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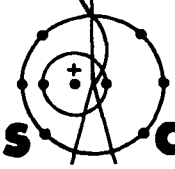
Low-Temperature Equation of State for Metals



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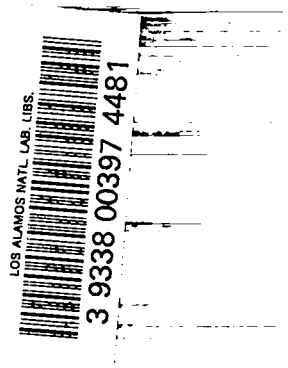

by

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

LOW-TEMPERATURE EQUATION OF STATE FOR METALS

by

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

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

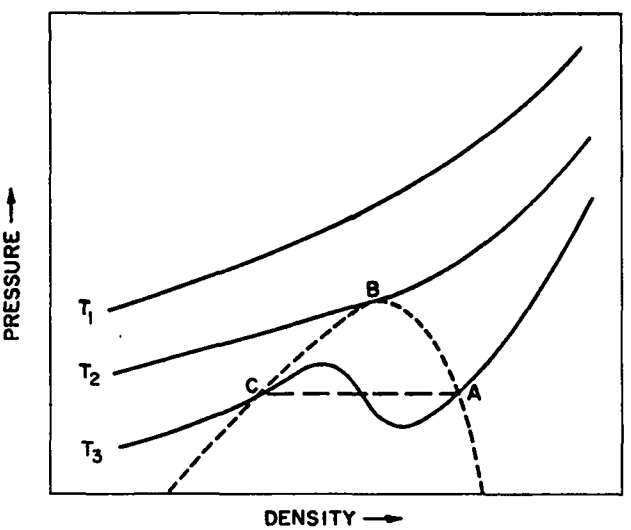

Fig. 1. Typical P-V diagram showing location of mixed-phase region.

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_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.

$$U_s = C_o + S \cdot U_p \quad , \tag{1}$$

and

$$\delta = S/(1 + S) \quad . \tag{2}$$

TABLE I

T = 0 ISOTHERM BOUNDARY CONDITIONS

Physical Constraints	Region I	Region II	Region III
$P_c(125) = P_{TF}(125)$	x		
$P_c(1) = 0$	x	x	
$P_c'(1) = P_H'(1) = 0.01\rho_o C_o^2$	x	x	
$P_c''(1) = P_H''(1) = 0.02\rho_o C_o^2(2S - 1)$	x	x	
$P_c(\delta) = -P_o$		x	x
$P_c'(\delta) = 0$		x	x
$P_c(0) = 0$			x
$\int_1^0 P_c/\eta^2 d\eta = \rho_o E_c$		x	x

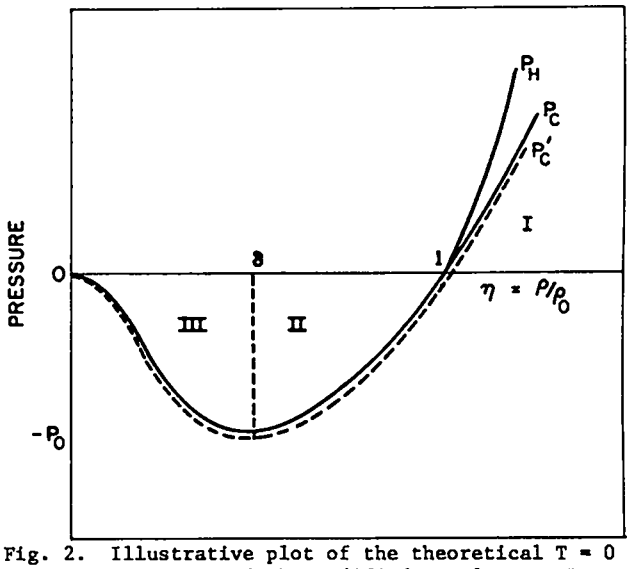

Fig. 2. Illustrative plot of the theoretical T = 0 curve P_c and the modified T = 0 curve P_c'.

The expression for P_c in region I is similar to the modified pressure function used by Barnes[1] 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.

