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Low-Temperature Equation of State for Metals



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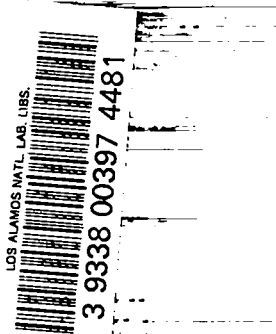


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Low-Temperature Equation of State for Metals

by

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



LOW-TEMPERATURE EQUATION OF STATE FOR METALS

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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

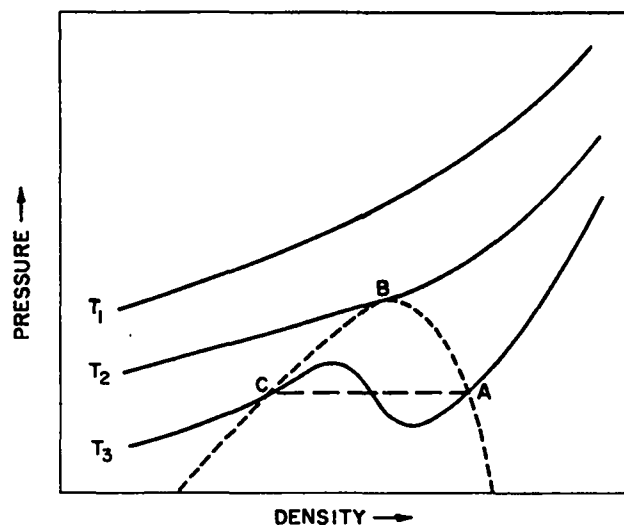


Fig. 1. Typical P-V diagram showing location of mixed-phase region.

the $T = 0$ calculation, resulted in the actual isotherm T_3 . By thermodynamic considerations, the stable path of the system through the mixed-phase region 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 effects. Obtaining the pressure and energy from the $T = 0$ curve is therefore the first step. The pressure 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_0 is the ultimate tensile strength, S and C_0 are obtained from the Hugoniot shock relationship shown in Eq. (1), and $P_c(125)$ comes from a Thomas-Fermi calculation.

$$U_s = C_0 + S \cdot U_p \quad (1)$$

and

$$\delta = S/(1 + S) \quad (2)$$

TABLE I

$T = 0$ ISOTHERM BOUNDARY CONDITIONS

Physical Constraints	Region		
	I	II	III
$P_c(125) = P_{TF}(125)$	x		
$P_c(1) = 0$	x	x	
$P'_c(1) = P'_H(1) = 0.01\rho_0 C_0^2$	x	x	
$P''_c(1) = P''_H(1) = 0.02\rho_0 C_0^2(2S - 1)$	x	x	
$P_c(\delta) = -P_0$		x	x
$P'_c(\delta) = 0$		x	x
$P_c(0) = 0$			x
$\int_1^0 P_c/\eta^2 d\eta = \rho_0 E_c$		x	x

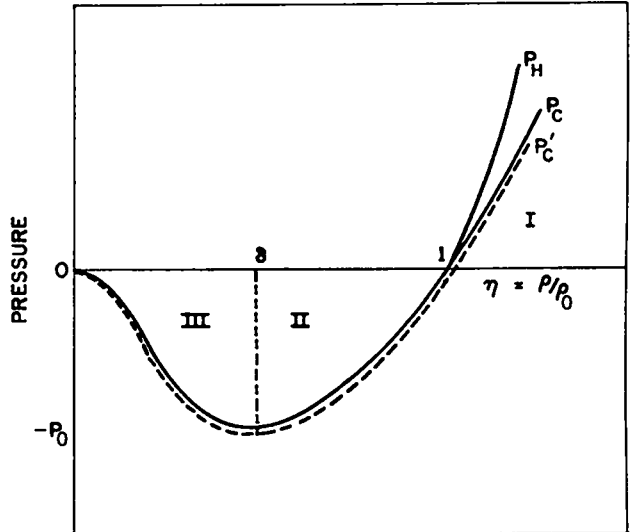


Fig. 2. Illustrative plot of the theoretical $T = 0$ curve P_c and the modified $T = 0$ curve P'_c .

The expression for P_c in region I is similar to the modified pressure function used by Barnes¹ and takes into account the attractive and repulsive nature of the interatomic forces. This formula is given in Eq. (3), where A , B_r , and B_a are derived from the boundary conditions.

$\eta > 1$

$$P_c = A\eta^{2/3} (\eta e^{B_r \eta^\nu} - e^{B_a \eta^\nu}) \quad (3)$$

$$\nu = 1 - \eta^{-1/3}$$

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 encountered in treating it as one region. The resultant equations are

$\delta \leq \eta \leq 1$

$$P_c = \eta^{4/3} (\eta^{1/3} - 1) \left[A + (\eta^{1/3} - \delta^{1/3}) \left[B + (\eta^{1/3} - \delta^{1/3}) \left[C + (\eta^{1/3} - 1) \left[D + (\eta^{1/3} - 1) E \right] \right] \right] \right] \quad (4)$$

and

$$\eta < \delta$$

$$P_c = P_o [K + 2 - (K + 1)\eta/\delta] (\eta/\delta)^{(K+1)} \quad (5)$$

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

$$\frac{1}{\rho_o} \int_1^x \frac{P_c}{\eta^2} d\eta = E_{cold} \quad (6)$$

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),

$$P_H = (P_c - \rho_o \gamma \eta E_c) / (1 - \gamma(\eta - 1)/2) \quad (7)$$

where γ is the Gruneisen ratio and is obtained from

$$\gamma = -\frac{1}{3} + \frac{1}{2} \frac{\eta^2 P_c'' + 2/3 \eta P_c' - 2/9 P_c}{\eta P_c' - 2/3 P_c} \quad (8)$$

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.

$$F_n = N_o kT [3\ln(\theta/T) - 1 + 1.5\ln(1 + \Psi)] \quad (9)$$

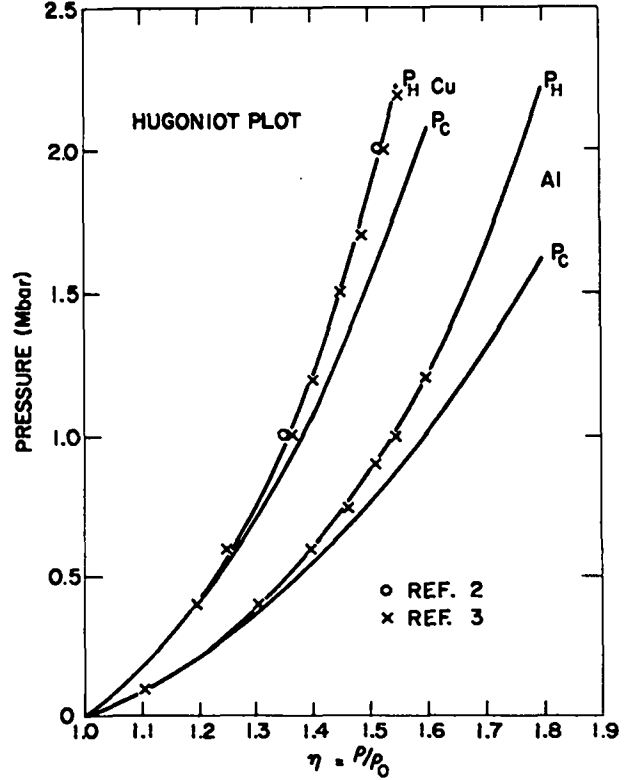


Fig. 3. Comparison of experimental and theoretical Hugoniot curves.

$$P_n = \rho N_o kT \left[\frac{3\Gamma + \Psi}{1 + \Psi} \right] \quad (10)$$

$$E_n = 1.5 N_o kT \left[\frac{2 + \Psi}{1 + \Psi} \right] \quad (11)$$

$$S_n = -N_o k [3\ln(\theta/T) - 4 + 1.5\ln(1 + \Psi) + 1.5\Psi/(1 + \Psi)] \quad (12)$$

and

$$\Psi = F(\rho, T)$$

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 . θ is the Debye temperature and Γ is the Gruneisen ratio, both functions of density. Ψ 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 Ψ 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

$$0 < r < r_1$$

$$V(r) = Ze/(1 + \alpha r)^2/r + Z^*e(r^2/2R^2 - B_0)/R \quad (13)$$

$$B_0 = (Z/Z^*)(R/r_1)/(1 + \alpha r_1)^2 - R/r_1 + 1.5 \quad (14)$$

$$\alpha = 0.6057 Z^{1/3} \quad , \quad (15)$$

and

$$r_1 < r < R$$

$$V(r) = Z^*e(R/r + r^2/2R^2 - 1.5)/R \quad . \quad (16)$$

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

TABLE II

REPRESENTATIVE VALUES OF INTERPOLATION FUNCTION

$\eta = \rho/\rho_0$	Ψ
0.05	137.01
0.1	40.88
0.2	9.50
0.3	3.70
0.4	1.489
0.5	0.7459
0.6	0.4135
0.7	0.2494
0.8	0.1621

Fermi-Dirac statistics for the electronic distribution. With this information, P_{el} and E_{el} can be found with the equations

$$P_{el} = (2/3\rho) \left(I_{3/2}(\mu)/I_{1/2}(\mu) \right) kT \quad , \quad (17)$$

$$E_{el} = (3P_e/\rho + E_S/2) \quad . \quad (18)$$

The electronic Gibbs free energy is

$$G_{el} = -\mu N \quad . \quad (19)$$

$I_{1/2}$ 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 μ 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

$$\begin{aligned} P_{Tot}(T) &= P_{el} + P_N + P_C \\ &= P_C + [P_{el}(T) - P_{el}(0.01)] \\ &\quad + [P_N(T) - P_N(0.01)] \quad . \quad (20) \end{aligned}$$

