Low-Temperature Equation of State for Metals
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by

A. L. Merts
N. H. Magee, Jr.
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ABSTRACT

A code has been developed that calculates an improved equation of state (EOS) for pure metals in the melt-vapor region. The theory behind the code incorporates contributions to the EOS from a zero temperature model as well as from thermal atomic and electronic calculations, but does not include the effects of polymorphic and higher-order phase transitions. Pressures and energies have been obtained for several metals with Z less than 26 over temperature ranges from 0.02 eV to 10 keV and densities from $10^{-26}$ g cm$^{-3}$ to 1000 g cm$^{-3}$. Comparison of calculated critical point parameters (temperature, pressure, and density) with experiment is difficult due to scarcity of experimental results, but such comparisons tend to show the calculated values to be too large, a feature shared with other theoretical results.

I. INTRODUCTION

Many applications require consistent and reasonably accurate equation-of-state (EOS) results over a large range of temperatures and densities. For temperatures above $10^5$K, adequate results are obtained from existing codes, but below those temperatures and at normal densities the codes are not able to handle the calculations in the melt-vapor region. Usually ideal gas conditions are assumed. This code was developed to obtain more accurate pressures and internal energies for pure metals in this mixed-phase region. The present version of the code is able to calculate this first-order phase transition, but cannot handle polymorphic or higher-order phase transitions. For this reason, metals such as iron and titanium cannot be accurately calculated at this time.

The pertinent aspects of the problem can be seen in Fig. 1. Three isotherms, $T_1$, $T_2$, and $T_3$, are shown on this P-V diagram, where $T_2$ and $T_3$ pass through the melt-vapor region shown by the dotted line and $T_1$ lies above it. Most existing codes produce isotherms similar to $T_1$ for all temperatures $T_1$, $T_2$, and $T_3$ and ignore the distortion of the pressure curve due to the presence of the mixed-phase region. Using more realistic models, especially for

Fig. 1. Typical P-V diagram showing location of mixed-phase region.
the \( T = 0 \) calculation, resulted in the actual iso-
therm \( T_3 \). By thermodynamic considerations, the sta-
ble path of the system through the mixed-phase re-
gion is not the isotherm \( T_3 \), but rather the dashed
line from A to C, where A and C are local minimum of
the Gibbs free energy. Therefore, to obtain the EOS
of the system it is necessary to calculate both the
boundary of the mixed-phase region and the isotherm.

II. THEORY

As mentioned above, the contributions to the
isotherm come from zero temperature and thermal ef-
fects. Obtaining the pressure and energy from the
\( T = 0 \) curve is therefore the first step. The pres-
sure curve was fitted to satisfy the experimental
shock Hugoniot, the cohesive energy of the metal,
and the ultimate tensile strength. The resultant
curve, labeled \( P_c \), is shown in Fig. 2, where \( P_H \)
is the Hugoniot curve. This isotherm has been split
into three regions for computational reasons, and
the boundary conditions for each region are listed
in Table I. In these equations, \( E_c \) is the cohesive
energy, \( P_o \) is the ultimate tensile strength, \( S \) and
\( C_o \) are obtained from the Hugoniot shock relationship
shown in Eq. (1), and \( P_c(125) \) comes from a Thomas-
Fermi calculation.

\[
U_s = C_o + S \cdot U_p
\]

and

\[
\delta = S/(1 + S)
\]

TABLE I

\( T = 0 \) ISOTHERM BOUNDARY CONDITIONS

<table>
<thead>
<tr>
<th>Physical Constraints</th>
<th>Region</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>I</td>
</tr>
<tr>
<td>( P_c(125) = P_{TF}(125) )</td>
<td>x</td>
</tr>
<tr>
<td>( P_c(1) = 0 )</td>
<td></td>
</tr>
<tr>
<td>( P_c'(1) = P_{H}'(1) = 0.02 \rho_o C_o^2 )</td>
<td>x</td>
</tr>
<tr>
<td>( P_c''(1) = P_{H}''(1) = 0.05 \rho_o C_o^2(2S - 1) )</td>
<td>x</td>
</tr>
<tr>
<td>( P_c(6) = -P_o )</td>
<td></td>
</tr>
<tr>
<td>( P_c'(6) = 0 )</td>
<td>( x )</td>
</tr>
<tr>
<td>( P_c'(0) = 0 )</td>
<td>( x )</td>
</tr>
<tr>
<td>( \rho_{o} ) ( c ) ( / \eta ) ( d \eta = \rho_o E_c )</td>
<td>( x )</td>
</tr>
</tbody>
</table>

The expression for \( P_c \) in region I is similar to
the modified pressure function used by Barnes\(^1\) and
takes into account the attractive and repulsive na-
ture of the interatomic forces. This formula is
given in Eq. (3), where \( A, B, r, \) and \( B_a \) are derived
from the boundary conditions.

\[
\eta > 1
\]

\[
P_c = A \eta^{2/3} \left[ B_p^V - e^{B_a} \right], \quad (3)
\]

\[
\nu = 1 - \eta^{-1/3}
\]

The expressions for \( P_c \) in the other two regions are
derived entirely from the boundary conditions with
the additional mathematical constraint that \( dP_c/d\eta \)
\( \leq 0 \) in region III. The negative portion of the curve
was split after mathematical difficulties were en-
countered in treating it as one region. The result-
ant equations are

\[
\delta < \eta \leq 1
\]

\[
P_c = \eta^{4/3} \left( (\eta^{1/3} - 1) \left[ A + (\eta^{1/3} - \delta^{1/3}) \left[ B + \right.ight.ight.

\[
\left. \left. (\eta^{1/3} - \delta^{1/3}) \right] C + (\eta^{1/3} - 1) \left[ D + \right.ight.

\[
\left. \left. (\eta^{1/3} - 1) \right] E \right]\right] \right] \right] \right]
\]

(4)
and

\[ \eta < \delta \]

\[ P_c = P_o [K + 2 - (K + 1)\eta/\delta]^{(K+1)\eta/6} \]

(5)

After the pressure is obtained, the energy contribution can be calculated easily from the relationship

\[ \frac{1}{P_o} \int_{1}^{X} \frac{P_c}{n} \, dn = E_{\text{cold}} \]

(6)

As a partial check on the calculation, it is possible to use the \( P_c \) curve for \( \eta \geq 1 \) to recalculate the Hugoniot curve and to compare it to experimental results. The relationship between \( P_H \) and \( P_c \) is given in Eq. (7),

\[ P_H = \frac{(P_c - P_o \gamma_n n_c)}{(1 - \gamma(n - 1)/2)} \]

(7)

where \( \gamma \) is the Gruneisen ratio and is obtained from

\[ \gamma = -\frac{1}{3} + \frac{1}{2} \frac{\eta^2 P''}{P_c} + \frac{2/3 \eta P' - 2/9 P}{n^2 P_c} - \frac{2/3 P_c}{\eta P_c} \]

(8)

Plots of the resultant \( P_H \) curves are shown in Fig. 3 where the experimental points are from averaged curves.\(^2,3\) As expected, comparison is quite good at normal and higher densities, well within experimental error.

For temperatures greater than zero, contributions to the pressure, energy, and entropy arise from atomic and electronic components. At present, treatment of the atomic EOS is similar to that used by Thompson,\(^4\) which in turn is based on the work of Kormer et al.\(^5\) Without going into detail, the important equations are given below.

\[ F_n = N_o kT[3\ln(\theta/T) - 1 + 1.5\ln(1 + \Psi)] \]

(9)

\[ P_n = \rho N_o kT \left[ \frac{3\Psi + \Psi}{1 + \Psi} \right] \]

(10)

\[ E_n = 1.5N_o kT \left[ \frac{2 + \Psi}{1 + \Psi} \right] \]

(11)

\[ S_n = -N_o k[3\ln(\theta/T) - 4 + 1.5\ln(1 + \Psi) + 1.5\Psi/(1 + \Psi)] \]

(12)

and

\[ P = F(\rho, T) \]

Fig. 3. Comparison of experimental and theoretical Hugoniot curves.

\( F_n \) is the nuclear-free energy and \( P_n, E_n, \) and \( S_n \) are the pressure, energy, and entropy, respectively, obtained by the normal thermodynamic relationships from \( F_n \). \( \theta \) is the Debye temperature and \( \Gamma \) is the Gruneisen ratio, both functions of density. \( \Psi \) is an interpolation function that transforms the equations smoothly from high to low temperatures and gives rise to a continuous if somewhat inaccurate transition for \( P_n, E_n, \) and \( S_n \). This is necessary
for the numerical methods used in the code. Table II shows the rapid variation of \( Y \) with density for aluminum at a constant temperature.

The electronic thermal contribution is a Thomas–Fermi–like treatment, but uses a modified and parameterized Thomas–Fermi potential to speed up the calculations. This potential, broken into two parts, is

\[
\begin{align*}
\alpha < r < r_1 & \quad V(r) = Z e / (1 + \alpha r)^2 / r + Z^* e (r^2 / 2R^2 - B_0) / R \\
& \quad (13) \\
B_0 & = (Z/Z^*)(R/r_1)^2 / (1 + \alpha r_1)^2 - R/r_1 + 1.5 \\
& \quad (14) \\
\alpha & = 0.6057 Z^{1/3} \\
& \quad (15)
\end{align*}
\]

and

\[
\begin{align*}
r_1 < r < R & \quad V(r) = Z^* e (R/r + r^2 / 2R^2 - 1.5) / R \\
& \quad (16)
\end{align*}
\]

\( R \) is the radius of the spherical atomic volume, \( r_1 \) is the radius at which Eqs. (9) and (10) join, \( Z^* \) is the "effective number" of free electrons, and \( e \) is the electronic charge. \( Z^* \) is calculated using Fermi–Dirac statistics for the electronic distribution. With this information, \( P_{el} \) and \( E_{el} \) can be found with the equations

\[
\begin{align*}
P_{el} & = (2/3p) (I_3/2(\mu)/I_1/2(\mu)) kT \\
& \quad (17) \\
E_{el} & = (3p e / \rho + E_S / 2) \\
& \quad (18)
\end{align*}
\]

The electronic Gibbs free energy is

\[
G_{el} = -\mu N \\
& \quad (19)
\]

\( I_{1/2} \) and \( I_{3/2} \) are the Fermi–Dirac integrals of order 1/2 and 3/2 and \( E_S \) is the electronic interaction energy. \( N \) is the number of free electrons and \( \mu \) is the electron degeneracy parameter.