$\eta > 1$

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

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

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

$\delta \leq \eta \leq 1$

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

and

$\eta < \delta$

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

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

$$\frac{1}{\rho_o}\int_1^x \frac{P_c}{\eta^2}\, d\eta = E_{cold} \quad . \tag{6}$$

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),

$$P_H = (P_c - \rho_o \gamma \eta E_c)/\left(1 - \gamma(\eta - 1)/2\right) \quad , \tag{7}$$

where γ is the Gruneisen ratio and is obtained from

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

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.

$$F_n = N_o kT[3\ell n(\theta/T) - 1 + 1.5\ell n(1 + \Psi)] \quad , \tag{9}$$

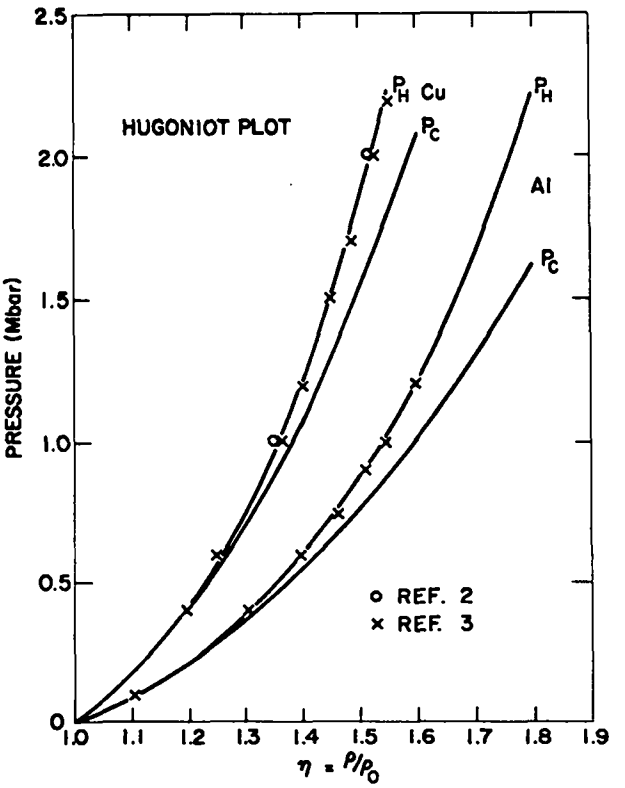

Fig. 3. Comparison of experimental and theoretical Hugoniot curves.

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

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

$$S_n = -N_o k[3\ell n(\theta/T) - 4 + 1.5\ell n(1 + \Psi) + 1.5\Psi/(1 + \Psi)] \quad , \tag{12}$$

and

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

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

$o < r < r_1$

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

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

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

and

$r_1 < r < R$

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

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

$\eta = \rho/\rho_o$	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

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

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

The electronic Gibbs free energy is

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

$I_{1/2}$ 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 $T \to 0$, 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

$$P_{Tot}(T) = P_{el} + P_N + P_c$$

$$= P_c + [P_{el}(T) - P_{el}(0.01)]$$

$$+ [P_N(T) - P_N(0.01)] \quad . \qquad (20)$$

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 ($P_{c'}$) 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_o 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

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

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

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

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.

$$P_{Tot} = P_{c'} + [P_N(T) - P_N(0.01)] + G(T,\rho)[P_{el}(T) - P_{el}(0.01)] \quad , \tag{23}$$

$$G_{Tot} = E_{c'} + [E_N(T) - E_N(0.01)] + \left[P_{c'} + \left(P_N(T) - P_N(0.01)\right)\right]/\rho - [T\,S_N(T) - 0.01\,S_N(0.01)] + G(T,\rho)[G_{el}(T) - G_{el}(0.01)] \quad . \tag{24}$$

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.

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

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.

