Green corrections are applied in the program.

Green writes,

$$\bar{g}^{S}_{FD}(u, \gamma^2, \eta) = \left(1 - \frac{2\gamma^2}{ul}\right)\left\{\frac{g_0(\omega)}{1 - e^{-4}} \log\left[\frac{\left(1 + e^{\eta}\right)\left(1 + e^{\eta - u - 2\gamma^2/l}\right)}{\left(1 + e^{\eta - u}\right)\left(1 + e^{\alpha - 2\gamma^2/l}\right)}\right. + \bar{g}_{FD}\left(\gamma^2, u, \eta - 2\gamma^2/l\right)\right.$$

where $\bar{g}_{FD}^{S}$, the un-normalized gaunt factor including screening, has been written in terms of the tabulated Karzas and Latter gaunt factors $\bar{g}_{FD}$ and $g_0(\omega)$, the asymptotic value of the unscreened hydrogenic gaunt factor for $E = 0$. $g_0(\omega_i)$ has been tabulated by Karzas and Latter also however the program uses a polynomial approximation to compute $g_0(\omega_i)$ as a function of ω_i. ω_i is defined by

$$\omega_i = \frac{u}{\gamma_i^2}$$

where u has its usual meaning and

$$\gamma_i^2 = \frac{Z_i^2}{(kT)}$$

η is the degeneracy parameter and l is a dimensionless length such that the screened potential is given by

$$V = \frac{2e^{-\rho/l}}{\rho} .$$

Results obtained from the polynomial for $g_0(\omega)$ we checked against Green's tabular values and agreement was only to one or two figures. Green states "In the classical case, l is just the Debye length divided by a_0/Z. At higher densities, insofar as the one-electron approximation can be applied, the potential that the electron sees must go into the Fermi-Thomas potential. Kidder (UCRL 5267-T, June 1958) discusses the behavior of this potential and points out the circumstances under which it may be approximated by the above potential, V, with a value for $l a_0/Z$ somewhat different from the Debye length."

The Los Alamos code uses the following for l,

$$l^{-1} = \frac{y_i}{R_D/a_0}$$

Finally, the screened gaunt factor used in the code is calculated under conditions of electron degeneracy, η, as

$$\bar{g}_{ff}\left(\gamma^2, u, \eta\right) = \frac{\sqrt{\pi}\, \bar{g}^{5}_{FD}\left(\gamma^2, u, \eta\right)}{2I_{1/2}(\eta)}$$

where $I_{1/2}(\eta)$ is the Fermi Dirac integral

$$I_{1/2}(\eta) = \int_0^\infty \frac{\sqrt{x}}{1 + e^{x-\eta}}\, dx \,.$$

In actual usage, three equations have been used in the code depending upon various degrees of degeneracy.

Cox states "for free-free absorption the nuclear charge seen by the free electron is taken as yi, and even if data for individual ions are known, the sum is only one term per element. This is possible because free-free absorption is never important when there is only partial ionization."

The factor, $2\pi^2 me^4/h^2$, here as before, cancels when using (kT) in Rydbergs and the form of the equation in the code is

$$D_{ff} = \sum_i \frac{X_i\, y_i^2}{(kT)_{Ryd}} \ln\left(1 + e^{\eta}\right) \bar{g}_{ff}\left(u, y_i^2/kT, \eta\right)$$

Scattering Ds(u)

Cox writes the following equation for $D_s(u)$

$$D_s(u) = \frac{\sigma_e \rho u^3}{A} = \sum_i X_i\, y_i\, \frac{u^3}{1 - e^{-u}} (kT) \frac{\sqrt{3}}{8} \left(\frac{2\pi e^2}{hc}\right)^3 \frac{h^2}{2\pi^2 mc^4}\, G(u) \,.$$

$G(u)$ is the ratio of effective electron-scattering cross-section, σ_{eff}, to the Thomson cross section for scattering of radiation by electrons, σ_0, given by Sampson (1959) that is

$$G(u) = \frac{\sigma_{eff}}{\sigma_0}$$

where

$$\sigma_0 = \frac{8\pi}{3}\left(\frac{e^2}{mc^2}\right)^2$$

Cox writes

$$\sigma_e = \sum_i X_i\, y_i\, \sigma_{eff}\, \frac{N}{\rho} = \sum_i X_i\, y_i\, \sigma_0\, G(u)\, \frac{N}{\rho}$$

where X_i are the number fractions of element i, y_i the number of free electrons from element i, N the particle density and ρ the matter density. u and A have these usual forms defined in equations 65 and 67 in his chapter in "Stellar Structures."