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_{c_0}) 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

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

$$G(T, \rho) = 2 / \left[1 + \exp \left(\frac{(10 - 10/(1 + \psi))}{T} \right) \right] , \quad (21)$$

which reduces the electronic EOS below 5.0 eV. ψ 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

$$P_{el} = G(T, \rho) [P_{el}(T) - P_{el}(0.01)] \quad (22)$$

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.

$$P_{Tot} = P_c + [P_N(T) - P_N(0.01)] + G(T, \rho) [P_{el}(T) - P_{el}(0.01)] \quad (23)$$

$$G_{Tot} = E_c + [E_N(T) - E_N(0.01)] + \left[P_c + (P_N(T) - P_N(0.01)) \right] / \rho - [T S_N(T) - 0.01 S_N(0.01)] + G(T, \rho) [G_{el}(T) - G_{el}(0.01)] \quad (24)$$

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.

$$\begin{pmatrix} P(\eta_2) - P(\eta_1) \\ G(\eta_2) - G(\eta_1) \end{pmatrix} = \begin{pmatrix} \partial P_1 / \partial \eta_1 & - \partial P_2 / \partial \eta_2 \\ \partial G_1 / \partial \eta_1 & - \partial G_2 / \partial \eta_2 \end{pmatrix} \begin{pmatrix} \Delta \eta_1 \\ \Delta \eta_2 \end{pmatrix} \quad (25)$$

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.

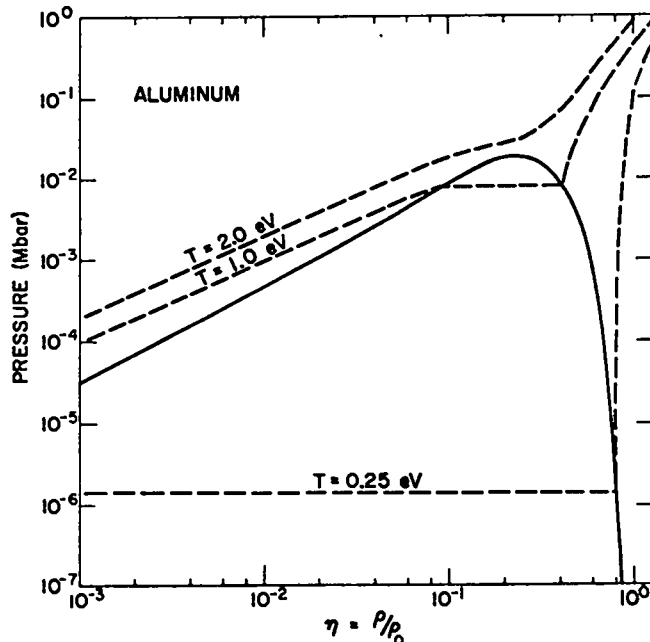


Fig. 4. Detailed plot of aluminum mixed-phase region and representative isotherms.

TABLE III
CRITICAL POINT PARAMETER COMPARISON

Element	LTEOS	Thompson ^{4,7}	Grosse ⁸	Adler & Young ⁶	Experimental ^b Results
Lithium	$T_c = 0.5351$ eV		0.3541	0.3301	0.2777 ± 0.052
	$P_c = 0.00184$ Mbars			0.002422	0.000689 ± 0.00014
	$\rho_c = 0.071$ gcm ⁻³			0.1470	0.1148 ± 0.0332
Beryllium	$T_c = 0.919$	0.785			
	$P_c = 0.0330$	0.0142			
	$\rho_c = 0.577$	0.318			
Sodium	$T_c = 0.5730$		0.2413	0.2270	0.2217 ± 0.03
	$P_c = 0.00202$		0.0004965	0.000921	0.000355 ± 0.00007
	$\rho_c = 0.1947$		0.1796	0.2692	0.2025 ± 0.04
Magnesium	$T_c = 0.7218$		0.3317	0.2937	
	$P_c = 0.0680$		0.00175	0.001929	
	$\rho_c = 0.7908$		0.4122	0.4615	
Aluminum	$T_c = 1.479$	0.904	0.7367	0.6162	
	$P_c = 0.0188$	0.00616		0.005458	
	$\rho_c = 0.679$	0.478		0.690	
Copper ^a	$T_c = 1.951$		0.7667	0.6570	
	$P_c = 0.0382$			0.0083	
	$\rho_c = 2.323$		1.048	2.318	

^aConverged on critical point, but did not converge on mixed-phase boundary.

^bExtrapolated to critical temperature from experimental data.⁹

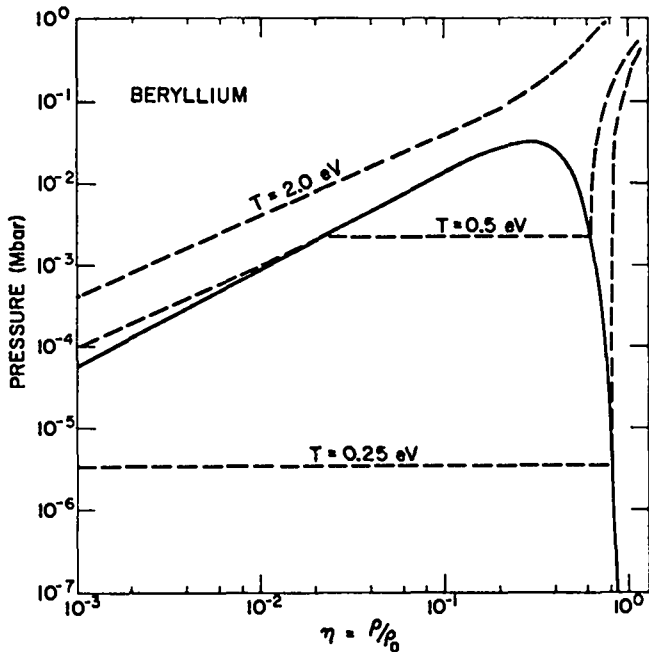


Fig. 5. Detailed plot of beryllium mixed-phase region and representative isotherms.

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APPENDIX A

SAMPLE CALCULATIONS FOR BERYLLIUM

INPUT FORMAT FOR LTEOS CODE

Column	Symbol	Identification
1-10	ATMNO	Atomic number of element
11-20	ATMWT	Atomic weight of element
21-30	RO	Normal density
31-40	S	Hugoniot S
41-50	CO	Hugoniot C ₀
51-60	PO	Tensile strength
61-70	U	Cohesive energy
71-80	H4	Debye temperature

Card #2 (2I4)

Column	Symbol	Identification
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

ATOMIC NUMBER = 4.00000E+00 NORMAL DENSITY(GM/CM3) = 1.8510CE+CC
 ATOMIC WEIGHT = 9.01300E+00 COLL DENSITY(GM/CM3) = 1.86269E+00
 HLGCAIET S = 1.12400E+00 COHESIVE ENERGY(EV) = 3.6000CE-01
 HLGCAIET CO = 7.97800E+00 TENSILE STRENGTH(MBARS) = 2.68132E-01
 PRESSURE(ETA)=12519MBARS1= 1.61688E+04
 DEBYE TEMPERATURE(EV) = 5.9950CE-02

T = 0 ISOTHERM CALCULATIONS

GRUNEISEN CAPPA = 1.24800E+00
 MINIMUM PRESSURE LOCATION(ETA) = 01 = 5.29190E-01

EQUATION CONSTANTS

ETA LESS THAN 1-----K = 2.08105E+00
 ETA BETWEEN 1 AND 1.-C1 = 3.27719E+00
 C2 = 9.30469E-01
 C3 = 3.22963E+00
 C4 = 1.33117E+01
 C5 = -9.52017E-01
 ETA GREATER THAN 1-----A = 1.06111E+00
 B = 1.98308E+00
 SA = 1.61437E+00

CHEMICAL POINT RESULTS

T-CRIT(EV) = 9.1872229E-01
 P-CRIT(MBARS) = 3.297336AE-02
 ETA-CRIT = 3.1165838E-01

MIXED PHASE BOUNDARY PARAMETERS

TEMPERATURE LEVEL	ETA	PRESSURE MBARS	ENERGY MBAR-CC/GM1	GROSS ENERGY
8.50000E-01	1.69901E-01 4.18183E-01	2.38846E-02 2.38846E-02	4.9C417E-01 3.9F695E-01	-7.7E167E-C1 -7.7E167E-C1
8.00000E-01	1.36211E-01 4.63464E-01	1.91285E-02 1.91286E-02	4.8E863E-01 3.64480E-01	-7.15158E-C1 -7.15158E-C1
7.50000E-01	1.09190E-01 4.95180E-01	1.50191E-02 1.50191E-02	4.81107E-01 3.36358E-01	-6.52694E-01 -6.52694E-C1
7.00000E-01	8.66888E-02 5.20803E-01	1.14631E-02 1.14630E-02	4.74144E-01 3.11048E-01	-5.91027E-01 -5.91027E-01
6.50000E-01	6.95349E-02 5.43805E-01	8.68340E-03 8.68340E-03	4.66471E-01 2.8F833E-01	-5.28294E-01 -5.28294E-01
6.00000E-01	5.09562E-02 5.68792E-01	5.94728E-03 5.94728E-03	4.58289E-01 2.63212E-01	-4.7C15AE-01 -4.7C15AE-01
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4.00000E-01	6.50173E-03 7.05108E-01	5.02442E-04 5.02442E-04	4.24942E-01 1.60163E-01	-2.5C157E-C1 -2.5C157E-01
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3.00000E-01	5.73357E-04 7.87749E-01	3.29620E-05 3.29619E-05	4.08862E-01 1.11225E-01	-1.56172E-C1 -1.56172E-01
2.50000E-01	6.95819E-05 8.29419E-01	3.31060E-06 3.31060E-06	4.00830E-01 8.86467E-02	-1.14614E-01 -1.14614E-01
2.00000E-01	2.49947E-06 8.70076E-01	9.41457E-08 9.41457E-08	3.92797E-01 6.75465E-02	-7.68600E-02 -7.68600E-02
1.50000E-01	6.87346E-09 9.09061E-01	1.90767E-10 1.90767E-10	3.84765E-01 4.86730E-02	-4.4C4C4E-02 -4.4C4C4E-02
1.00000E-01	1.80778E-14 9.45941E-01	3.22543E-16 3.22543E-16	3.76732E-01 3.03235E-02	-1.7F157E-C2 -1.78157E-02
7.50000E-02	1.40992E-20 9.63505E-01	1.81679E-22 1.81679E-22	3.72716E-01 2.16730E-02	-7.7C452E-03 -7.7C452E-03
5.00000E-02	1.71580E-34 9.80462E-01	1.36058E-36 1.36058E-36	3.68700E-01 1.31040E-02	-6.53067E-04 -6.53067E-04