III. CALCULATIONS AND RESULTS

Although the theory has now been fully outlined, several important boundary conditions must be established before the actual calculations can be undertaken. First, the electronic model does not approach zero pressure or internal energy as \( T \rightarrow 0 \), therefore a zero temperature reference point must be chosen. The temperature 0.01 eV was picked as the pressure, etc., had become essentially constant for all lower temperatures. To remain consistent, it was necessary to use the same reference point for the nuclear model. Thus, for example, the total pressure would now become

\[
P_{Tot}(T) = P_{el} + P_{N} + P_{C} \\
& \quad (20)
\]

Next, the \( T = 0 \) curve is based on Hugoniot parameters, etc., obtained at ambient temperatures where there are thermal contributions to the EOS. Assuming this temperature to be 0.02 eV, the "cold" curve \( P_C \) in Fig. 2 actually includes some thermal effects. To take this into account, the pressure curve has been adjusted to give a total pressure of zero at normal density and 0.02 eV. Therefore, the \( P_C \) curve is the \( T = 0.02 \) eV curve, the true \( T = 0 \) curve \( (P_{N}) \) lies just below the \( P_C \) curve and crosses the horizontal axis at a density greater than normal density. This gives a slightly denser reference

<table>
<thead>
<tr>
<th>( n = \rho / \rho_0 )</th>
<th>( \Psi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>137.01</td>
</tr>
<tr>
<td>0.1</td>
<td>40.88</td>
</tr>
<tr>
<td>0.2</td>
<td>9.50</td>
</tr>
<tr>
<td>0.3</td>
<td>3.70</td>
</tr>
<tr>
<td>0.4</td>
<td>1.489</td>
</tr>
<tr>
<td>0.5</td>
<td>0.7459</td>
</tr>
<tr>
<td>0.6</td>
<td>0.4135</td>
</tr>
<tr>
<td>0.7</td>
<td>0.2494</td>
</tr>
<tr>
<td>0.8</td>
<td>0.1621</td>
</tr>
</tbody>
</table>
density $R_0$ for the cold curve, consistent with the fact that a metal will contract slightly as it is cooled.

A final modification now must be made to the electronic model because it does not allow for the transition from a free electron gas to a solid. The model produces too large a contribution at low temperatures and therefore has been multiplied by

$$G(T,\rho) = 2 \left[ \frac{1 + \exp (10 - 10/(1 + \Psi))/\rho}{\rho} \right]$$

which reduces the electronic EOS below 5.0 eV. $\Psi$ is the same as in the nuclear model and the coefficient 10 was chosen as an average ionization energy for the light metals. Thus, the final electronic pressure is now

$$P_{el} = G(T,\rho)\left[ P_{el}(T) - P_{el}(0.01) \right]$$

(22)

As mentioned previously, the pressure and Gibbs free energy were used to define the mixed-phase region. With the above modifications, these quantities can now be defined.

$$P_{Tot} = P_c + \left[ P_N(T) - P_N(0.01) \right]$$

$$+ G(T,\rho)\left[ P_{el}(T) - P_{el}(0.01) \right]$$

(23)

$$G_{Tot} = E_c + \left[ P_N(T) - P_N(0.01) \right]$$

$$+ \left[ \left( P_c + \left( P_N(T) - P_N(0.01) \right) \right) /\rho \right.$$

$$- \left( T S_N(T) - 0.01 S_N(0.01) \right]$$

$$+ G(T,\rho)\left[ G_{el}(T) - G_{el}(0.01) \right]$$

(24)

Looking at Fig. 1 again, the logical place to start the calculations is the critical point, where the $T_2$ isotherm just passes through the melt–vapor region. This point is located by finding the zero points of the first and second derivatives of the pressure with respect to density. In approaching the critical point, extreme care must be exercised to remain below the critical temperature and above the critical density during the search to ensure convergence. Comparison of the calculated critical point parameters to those of other theoretical models and experiment is outlined in Table III.

When the critical point has been established, the other boundary points (A and C in Fig. 1) are found by simultaneously equating the Gibbs free energy and the pressure at the upper and lower densities. Expanding Eqs. (23) and (24) in first-order Taylor series, we obtain the calculational technique used to determine the correct densities.

$$\left( P(\eta_2) - P(\eta_1) \right) / G(\eta_2) - G(\eta_1) = \left( \frac{\Delta P_1}{\Delta \eta_1} - \frac{\Delta P_2}{\Delta \eta_2} \right) \Delta \eta_1$$

(25)

After the boundary is set up, the isotherms can be calculated easily for the metal. Outside the mixed-phase region, the pressure and energy are calculated normally as outlined in previous sections. Inside the mixed-phase region, the pressure is a constant (equal to the value on the boundary) whereas the energy is a linear interpolation between the values at the upper and lower densities. The mixed-phase region and representative isotherms are shown for aluminum and beryllium in Figs. 4 and 5. A sample input and output is provided in Appendix A for users, whereas the code is listed in Appendix B.

IV. DISCUSSION OF RESULTS

Table III shows that the calculated temperatures and pressures are consistently higher than the experimental values for the few elements that can be compared. This is to be expected for our calculations because the experimental results are for the soft metals, whereas the electronic effects are relatively more important than for other metals. Thus, our modification of the present thermal electronic model plus our present inability to separate out the electronic effects in the cohesive energy and Hugoniot parameters leads to the overly high values. We hope that this discrepancy will be reduced when the electronic model is improved in the
next version of the code where a more accurate quantum theory using the method of quantum defects will be employed instead of the present model. The effect of the thermal electronic effect on the $T = 0$ isotherm parameters (cohesive energy, Hugoniot parameters, etc.) will also be examined in more detail.

In spite of the above difficulties, the code is a useful one for two reasons. First, it is quite general and is able to produce useful results for most metals below $Z = 30$ with only eight input parameters. Second, the calculated isotherms are consistent for all densities and all temperatures above 0.01 eV, and although somewhat inaccurate in the immediate vicinity of the critical point, they are quite accurate for most of the solid and vapor regions. Thus, we hope that users will find the code helpful while an updated version is being prepared.

![Figure 4](image)

**Fig. 4.** Detailed plot of aluminum mixed-phase region and representative isotherms.

<table>
<thead>
<tr>
<th>Element</th>
<th>LTOES</th>
<th>Thompson (4,7)</th>
<th>Grosse (8)</th>
<th>Adler &amp; Young (6)</th>
<th>Experimental a, b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lithium</td>
<td>$T_c = 0.5351$ eV</td>
<td>0.3541</td>
<td>0.3301</td>
<td>0.2777 ± 0.052</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$P_c = 0.00184$ Mbars</td>
<td></td>
<td>0.002422</td>
<td>0.000689 ± 0.00014</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\rho_c = 0.071$ g/cm$^3$</td>
<td></td>
<td>0.1470</td>
<td>0.1148 ± 0.0332</td>
<td></td>
</tr>
<tr>
<td>Beryllium</td>
<td>$T_c = 0.919$</td>
<td>0.785</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$P_c = 0.0330$</td>
<td>0.0142</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\rho_c = 0.577$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sodium</td>
<td>$T_c = 0.5730$</td>
<td>0.2413</td>
<td>0.2270</td>
<td>0.2217 ± 0.03</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$P_c = 0.00202$</td>
<td>0.0004965</td>
<td>0.000921</td>
<td>0.000355 ± 0.00007</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\rho_c = 0.1947$</td>
<td>0.1796</td>
<td>0.2692</td>
<td>0.2025 ± 0.04</td>
<td></td>
</tr>
<tr>
<td>Magnesium</td>
<td>$T_c = 0.7218$</td>
<td>0.3317</td>
<td>0.2937</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$P_c = 0.0680$</td>
<td>0.00175</td>
<td>0.001929</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\rho_c = 0.7908$</td>
<td>0.4122</td>
<td>0.4615</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Aluminum</td>
<td>$T_c = 1.479$</td>
<td>0.904</td>
<td>0.7367</td>
<td>0.6162</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$P_c = 0.0188$</td>
<td>0.00616</td>
<td>0.005458</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\rho_c = 0.679$</td>
<td>0.478</td>
<td>0.690</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Copper a</td>
<td>$T_c = 1.951$</td>
<td>0.7667</td>
<td>0.6570</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$P_c = 0.0382$</td>
<td>0.0083</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\rho_c = 2.323$</td>
<td>1.048</td>
<td>2.318</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

a Converged on critical point, but did not converge on mixed-phase boundary.
b Extrapolated to critical temperature from experimental data.