σ_e is the absorption coefficient for electron scattering/gm and is summed over all elements in the mixture. The induced emission correction $(1 - e^{-u})$ for pure absorption processes should not be applied to free-electron scattering and is therefore put into $Ds(u)$ to cancel out the factor in the weighting function $w(u)$.

$G(u)$, which is the same as $G(t, t')$ in equation (31) in Sampson (1959) can be represented by the following expression (as derived by Cox)

$$G(u) = 1 + \frac{1}{B(T)}\left(c_0 + c_2 u + c_2 u^2 + c_3 u^3 + c_4 u^4 + c_5 u^5\right)$$

where

$$B(T) = 1 + 1.875T + 0.8203125T^2 - 0.3076617188T^3 + 0.367270229T^4 - 0.51549911T^5$$

$$c_0 = +(2T + 8.75T^2 + 14.76525T^3 + 6.7675781T^4 - 2.7493286T^5)$$

$$c_1 = -(3.2T + 26.6T^2 + 122.85T^3 + 351.91406T^4 + 549.86572T^5)$$

$$c_2 = +(10.5T^2 + 141.4875T^3 + 1011.8883T^4 + 4600.3966T^5)$$

$$c_3 = -(31.4714285T^3 + 620.31607T^4 + 6341.6191T^5)$$

$$c_4 = +(88.114286T^4 + 2380.7571T^5)$$

$$c_5 = -(234.85714T^5).$$

T is in units of mc^2 and is $T = (kT)_{kv}/510.974$ kv/mc^2. This is the form used in the code.

The equation used in the program for D_s is

$$D_s(u) = y \frac{u^3}{1 - e^{-u}} \frac{\sqrt{3}}{8} \left(\frac{2\pi e^2}{hc}\right)^3 (kT)\, G(u)$$

where the factor

$$\frac{h^2}{2\pi^2 me^4}$$

is, of course, included in the temperature conversion for (kT) in Rydbergs. The total number of free electrons per average atom, y, is

$$y = \sum_i X_i y_i$$

H^- Bound-Free Absorption $D^{(u)}_{H^-_{bf}}$

Cox writes in equation (147)

$$D^{(u)}_{H^-_{bf}} = \frac{K_{H^-_{bf}} \rho u^3}{A} = \sigma_{H^-_{bf}} \frac{X_{H^-}}{X_{H^-}} X_H X_{H^-} \frac{3\sqrt{3}\, mc}{2^4\, hc^2} (kT)\, u^3$$

where, using the Saha ionization equation at the temperature and density of interest with the known ionization energy of .75 ev for the H^- ion gives the following for the ratio of the H^- ion abundance per neutral hydrogen atom,

$$\frac{X_{H^-}}{X_{H^\circ}} = 4.158 \times 10^{-10}\, P_e\, \theta^{5/2}\, e^{1.726\theta}$$

where θ = 5040/T°K and other units are in cgs.

The bound-free H^- cross sections, $\sigma_{H^-_{bf}}$, used are published by Gelfman (1962), and here as with the H^-_{ff} absorption, the H^- ion is not allowed to exist above T = 2V = 23, 210°K.

The tables, have Avogadros Number, N_0, included in them, or $N_0 \sigma_{H^-_{bf}}$ and are tabulated as a function

$$\left((kT)_{Ryd} \cdot u - E_0\right)$$

The form of the equation used in the code is as follows.

$$D_{H^-_{bf}} = N_0 \sigma_{H^-_{bf}} \frac{X_{H^-}}{X_{H^\circ}} u^3 X_H X_{H^\circ} \frac{\rho}{\mu_c} \frac{a_0 V}{AV}$$

Equivalence between this and Cox's published equation can be seen from the following.