TEMPERATURE = 2.50000E-01

MHC	PRESSURE	ENERGY
1.85100E-03	3.31060E-06	4.00480E-01
9.25500E-03	3.31060E-06	3.78974E-01
1.85100E-02	3.31060E-06	3.97092E-01
9.25500E-02	3.31060E-06	3.87935E-01
1.85100E-01	3.31060E-06	3.63715E-01
9.25500E-01	3.31060E-06	2.12646E-01
1.00000E+00	3.31060E-06	1.97496E-01
1.70000E+00	3.31060E-06	1.56824E-01
1.40000E+00	3.31060E-06	1.16152E-01
1.60000E+00	3.01474E-02	8.45633E-02
1.80000E+00	1.38703E-01	7.83431E-02
1.85000E+00	1.69591E-01	7.79640E-02
1.86000E+00	1.75965E-01	7.79566E-02
1.90000E+00	2.92364E-01	7.81171E-02
2.00000E+00	2.74690E-01	7.97478E-02
2.50000E+00	7.77196E-01	1.18446E-01
3.00000E+00	1.49455E+00	1.70767E-01
5.00000E+00	6.65427E+00	5.68353E-01

TEMPERATURE = 5.00000E-01

MHC	PRESSURE	ENERGY
1.85100E-03	9.71364E-05	4.40992E-01
9.25500E-03	4.85540E-04	4.44097E-01
1.85100E-02	9.71194E-04	4.41033E-01
9.25500E-02	2.26903E-03	4.31310E-01
1.85100E-01	2.26903E-03	4.17362E-01
9.25500E-01	2.26903E-03	2.60780E-01
1.00000E+00	2.26903E-03	2.45528E-01
1.70000E+00	1.47961E-02	2.06932E-01
1.40000E+00	1.01439E-01	1.81074E-01
1.60000E+00	2.04175E-01	1.66524E-01
1.80000E+00	3.27082E-01	1.61128E-01
1.85000E+00	3.53883E-01	1.60888E-01
1.86000E+00	3.60378E-01	1.60906E-01
1.90000E+00	3.87292E-01	1.61160E-01
2.00000E+00	4.61129E-01	1.62971E-01
2.50000E+00	9.70215E-01	1.94038E-01
3.00000E+00	1.71090E+00	2.54353E-01
5.00000E+00	6.95484E+00	6.71438E-01

APPENDIX B

LISTING OF THE LTEOS CODE

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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,AK,
1   EREF,TREF,SAVE(50),  P0,THETIN,RHOIN,PTOT,ETOT,RCOLD
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***** CALCULATES THE MIXED PHASE BOUNDARY *****
6 CALL CRTBND
C***** CALCULATES DESIRED ISOTHERMS OR TEMPERATURE DENSITY POINTS *****
READ (10,1) NTHETA,NRHO
1  FORMAT(2I4)
   IF(NTHETA) 11,6,4
4  READ(10,2)(THETA(I),I=1,NTHETA)
   READ (10,2) (RHO(I),I=1,NRHO)
2  FORMAT(6E12. 5)
   DO 10 I = 1,NTHETA
     PRINT 3,THETA(I)
3  FORMAT(1H1,2X,*TEMPERATURE = *,1PE12. 5//7X,*RHO*,7X,*PRESSURE*,5X,
1  *ENERGY*/)
   THETIN = THETA(I)
   DO 10 J = 1,NRHO
     RHOIN = RHO(J)
     CALL ISOCAL
     PRINT 5,RHOIN,PTOT,ETOT
5  FORMAT(2X,1P10E12. 5)
10 CONTINUE
   GO TO 6
11 STOP
END
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,AK,
1   EREF,TREF,SAVE(50),  P0,THETIN,RHOIN,PTOT,ETOT,RCOLD
DIMENSION GEN(20),C(2,2),AP(2),RP(2),IROW(2),TEMP(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., .05., .005., .0005,
1 ., .1., .2. /
DIMENSION COLDP(12)
DATA COLDP/. 9524., . 96154., . 97087., . 98039., . 990991,1. 0000,1. 0417,1. 087,
1 1. 1364,1. 1905,1. 250,1. 66666/
C
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
C

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C***** SETS UP T=0 CALCULATION *****
200 READ (10,1) ATMNO,ATMWT,R0,S,C0,P0,U,H4
1  FORMAT(8E10.3)
   IF(ATMNO .GT. 25. .AND. ATMNO .LT. 27.) GO TO 990
   IF(ATMWT .EQ. 0) GO TO 1001
   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,RCOLD,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 CO =
4  *,E12.5,* TENSILE STRENGTH(MBARS) = *,E12.5/32X,* PRESSURE(ET
5  A=125)(MBARS)= *,E12.5/32X,* DEBYE TEMPERATURE(EV) = *,E12.5/)
   PRINT 8,GAMMA,D1,AK,C1,C2,C3,C4,C5,A,B1,B2
8  FORMAT(1H0,/*-----
6  /* 22X,*T = 0 ISOTHERM CALCULATIONS*/* GRUNEISEN GAMMA = *,
11PE12.5/* 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 = *,E12.5
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)