6
Fig. 5. Detailed plot of beryllium mixed-phase region and representative isotherms.

REFERENCES


APPENDIX A

SAMPLE CALCULATIONS FOR BERYLLIUM

<table>
<thead>
<tr>
<th>Column</th>
<th>Symbol</th>
<th>Identification</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>ATMNO</td>
<td>Atomic number of element</td>
</tr>
<tr>
<td>11-20</td>
<td>ATMWT</td>
<td>Atomic weight of element</td>
</tr>
<tr>
<td>21-30</td>
<td>RO</td>
<td>Normal density</td>
</tr>
<tr>
<td>31-40</td>
<td>S</td>
<td>Hugoniot S</td>
</tr>
<tr>
<td>41-50</td>
<td>CO</td>
<td>Hugoniot C_p</td>
</tr>
<tr>
<td>51-60</td>
<td>P0</td>
<td>Tensile strength</td>
</tr>
<tr>
<td>61-70</td>
<td>U</td>
<td>Cohesive energy</td>
</tr>
<tr>
<td>71-80</td>
<td>H4</td>
<td>Debye temperature</td>
</tr>
</tbody>
</table>

Card #2 (2I4)

<table>
<thead>
<tr>
<th>Column</th>
<th>Symbol</th>
<th>Identification</th>
</tr>
</thead>
</table>
| 1-4    | NTHETA | Number of temperature points*
| 5-8    | NRHO   | Number of density points

*Note—if zero, go to next element.

Card #3 (6E12.5)

List all temperature points, if any, in the above format.

Card #4 (6E12.5)

List all density points in the above format.
### II. OUTPUT FROM LTEOS

#### INPUT PARAMETERS

<table>
<thead>
<tr>
<th>Artist Number</th>
<th>4.00000E+00</th>
<th>Normal Density/CPM</th>
<th>1.65100E+00</th>
</tr>
</thead>
<tbody>
<tr>
<td>Artic Weight</td>
<td>9.01300E+00</td>
<td>Calc Density/CPM</td>
<td>1.82860E+00</td>
</tr>
<tr>
<td>HCCPict S</td>
<td>1.11670E+00</td>
<td>Osmotic Envelope</td>
<td>3.40000E+01</td>
</tr>
<tr>
<td>HCCPict CO</td>
<td>7.94900E+00</td>
<td>Tensile Strength/MPA</td>
<td>2.68132E+01</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Pressure/ATMR/MPA</td>
<td>1.61260E+00</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Debye Temperature/MPA</td>
<td>6.99500E+02</td>
</tr>
</tbody>
</table>

#### COLLECTED PARAMETERS (Method 1)

- T = 0 ISOTHEM CALCULATIONS
- Eta Between C1 and C2: 1.27719E+02
- Critical Point Results

#### CRITICAL POINT RESULTS

<table>
<thead>
<tr>
<th>C-critical</th>
<th>9.187229E-01</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-critical</td>
<td>1.297331E+02</td>
</tr>
<tr>
<td>C-at</td>
<td>7.116931E-01</td>
</tr>
</tbody>
</table>

### PRED PHASE EQUANCY PARAMETERS

#### TEMPERATURE / 7.50000E+01

<table>
<thead>
<tr>
<th>Temperature</th>
<th>ETA</th>
<th>Pressure</th>
<th>Energy</th>
<th>Gibbs Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.50000E-01</td>
<td>1.64900E-01</td>
<td>2.18486E+02</td>
<td>4.93417E+01</td>
<td>-7.78167E+01</td>
</tr>
<tr>
<td>8.50000E-01</td>
<td>1.65012E-01</td>
<td>2.18486E+02</td>
<td>4.93417E+01</td>
<td>-7.78167E+01</td>
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#### Pressure / Gibbs Energy

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APPENDIX B

LISTING OF THE LTEOS CODE
PROGRAM LTEOS (INPUT, OUTPUT, TAPE9 = OUTPUT, TAPE10 = INPUT)

COMMON /BLK/ AO, A1, E3, E4, F1, R, R2, S2, TO, X, Y, Z, Z9, Z10, Q(8), J1, N, QN, Q

1 N3, TO1, Q3(7), RQB, TO32, ITRAN, Z11, Y5, FNZR2

COMMON ATMWT, ATMNO, H4, GAMMA, R0

COMMON ECMAT(200), ETAMAT(200), A, B1, B2, C1, C2, C3, C5, C4, D1, A, K,
1 EREF, TREF, SAVE(50), P0, THETIN, RHOIN, PTOT, ETOT, RCOLD
2 DIMENSION THETA(100), RHO(100)

C
C THIS SECTION OF THE CODE SETS UP THE MIXED PHASE REGION AND INPUTS
C THE TEMPERATURE AND DENSITY FOR THE ISOTHERMS
C
C C***** CALCULATES THE MIXED PHASE BOUNDARY ********************

6 CALL CRTBND

C***** CALCULATES DESIRED ISOTHERMS OR TEMPERATURE DENSITY POINTS *****

READ (10, 1) NTHETA, NRHO
1 FORMAT (214)
2 IF (NTHETA) 11, 6, 4
3 READ (10, 2) (THETA(I), I = 1, NTHETA)
4 READ (10, 2) (RHO(I), I = 1, NRHO)
5 FORMAT (6E12. 5)
6 DO 10 I = 1, NTHETA
7 PRINT 3, THETA(I)
8 FORMAT (1H1, 2X, *TEMPERATURE = *, 1PE12. 5//7X, *RHO*, 7X, *PRESSURE*, 5X,
1 1 *ENERGY*/)
9 THETIN = THETA(I)
10 DO 10 J = 1, NRHO
11 PRINT 5, RHOIN, PTOT, ETOT
12 PRINT 5, RHOIN, PTOT, ETOT
13 FORMAT (2X, 1P1OE12. 5)
14 CONTINUE

CALL ISOCAL

C MAIN SUBROUTINE - IT CALCULATES (IN THIS ORDER) THE T=0 CURVE, THE
C CRITICAL POINT, THE MIXED PHASE REGION AND THE ISOTHERM PRESSURES
C AND ENERGIES

SUBROUTINE CRTBND

COMMON /BLK/ AO, A1, E3, E4, F1, R, R2, S2, TO, X, Y, Z, Z9, Z10, Q(8), J1, N, QN, Q

1 N3, TO1, Q3(7), RQB, TO32, ITRAN, Z11, Y5, FNZR2

COMMON ATMWT, ATMNO, H4, GAMMA, R0

COMMON ECMAT(200), ETAMAT(200), A, B1, B2, C1, C2, C3, C5, C4, D1, A, K,
1 EREF, TREF, SAVE(50), P0, THETIN, RHOIN, PTOT, ETOT, RCOLD
2 DIMENSION GEN(20), C(2, 2), AP(2), RP(2), IROW(2), TEM(2), TSTORE(100),
1 ETA1(100), ETA2(100), PRESS1(100), PRESS2(100), ENERG1(100),
2 ENERG2(100), PCHECK(50), GCHECK(50)

DATA (GEN(I), I = 1, 14) / 0., 5.1, 2., 4., 8., 16., 1., 0.5., 0.05., 0.005., 0.0005. /
1 .1., .2. /

DIMENSION COLDP(12)

DATA COLDP/ 9524., 96154., 97087., 98039., 990991.1., 0.0001.0.0417., 1.087, /
1 1.1364., 1.1905., 1.250, 1.66666/
C***** SETS UP T=0 CALCULATION                                29AP72

200 READ (10,1) ATMNO,ATMWt,R0,S,C0,P0,U,H4

1 FORMAT(8E10.3)       LTEO S

   IF(ATMNO .GT. 25 . AND. ATMNO .LT. 27.) GO TO 990       LTEO S
   IF(ATMWt . EQ. 0) GO TO 1001                                LTEO S
   B = 125. *R0
   CALL EOS(0,B,,01,PUPPER,EUPPER)
   PUPPER = PUPPER*PSI(125.,.01)
   CALL COLCOF(S,C0,PUPPER,U)
   PRINT 4,ATMNO,R0,ATMWt,R0,COLD,S,U,C0,P0,PUPPER,H4

4 FORMAT(1H1,28X,"INPUT PARAMETERS"/* ATOMIC NUMBER = *,1PE12.5,
   1 * NORMAL DENSITY(GM/CM3) = *,E12.5/* ATOMIC WEIGHT = *,
   2 E12.5,* COLD DENSITY(GM/CM3) = *,E12.5/* HUGONIOT S = *
   3,E12.5,* COHESIVE ENERGY(EV) = *,E12.5/* HUGONIOT C0 =
   4 *,E12.5,* TENSILE STRENGTH(MBARS) = *,E12.5/32X,* PRESSURE(ET
   5 A=125)(MBARS)= *,E12.5/32X,* DEBYE TEMPERATURE(EV) = *,E12.5/ 4APR72
   PRINT 8,GAMMA,D1,AK,C1,C2,C3,C4,C5,A,B1,B2

8 FORMAT(1H0,"-----------------------------------------------------
   6 /* 22X,\"T = 0 ISOTHERM CALCULATIONS\"/* GRUNEISEN GAMMA = *
   1 1PE12.5,/* MINIMUM PRESSURE LOCATION(ETA) = D1 = *,E12.5,/
   2 EQUATION CONSTANTS\"/* ETA LESS THAN D1---- --K = *,E12.5/\" ETA
   3 BETWEEN D1 AND 1. -C1 = *,E12.5/24X,*C2 = *,E12.5/24X,*C3 = *
   4 /24X,*C4 = *,E12.5/24X,*C5 = *,E12.5/\" ETA GREATER THAN 1.---- A
   5 = *,E12.5/24X,*BR = *,E12.5/24X,*BA = *,E12.5)          EXPLA

C************ START OF CRITICAL POINT SEARCH SECTION *************** LTEO S

   TO = .05
   ESTART = AK*D1/(AK + 1.) + .11*D1
   EREF = 0.
   TREF = 0.
   DELT = 1.
   ITEMP = 8
   IRHO = 8
   DELRHO = GEN(IRHO)