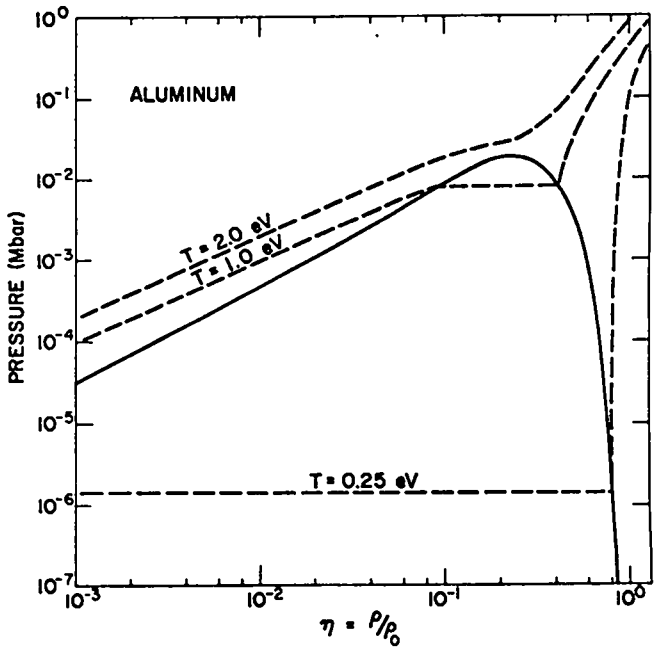

Fig. 4. Detailed plot of aluminum mixed-phase region and representative isotherms.

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
	ρ_c =	0.071 gcm^{-3}			0.1470	0.1148 ± 0.0332
Beryllium	T_c =	0.919	0.785			
	P_c =	0.0330	0.0142			
	ρ_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
	ρ_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	
	ρ_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	
	ρ_c =	0.679	0.478		0.690	
Copper[a]	T_c =	1.951		0.7667	0.6570	
	P_c =	0.0382			0.0083	
	ρ_c =	2.323		1.048	2.318	

[a] Converged on critical point, but did not converge on mixed-phase boundary.

[b] Extrapolated to critical temperature from experimental data.[9]

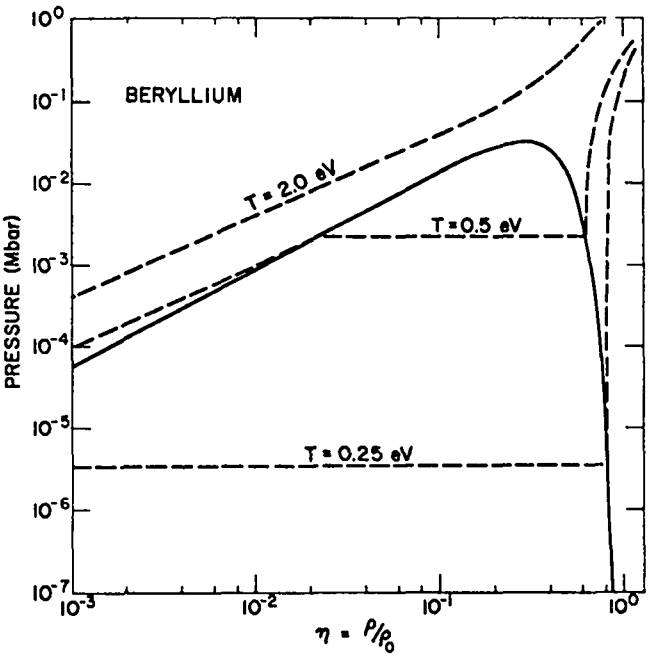

Fig. 5. Detailed plot of beryllium mixed-phase region and representative isotherms.

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APPENDIX A

SAMPLE CALCULATIONS FOR BERYLLIUM

. INPUT FORMAT FOR LTEOS CODE

Card #1 (8F10.8)

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_o
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+00
ATOMIC WEIGHT	= 9.01300E+00	COLD DENSITY(GM/CM3)	= 1.8626SE+00
MUSCNICT S	= 1.12400E+00	COHESIVE ENERGY(EV)	= 3.60CCOE-01
MUSCNICT CO	= 7.99800E+00	TENSILE STRENGTH(MBARS)	= -2.68132E-01
		PRESSURE(ETA=1251(MBARS)	= 1.61C68E+04
		DEBYE TEMPERATURE(EV)	= 9.9950CE-02

T = 0 ISOTHERM CALCULATIONS

GRUNEISEN GAMMA = 1.24800E+00
MINIMUM PRESSURE LOCATION(ETA) = D1 = 5.29190E-01

EQUATION CONSTANTS

ETA LESS THAN C1--------K	=	2.08105E+00
ETA BETWEEN C1 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
BR	=	1.9830AE+00
BA	=	1.61437E+00