C***** START OF CRITICAL POINT SEARCH SECTION *****
   TO = .05
   ESTART = AK*D1/(AK + 1.) + .11*D1
   EREF = 0.
   TREF = 0.
   DELT = 1.
   ITEMP = 8
   IRHO = 8
   DELRHO = GEN(IRHO)
3  S8 = 1.
   CALL PDPCAL(TO,ESTART,PRES,PRESP,S0,1)
   SREF = S0
   IF(S8*SREF .GT. 0) GO TO 6
   ESTART = 1.
   PRINT 5
5  FORMAT(1X,*AM RESTARTING ETA AT 1.* )
   GO TO 3
6  ESTART = ESTART*(1. - DELRHO)
   CALL PDPCAL(TO,ESTART,PRES,PRESP,S0,1)
   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,PRESP,S0,1)
   SREF = S0

```

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29AP72
LTEOS
LTEOS
LTEOS
LTEOS
LTEOS
LTEOS
21AP72
LTEOS
4APR72
LTEOS
LTEOS
4APR72
LTEOS
LTEOS
4APR72
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29AP72
LTEOS

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IF(ABS(SREF) .LT. 1.E-5) GO TO 15	LTEOS
S8 = ABS(SREF)/SREF	LTEOS
DELRHO = S8*ABS(DELRHO/10.)	LTEOS
IF(ABS(DELRHO) .GT. .000001) GO TO 6	LTEOS
PRINT 11,ESTART,PRES,S0	LTEOS
11 FORMAT(1X,*CAN NOT CONVERGE ON ZERO SECOND DERV., ETA =*,1PE12.5,	LTEOS
1 *PRESSURE =*,E12.5,* AND P SEC. DERV. =*,E12.5)	LTEOS
GO TO 1000	LTEOS
15 IF(PRESP .LT. 0) GO TO 20	LTEOS
PRINT 16,ESTART	LTEOS
16 FORMAT(1X,*FIRST DERV. IS POS. AND SEC. DERV. IS NEG. ANT ETA =*,	LTEOS
1 1PE12.5, * RESTART*)	LTEOS
IF(PRESP .LT. 1.E-4) GO TO 40	29AP72
GO TO 1000	LTEOS
20 IF(ABS(PRESP) .LT. 1.E-5) GO TO 40	LTEOS
DO 25 I = 1,2	LTEOS
AI = I	LTEOS
E = ESTART*(1. + (AI - 1.5)*.001)	LTEOS
B = E*R0	LTEOS
CALL EOS(0,B,.01,PLOWER,ELOWER)	LTEOS
25 SAVE(I) = PLOWER	LTEOS
CALL COLD(ESTART,PCOLD,PPCOLD,ECOLD,EPCOLD)	LTEOS
28 PPREF = PRESP	LTEOS
26 TSAVE = T0	LTEOS
T0 = T0 + DELT*T0	LTEOS
CALL PDPCAL(T0,ESTART,PRES,PRESP,S0,0)	29AP72
IF(PRESP .GT. 0) GO TO 30	LTEOS
IF(ABS(PRESP) .LT. 1.E-5) GO TO 35	LTEOS
IF(T0 .LT. 10.) GO TO 28	LTEOS
PRINT 27,T0,ESTART	LTEOS
27 FORMAT(1X,*TEMP. IS TOO LARGE,START AGAIN. T0 = *,1PE12.5,* ETA =*	LTEOS
1 ,E12.5)	LTEOS
GO TO 1000	LTEOS
30 T0 = TSAVE + (T0 - TSAVE)*ABS(PPREF/(PPREF-PRESP))* .95	LTEOS
CALL PDPCAL(T0,ESTART,PRES,PRESP,S0,0)	29AP72
IF(PRESP .GT. 0) GO TO 30	LTEOS
IF(ABS(PRESP) .LT. 1.E-5) GO TO 35	LTEOS
DELT = .01*DELT	LTEOS
IF(DELT .GT. .000001) GO TO 26	LTEOS
PRINT 31,T0,PRESP	LTEOS
31 FORMAT(1X,*CAN NOT CONVERGE ON LOCATION OF ZERO SLOPE*,1PE12.5)	LTEOS
GO TO 1000	LTEOS
35 DELT = GEN(ITEMP)	LTEOS
ITEMP = ITEMP + 1	LTEOS
CALL PDPCAL(T0,ESTART,PRES,PRESP,S0,1)	29AP72
IF(ABS(S0) .LT. 1.E-5) GO TO 40	LTEOS
SREF = S0	LTEOS
S8 = ABS(SREF)/SREF	LTEOS
DELRHO = S8*GEN(IRHO)	LTEOS
IRHO = IRHO + 1	LTEOS
GO TO 6	LTEOS
40 CALL PGCAL(0,ESTART,T0,PCRIT,PPTOT,ECRIT,GTOT,GPTOT)	21AP72
PRINT 41,T0,PCRIT,ESTART	21AP72

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41  FORMAT(1H0,/*-----
1  */22X,*CRITICAL POINT RESULTS*// T-CRIT(EV) = *,1PE15.7/* P-
2  CRIT(MBARS) = *,E15.7/* ETA-CRIT = *,E15.7)
    TCRT = T0
    ETACRT = ESTART
C
C***** START OF MIXED PHASE BOUNDARY CALCULATION *****
C
    ETA1(1) = ETACRT
    ETA2(1) = ETACRT
    PRESS1(1) = PCRT
    PRESS2(1) = PCRT
    ENERG1(1) = ECRIT
    ENERG2(1) = ECRIT
    TSTORE(1) = TCRT
    ITEMP = 2
    PRINT 42
42  FORMAT(1H1,1X,*MIXED PHASE BOUNDARY PARAMATERS*//3X,*TEMPERATURE*,
1  8X,*ETA*,9X,*PRESSURE*,7X,*ENERGY*,5X,*GIBBS ENERGY*/7X,*(EV)*,24X
2  ,*(MBAR)*,5X,*(MBAR-CC/GM)*//)
    ICYCLE = 1
    DELTP = .05
    DELT = .1
    IF(T0 .LE. 1.) DELT = .05
    MTEMP = 10.*T0
    TEM = MTEMP
    T0 = TEM/10.
    IF(TCRT - T0 .LT. DELT) T0 = T0 - DELT
    E = ESTART - .15
    IF(E .LT. 0.) E = .01
    CALL PGCAL(0,E,T0,PTO,PPTOT,ETOT,GTOT,GPTOT)
    DO 45 I = 1,100
    E = E + .01
    CALL PGCAL(0,E,T0,PNEW,PPTOT,ETOT,GTOT,GPTOT)
    IF (PNEW .GT. PTO ) GO TO 45
    SAVE(1) = E - .06
    ELOW = E + .01
    GO TO 46
45  PTO = PNEW
    PRINT 43
43  FORMAT(* FAILED TO FIND STARTING POINT FOR CRITICAL BOUNDARY*)
46  PTO = PNEW
    DO 48 I = 1,100
    E = E + .01
    CALL PGCAL(0,E,T0,PNEW,PPTOT,ETOT,GTOT,GPTOT)
    IF(PNEW .LT. PTO ) GO TO 48
    SAVE(2) = E + .03
    EHIGH = E - .01
    GO TO 50
48  PTO = PNEW
50  CONTINUE
    DO 60 I = 1,50
    S8 = 1.
    DO 55 J = 1,2

```


E = SAVE(J)	LTEOS
CALL PGCAL(1,E,TO,PTOT,PPTOT,ETOT,GTOT,GPTOT)	20APR72
C(2,J) = S8*PPTOT	LTEOS
I1 = 8 + 2*J	LTEOS
SAVE(I1) = PTOT	LTEOS
C(1,J) = S8*GPTOT	20APR72
I3 = 20 + 2*J	LTEOS
I2 = I1 + 1	LTEOS
SAVE(I3) = ETOT	LTEOS
SAVE(I2) = GTOT	20APR72
55 S8 = -1.	LTEOS
GCHECK(I) = SAVE(I1)	LTEOS
PCHECK(I) = SAVE(I2)	LTEOS
AP(1) = SAVE(I3) - SAVE(I1)	LTEOS
AP(2) = SAVE(I2) - SAVE(I0)	LTEOS
IF(ABS(AP(1)/SAVE(I1)) .LT. 1.E-6) GO TO 57	LTEOS
56 IF(I .LE. 3) GO TO 75	LTEOS
IF(ABS((GCHECK(I) - GCHECK(I-2))/GCHECK(I)) .GT. 1.E-10) GO TO 75	LTEOS
IF(ICYCLE .GT. 1) GO TO 81	LTEOS
ICYCLE = 2	LTEOS
TCYCLE = T0	LTEOS
T0 = T0 + .005	LTEOS
GO TO 50	LTEOS
57 IF(ABS(AP(2)/SAVE(I0)) .LT. 1.E-5) GO TO 105	LTEOS
IF(I .LT. 3) GO TO 75	LTEOS
IF(ABS((PCHECK(I)- PCHECK(I-2))/PCHECK(I)) .LT. 1.E-10) GO TO 64	LTEOS
75 CONTINUE	LTEOS
CALL MATINV(C,2,2,IROW,TEMP)	LTEOS
CALL MATMPY(2,2,1,C,2,AP,2,RP,2)	LTEOS
SAVE(1) = SAVE(1) + RP(1)	4APR72
SAVE(2) = SAVE(2) + RP(2)	4APR72
85 IF(SAVE(1) .GT. ETACRT) GO TO 95	LTEOS
IF(SAVE(2) .LT. ETACRT) GO TO 95	LTEOS
IF(SAVE(1) .LT. 0) SAVE(1) = (SAVE(1) - RP(1))/2.	LTEOS
IF(SAVE(1) .GT. ELOW) SAVE(1) = ELOW - .01	18APR72
IF(SAVE(2) .LT. EHIGH) SAVE(2) = EHIGH + .01	18APR72
60 CONTINUE	LTEOS
IF(ABS(AP(1)/SAVE(I1)) .GT. 1.E-6) GO TO 89	LTEOS
64 IF(SAVE(I0) .GT. 1.E-8) GO TO 89	LTEOS
IPOS = 0	LTEOS
IF(SAVE(I0) .LT. SAVE(I2)) IPOS = 1	LTEOS
SIG = ABS(SAVE(I0) - SAVE(I2))/(SAVE(I0) - SAVE(I2))	LTEOS
STEP = 1.E-7	LTEOS
74 ITEM = 1	LTEOS
DO 76 I4 = 1,11	LTEOS
AI4 = I4	LTEOS
ETE = SAVE(2)*(1. + SIG*STEP*AI4)	LTEOS
CALL PGCAL(1,ETE,TO,PTEMP,PPTOT,ETOT,GTEM,GPTOT)	4APR72
IPOSP = 0	LTEOS
IF(SAVE(I0) .LT. PTEMP) IPOSP = 1	LTEOS
IF(IPOS .NE. IPOSP) GO TO 62	LTEOS
ITEM = ITEM + 1	LTEOS
76 CONTINUE	LTEOS

PRINT 78,TO,ETE,PTEMP,ETOT,GTEM	EXPLA
78 FORMAT(1X,*CAN NOT FIND CROSS POINT*,1P6E15.7)	LTEOS
GO TO 150	LTEOS
62 IF(ITEM .GT. 1) GO TO 77	LTEOS
STEP = STEP/10.	LTEOS
IF(STEP .GT. 1.E-14) GO TO 74	4APR72
IF(SIG .LT. 0) ETE = SAVE(2)	4APR72
77 IF(ABS((GTEM - SAVE(13))/SAVE(13)) .GT. 1.E-5) GO TO 69	4APR72
SAVE(12) = SAVE(10)	LTEOS
65 DO 82 I4 = 1,200	4APR72
AI4 = I4	LTEOS
ETE1 = ETE*(1. + STEP*AI4)	LTEOS
SAVE(2) = ETE1*(1. - STEP)	LTEOS
CALL PGCAL(1,ETE1,TO,PTEMP,PPTOT,ETOT,GTEM,GPTOT)	20APR72
IF(ABS((GTEM - SAVE(13))/SAVE(13)) .LT. 1.E-8) GO TO 105	LTEOS
82 CONTINUE	LTEOS
GO TO 105	LTEOS
69 PRINT 70	LTEOS
70 FORMAT(1X,*NUMERIC PROBLEMS PREVENT CONVERGENCE*)	LTEOS
GO TO 65	LTEOS
81 PRINT 70	LTEOS
GO TO 111	LTEOS
89 PRINT 90	LTEOS
90 FORMAT(1X,*CAN NOT CONVERGE IN 50 TRIES*)	LTEOS
IF(ICYCLE .GT. 1) GO TO 150	29AP72
ICYCLE = 2	29AP72
TCYCLE = TO	29AP72
TO = TO + .01	29AP72
GO TO 50	29AP72
95 PRINT 100,SAVE(1),ETACRT,SAVE(2)	LTEOS
100 FORMAT(1X,*ETAS ARE CROSSING CRITICAL ETA*,1P3E12.5)	LTEOS
GO TO 150	4APR72
105 TSTORE(ITEMP) = TO	LTEOS
ETA1(ITEMP) = SAVE(1)	LTEOS
ETA2(ITEMP) = SAVE(2)	LTEOS
PRESS1(ITEMP) = SAVE(10)	LTEOS
PRESS2(ITEMP) = SAVE(12)	LTEOS
ENERG1(ITEMP) = SAVE(22)	LTEOS
ENERG2(ITEMP) = SAVE(24)	LTEOS
PRINT 110,TO,ETA1(ITEMP),PRESS1(ITEMP),ENERG1(ITEMP),SAVE(11),	LTEOS
1 ETA2(ITEMP),PRESS2(ITEMP),ENERG2(ITEMP),SAVE(13)	LTEOS
110 FORMAT(2X,5(1PE12.5,2X)/16X,4(E12.5,2X)/)	LTEOS
ITEMP = ITEMP + 1	LTEOS
111 IF(ICYCLE .GT. 1) TO = TCYCLE	4APR72
ICYCLE = 1	4APR72
112 IF(TO .LT. .11) DELTP = .025	LTEOS
TO = TO - DELTP	LTEOS
IF(TO .LT. .049) GO TO 150	4APR72
EFAC = 2.	LTEOS
IF(TO .LT. .2) EFAC = 1.	LTEOS
SAVE(1) = SAVE(1)/EXP(TCRIT/(EFAC*TO))	LTEOS
SAVE(2) = ETA2(ITEMP-1)*1.20	LTEOS
IF(ITEMP .GT. 6) SAVE(2) = 2.*ETA2(ITEMP-1) - ETA2(ITEMP-2)	LTEOS