   S8 = 1.
   CALL PDPCAL(TO,ESTART,PRES,PRES,P,S0,1)  29AP72
   SREF = S0
   IF(S8*SREF .GT. 0) GO TO 6
   ESTART = 1.
   PRINT 5

5 FORMAT(1X,*AM RESTARTING ETA AT 1.*)               LTEO S
   GO TO 3

6 ESTART = ESTART*(1. - DELRHO)
   CALL PDPCAL(TO,ESTART,PRES,PRES,P,S0,1)  29AP72
   IF(S8*S0 . LT. 0) GO TO 10
   SREF = S0
   IF(ESTART .GT. .05) GO TO 6
   PRINT 7,ESTART

7 FORMAT(1X,*CAN NOT FIND NEG. SEC. DERV. DOWN TO ETA = *,1PE12.5)
   GO TO 1000

10 IF(ABS(S0) . LT. 1.E-5) GO TO 15
   ESTART = ESTART*(1. + DELRHO*(1. - ABS(SREF/(SREF- S0))))
   CALL PDPCAL(TO,ESTART,PRES,PRES,P,S0,1)
   SREF = S0

11
IF(ABS(SREF) .LT. 1.E-5) GO TO 15
S8 = ABS(SREF)/SREF
DELRHO = S8*ABS(DELRHO/10.)
IF(ABS(DELRHO) .GT. 1E-02) GO TO 6
PRINT 11,ESTART,PRES,S0
FORMAT(1X,*CAN NOT CONVERGE ON ZERO SECOND DERIV., ETA =*,1PE12.5,
*PRESSURE =*,E12.5,* AND P SEC. DERIV. =*,E12.5)
GO TO 1000
15 IF(PRESP .LT. 0) GO TO 20
PRINT 16,ESTART
16 FORMAT(1X,*FIRST DERIV. IS POS. AND SEC. DERIV. IS NEG. ANT ETA =*,
1PE12.5, * RESTART*)
IF(PRESP .LT. 1.E-4) GO TO 40
GO TO 1000
20 IF(ABS(PRESP) .LT. 1.E-5) GO TO 40
DO 25 I = 1,2
AI = I
E = ESTART*(1. + (AI - 1.5)*.001)
B = E*R0
CALL EOS(0,B,01,PLOWER,ELOWER)
SAVE(I) = PLOWER
CALL COLD(ESTART,PCOLD,PPCOLD,ECOLD,EPCOLD)
PPREF = PRESP
25 SAVE(I) = PLOWER
CALL COLD(ESTART,PCOLD,PPCOLD,ECOLD,EPCOLD)
PREF = PRESP
26 TSAVE = T0
TO = T0 + DELT*T0
CALL PDPCAL(T0,ESTART,PRES,PREF,S0,0)
IF(PRESP .GT. 0) GO TO 30
IF(ABS(PRESP) .LT. 1.E-5) GO TO 35
IF(TO .LT. 10.) GO TO 28
PRINT 27,T0,ESTART
FORMAT(1X,*TEMP. IS TOO LARGE,START AGAIN. TO = *,1PE12.5,* ETA =*
1,E12.5)
GO TO 1000
30 TO = TSAVE + (T0 - TSAVE)*ABS(PREF/(PREF-PRESP))* .95
CALL PDPCAL(T0,ESTART,PRES,PREF,S0,0)
IF(PRESP .GT. 0) GO TO 30
IF(ABS(PRESP) .LT. 1.E-5) GO TO 35
DELT = .01*DELT
IF(DELT .GT. .000001) GO TO 26
PRINT 31,T0,PRESP
35 FORMAT(1X,*CAN NOT CONVERGE ON LOCATION OF ZERO SLOPE*,1PE12.5)
GO TO 1000
35 DELT = GEN(ITEMP)
ITEMP = ITEMP + 1
CALL PDPCAL(T0,ESTART,PRES,PREF,S0,1)
IF(ABS(S0) .LT. 1.E-5) GO TO 40
SREF = S0
S8 = ABS(SREF)/SREF
DELRHO = S8*GEN(IRHO)
IRHO = IRHO + 1
GO TO 6
40 CALL PGCAL(0,ESTART,T0,PCRIT,PPTOT,ECRIT,GTOT,GPTOT)
PRINT 41,T0,PCRIT,ESTART
START OF MIXED PHASE BOUNDARY CALCULATION ***************

ETA1(1) = ETACRT
ETA2(1) = ETACRT
PRESS1(1) = PCRTI
PRESS2(1) = PCRTI
ENERG1(1) = ECRIT
ENERG2(1) = ECRIT
TSTORE(1) = TCRIT
IITEMP = 2
PRINT 42

ICYCLE = 1
DELP = .05
DELT = .1
IF(TO . LE. 1.) DELT = .05
MTEMP = 10. *TO
TEM = MTEMP
TO = TEM/10.
IF(TCRIT - TO . LT. DELT) TO = TO - DELT
E = ESTART - .15
IF(E .LT. 0.) E = .01
CALL PGCAL(O,E,TO,PNEW,PPTOT,ETOT,GTOT,GPTOT)
DO 45 I = 1,100
E = E + .01
CALL PGCAL(O,E,TO,PNEW,PPTOT,ETOT,GTOT,GPTOT)
IF (PNEW . GT. Fro ) GO TO 45
SAVE(1) = E - .06
ELOW = E+ .01
GO TO 46
45 Fro = PNEW
PRINT 43

P0 = PNEW
PRINT 43

FORMAT(* FAILED TO FIND STARTING POINT FOR CRITICAL BOUNDARY*)

PT0 = PNEW
DO 48 I = 1,100
E = E + .01
CALL PGCAL(O,E,TO,PNEW,PPTOT,ETOT,GTOT,GPTOT)
IF(PNEW . LT. PTO ) GO TO 48
SAVE(1) = E - .06
ELOW = E + .01
GO TO 46
48 PTO = PNEW

CONTINUE
DO 55 J = 1,2

18APR72 13
E = SAVE(J)
CALL PGCAL(1,E,T0,PTOT,PPTOT,ETOT,GTOT,GPTOT)
C(2,J) = S8*PPTOT
I1 = 8 + 2*J
SAVE(I1) = PTOT
C(1,J) = S8*GTOT
I3 = 20 + 2*J
I2 = I1 + 1
SAVE(I3) = ETOT
SAVE(I2) = GTOT

55 S8 = -1.
GCHECK(I) = SAVE(I1)
PCHECK(I) = SAVE(I2)
AP(1) = SAVE(I3) - SAVE(I1)
AP(2) = SAVE(I2) - SAVE(10)
IF(ABS(AP(1)/SAVE(I1)) . LT. 1. E-6) GO TO 57

56 IF(1 . LE. 3) GO TO 75
IF(ABS((GCHECK(I) - GCHECK(I-2))/GCHECK(I)) . GT. 1. E-10) GO TO 75
IF(ICYCLE . GT. 1) GO TO 81
ICYCLE = 2
TCYCLE = T0
T0 = T0 + .005
GO TO 50

57 IF(ABS(AP(2)/SAVE(10)) . LT. 1. E-5) GO TO 105
IF(1 . LT. 3) GO TO 75
IF(ABS((PCHECK(I)-PCHECK(I-2))/PCHECK(I)) . LT. 1. E-10) GO TO 64

75 CONTINUE
CALL MATINV(C,2,2,1ROW,TEMP)
CALL MATMPY(2,2,1,C,2&,2,RP,2)
SAVE(1) = SAVE(1) + RP(1)
SAVE(2) = SAVE(2) + RP(2)

85 IF(SAVE(1) . GT. ETACRT) GO TO 95
IF(SAVE(2) . LT. ETACRT) GO TO 95
IF(SAVE(1) . LT. 0) SAVE(1) = (SAVE(1) - RP(1))/2.
IF(SAVE(1) . GT. ELOW) SAVE(1) = ELOW - .01
IF(SAVE(2) . LT. EHIGH) SAVE(2) = EHIGH + .01

60 CONTINUE
IF(ABS(AP(1)/SAVE(I1)) . GT. 1. E-6) GO TO 89

64 IF(SAVE(10) . GT. 1. E-8) GO TO 89
IPOS = 0
IF(SAVE(10) . LT. SAVE(12)) IPOS = 1
SIG = ABS(SAVE(10) - SAVE(12))/(SAVE(10) - SAVE(12))
STEP = 1. E-7

74 ITEM = 1
DO 76 I4 = 1,11
AI4 = I4
ETE = SAVE(2)*(1. + SIG*STEP*AI4)
CALL PGCAL(1,ETE,T0,PTEM,PPTOT,ETOT,GTEM,GPTOT)
IPOS = 0
IF(SAVE(10) . LT. PTEMP) IPOS = 1
IF(IPOS . NE. IPOS) GO TO 62
ITEM = ITEM + 1