CRITICAL POINT RESULTS

T-CRIT(EV)	=	9.1872229E-01
P-CRIT(MBARS)	=	3.2933364E-02
ETA-CRIT	=	3.1165838E-01

MIXED PHASE BOUNDARY PARAMETERS

TEMPERATURE (EV)	ETA	PRESSURE (MBAR)	ENERGY (MBAR-CC/GM)	GIBBS ENERGY
8.50000E-01	1.69901E-01	2.38846E-02	4.9C417E-01	-7.78167E-C1
	4.18183E-01	2.38846E-02	3.9P695E-01	-7.78167E-01
8.00000E-01	1.36011E-01	1.91285E-02	4.86863E-01	-7.15158E-C1
	4.63464E-01	1.91286E-02	3.64480E-01	-7.15158E-01
7.50000E-01	1.09190E-01	1.50191E-02	4.81107E-01	-6.52694E-01
	4.95180E-01	1.50191E-02	3.36358E-01	-6.52694E-C1
7.00000E-01	8.66888E-02	1.14631E-02	4.74144E-01	-5.91027E-01
	5.20803E-01	1.14630E-02	3.11048E-01	-5.91027E-01
6.50000E-01	6.95349E-02	8.68340E-03	4.66421E-01	-5.28294E-01
	5.43805E-01	8.68340E-03	2.8P833E-01	-5.28294E-01
6.00000E-01	5.09562E-02	5.94728E-03	4.58289E-01	-4.7C158E-01
	5.68792E-01	5.94728E-03	2.63212E-01	-4.7C158E-01
5.50000E-01	3.62457E-02	3.89026E-03	4.49893E-01	-4.11919E-01
	5.97712E-01	3.89026E-03	2.38036E-01	-4.11919E-C1
5.00000E-01	2.33062E-02	2.26903E-03	4.41425E-01	-3.56427E-01
	6.30227E-01	2.26903E-03	2.11430E-01	-3.56427E-01
4.50000E-01	1.34442E-02	1.17302E-03	4.33092E-01	-3.02165E-C1
	6.66239E-01	1.17302E-03	1.85513E-01	-3.02165E-01
4.00000E-01	6.50173E-03	5.02442E-04	4.24942E-01	-2.5C157E-C1
	7.05108E-01	5.02442E-04	1.60163E-01	-2.5C157E-01
3.50000E-01	2.32688E-03	1.56810E-04	4.16894E-01	-2.02286E-01
	7.45954E-01	1.56809E-04	1.34353E-01	-2.02286E-C1
3.00000E-01	5.73357E-04	3.29620E-05	4.08862E-01	-1.56172E-C1
	7.87749E-01	3.29619E-05	1.11225E-01	-1.56172E-01
2.50000E-01	6.95819E-05	3.31060E-06	4.0C830E-01	-1.14614E-01
	8.29419E-01	3.31060E-06	8.84467E-02	-1.14614F-01
2.00000E-01	2.49947E-06	9.41457E-08	3.92797E-01	-7.68600E-02
	8.70076E-01	9.41457E-08	6.75465E-02	-7.68600E-02
1.50000E-01	6.87346E-09	1.90767E-10	3.84765E-01	-4.4C404E-02
	9.09063E-01	1.90767E-10	4.86730E-02	-4.4C404E-02
1.00000E-01	1.8077AF-14	3.22543E-16	3.76732E-01	-1.7P157E-C2
	9.45941E-01	3.22543E-16	3.03235E-02	-1.78157E-02
7.50000E-02	1.40992E-20	1.81679E-22	3.72716E-01	-7.7C452E-03
	9.63505E-01	1.81679E-22	2.16730E-02	-7.7C452E-03
5.00000E-02	1.71580E-34	1.36058E-36	3.68700E-01	-6.53067E-04
	9.80462E-01	1.36058E-36	1.31040E-02	-6.53067E-04

TEMPERATURE = 7.50000E-01

RHO	PRESSURE	ENERGY
1.851001-03	3.31060E-06	4.00480F-01
9.255001-03	3.31060F-06	3.98974E-01
1.851001-02	3.31060E-06	3.97092E-01
9.255001-02	3.31060E-06	3.87035E-01
1.851001-01	3.31060E-06	3.63214E-01
9.255001-01	3.31060E-06	2.12646E-01
1.000001+00	3.31060F-06	1.97496E-01
1.200001+00	3.31060E-06	1.96824E-01
1.400001+00	3.31060E-06	1.16152E-01
1.600001+00	3.01474F-02	8.45633E-02
1.800001+00	1.38703E-01	7.83431E-02
1.850001+00	1.69591E-01	7.79640E-02
1.860001+00	1.75965F-01	7.79566E-02
1.900001+00	2.02364E-01	7.81171E-02
2.000001+00	2.74690E-01	7.97428E-02
2.100001+00	7.72196E-01	1.10446E-01
3.000001+00	1.49655E+00	1.70767E-01
5.000001+00	6.65427E+00	5.88353E-01