	IF(SAVE(2) .GT. 1.) SAVE(2) = .99	LTEOS
	GO TO 50	LTEOS
C		LTEOS
150	NBOUND = ITEMP - 1	LTEOS
	PTO = PRESS1(NBOUND)	4APR72
	E = ETA2(NBOUND)	4APR72
	DO 155 I = 1,100	4APR72
	E = E - .01	4APR72
	CALL PGCAL(0,E,TSTORE(NBOUND),PTOT,PPTOT,ETOT,GTOT,GPTOT)	4APR72
	IF(PTOT .GT. PTO) GO TO 156	4APR72
155	PTO = PTOT	4APR72
156	EBOUND = E + .01	4APR72
	GO TO 160	LTEOS
990	PRINT 991	LTEOS
991	FORMAT(* IRON IS NOT AVAILABLE AT PRESENT TIME*)	EXPLA
160	RETURN	LTEOS
C	***** ISOTHERM CALCULATION *****	EXPLA
	ENTRY ISOCAL	EXPLA
	E = RHOIN/R0	LTEOS
	IF(THETIN .LT. .01) THETIN = .01	4APR72
	IF(THETIN .GT. TCRIT) GO TO 240	LTEOS
	DO 205 IJ = 1,NBOUND	LTEOS
	IF(THETIN .GE. TSTORE(IJ)) GO TO 207	LTEOS
205	CONTINUE	LTEOS
	IF(E .GT. EBOUND) GO TO 240	4APR72
	PTOT = 0.	4APR72
	ETOT = 0.	4APR72
	GO TO 1001	4APR72
207	TINTER = (TSTORE(IJ)- THETIN)/(TSTORE(IJ)- TSTORE(IJ- 1))	LTEOS
	ETAHI = ETA2(IJ) - TINTER*(ETA2(IJ) - ETA2(IJ- 1))	LTEOS
	ETALO = ETA1(IJ) - TINTER*(ETA1(IJ) - ETA1(IJ- 1))	LTEOS
	IF(E .GT. ETAHI) GO TO 240	LTEOS
	IF(E .LT. ETALO) GO TO 240	LTEOS
	PTOT = PRESS1(IJ) - TINTER*(PRESS1(IJ) - PRESS1(IJ- 1))	LTEOS
	ENGHI = ENERG2(IJ) - TINTER*(ENERG2(IJ) - ENERG2(IJ- 1))	LTEOS
	ENGLO = ENERG1(IJ) - TINTER*(ENERG1(IJ) - ENERG1(IJ- 1))	LTEOS
	ETOT = ENGHI - (ENGHI- ENGLO)*(ETAHI - E)/(ETAHI - ETALO)	LTEOS
	GO TO 1001	LTEOS
240	CALL PGCAL(0,E,THETIN,PTOT,PPTOT,ETOT,GTOT,GPTOT)	29AP72
	GO TO 1001	LTEOS
1000	PRINT 1002	LTEOS
1002	FORMAT(1X,*CAN NOT WORK THIS CASE*)	LTEOS
1001	RETURN	LTEOS
	END	LTEOS
	SUBROUTINE EOS(I5,DENSITY,TEMPTUR,P2,U)	LTEOS
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
	DATA Q/0. ,. 5,1. ,2. ,4. ,8. ,16. ,.1 E+ 200/	LTEOS
	DATA Q3/0. ,. 125,1. ,8. ,64. ,512. ,4096. /	LTEOS
C		EXPLA
C	ELECTRONIC EQUATION OF STATE MAIN SUBROUTINE - FIND PRESSURE,	EXPLA
C	INTERNAL ENERGY AND ELECTRONIC GIBBS FREE ENERGY FOR SPECIFIC	EXPLA

C	TEMPERATURE AND DENSITY	EXPLA
C		EXPLA
	Z=ATMNO	LTEOS
	A=ATMWT	LTEOS
	TO=TEMPTUR	LTEOS
	RO=DENSITY	LTEOS
	KKK=0	LTEOS
	Z9=Z**. 3333333	LTEOS
	Z11=1. /Z9	LTEOS
	R=(2. 67404715*A/RO)**. 3333333	LTEOS
	Z10=R*Z9	LTEOS
	RQB=R**3	LTEOS
15	CONTINUE	LTEOS
	TO32=SQRT(TO)*TO	LTEOS
	TO1=1. /TO	LTEOS
	AO=. 6057*Z9	LTEOS
	DO 1 I=2,8	LTEOS
	IF (Z10. LT. Q(I)) GO TO 2	LTEOS
1	CONTINUE	LTEOS
2	J1=I	LTEOS
	N=I- 1	LTEOS
	QN=Q(N)	LTEOS
	QN3=QN**3	LTEOS
	ITRAN=1	LTEOS
	IF (Z10. LT. 16.) ITRAN=2	LTEOS
	R2=R	LTEOS
	FNZR2=1. /(1. + AO*R2)	LTEOS
	FNZR2=FNZR2**2*(2. *AO*R2*FNZR2+ 1.)*Z	LTEOS
	F1=236. 34647*FNZR2/(RQB*TO32)	LTEOS
	CALL SUB400	LTEOS
	E3=E4	LTEOS
	CALL SUB1100	LTEOS
	Z2=S2	LTEOS
	R2=R2*. 99	LTEOS
	FNZR2=1. /(1. + AO*R2)	LTEOS
	FNZR2=FNZR2**2*(2. *AO*R2*FNZR2+ 1.)*Z	LTEOS
	F1=236. 34647*FNZR2/(RQB*TO32)	LTEOS
	CALL SUB400	LTEOS
	E3=E4	LTEOS
	CALL SUB1100	LTEOS
	Z3=S2	LTEOS
	IF (Z2/Z. GE. 1.) GO TO 3	LTEOS
	ISW=1	LTEOS
	R2=. 1	LTEOS
	Z2=Z	LTEOS
	GO TO 4	LTEOS
3	ISW=2	LTEOS
	R2=R/3.	LTEOS
	IF (Z2/Z3. LT. 1.) GO TO 8	LTEOS
4	R3=R2	LTEOS
	FNZR2=1. /(1. + AO*R2)	LTEOS
	FNZR2=FNZR2**2*(2. *AO*R2*FNZR2+ 1.)*Z	LTEOS
	F1=236. 34647*FNZR2/(RQB*TO32)	LTEOS

	CALL SUB400	LTEOS
	E3=E4	LTEOS
	CALL SUB1100	LTEOS
	Z4=Z2- S2	LTEOS
	IF (ABS(Z4/Z2). LT. 1. E- 10) GO TO 5	LTEOS
	R2=R3*. 99	LTEOS
	FNZR2=1. /(1. + AO*R2)	LTEOS
	FNZR2=FNZR2**2*(2. *AO*R2*FNZR2+ 1.)*Z	LTEOS
	F1=236. 34647*FNZR2/(RQB*TO32)	LTEOS
	CALL SUB400	LTEOS
	E3=E4	LTEOS
	CALL SUB1100	LTEOS
	Z3=Z2- S2	LTEOS
	R2=R3- . 01*R3*Z4/(Z4- Z3)	LTEOS
	GO TO 4	LTEOS
5	GO TO (9,6), ISW	LTEOS
6	PRINT 10	LTEOS
	PRINT 11	LTEOS
7	X=E3	LTEOS
	CALL SUB600	LTEOS
	CALL SUB1100	LTEOS
	Z4=Z- S2	LTEOS
	IF (ABS(Z4/Z). LT. 1. E- 10) GO TO 9	LTEOS
	E3=. 99*E3	LTEOS
	X=E3	LTEOS
	CALL SUB600	LTEOS
	CALL SUB1100	LTEOS
	Z3=Z- S2	LTEOS
	E3=(1. 010101- . 01010101*Z4/(Z4- Z3))*E3	LTEOS
	GO TO 7	LTEOS
8	PRINT 12	LTEOS
	PRINT 13	LTEOS
	STOP 276	LTEOS
9	X=E4	LTEOS
	CALL SUB600	LTEOS
	CALL SUB800	LTEOS
	ETE = RO/RO	21AP72
	PS = PSI(ETE,TEMPTUR)	21AP72
	IF(I5 .EQ. 0) PS = 1.	21AP72
	PO=FNZR2*TO/RQB*Y5/Y*1. 722*PS	21AP72
	IF (KKK. GT. 0) GO TO 20	LTEOS
	P1=PO	LTEOS
20	CONTINUE	LTEOS
	R5=AO*R2	LTEOS
	R6=AO*R	LTEOS
	R7=R2/R	LTEOS
	R8=1. + R5	LTEOS
	Z5=FNZR2/Z	LTEOS
	B1=ALOG(R8)	LTEOS
	V1=(Z5/R6**2)*(1. /R8+ B1- 1.)	LTEOS
	V2=Z5**2*R7**3*(R7**2*. 1- A1*. 333333)	LTEOS
	V3=- . 4*R6/R8**5	LTEOS
	V4=Z5/R6**2	LTEOS