76 CONTINUE
PRINT 78,T0,ETE,PTEMP,ETOT,GTEM
78 FORMAT(1X,"CAN NOT FIND CROSS POINT",1P6E15.7)
GO TO 150
62 IF(ITEM .GT. 1) GO TO 77
STEP = STEP/10.
IF(STEP .GT. 1.E-14) GO TO 74
IF(SIG .LT. 0) ETE = SAVE(2)
77 IF(ABS(GTEM - SAVE(13))/SAVE(13) .GT. 1.E-5) GO TO 69
SAVE(12) = SAVE(10)
65 DO 82 I4 = 1,200
A14 = I4
ETE1 = ETE*(1. + STEP*A14)
SAVE(2) = ETE1*(1. - STEP)
CALL PGCAL(1,ETE1,T0,PTEMP,PPTOT,ETOT,GTEM,GPTOT)
IF(ABS(GTEM - SAVE(13))/SAVE(13) .LT. 1.E-8) GO TO 105
82 CONTINUE
GO TO 105
69 PRINT 70
70 FORMAT(1X,"NUMERIC PROBLEMS PREVENT CONVERGENCE")
GO TO 65
81 PRINT 70
GO TO 111
89 PRINT 90
90 FORMAT(1X,"CAN NOT CONVERGE IN 50 TRIES")
IF(ICYCLE .GT. 1) GO TO 150
ICYCLE = 2
TCYCLE = T0
T0 = T0 + .01
GO TO 50
95 PRINT 100,SAVE(1),ETACRT,SAVE(2)
100 FORMAT(1X,"ETAS ARE CROSSING CRITICAL ETA",1P3E12.5)
GO TO 150
105 TSTORE(ITEMP) = T0
ETA1(ITEMP) = SAVE(1)
ETA2(ITEMP) = SAVE(2)
PRESS1(ITEMP) = SAVE(10)
PRESS2(ITEMP) = SAVE(12)
ENERG1(ITEMP) = SAVE(22)
ENERG2(ITEMP) = SAVE(24)
PRINT 110,T0,ETA1(ITEMP),PRESS1(ITEMP),ENERG1(ITEMP),SAVE(11),
1 ETA2(ITEMP),PRESS2(ITEMP),ENERG2(ITEMP),SAVE(13)
110 FORMAT(2X,1P1E12.5,1X,4(E12.5,2X)/)
ITEMP =ITEMP + 1
111 IF(ICYCLE .GT. 1) T0 = TCYCLE
ICYCLE = 1
112 IF(T0 .LT. .11) DELTP = .025
T0 = T0 - DELTP
IF(T0 .LT. .049) GO TO 150
EFAC = 2.
IF(T0 .LT. .2) EFAC = 1.
SAVE(1) = SAVE(1)/EXP(TCRIT/(EFAC*T0))
SAVE(2) = ETA2(ITEMP-1)*1.20
112 IF(ITEM .GT. 6) SAVE(2) = 2.*ETA2(ITEMP-1) - ETA2(ITEMP-2)
IF(SAVE(2) .GT. 1.) SAVE(2) = .99
GO TO 50

C
150 NBOUND = ITEMP - 1
PTO = PRESS1(NBOUND)
E = ETA2(NBOUND)
DO 155 I = 1,100
E = E - .01
CALL PGCAL(0,E,TSTORE(NBOUND),PTOT,PPTOT,ETOT,GTOT,GPTOT)
IF(PTOT .GT. PTO) GO TO 156
155 PTO = PTOT
156 EBOUND = E + .01
GO TO 160
990 PRINT 991
991 FORMAT(* IRON IS NOT AVAILABLE AT PRESENT TIME*)
RETURN
C
ENTRY ISOCAL
E = RHOIN/R0
IF(THETIN .LT. .01) THETIN = .01
IF(THETIN .GT. TCRIT) GO TO 240
DO 205 IJ = 1,NBOUND
IF(THETIN .GE. TSTORE(IJ)) GO TO 207
CONTINUE
IF(E .GT. EBOUND) GO TO 240
PTOT = 0.
ETOT = 0.
GO TO 1001
205 CONTINUE
IF(E .GT. EBOUND) GO TO 240
PTOT = PRESS1(IJ) - TINTER* (PRESS1(IJ) - PRESS1(IJ- 1))
ENGHI = ENERG2(IJ) - TINTER* (ENERG2(IJ) - ENERG2(IJ- 1))
ENGLO = ENERG1(IJ) - TINTER* (ENERG1(IJ) - ENERG1(IJ- 1))
ETOT = ENGHI - (ENGHI- ENGLO)*(ETAHI - E)/(ETAHI - ETALO)
GO TO 1001
207 TINTER = (TSTORE(IJ)- THETIN)/(TSTORE(IJ)- TSTORE(IJ- 1))
ETAHI = ETA2(IJ) - TINTER*(ETA2(IJ) - ETA2(IJ- 1))
ETALO = ETA1(IJ) - TINTER*(ETA1(IJ) - ETA1(IJ- 1))
IF(E .GT. ETAHI) GO TO 240
IF(E .LT. ETALO) GO TO 240
CALL PGCAL(0,E,THETIN,PTOT,PPTOT,ETOT,GTOT,GPTOT)
GO TO 1001
240 PRINT 1002
1002 FORMAT(1X,*CAN NOT WORK THIS CASE*)
RETURN
C
ENTRY ISOCAL
E = RHOIN/R0
IF(THETIN .LT. .01) THETIN = .01
IF(THETIN .GT. TCRIT) GO TO 240
DO 205 IJ = 1,NBOUND
IF(THETIN .GE. TSTORE(IJ)) GO TO 207
CONTINUE
IF(E .GT. EBOUND) GO TO 240
PTOT = 0.
ETOT = 0.
GO TO 1001
205 CONTINUE
IF(E .GT. EBOUND) GO TO 240
PTOT = PRESS1(IJ) - TINTER* (PRESS1(IJ) - PRESS1(IJ- 1))
ENGHI = ENERG2(IJ) - TINTER* (ENERG2(IJ) - ENERG2(IJ- 1))
ENGLO = ENERG1(IJ) - TINTER* (ENERG1(IJ) - ENERG1(IJ- 1))
ETOT = ENGHI - (ENGHI- ENGLO)*(ETAHI - E)/(ETAHI - ETALO)
GO TO 1001
207 TINTER = (TSTORE(IJ)- THETIN)/(TSTORE(IJ)- TSTORE(IJ- 1))
ETAHI = ETA2(IJ) - TINTER*(ETA2(IJ) - ETA2(IJ- 1))
ETALO = ETA1(IJ) - TINTER*(ETA1(IJ) - ETA1(IJ- 1))
IF(E .GT. ETAHI) GO TO 240
IF(E .LT. ETALO) GO TO 240
CALL PGCAL(0,E,THETIN,PTOT,PPTOT,ETOT,GTOT,GPTOT)
GO TO 1001
240 PRINT 1002
1002 FORMAT(1X,*CAN NOT WORK THIS CASE*)
RETURN
C
ENTRY ISOCAL
E = RHOIN/R0
IF(THETIN .LT. .01) THETIN = .01
IF(THETIN .GT. TCRIT) GO TO 240
DO 205 IJ = 1,NBOUND
IF(THETIN .GE. TSTORE(IJ)) GO TO 207
CONTINUE
IF(E .GT. EBOUND) GO TO 240
PTOT = 0.
ETOT = 0.
GO TO 1001
205 CONTINUE
IF(E .GT. EBOUND) GO TO 240
PTOT = PRESS1(IJ) - TINTER* (PRESS1(IJ) - PRESS1(IJ- 1))
ENGHI = ENERG2(IJ) - TINTER* (ENERG2(IJ) - ENERG2(IJ- 1))
ENGLO = ENERG1(IJ) - TINTER* (ENERG1(IJ) - ENERG1(IJ- 1))
ETOT = ENGHI - (ENGHI- ENGLO)*(ETAHI - E)/(ETAHI - ETALO)
GO TO 1001
207 TINTER = (TSTORE(IJ)- THETIN)/(TSTORE(IJ)- TSTORE(IJ- 1))
ETAHI = ETA2(IJ) - TINTER*(ET
C TEMPERATURE AND DENSITY