The average atom density, N, can be written as

$$N = \frac{Ne}{y} = \rho \frac{N_0}{\mu_c}$$

where Ne is the electron density, y the average number of free electrons per average atom, ρ, the density, and μc, the cold gram molecular weight. The quantity a_0 V/AV is just A^{-1} in centimeters, and therefore

$$N_0 \frac{\rho}{\mu_c} \left(\frac{a_0 V}{AV}\right) = \frac{3\sqrt{3}\, mc}{2^4\, hc^2} (kT)$$

<u>H^- Free-Free Absorption $D^{(u)}_{H^-_{ff}}$</u>

Cox writes in equation 148 in "Stellar Structures"

$$D_{H^-_{ff}} = \frac{K_{H^-_{ff}}\, \rho u^3}{A} = \left(\frac{K_{H^-_{ff}}}{P_e\, X_{H^\circ}}\right) P_e\, X_{H^\circ}\, X_H\, u^3\, \frac{3\sqrt{3}\, mc}{2^4\, he^2} (kT)$$

where the absorption coefficient per gram, $K_{H^-_{ff}}$, is tabulated by Ohmura and Ohmara (1960, 1961). The quantity tabulated in their article is the continuous absorption coefficient of the negative hydrogen ion per neutral hydrogen atom and per unit electron pressure for free-free transitions after allowing for stimulated emission factor.

Cox has tabulated the following quantity for use in the code

$$\left[\frac{(\Delta k^2)^3\, K_{H^-_{ff}}\, N_0}{P_e\, X_{H^\circ}}\right].$$

where $(\Delta k^2) = u(kT)_{Ryd.}$ and is tabulated as a function of $(kT)_{kv}$ and (Δk^2).

The form of the equation in the code is then

$$D_{H^-_{fG}} = \theta^{-3}_{Ryd} \left[\frac{\left(\Delta k^2\right)^3 K_{H^-_{ff}} N_0}{P_e X_{H^\circ}}\right] P_e X_{H^\circ} X_H \left(\frac{\rho}{\mu_c} \frac{a_0 V}{AV}\right)$$

The equivalence of this equation with that by Cox is of course seen as before by knowing that

$$\frac{3\sqrt{3}\, mc}{2^4 a_e^2} (kT) = N_0 \frac{\rho}{\mu_c} \left(\frac{a_0 V}{AV}\right)$$

<u>H_2^+ Absorption $D_{H_2^+}(u)$ and H+H Abs $D_{H^+}(u)H$</u>

Cox writes (equation 149) for molecular effects

$$D_m(u) = \frac{K_m \rho u^3}{A} = DH_2^+ + D_{H+H}$$

a) DH_2^+

$$DH_2^+ = A_{H2^+} N_t^2 X_H^2 X_{H^\circ} X_{H^+} u^3 \frac{3\sqrt{3}\, mc\, (kT)}{2^4 he^2 N_t}$$

$A_{H_2^+}$ is tabulated by Bates (1952) and are only applied in the temperature range (2500 - 12,000°K). The code has

$$D_{H_e^+} = K_{H_2^+} u^3 X_H^2 XB_H X(H, t) \left(\frac{\rho}{\mu_c}\right)^2 \left(N_0^2 \times 10^{-39}\right) \left(\frac{a_0 V}{AV}\right)$$

Since

$$\frac{\rho}{\mu_c} = \frac{N_t}{N_0} \quad \text{and} \quad \frac{3\sqrt{3}}{2^4}\frac{mc}{he^2}(kT) = N_0 \frac{\rho}{\mu_c}\left(\frac{a_0 V}{AV}\right)$$

The tabulated values of $K_{H_2^+}$ are scaled by 10^{-39}.