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V4=V4*((- 3. *R5**3+ 9. *R5**2+ 18. *R5+ 8. )/(6. *R8**3)- 4. /3. + B1)
V5=(- A1*Z5*2. )*((1. - (1. + 3. *R5)/R8**3)/6. )
V6=(Z5/2. )*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(I5 . EQ. 1) GO TO 25
P2 = P1
U = U1
GO TO 35
25 TO = . 01
   KKK=1
   GO TO 15
30 U=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/ 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 INNER JOIN RADIUS OF ELECTRONIC POTENTIAL
C
X1 = S/R
A1=(Z/FNZR2)*(R/R2/(1. + AO*R2)**2)- R/R2+ 1. 5
FNI=27. 2*Z/R
FNI=FNI*(1. /X1)*(1. /(1. + AO*R*X1)**2)
FNI=FNI+ 27. 2*FNZR2*(X1**2/2. - A1)/R
RETURN
END
SUBROUTINE SUB600
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 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

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	RETURN	LTEOS
2	IF (X. GE. - 2.) GO TO 3	LTEOS
	W1=EXP(X)	LTEOS
	W2=W1*W1	LTEOS
	Y=W1*(. 886227- . 2852038*W1+ . 17055438*W2)	LTEOS
	RETURN	LTEOS
3	T=(X+ 2.)/6.	LTEOS
	Q1=3. 09954*T	LTEOS
	Y=. 115137+ 5. 66425*T	LTEOS
	Y=Y+ (T- 1.)*T*(6. 46229- 1. 4536*EXP(- Q1))	LTEOS
	RETURN	LTEOS
	END	LTEOS
	FUNCTION FNO (S)	LTEOS
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
C		EXPLA
C	CALCULATES OUTER IONIC RADIUS OF ELECTRONIC POTENTIAL	EXPLA
C		EXPLA
	X1 = S/R	EXPLA
	FNO=(27. 2*FNZR2/R)*(1. /X1+ X1**2/2. - 1. 5)	LTEOS
	RETURN	LTEOS
	END	LTEOS
	SUBROUTINE SUB800	LTEOS
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
C		EXPLA
C	CALCULATES THE FERMI DIRAC INTEGRAL OF ORDER 3/2	EXPLA
C		EXPLA
	IF(X . LT. 4.) GO TO 1	EXPLA
	Y5=SQRT(X)*(. 4*X**2+ 2. 467401- . 7102746/X**2)	LTEOS
	Y5=Y5- SQRT(X)*2. 771862/X**4	LTEOS
	RETURN	LTEOS
1	IF (X. GT. - 2.) GO TO 2	LTEOS
	X5=EXP(X)	LTEOS
	X6=X5*X5	LTEOS
	Y5=1. 32934*X5	LTEOS
	Y5=Y5*(1. - . 176777*X5+ . 06415*X6)	LTEOS
	RETURN	LTEOS
2	T=(X+ 2.)*. 166667	LTEOS
	Q1=3. 09954*T	LTEOS
	Y5=. 115137*T+ 5. 66425/2. *T**2	LTEOS
	Y6=EXP(- Q1)	LTEOS
	Y7=6. 46229*T**2*(T*. 333333- . 5)+ Y5	LTEOS
	Y5=(2. - Y6*(Q1**2+ 2. *Q1+ 2.))*. 03358213	LTEOS
	Y5=Y5- (1. - Y6*(Q1+ 1.))*. 10408916	LTEOS
	Y5=- 1. 4536*Y5	LTEOS
	Y5=((Y5+ Y7)*6. + . 11720928)	LTEOS
	Y5=Y5*1. 5	LTEOS
	RETURN	LTEOS
	END	LTEOS
	SUBROUTINE SUB1100	LTEOS

	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
C		EXPLA
C	THIS SUBROUTINE DOES THE INTEGRATION OF THE ELECTRONIC POTENTIAL	EXPLA
C	USING QUADRATURE FORMULAS	EXPLA
C		EXPLA
	S1 = 0.	EXPLA
	IF (N. LT. 2) GO TO 4	LTEOS
	DO 3 J=2,N	LTEOS
	S=Q(J)/Z9	LTEOS
	IF (. 73*S/R2. GT. 1.) GO TO 1	LTEOS
	X=FNI(. 73*S)*TO1+ E3	LTEOS
	GO TO 2	LTEOS
1	X=FNO(. 73*S)*TO1+ E3	LTEOS
2	CALL SUB600	LTEOS
	S1=S1+ Y*(Q3(J)- Q3(J-1))/Z	LTEOS
3	CONTINUE	LTEOS
4	CONTINUE	EXPLA
	GO TO (5,10), ITRAN	LTEOS
5	CONTINUE	LTEOS
C	R 16 (LOW DENSITY CASE)	LTEOS
	S=(16. + . 46*(Z10- 16.)*. 5)*Z11	LTEOS
	S9=(16. + (Z10- 16.)*. 5)*Z11	LTEOS
	IF (S/R2. LT. 1.) GO TO 6	LTEOS
	X=FNO(S)*TO1+ E3	LTEOS
	CALL SUB600	LTEOS
	GO TO 7	LTEOS
6	X=FNI(S)*TO1+ E3	LTEOS
	CALL SUB600	LTEOS
7	S1=S1+ Y*(S9**3- Q3(N))/Z	LTEOS
	S=(S9+ . 46*(R- 16. *Z11)*. 5)	LTEOS
	IF (S/R2. LT. 1.) GO TO 8	LTEOS
	X=FNO(S)*TO1+ E3	LTEOS
	CALL SUB600	LTEOS
	GO TO 9	LTEOS
8	X=FNI(S)*TO1+ E3	LTEOS
	CALL SUB600	LTEOS
9	S1=S1+ Y*(RQB- S9**3)	LTEOS
	GO TO 14	LTEOS
10	IF (J1. LT. 3) GO TO 15	LTEOS
	S=(Q(N)+ (Z10- Q(N))* . 46)*Z11	LTEOS
11	IF (S/R2. LT. 1.) GO TO 12	LTEOS
	X=FNO(S)*TO1+ E3	LTEOS
	CALL SUB600	LTEOS
	GO TO 13	LTEOS
12	X=FNI(S)*TO1+ E3	LTEOS
	CALL SUB600	LTEOS
13	S1=S1+ Y*(RQB- Q3(N))/Z	LTEOS
14	S1=S1/3.	LTEOS
	S2=S1*1. 2693229E- 2*TO32	LTEOS
	RETURN	LTEOS
15	S=. 73*R	LTEOS

	GO TO 11	LTEOS
	END	LTEOS
	SUBROUTINE SUB400	LTEOS
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
C		EXPLA
C	FINDS ETA GIVEN THE FERMI DIRAC INTEGRAL OF ORDER 1/2 FROM AN	EXPLA
C	APPROXIMATION FORMULA	EXPLA
C		EXPLA
	IF(F1 .LT. 5.77939) GO TO 3	LTEOS
	E4=1.5*F1**.666667	LTEOS
1	X=E4	LTEOS
	CALL SUB600	LTEOS
	F2=F1-Y	LTEOS
	IF (ABS(F2/F1).LT.1.E-10) GO TO 2	LTEOS
	F3=1.-.4112335/X**2-1.7756865/X**4	LTEOS
	F3=F3-29.1045555/X**6	LTEOS
	F3=-F3*SQRT(X)	LTEOS
	E4=E4-F2/F3	LTEOS
	GO TO 1	LTEOS
2	E4=X	LTEOS
	RETURN	LTEOS
3	IF (F1.GT..115137) GO TO 6	LTEOS
	E4=1.128379186*F1	LTEOS
4	E5=E4*E4	LTEOS
	E2=.886226925*E4*(1.-.321818*E4+.19245*E5)	LTEOS
	F2=F1-E2	LTEOS
	IF (ABS(F2/F1).LT.1.E-10) GO TO 5	LTEOS
	F3=-.886226925*(1.-.643636*E4+.57735*E5)	LTEOS
	E4=E4-F2/F3	LTEOS
	GO TO 4	LTEOS
5	E4=ALOG(E4)	LTEOS
	RETURN	LTEOS
6	T=.9999	LTEOS
7	X=6.*T-2.	LTEOS
	CALL SUB600	LTEOS
	F2=Y	LTEOS
	F2=F1-F2	LTEOS
	IF (ABS(F2/F1).LT.1.E-10) GO TO 8	LTEOS
	W=EXP(-3.09954*T)	LTEOS
	F3=5.66425+T*(T-1.)*1.4536*3.09954*W	LTEOS
	F3=-F3-(2.*T-1.)*(6.46229-1.4536*W)	LTEOS
	T=T-F2/F3	LTEOS
	GO TO 7	LTEOS
8	E4=6.*T-2.	LTEOS
	RETURN	LTEOS
	END	LTEOS
	FUNCTION PSI(E,T0)	21AP72
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
C		21AP72