Z=ATMNO
A=ATMWT
TO=TEMPTUR
RO=DENSITY
KKK=O
Z9=Z**.3333333
Z11=1./Z9
R=(2.6740715*A/RO)**.3333333
Z10=R*Z9
RQB=R**3

15 CONTINUE
TO32=SQRT(TO)*TO
TO1=1./TO
AO=.6057*Z9
DO 1 I=2,8
IF (Z10.LT.Q(I)) GO TO 2
1 CONTINUE
2 J1=I
N=I-1
QN=Q(N)
QN3=QN**3
ITRAN=1
IF (Z10.LT.16.) ITRAN=2
R2=R
FNZR2=1./(1. + AO*R2)
FNZR2=FNZR2**2*(2.*AO*R2*FNZR2+1.)*Z
F1=236.34647*FNZR2/(RQB*TO32)
CALL SUB400
E3=E4
CALL SUB1100
Z2=S2
R2=R2*.99
FNZR2=1./(1. + AO*R2)
FNZR2=FNZR2**2*(2.*AO*R2*FNZR2+1.)*Z
F1=236.34647*FNZR2/(RQB*TO32)
CALL SUB400
E3=E4
CALL SUB1100
Z3=S2
IF (Z2/Z.GE.1.) GO TO 3
ISW=1
R2=.1
Z2=Z
GO TO 4
3 ISW=2
R2=R/3.
IF (Z2/Z.GE.1.) GO TO 8
4 R3=R2
FNZR2=1./(1. + AO*R2)
FNZR2=FNZR2**2*(2.*AO*R2*FNZR2+1.)*Z
F1=236.34647*FNZR2/(RQB*TO32)
CALL SUB400
E3=E4  
CALL SUB1100
Z4=Z2-S2  
IF (ABS(Z4/Z2). LT. 1.E-10) GO TO 5
R2=R3*.99  
FNZR2=1. / (1. + AO*R2)  
FNZR2=FNZR2**(2.*AO*R2*FNZR2+1.)*Z  
F1=236.34647*FNZR2/(RQB*TO32)  
CALL SUB400
E3=E4  
CALL SUB1100
Z4=Z2-S2  
R2=R3-.01*R3*Z4/(Z4-Z3)  
GO TO 4
5  GO TO (9,6), ISW  
6  PRINT 10  
   PRINT 11  
7  X=E3  
   CALL SUB600  
   CALL SUB1100
Z4=Z2-S2  
IF (ABS(Z4/Z). LT. 1.E-10) GO TO 9
E3=.99*E3
   X=E3  
   CALL SUB600  
   CALL SUB1100
Z3=Z2-S2  
E3=(1.010101-.010101*Z4/(Z4-Z3))*E3
GO TO 7
8  PRINT 12  
   PRINT 13  
   STOP 276  
9  X=E4  
   CALL SUB600  
   CALL SUB800
ETE=RO/R0  
PS=PSI(ETE,TEMPTUR)  
IF (15 . EQ. 0) PS = 1.  
   PO=FNZR2*TO/RQB*Y5/Y*1.722*PS  
   IF (K81G. GT. 0) GO TO 20  
P1=PO
20 CONTINUE  
R5=AO*R2  
R6=AO*R  
R7=R2/R  
R8=1.+R5  
Z5=FNZR2/Z  
B1=ALOG(R8)  
V1=(Z5/R6**2)*(1./R8+B1-1.)  
V2=Z5**2*R7**3*(R7**2*.1-A1*.33333)  
V3=.4*R6/R8**5  
V4=Z5/R6**2
V4 = V4'((-3*R5**3+9.*R5**2+18.*R5+8.)/(6.*R8**3)-4./3.+ B1)
V5 = (-A1**2337/X)**X
V6 = (Z10/2.)*R7**2+(2.*R6/3.)*(-1./R8**3)
V7 = (Z5**5.)*(1.-R7**2)
V8 = 1.-R7**2*(5.-5.*R7+.1*R7**3)
VO = Z**2*(V1+V2+V3+V4+V5+V6+V7)-FNZR2**2*V8
UO = (39.383*VO)/(R*A)*PS
IF(KKK,GT.0) GO TO 30
U1 = 1.5*(P1/RO)+UO*.5
IF(15.EQ.1) GO TO 25
P2 = P1
U = U1
GO TO 35
25 TO = .01
KKK = 1
GO TO 15
30 U1 = 1.5*(PO/RO)+UO*.5
P2 = P1-PO
U = U1-U
35 RETURN
C
10 FORMAT (* LOW TEMP. LOW DENSITY-ACCURACY*)
11 FORMAT (* DISCONTINUOUS POTENTIAL POSSIBLE*)
12 FORMAT (* NO UNIQUE SOL. CAN BE FOUND*)
13 FORMAT (* SEE LINE 214*)
END
FUNCTION FNI (S)
COMMON /BLK/ A0,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,RO
CALCULATES INNER JOIN RADIUS OF ELECTRONIC POTENTIAL
C
X1 = S/R
A1 = (Z/FNZR2)*(R/R2/(1. + AO*R2)**2)- R/R2+ 1. 5
FN1 = 27. 2*Z/R
FN1 = FN1*(1./X1)*(1./AO* R*X1)**2)
FN1 = FN1+ 27. 2*FNZR2*(X1**2/2.- A1)/R
RETURN
END
SUBROUTINE SUB600
COMMON /BLK/ A0,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,RO
CALCULATES THE FERMI DIRAC INTEGRAL OF ORDER 1/2
C
IF(X .LE. 4.) GO TO 2
Y = 666667*SQRT(X)*X
Y1 = (1.+1.2337/X**2+1.06541/X**4)
IF (X.GT.1.E+6) GO TO 1
Y1 = Y1+ 9.70152/X**6
1 Y = Y*Y1
RETURN
2 IF (X .GE. -2.) GO TO 3
W1=EXP(X)
W2=W1*W1
Y=W1*(- 886227-. 2852038*W1 + . 17055438*W2)
RETURN
3 T=(X+2.)/6.
Q1=3.09954*T
Y=. 115137+ 5.66425*T
Y=Y+ (T-1.)*T*(6.46229-1. 4536*EXP(-Q1))
RETURN
END
FUNCTION FNO (S)
COMMON /BLK/ AOJU,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
N,QN,Q
N3,T01,Q3(7),RQB,T032,1TRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,R0
CALCULATES OUTER IONIC RADIUS OF ELECTRONIC POTENTIAL
X1 = S/R
FNO=(27.2*FNZR2/R)*(1./X1+ X1**2/2.- 1.5)
RETURN
END
SUBROUTINE SUB800
COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
N3,T01,Q3(7),RQB,T032,1TRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,R0
CALCULATES THE FERMI DIRAC INTEGRAL OF ORDER 3/2
IF(X .LT. 4.) GO TO 1
X5=SQRT(X)*(.4*X**2+ 2.467401-. 7102746/X**2)
Y5=Y5- SQRT(X)**2.771862/X**4
RETURN
1 IF (X. GT. -2.) GO TO 2
X5=EXP(X)
X6=X5*X5
Y5=1. 32934*X5
Y5=Y5*(1.- .176777*X5+. 06415*X6)
RETURN
2 T=(X+2.)*. 166667
Q1=3.09954*T
Y5=. 115137*T+ 5.66425/2.*T**2
Y6=EXP(-Q1)
Y7=6.46229*T**2*(T*. 333333-. 5)+ Y5
Y5=(2.- Y6*(Q1**2+ 2.*Q1+ 2.))*0.03358213
Y5=Y5-(1.- Y6*(Q1+ 1.))*1. 0408916
Y5=1.4536*Y5
Y5=(Y5+ Y7)*6. + . 11720928
Y5=Y5*1.5
RETURN
END
SUBROUTINE SUB1100
COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,R0

C
C THIS SUBROUTINE DOES THE INTEGRATION OF THE ELECTRONIC POTENTIAL
C USING QUADRATURE FORMULAS

S1 = 0.
IF (N. LT. 2) GO TO 4
DO 3 J=2,N
   S=Q(J)/Z9
   IF (.73*S/R2.GT.1.) GO TO 1
   X=FNI(.73*S)*TO1+ E3
   GO TO 2
1   X=FNO(.73*S)*TO1+ E3
2   CALL SUB600
   S1=S1+ Y*(Q3(J)- Q3(J-1))/Z
3   CONTINUE
4   CONTINUE
   GO TO (5,10), ITRAN
5   CONTINUE
C
R 16 (LOW DENSITY CASE)
S=(16. + .46*(Z10-16.)*.5)*Z11
S9=(16. + (Z10-16.)*.5)*Z11
IF (S/R2.LT.1.) GO TO 6
   X=FNO(S)*TO1+ E3
   CALL SUB600
   GO TO 7
6   X=FNI(S)*TO1+ E3
   CALL SUB600
   S1=S1+ Y*(S9**3- Q3(N)/Z)
   S=(S9+ .46*(R-16.)*Z11)*.5
   IF (S/R2.LT.1.) GO TO 8
   X=FNO(S)*TO1+ E3
   CALL SUB600
   GO TO 9
8   X=FNI(S)*TO1+ E3
   CALL SUB600
   S1=S1+ Y*(RQB- S9**3)
   GO TO 14
10  IF (J1.LT.3) GO TO 15
   S=(Q(N)+ (Z10- Q(N))*.46)*Z11
11  IF (S/R2.LT.1.) GO TO 12
   X=FNO(S)*TO1+ E3
   CALL SUB600
   GO TO 13
12  X=FNI(S)*TO1+ E3
   CALL SUB600
13  S1=S1+ Y*(RQB- Q3(N)/Z)
   S1=S1/3.
14  S2=S1*1.2693229E-2*TO32
   RETURN
15  S=.73*R
GO TO 11
END

SUBROUTINE SUB400
COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,R0

C FINDS ETA GIVEN THE FERMI DIRAC INTEGRAL OF ORDER 1/2 FROM AN
C APPROXIMATION FORMULA
C
IF(F1 . LT. 5.77939) GO TO 3
E4=1.5*F1**.666667
X=E4
CALL SUB600
F2=F1-Y
IF (ABS(F2/F1). LT. 1. E-10) GO TO 2
F3=1.-.4112335/X**2-1.7756865/X**4
F3=F3-29.1045555/X**6
F3=-F3*SQRT(X)
E4=E4-F2/F3
GO TO 1
2 E4=X
RETURN
3 IF (F1.GT.115137) GO TO 6
E4=1.128379186*F1
4 E5=E4*E4
E2=.886226925*E4*(1.-.321818*E4+.19245*E5)
F2=F1-E2
IF (ABS(F2/F1). LT. 1. E-10) GO TO 5
F3=-.886226925*(1.-.643636*E4+.57735*E5)
E4=E4-F2/F3
GO TO 4
5 E4=ALOG(E4)
RETURN
6 T=.9999
7 X=6.*T-2.
CALL SUB600
F2=Y
F2=F1-F2
IF (ABS(F2/F1). LT. 1. E-10) GO TO 8
W=EXP(-3.09954*T)
F3=.66425+T*(T-1.)*1.4536*3.09954*W
F3-=F3-(2.*T-1.)*(6.46229-1.4536*W)
T=T-F2/F3
GO TO 7
8 E4=6.*T-2.
RETURN
FUNCTION PSI(E,T0)
COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2
COMMON ATMWT,ATMNO,H4,GAMMA,R0

C
C CALCULATES THE MODIFICATION FUNCTION FOR THE ELECTRONIC PRESSURE, ETC. TO COMPENSATE FOR THERMAL EFFECTS AND MODEL PROBLEMS