b) D_{H+H}

Here, Cox writes

$$D_{H+H} = A_{H+H}\left(P_g - P_e\right)^2 X_H^2 X_{H_0}^2 u^3 \frac{3\sqrt{3}\,mc(kT)}{2^4\,he^2\,N_t}$$

where A_{H+H} is tabulated by Zwaan (1962) and is applied in the temperature range (3000 - 8000°K). The code has

$$D_{H+H} = 10^{\log A_{H+H}} u^3 \left(P - P_e\right)^2 X_H^2 \frac{a_0 V}{AV} XB_H^2$$

TEMPERATURES ABOVE 10^{8}°K

In the temperature region 10^8°K up to above $kT = mc^2$, Compton scattering by electrons is the most important process in determining the opacity (Sampson, 1959), and Cox uses the following for the opacity resulting from Compton scattering alone.

$$\kappa_c = \frac{N_{(e+p)}\,\sigma_0}{\rho}\,\bar{G}(T) \tag{1}$$

This equation neglects absorption and $N_{(e+p)}$ = density of electrons and positrons $\bar{G}(T)$ is

$$\bar{G}(T) = \left\{\frac{15}{4\pi^4}\int_0^\infty u^4\,e^u\left(e^4 - 1\right)^{-2}\left[G(u, T')\right]^{-1} du\right\}^{-1},$$

and is the Rosseland mean of $G(u, T')$. $G(u, T')$ is the ratio of the effective Compton cross-section, defined by Sampson, to σ_0, the Thomson cross-section for scattering of radiation by electrons. T' is in units of mc^2 and $u = h\nu/kT$

$$\sigma_0 = \frac{8\pi}{3}\left(\frac{e^2}{mc^2}\right)^2 = 6.65209 \times 10^{-25}\ \text{cm}^2$$

For the temperature range $20\ \text{kv} \leq kT \leq 125\ \text{kv}$, Sampson derived the following polynomial fit for $\bar{G}(T)$, T is in units of kv

$$\bar{G}(T) = -0.13887 + 4.9871(T)^{-1/2} - 5.9479(T)^{-1} - 2.362(T)^{-3/2}$$

Equation (1) can be written as

$$\kappa_c = \frac{N_{(e+P)}}{N_0}\frac{\sigma_0 N_0}{\rho}\bar{G}(T) = 0.40077\frac{N_{(e+p)}}{\rho N_0}\bar{G}(T)$$

From equation 132 in Cox's chapter

$$\frac{N_e}{\rho N_0} = \frac{y}{\mu_c}$$

where he has neglected any positron concentration and therefore obtains the following equation for κ_c

$$\kappa_c = \frac{y}{\mu_c}\bar{G}(T) \tag{2}$$

where

$$\bar{G}(T) = -0.055655 + 1.9987T^{-1/2} - 2.3837T^{-1} - 0.94662T^{-3/2}$$

Cox uses equation (2) down to $kT = 14\ \text{kv}$ which gives rise to a small difference in the computation of $\bar{G}(T)$ and therefore to the radiative opacity, κ_c, as well. $\bar{G}(T)$ was checked at $kT = 14\ \text{kv}$ to compare the result using the above polynomial with the tabulated value published by Sampson. Sampson's value was obtained by numerically integrating the integral representation for $\bar{G}(T)$.

$$\bar{G}(T)_{\text{Sampson}} = 0.7279 \qquad (kT = 14\,\text{kv})$$

$$\bar{G}(T)_{\text{Cox}} = 0.7241 \qquad (kT = 14\,\text{kv})$$

ELECTRON CONDUCTIVE OPACITY

At very high densities where electron degeneracy becomes important, one must consider electron conductions with radiation flow for transportation of energy.