C	CALCULATES THE MODIFICATION FUNCTION FOR THE ELECTRONIC PRESSURE,	21AP72
C	ETC. TO COMPENSATE FOR THERMAL EFFECTS AND MODEL PROBLEMS	21AP72
C		21AP72
	IF(E .LT. 1.) GO TO 1	21AP72
	DEBYE = H4*EXP((GAMMA/E - (3. *E-1.)/(3. *E**2))*(E-1.))*E**.6666667	21AP72
	GO TO 10	21AP72
1	IF(E .GT. 1.E-10) GO TO 5	21AP72
	T = H4*EXP(1.5 - 2. *GAMMA)	21AP72
	SI = .018596*(R0/ATMWT)**(2./3.)*T0*T/(ATMWT*E**(4./3.))	21AP72
	GO TO 15	21AP72
5	DEBYE = H4*E*EXP(((3. *GAMMA-2.)+ .5*(1.-2. *GAMMA)*(E+1.))*(E-1.))	21AP72
10	SI = .018596*(T0/DEBYE**2)*(E*R0/ATMWT)**.6666667/ATMWT	21AP72
15	EXT = (10. - 10./(1. + SI))/T0	21AP72
	IF(EXT .LT. 700.) GO TO 20	21AP72
	PSI = 0.	21AP72
	GO TO 25	21AP72
20	PSI = 2./(1. + EXP(EXT))	21AP72
25	RETURN	21AP72
	END	21AP72
	SUBROUTINE COLD(ESAVE,PCOLD,PPCOLD,ECOLD,EPCOLD)	4APR72
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
	COMMON ECMAT(200),ETAMAT(200),A,B1,B2, C1,C2,C3,C5,C4,D1,AK,	21AP72
1	EREF,TREF,SAVE(50), P0,THETIN,RHOIN,PTOT,ETOT,RCOLD	21AP72
C		EXPLA
C	FOR A SPECIFIC TEMPERATURE AND DENSITY, THE SUBROUTINE FINDS THE	EXPLA
C	T=0 PRESSURE AND INTERNAL ENERGY	EXPLA
C		EXPLA
	TH = 1./3.	EXPLA
	TI = 2./3.	LTEOS
	E = R0*ESAVE/RCOLD	4APR72
	IF(E .LT. 1.) GO TO 5	LTEOS
	E1 = 1. - 1./E**TH	LTEOS
	E2 = EXP(E1*B1)	LTEOS
	E3 = EXP(E1*B2)	LTEOS
	PCOLD = A*(E**E**TI*E2 - E**TI*E3)	LTEOS
	G1 = E2*(5. *E**TI/3. + B1*E**TH/3.)	LTEOS
	G2 = E3*(2./(3. *E**TH) + B2/(3. *E**TI))	LTEOS
	PPCOLD = A*(G1 - G2)	LTEOS
	G3 = (E**TI - B1*E**TH)*E2 - B1**2*EXP(B1)*(EPIN(B1)- EPIN(B1/E**TH))	LTEOS
	G4 = G3 + B1 - 1. + 2./B2*(1. - E3)	LTEOS
	ECOLD = 1.5*A*G4/R0	LTEOS
	GO TO 21	LTEOS
5	IF(E .LT. D1) GO TO 10	LTEOS
	E1 = 1. - E**TH	LTEOS
	E2 = E**TH - D1**TH	LTEOS
	E3 = 5. *E**TI - 4. *E**TH	LTEOS
	G3 = C2 + E2*(C3 - E1*(C4 - C5*E1))	LTEOS
	PCOLD = -E*E**TH*E1*(C1 + E2*G3)	LTEOS
	G5 = -4. *E**TH*E1**3*E2**2+ 3. *E**TI*E1**2*E2**2- 2. *E**TI*E1**3*E2	LTEOS
	G4 = 4. *E**TH*E1**2*E2**2- 2. *E**TI*E1*E2**2+ 2. *E**TI*E1**2*E2	LTEOS
	G3 = E3*E2**2 - 2. *E**TI*E1*E2	LTEOS

	G2 = E3*E2 - E**TI*E1	LTEOS
	PPCOLD = (C1*E3 + C2*G2 + C3*G3 + C4*G4 + C5*G5)/3.	LTEOS
	GO TO 20	LTEOS
10	PCOLD = P0*(AK+2. - (AK+1.)*E/D1)*(E/D1)**(AK+1.)	LTEOS
	PPCOLD = P0*(AK+1.)*(AK+2.)/D1*((E/D1)**AK - (E/D1)**(AK+1.))	LTEOS
20	ECOLD = 0.	LTEOS
21	CONTINUE	LTEOS
	IF(E .GT. 1.) GO TO 50	LTEOS
	IF(E .LT. D1) GO TO 40	LTEOS
	IF(E .GT. ETAMAT(1)) GO TO 30	LTEOS
	DO 25 I = 2,200	LTEOS
	IF(E .GT. ETAMAT(I)) GO TO 35	LTEOS
25	CONTINUE	LTEOS
30	ECOLD = ECMAT(1)*(E - ETAMAT(1))/(1. - ETAMAT(1))/R0	LTEOS
	GO TO 50	LTEOS
35	ECOLD = (ECMAT(I) + (E - ETAMAT(I))*(ECMAT(I) - ECMAT(I-1))/ 1 (ETAMAT(I-1) - ETAMAT(I)))/R0	LTEOS
	GO TO 50	LTEOS
40	ECOLD = (ECMAT(200) + P0*((AK+2.)*(E/D1)**AK - AK*(E/D1)**(AK+1.) 1 - 2.)/(D1*AK))/R0	LTEOS
50	RETURN	LTEOS
	END	LTEOS
50	RETURN	LTEOS
	END	LTEOS
	SUBROUTINE PDPICAL(TO,E,PRES,PRESPP,PRESPP,I5)	29AP72
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
	COMMON ECMAT(200),ETAMAT(200),A,B1,B2, C1,C2,C3,C5,C4,D1,AK,	21AP72
1	EREF,TREF,SAVE(50), P0,THETIN,RHOIN,PTOT,ETOT,RCOLD	21AP72
	DIMENSION AP(20),P(3,3),RP(3),D(3),TEMP(3),IROW(3)	LTEOS
C		29AP72
C	FINDS THE FIRST AND SECOND DERIVATIVES OF THE PRESSURE WITH	29AP72
C	RESPECT TO DENSITY AT A CONSTANT TEMPERATURE	29AP72
C		29AP72
	PRESPP = 0.	29AP72
	IF(I5 .EQ. 0) GO TO 5	29AP72
	IF(TO .NE. TREF) GO TO 1	LTEOS
	IF(ABS((E-EREF)/E) .LT. .07) GO TO 5	LTEOS
1	I1 = 1	LTEOS
	TREF = T0	LTEOS
	EREF = E	LTEOS
	DO 3 I = 1,3	LTEOS
	AI = I	LTEOS
	EP = E*(1. + (AI-2.)*.07)	LTEOS
	P(I,1) = 1.	LTEOS
	P(I,2) = EP	LTEOS
	P(I,3) = EP**2	LTEOS
	DO 2 J = 1,2	LTEOS
	AJ = J	LTEOS
	B = EP*(1. + (AJ - 1.5)*.001)*R0	21AP72
	CALL EOS(1,B,TO,AP(I1),ETOT)	21AP72
2	I1 = I1 + 1	LTEOS

	W = 2. *SI/(3. *E) - 2. *SI*DEBYEP/DEBYE	LTEOS
	ET = 1. 5*B*TO*(2. + SI)/(1. + SI)	LTEOS
	ETP = -ET*W/((1. + SI)*(2. + SI))	LTEOS
	PT = R0*E*B*TO*(3. *GAMP + SI)/(1. + SI)	LTEOS
	PTP = PT/E-PT*W/(1. + SI)+PT*(3. *GAMPP+W)/(3. *GAMP+SI)	LTEOS
	ST=-TO*B*(3. *ALOG(DEBYE/TO)- 4. + 1. 5*ALOG(1. + SI) + 1. 5*SI/(1. + SI))	LTEOS
	STP = -B*(3. *DEBYEP/DEBYE+ 3. *W/(1. + SI)- 3. *SI*W/(2. *(1. + SI)**2))*TO	LTEOS
20	IF(IPRES .GT. 0) GO TO 30	LTEOS
	IPRES = IPRES + 1	LTEOS
	SI = SI	LTEOS
	ET1 = ET	LTEOS
	PT1 = PT	LTEOS
	ST1 = ST	LTEOS
	ETP1 = ETP	LTEOS
	PTP1 = PTP	LTEOS
	STP1 = STP	LTEOS
	T1 = TO	LTEOS
	TO = .01	LTEOS
	GO TO 2	LTEOS
30	TO = T1	LTEOS
	SI = SI	LTEOS
	ET = ET1 - ET	LTEOS
	PT = PT1 - PT	LTEOS
	ST = ST1 - ST	LTEOS
	PTP = PTP1 - PTP	LTEOS
	ETP = ETP1 - ETP	LTEOS
	STP = STP1 - STP	LTEOS
	RETURN	LTEOS
	END	LTEOS
	SUBROUTINE COLCOF(S,C0,PUPPER,U)	LTEOS
	COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1	N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1
	COMMON ATMWT,ATMNO,H4,GAMMA,R0	21AP72
	COMMON ECMAT(200),ETAMAT(200),A,B1,B2, C1,C2,C3,C5,C4,D1,AK,	21AP72
1	EREF,TREF,SAVE(50), P0,THETIN,RHOIN,PTOT,ETOT,RCOLD	21AP72
	DIMENSION RP(3),P(3,3),D(3),TEMP(3),IROW(3),PTEST(10),ETEST(10)	LTEOS
	EQUIVALENCE (ECMAT,TEMP),(ETAMAT,IROW)	LTEOS
C		EXPLA
C	SETS UP THE CONSTANTS FOR THE T=0 CURVE (MODIFIED TO TAKE INTO	EXPLA
C	ACCOUNT LOW TEMPERATURE CONTRIBUTIONS)	EXPLA
C		EXPLA
	D1 = S/(S+ 1.)	LTEOS
	RCOLD = R0	4APR72
	RSAVE = R0	4APR72
	PSAVE = P0	4APR72
	NTRY = 1	4APR72
2	R0 = RCOLD	4APR72
	A0 = PUPPER	LTEOS
	B0 = 0. 01*R0*C0**2	LTEOS
	D0 = .02*R0*C0**2*(2. *S - 1.)	LTEOS
	THIRD = 1./3.	LTEOS
	TTHIRD = 2. *THIRD	LTEOS