C

IF(E .LT. 1.) GO TO 1
DEBYE = H4*EXP((GAMMA/E - (3. *E-1.)/(3. *E**2))*(E-1.))*E**.6666667
GO TO 10
1 IF(E .GT. 1. - E-10) GO TO 5
T = H4*EXP(1.5 - 2. *GAMMA)
SI = .018596*(R0/ATMW)***(2./3.)*T0*T/((ATMW)**(4./3.))
GO TO 15
5 DEBYE = H4*E*EXP(((3. *GAMMA-2.)+.5*(1. - 2. *GAMMA)*E)/E**2)
SI = .018596*(T0/DEBYE)**(2.)*E*R0/ATMW
GO TO 20
EXT = (10. - 10.)/(1. + SI)/T0
IF(EXT . LT. 700. ) GO TO 20
PSI = 0.
GO TO 25
20 PSI = .2./(1. + EXP(EXT))
25 RETURN

END

SUBROUTINE COLD(ESAVE,PCOLD,PPCOLD,ECOLD,EPCOLD)

COMMON /BLK/ AO,A1 ,E3,E4,Fl,R,R2,S2,T0,X,Y,Z,Z9,Z10,Q(8),l,N,Q

COMMON ATMWT,TMN0,H4,GAMMA,RO

COMMON ECMAT(200),ETAMAT(200),A,B1,B2,C1,C2,C3,C5,C4,DI,AK,

C FOR A SPECIFIC TEMPERATURE AND DENSITY, THE SUBROUTINE FINDS THE T=0 PRESSURE AND INTERNAL ENERGY
C

TH = 1./3.
TI = 2./3.
E = R0*ESAVE/RCOLD
IF(E .LT. 1.) GO TO 5
E1 = 1. - 1./E**TH
E2 = EXP(E1*B1)
E3 = EXP(E1*B2)
PCOLD = A*(E**E**TI*E2 - E**TI*E3)
PPCOLD = A*(G1 - G2)
G3 = (E**TI - B1*E**TH)*E2 - B1**2*EXP(B1)*(EPIN(B1) - EPIN(E1/E**TH))
G4 = G3 + B1 - 1. + 2. /B2*(1. - E3)
ECOLD = 1.5*A*G4/R0
GO TO 21
5 IF(E .LT. D1) GO TO 10
E1 = 1. - E**TH
E2 = E**TH - D1**TH
G3 = C2 + E2*(C3 - E1*(C4 - C5*E1))
PPCOLD = -E**E**TH*E1*(C1 + E2*G3)
G3 = E3*E2**2 - 2. *E**TI*E1*E2

RETURN

END
G2 = E3*E2 - E**TI*E1
PPCOLD = (C1*E3 + C2*G2 + C3*G3 + C4*G4 + C5*G5)/3.
GO TO 20
10 PPCOLD = P0*(AK+2. - (AK+1.)*E/D1)**(AK+1.)
PPCOLD = P0*(AK+1.)*(AK+ 2.)/(E/D1)**AK - (E/D1)**(AK+ 1.)
20 ECOLD = 0.
21 CONTINUE
IF(E .GT . 1.) GO TO 50
IF(E .LT. D1) GO TO 40
IF(E .GT. ETAMAT(I)) GO TO 30
DO 25 I = 2,200
IF(E .GT. ETAMAT(I)) GO TO 35
CONTINUE
25 CONTINUE
30 ECOLD = ECMAT(I)*(E - ETAMAT(I))/(AK + 1. - ETAMAT(I))/R0
GO TO 50
35 ECOLD = (ECMAT(I) + (E - ETAMAT(I))*ECMAT(I) - ECMAT(I-1))/
1 (ETAMAT(I-1) - ETAMAT(I))/R0
GO TO 50
40 ECOLD = (ECMAT(200) + P0*((AK+2.)*(E/D1)**AK - AK*(E/D1)**(AK+1.))
1 - 2.)/(D1*AK))/R0
50 RETURN
50 RETURN
END
SUBROUTINE PDPCAL(T0,E,PRES,pREsp,pREspp,15)
COMMON /BLK/ AO,A1,E3,E4,F1,R2,S2,T0,x,y, Zz9,z10,Q(8)J 1,N,QN,Q
COMMON ATMWT,ATMN0,H4,GAMMA,R0
COMMON ECMAT(200),ETAMAT( 200),A,B1 ,B2, Cl ,C2,C3,C5 ,C4J31 AK,
EREF,TREF,SAVE( 50), PO,THETIN,RHOIN,PTOT, ETOT,RCOLD
DIMENSION AP(20),P(3,3),RP( 3),D(3),TEMP(3),IROW(3)
C FINDS THE FIRST AND SECOND DERIVATIVES OF THE PRESSURE WITH
C RESPECT TO DENSITY AT A CONSTANT TEMPERATURE
C
PRESSPP = 0.
IF(I5 . EQ. 0) GO TO 5
IF(T0 . NE. TREF) GO TO 1
IF(ABS((E- EREF)/E) . LT. . 07) GO TO 5
1 11=1
TREF = T0
EREF = E
DO 3 I = 1,3
AI = I
EP = E*(1. + (AI-2.)*.07)
P(I,1) = 1.
P(I,2) = EP
P(I,3) = EP**2
DO 2 J = 1,2
AJ = J
B = EP*(1. + (AJ - 1.5)*.001)*R0
CALL EOS(I,B,T0,AP(I1),ETOT)
2 II = II + 1
\[ \text{IPRES} = 0 \]

\[ \text{B} = 0.9653/\text{ATMW} \]

\[ \text{IF}(\text{E} < 1.) \text{ GO TO 1} \]

\[ \text{GAMP} = \text{GAMMA}/\text{E} + 0.6666667*(\text{E} - 1.)/\text{E}^2 \]

\[ \text{GAMPP} = 4.0*\text{E} - 1.)/(3.*\text{E}^3) \]

\[ \text{DEBYE} = \text{H}^4*\text{EXP}(\text{GAMMA}/\text{E} - (3.*\text{E} - 1.))/(3.*\text{E}^2)*\text{E}^2 \]

\[ \text{DEBYEP} = 2.0*\text{DEBYE}/(3.*\text{E} + \text{E}^2) \]

\[ \text{ET} = 1.5*\text{B}^2*\text{T} \]

\[ \text{ETP} = 0. \]

\[ \text{PT} = \text{R}^0*\text{E}^2*\text{T}^2 \]

\[ \text{T} = \text{H}^4*\text{EXP}(1.5 - 2.*\text{GAMMA}) \]

\[ \text{SI} = 0.018596*(\text{R}^0/\text{ATMW})*(2.*\text{T} + 3.*)/\text{ATMW}^2*\text{E}^4/(4.*\text{R}^0) \]

\[ \text{ST} = -\text{B}^2/\text{ALOG}(0.018596*T0/\text{ATMW})^2+1.5*R^0/E/\text{ATMW}/T0^2*3 - 2.5*T0 \]

\[ \text{STP} = -\text{B}/\text{E}^2 \]

\[ \text{GO TO 20} \]

\[ \text{G5} = \text{GAMMA} - 1. \]

\[ \text{G6} = 1. - 2.*\text{GAMMA} \]

\[ \text{GAMP} = \text{E}^2*(\text{G5} + \text{G6}^2) \]

\[ \text{GAMPP} = \text{G5}^2 + \text{G6}^2*2.0*\text{E} - 1. \]

\[ \text{DEBYE} = \text{H}^4*\text{EXP}(3.*\text{GAMMA}-2.*E+1.)*\text{E}^2 \]

\[ \text{DEBYEP} = \text{DEBYE}/\text{E} + \text{DEBYE}^2*(3.*\text{GAMMA} - 2. + \text{E}^2/\text{E}^2) \]

\[ \text{SI} = 0.018596*T0/\text{DEBYE}^2*2.0*(\text{R}^0/\text{ATMW})^4*6666667/\text{ATMW} \]

\[ \text{DO 1,3} \]

\[ \text{AI} = 1 \]

\[ \text{EP} = \text{E}^{1.*\text{AI} - 2.0} \]

\[ \text{CALL PTHERM} \]

\[ \text{CALL COLD} \]

\[ \text{CALL EOS} \]

\[ \text{IF}(\text{I5} = 0) \text{ GO TO 7} \]

\[ \text{PRESPP} = \text{D}^2 + \text{E}^2*\text{D}^3 + \text{D}^4 \]

\[ \text{PRES} = \text{D}^5 \]

\[ \text{RETURN} \]

\[ \text{END} \]
\[ W = 2 \cdot \frac{S_1}{(3 \cdot E)} - 2 \cdot \frac{S_1 \cdot \text{DEBYEP/DEBYE}}{(1 + S_1)(2 + S_1)} \]

\[ ET = 1.5 \cdot B \cdot T_0 \cdot \frac{(2 + S_1)}{(1 + S_1)} \]

\[ ETP = -ET \cdot W / (1 + S_1)^2 \]

\[ PT = R_0 \cdot B \cdot T_0 \cdot (3 + \text{GAMP} + S_1) / (1 + S_1) \]

\[ PTP = PT / E - PT \cdot W / (1 + S_1) + PT \cdot (3 \cdot \text{GAMP} + W) / (3 + S_1) \]

\[ ST = T_0 \cdot B \cdot (3 \cdot \text{ALOG(DEBYE/T0)} - 4 + 1.5 \cdot \text{ALOG}(1 + S_1) + 1.5 \cdot \frac{S_1}{(1 + S_1)^2}) \]

\[ STP = -B \cdot \frac{(3 \cdot \text{DEBYEP/DEBYE} + 3 \cdot \frac{W}{(1 + S_1)} - 3 \cdot \frac{S_1 \cdot W}{2 \cdot (1 + S_1)^2})}{V} \]

\[ \text{IF}(\text{IPRES} \cdot \text{GT} \cdot 0) \text{ GO TO 30} \]

\[ \text{IPRES} = \text{IPRES} + 1 \]