The conductive flux can be expressed in the form following Mestel, (1950)

$$F_c = -\frac{4ac}{3}\frac{T^3}{\kappa_c \rho}\frac{\partial T}{\partial x} = \nu_c \frac{\partial T}{\partial x}$$

where the conductivity ν_c is obtained (Cox, p. 222) from one of the three cases:

1) $\eta < -4$ (non-degenerate gas)

$$\nu_c = \frac{128\, mk^5\, T^4\, e^{\eta}}{h^3\, e^4\, \rho N_0 \sum_i \frac{y_i^{\,2} X_i\, \Theta_i}{\mu_c}}$$

where

$$\Theta_i = \frac{1}{2}\ln\frac{2}{1-\cos\omega_i}$$

and ω_i is given by

$$\omega_i = \frac{[\theta Z^{1/3}]}{y_i^{1/3}}$$

and for this non-degenerate case

$$\theta Z^{1/3} = 0.58926\, e^{\eta/3}$$

2) $\eta \geq 8$ (high degeneracies)

$$\nu_e = \frac{16\pi^2 mk^5 T^4 \left(\eta^{3/2} + \frac{\pi^2}{8}\eta^{-1/2}\right)^2 \left(1 + 9.376\left(\eta^{3/2} + \frac{\pi^2}{8}\eta^{-1/2}\right)\right)^{-4/3}}{9h^3 e^4 \rho N_0 \sum_i \frac{y_i^2 X_i \Theta_i}{\mu_e}\left(1 + X^2\right)}$$

and

$$X^2 = \left[1.02715 \times 10^{-6}\frac{y\rho}{\mu_c}\right]^{2/3}; \qquad \frac{8\pi}{3}\frac{m^3 c^3}{h^3 N_0} = \frac{10^6}{1.02715}$$

where Θ_i and θ_i are given as before with the exception,

i) $[\theta Z^{1/3}]$ is obtained by interpolation from a table by (Cox, p. 223) of conductivity integrals for the interval $-4 \leq \eta \leq 30$

ii) $[\theta Z^{1/3}] = .84753, \ \eta > 30$

3) $(-4 \leq \eta \leq 8)$ (partial degeneracy)

Cox has tabulated the quantity

$$\nu_c \rho \sum_i \frac{y_i^2 X_i \Theta_i}{T^4 e^\eta}$$

for this case. Therefore one calculates Θ_i, as specified in 2) and divides out the known quantities to obtain ν_c.

Now κ_e is obtained from the flux equation

$$\kappa_e = \frac{4ac}{3} \left(\frac{T^3}{\rho \nu_c} \right)$$

a = radiation constant = 5.6692×10^{-5} erg cm^{-3} deg^{-4}

c = velocity of light = 2.997929×10^{10} cm sec^{-1}

The conductive opacity is then added in the following manner to the radiative opacity to give a total continuous opacity κ_T by

$$\frac{1}{\kappa_T} = \frac{1}{\kappa_R} + \frac{1}{\kappa_c}$$

REFERENCES

Bates, D. R.	1952	M. N. 112, 40
Chandrasekhar, S.	1939	Introduction to the Study of Stellar Structure, (Chicago University Press)
Cox, A. N.	1965	Stellar Structure, Chapter 3, University of Chicago

Geltman, S.	1962	Ap. J., 136, 935
Green, J. M.	1958	The Rand Corporation, report AECU-4133
	1960	The Rand Corporation, report RM-2580-AEC
John, T. L.	1960a	Ap. J., 131, 743
	1960b	M. N. 121, 41
Karzas, W. J.; and Latter, R.	1958a	Rand Corporation, report AECU 3703
	1958b	Rand Corporation, report RM-2091-AEC
Marshak, R. E.; Morse, P. M. and York, H.	1950	Ap. J., 111, 214
Mayer, H.	1947	Los Alamos Scientific Laboratory, report LA-647
Mestel, L.	1950	Proc. Cambridge Phil. Soc., 46, 331
Moore, C. E.	1949	National Bureau of Standards, Circ. 467,1
	1952	Ibid, 2
Ohmura, T. and Ohmura, H.	1960	Ap. J., 131, 8
	1961	Phys. Rev., 121, 513
Sampson, D. H.	1959	Ap. J., 129, 734
Stromgren, B.	1932	Zs, f. Ap., 4, 118
	1933	Zs. f. Ap., 7, 222
Zwaan, C.	1962	B.A.N., 16, 225
Stewart, J.	1963	List of Equations and Flow Charts of the L.A. OPACITY and IONIC codes (unpublished)