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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)
  P(2,1) = 1. + B1/3. - B2/3.
  P(3,1) = 1.333333 + TTHIRD*B1 + B1**2/9. - B2**2/9.
  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
1  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.
  P(3,3) = -2.*B2*A/9.
  CALL MATINV(P,3,3,IROW,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)
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,DELEE)
  CALL P THERM(D1,.02,PT,PTP,ET,ETP,ST,STP,SI)
  DELPEP = DELPE + PT
  P0 = PSAVE - DELPEP
  R0 = RSAVE
  CALL EOS(1,RSAVE,.02,DELPE,DELEE)
  CALL P THERM(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
  G1 = 9.*D0 - 6.*C1 - (2.+6.*D2)*C2 - (6.*D2**2+4.*D2)*C3
  C4 = G1/(2.*D2**2)
  G1 = 20.*R0*U - 30.*C1-(30.*D2-20.)*C2-(15.-40.*D2+30.*D2**2)*C3
  C5 = (G1-(30.*D2-12.-20.*D2**2)*C4)/(10.-24.*D2+15.*D2**2)
C***** PRESSURE CALCULATION FOR ETA LT. S/(S+1) *****
  IF(NTRY .GT. 1) GO TO 105
  E = 1.
  NTRY = 2
  DO 100 I = 1,10
  CALL COLD(E,PTEST(I),PPCOLD,ECOLD,EPCOLD)

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ETEST(I) = E	4APR72
IF(- PTEST(I) .LT. DELPEP) GO TO 100	4APR72
ITRY = I	4APR72
GO TO 106	4APR72
100 E = E - .005	4APR72
PRINT 104	4APR72
104 FORMAT(* DID NOT BRACKET CROSSPOINT*)	4APR72
STOP	4APR72
106 ETA =ETEST(ITRY)+(ETEST(ITRY- 1)- ETEST(ITRY))*(- PTEST(ITRY)- DELPEP)	4APR72
1 /(- PTEST(ITRY)+ PTEST(ITRY- 1))	4APR72
RCOLD = R0/ETA	4APR72
GO TO 2	4APR72
105 E = RSAVE/R0	4APR72
CALL COLD(E,PCOLD,PPCOLD,ECOLD,EPCOLD)	4APR72
IF(ABS((PCOLD+ DELPEP)/DELPEP) .LT. 1.E-6) GO TO 150	4APR72
RCOLD = RSAVE*RCOLD/(RSAVE- RCOLD*(PCOLD+ DELPEP)/PPCOLD)	4APR72
GO TO 2	4APR72
150 F = 0.	4APR72
G1 = (1. - D1)/800.	LTEOS
D2 = 1.	LTEOS
DO 25 I = 1,200	LTEOS
DO 20 J = 1,4	LTEOS
AJ = J	LTEOS
E = D2 - G1*AJ	LTEOS
E1 = 1. - E**THIRD	LTEOS
E2 = E**THIRD - D1**THIRD	LTEOS
IF(E .NE. 0) GO TO 19	LTEOS
ECMAT(I) = F	LTEOS
ETAMAT(I) = E	LTEOS
GO TO 25	LTEOS
19 T1 = E1*(C1 + E2*(C2 + E2*(C3 - E1*(C4 - C5*E1))))	LTEOS
20 F = F + G1*T1/E**TTHIRD	LTEOS
ECMAT(I) = F - G1*T1/(2. *E**TTHIRD)	LTEOS
ETAMAT(I) = E	LTEOS
25 D2 = E	LTEOS
AK = -2. *P0/(D1*(R0*U - ECMAT(200)))	LTEOS
PAK = R0*U - ECMAT(200)	29AP72
D2 = D1/400.	LTEOS
DO 30 I = 1,400	LTEOS
AJ = I	LTEOS
E = D2*AJ	LTEOS
T1 = P0*(AK+ 2. - (AK+ 1.)*E/D1)*(E/D1)**(AK+ 1.)/E**2	LTEOS
30 F = F - T1*D2	LTEOS
UINT = (F + T1*D2/2.)/R0	LTEOS
IF(ABS((U - UINT)/U) .GT. .001) WRITE(9,31) U,UINT	LTEOS
31 FORMAT(3X,*THE COHESIVE ENERGY *,E13.6,*DOES NOT AGREE WELL WITH	LTEOS
1 THE CALCULATED ENERGY *,E13.6)	LTEOS
50 R0 = RSAVE	4APR72
RETURN	4APR72
END	LTEOS
SUBROUTINE PGCAL(I5,EP,T0,PTOTA,PPTOT,ETOTA,GTOT,GPTOT)	29AP72
COMMON /BLK/ AO,A1,E3,E4,F1,R,R2,S2,TO,X,Y,Z,Z9,Z10,Q(8),J1,N,QN,Q	COM1
1 N3,TO1,Q3(7),RQB,TO32,ITRAN,Z11,Y5,FNZR2	COM1

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COMMON ATMWT,ATMNO,H4,GAMMA,R0                                21AP72
COMMON ECMAT(200),ETAMAT(200),A,B1,B2, C1,C2,C3,C5,C4,D1,AK, 21AP72
1  EREF,TREF,SAVE(50), P0,THETIN,RHOIN,PTOT,ETOT,RCOLD      21AP72
   DIMENSION AP(5)                                           29AP72
C                                                                 29AP72
C  CALCULATES THE PRESSURE, INTERNAL ENERGY, AND GIBBS FREE ENERGY 29AP72
C  AND FIRST DERIVATIVE WITH RESPECT TO DENSITY OF ABOVE FOR INPUT 29AP72
C  TEMPERATURES AND DENSITIES                                29AP72
C                                                                 29AP72
   IF(I5 .EQ. 0) GO TO 11                                     29AP72
   DO 10 I = 1,2                                             LTEOS
   AI = I                                                    LTEOS
   B = EP*(1. + (AI - 1.5)*.001)*R0                          29AP72
   CALL EOS(0,B,.01,PLOWER,ELOWER)                           LTEOS
   GUN = 0.                                                  29AP72
   GUN = FNZR2*E4*.01                                       29AP72
2  CALL EOS(0,B,T0,PUPPER,EUPPER)                             LTEOS
   E = B/R0                                                 29AP72
   F = PSI(E,T0)                                           29AP72
   AP(I) = (PUPPER - PLOWER)*F                               29AP72
10  AP(I+2) = -(FNZR2*E4*T0 - GUN)*F                         29AP72
11  B = EP*R0                                               29AP72
   CALL PHERM(EP,T0,PT,PTP,ET,ETP,ST,STP,SI)                29AP72
   CALL COLD(EP,PCOLD,PPCOLD,ECOLD,EPCOLD)                   29AP72
   CALL EOS(1,B,T0,DELPE,DELEE)                              29AP72
   PTOTA = PT + PCOLD + DELPE                                29AP72
   PPTOT = PTP + PPCOLD + (AP(2) - AP(1))/(.001*EP)         29AP72
   ETOTA = ET + ECOLD + DELEE                                29AP72
   GTOT = ET + ECOLD - ST + (PT+PCOLD)/(R0*EP) + (AP(4)+AP(3))/2.* 29AP72
1  .9653/ATMWT                                              29AP72
   GPTOT = ETP - STP - PT/(R0*EP**2) + (PTP+PPCOLD)/(R0*EP) + (AP(4)- 29AP72
1  AP(3))/(.001*EP)*.9653/ATMWT                             29AP72
   RETURN                                                    LTEOS
   END                                                       LTEOS
   FUNCTION EPIN(AX)                                         LTEOS
   DIMENSION MESSG(6)                                       LTEOS
   DATA P0/1.0/,P1/0.16515516520352/,P2/0.23785541396286E-1/,  LTEOS
1  P3/0.92333053076239E-3/,P4/0.9713386753293E-5/,         LTEOS
2  Q0/1.0/,Q1/0.4151551652034/,Q2/0.72018777145175E-1/,   LTEOS
3  Q3/0.62805155999224E-2/,Q4/0.23666563141677E-3/,(MESSG(I),I=1,6)/  LTEOS
4  48HE1(X) X.LE.0 NOT ALLOWED RESULT=LARGEST NUMBER/,    LTEOS
5  OMEGA/1.E256/                                           LTEOS
C                                                                 EXPLA
C  EXPONENTIAL INTEGRAL                                     EXPLA
C                                                                 EXPLA
   X=AX                                                      LTEOS
   IF (X.GT.1.0)GO TO 30                                     LTEOS
   IF(X.LE.0.0) GO TO 20                                     LTEOS
10  E1=X*(P0+ X*(P1+ X*(P2+ X*(P3+ X*P4))))/(Q0+ X*(Q1+ X*(Q2+ X*(Q3+ X*Q4))))  LTEOS
1  - ALOG(X)- 0.57721566490153                               LTEOS
   RETURN                                                    LTEOS
20  CALL LABRT(1,MESG,0)                                     LTEOS
   E1=OMEGA                                                  LTEOS

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

LTEOS
LTEOS
LTEOS
LTEOS
LTEOS