\[ S_1 = S_1 \]

\[ ET_1 = ET \]

\[ PT_1 = PT \]

\[ ST_1 = ST \]

\[ ETP_1 = ETP \]

\[ PTP_1 = PTP \]

\[ STP_1 = STP \]

\[ T_1 = T_0 \]

\[ T_0 = .01 \]

\[ \text{GO TO 2} \]

\[ \text{IF}(\text{IPRES} \cdot \text{GT} \cdot 0) \text{ GO TO 30} \]

\[ \text{RETURN} \]

\[ \text{END} \]

\[ \text{SUBROUTINE COLCOF(S,C0,PUPPER,U)} \]

\[ \text{COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,T0,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q} \]

\[ \text{COMMON ATMWT,ATMNO,H4,GMMA,R0} \]

\[ \text{COMMON ECMAT(200),ETAMAT(200),A,B1,B2, C1,C2,C3,C5,C4,D1,AK,} \]

\[ \text{EREF,TREF,SAVE(30), P0,THETIN,RHOIN,PTOT,ETOT,RCOLD} \]

\[ \text{DIMENSION R(3),P(3,3),D(3),TEMP(3),IROW(3),PTEST(10),ETEST(10)} \]

\[ \text{EQUIVALENCE (ECMAT,TEMP),(ETAMAT,IROW)} \]

\[ \text{SETS UP THE CONSTANTS FOR THE T=0 CURVE (MODIFIED TO TAKE INTO} \]

\[ \text{ACCOUNT LOW TEMPERATURE CONTRIBUTIONS)} \]

\[ D1 = S/(S+1.) \]

\[ RCOLD = R0 \]

\[ RSAVE = R0 \]

\[ PSAVE = P0 \]

\[ NTRY = 1 \]

\[ R0 = RCOLD \]

\[ A0 = PUPPER \]

\[ B0 = 0.01 \cdot R0 \cdot C0 \cdot 2 \]

\[ D0 = .02 \cdot R0 \cdot C0 \cdot 2 \cdot (2 \cdot S - 1.) \]

\[ THIRD = 1./3. \]

\[ TTHIRD = 2. \cdot THIRD \]
C******** PRESSURE CALCULATION FOR ETA GT. 1 **********

A = B0
B1 = 1.25 * ALOG(A0/(3100. * B0))
B2 = B1
DO 5 J = 1, 100
P(1,1) = 3125. * EXP(.8 * B1) - 25. * EXP(.8 * B2)
RP(1) = A0 - P(1,1)*A
RP(2) = B0 - P(2,1)*A
RP(3) = D0 - P(3,1)*A
IF (ABS(RP(1)/A0) . GT. .00001 ) GO TO 1
IF (ABS(RP(2)/B0) . GT. .00001) GO TO 1
IF (ABS(RP(3)/D0) . LE. .00001) GO TO 15
P(1,2) = 2500. * A* EXP(.8*B1)
P(2,2) = A/3.
P(3,2) = A*(TTHIRD + 2.*B1/9.)
P(1,3) = -20.*A* EXP(.8*B2)
P(2,3) = -A/3.
CALL MATINV(P,3,1,ROW,TEMP)
CALL MATMPY(3,3,1,P,3,Rp,3,D,3)
A = A + D(1)
B1 = B1 + D(2)
5 B2 = B2 + D(3)
WRITE (9,10)
FORMAT(3X,*HAVE DONE 100 ITERATIONS, CAN NOT CONVERGE*)
GO TO 50
15 GAMMA = (D0 + TTHIRD * B0)/(2.* B0) - 3333333333
B = R0*D1
CALL EOS(1,B,.02,DELPE,DELPE)
CALL PTHERM(D1,.02,PT,PTP,ET,ETP,ST,STP,SI)
DELPEP = DELPE + PT
P0 = PSAVE - DELPEP
R0 = RSAVE
CALL EOS(1,RSAVE,.02,DELPE,DELPE)
CALL PTHERM(1,.02,PT,PTP,ET,ETP,ST,STP,SI)
DELPEP = DELPE + PT
R0 = RCOLD
C******** PRESSURE CALCULATION FOR S/(S+1) LT. ETA LT. 1 **********

D2 = 1. - D1**THIRD
C1 = - P0/(D1*D1**THIRD*D2)
C2 = C1**5. *D1**THIRD - 4.)/(D1**THIRD*D2)
C3 = (3.*B0 - C1 - C2**D2)/D2**2
C4 = G1/(2.*D2**2)
C******** PRESSURE CALCULATION FOR ETA LT. S/(S+1) **********
ETEST(I) = E
IF(- PTEST(I) . LT. DELPEP) GO TO 100
ITRY = I
GO TO 106
100 E = E - .005
PRINT 104
104 FORMAT(* DID NOT BRACKET CROSSPOINT*)
STOP
106 ETA = ETEST(ITRY) + (ETEST(ITRY-1) - ETEST(ITRY)) * (- PTEST(ITRY) - DELPEP)
RCOLD = R0/ETA
GO TO 2
105 E = RSAVE/R0
CALL COLD(E,PCOLD,PPCOLD,ECOLD,EPCOLD)
IF(ABS(PCOLD+DELPEP)/DELPEP) . LT. 1.E-6) GO TO 150
RCOLD = RSAVE*RCOLD/(RSAVE-RCOLD*(PCOLD+DELPEP)/PPCOLD)
GO TO 2
150 F = 0.
G1 = (1. - D1)/800.
D2 = 1.
DO 25 I = 1,200
DO 20 J = 1,4
AJ = J
E = D2 - G1*AJ
E1 = 1. - E**THIRD
E2 = E**THIRD - D1**THIRD
IF(E . NE. 0) GO TO 19
ECMAT(I) = F
ETAMAT(I) = E
GO TO 25
19 T1 = E1*(C1 + E2*(C2 + E2*(C3 - E1*(C4 - C5*E1))))
20 F = F + G1*T1/E**THIRD
ECMAT(I) = F - G1*T1/(2.*E**THIRD)
ETAMAT(I) = E
25 D2 = E
AK = -2.*PO/(D1*(R0*U - ECMAT(200)))
PAK = R0*U - ECMAT(200)
D2 = D1/400.
DO 30 I = 1,1400
AJ = I
E = D2*AJ
T1 = PO*(AK+2.-(AK+1.)*E/D1)*(E/D1)**(AK+1.)/E**2
30 F = F - T1*D2
UINT = (F + T1*D2/2.)/R0
IF(ABS(U - UINT)/U) . GT. .001) WRITE(9,31) U,UINT
31 FORMAT(3X,*THE COHESIVE ENERGY *,E13.6,*DOES NOT AGREE WELL WITH
1 THE CALCULATED ENERGY *,E13.6)
50 R0 = RSAVE
RETURN
END
SUBROUTINE PGCAL(I5,EP,T0,PTOTA,PPTOT,ETOTA,GTOT,GPTOT)
COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2
COMMON ATMWT, ATMNO, H4, GAMMA, R0
COMMON ECMAT(200), ETAMAT(200), A, B1, B2, C1, C2, C3, C5, C4, D1, AK,
DIMENSION AP(5)

1 EREF, TREF, SAVE(50), P0, THETIN, ROHIN, PTOT, ETOT, RCOLD

CALCULATES THE PRESSURE, INTERNAL ENERGY, AND GIBBS FREE ENERGY
AND FIRST DERIVATIVE WITH RESPECT TO DENSITY OF ABOVE FOR INPUT
TEMPERATURES AND DENSITIES

IF(I5 . EQ. 0) GO TO 11
DO 10 I = 1, 2
AI = I
B = EP*(1. + (AI - 1.5)*.001)*R0
CALL EOS(0, B, .01, PLOWER, ELOWER)
GUN = 0.
GUN = FNZR2*E4*.01
2 CALL EOS(0, B, T0, PUPPER, EUPPER)
E = B/R0
F = PSI(E, T0)
AP(I) = (PUPPER - PLOWER) . F
AP(I + 2) = - (FNZR2*E4*T0 - GUN)*F
10 AP(I + 2) = - (FNZR2*E4*T0 - GUN)*F
11 B = EP*R0
CALL PTERM(E, T0, PT, PTP, ET, ETP, ST, STP, SI)
CALL COLD(E, PCOLD, PPCOLD, ECOLD, EPCOLD)
CALL EOS(1, B, T0, DELPE, DELEE)
PTOTA = PT + PCOLD + DELPE
PPTOT = PTP + PPCOLD + (AP(2) - AP(1))/(.001*EP)
ETOTA = ET + ECOLD + DELEE
GTOT = ET + ECOLD - ST + (PT + PCOLD)/(RO*EP) + (AP(4) + AP(3))/2.*.9653/ATMWT
GPTOT = ETP - STP - PT/(RO*EP**2) + (PTP + PPCOLD)/(RO*EP) + (AP(4) -
1 AP(3))/(.001*EP)**.9653/ATMWT
RETURN

FUNCTION EPIN(AX)
DIMENSION MESG(6)
DATA P0/1. O, P1/0. 16515516520352, P2/0. 23785541396286, 1/
1 P3/0. 92333053076239, 3, P4/0. 9713386753293E-5, /
2 Q0/1. O, Q1/0. 4151551652034, Q2/0. 72018777145175E-1, /
3 Q3/0. 6280515599224, E-2, Q4/0. 23666563141677, 3, (MESG(I), I = 1, 6)/
4 48HE1(X). X. LE. 0. NOT ALLOWED RESULT=LARGEST NUMBER/, 
5 OMEGA/1. E256/

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA

EXPLA
RETURN

30 E1 = GAMMA(0., X)
EPIN = E1
RETURN
END