TEMPERATURE = 5.00000E-01

RHO	PRESSURE	ENERGY
1.851001-03	9.71364E-05	4.40992E-01
9.255001-03	4.85540E-04	4.40997E-01
1.851001-02	9.71194F-04	4.41053E-01
9.255001-02	2.26903E-03	4.31310E-01
1.851001-01	2.26903E-03	4.17162E-01
9.255001-01	2.26903E-03	2.60780E-01
1.000001+00	2.26903E-03	2.45528E-01
1.200001+00	1.49961E-02	2.06932E-01
1.400001+00	1.01439E-01	1.81076E-01
1.600001+00	2.04175E-01	1.66524E-01
1.800001+00	3.22082F-01	1.61128E-01
1.850001+00	3.53883E-01	1.60888E-01
1.860001+00	3.60378E-01	1.60906E-01
1.900001+00	3.87292E-01	1.61160E-01
2.000001+00	4.61129E-01	1.62971E-01
2.500001+00	9.70215E-01	1.94038E-01
3.000001+00	1.71090E+00	2.54353F-01
5.000001+00	6.95484E+00	6.71438E-01

APPENDIX B

LISTING OF THE LTEOS CODE

```
      PROGRAM LTEOS(INPUT,OUTPUT,TAPE9=OUTPUT,TAPE10=INPUT)                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 THETA(100),RHO(100)                                        LTEOS
C                                                                          EXPLA
C     THIS SECTION OF THE CODE SETS UP THE MIXED PHASE REGION AND INPUTS    EXPLA
C     THE TEMPERATURE AND DENSITY FOR THE ISOTHERMS                        EXPLA
C                                                                          EXPLA
C***** CALCULATES THE MIXED PHASE BOUNDARY ******************************  EXPLA
    6 CALL CRTBND                                                          LTEOS
C***** CALCULATES DESIRED ISOTHERMS OR TEMPERATURE DENSITY POINTS ******   EXPLA
      READ (10,1) NTHETA,NRHO                                              LTEOS
    1 FORMAT(2I4)                                                          LTEOS
      IF(NTHETA) 11,6,4                                                    LTEOS
    4 READ(10,2)(THETA(I),I=1,NTHETA)                                      LTEOS
      READ (10,2) (RHO(I),I=1,NRHO)                                        LTEOS
    2 FORMAT(6E12. 5)                                                      LTEOS
      DO 10 I = 1,NTHETA                                                   LTEOS
      PRINT 3,THETA(I)                                                     LTEOS
    3 FORMAT(1H1,2X,*TEMPERATURE = *,1PE12. 5//7X,*RHO*,7X,*PRESSURE*,5X,  LTEOS
     1 *ENERGY*/)                                                          LTEOS
      THETIN = THETA(I)                                                    LTEOS
      DO 10 J = 1,NRHO                                                     LTEOS
      RHOIN = RHO(J)                                                       LTEOS
      CALL ISOCAL                                                          LTEOS
      PRINT 5,RHOIN,PTOT,ETOT                                              LTEOS
    5 FORMAT(2X,1P10E12. 5)                                                LTEOS
   10 CONTINUE                                                             LTEOS
      GO TO 6                                                              LTEOS
   11 STOP                                                                 LTEOS
      END                                                                  LTEOS
      SUBROUTINE CRTBND                                                    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 GEN(20),C(2,2),AP(2),RP(2),IROW(2),TEMP(2),TSTORE(100),    LTEOS
     1 ETA1(100),ETA2(100),PRESS1(100),PRESS2(100),ENERG1(100),            LTEOS
     2 ENERG2(100),PCHECK(50),GCHECK(50)                                   LTEOS
      DATA (GEN(I),I=1,14)/0,. 5,1. ,2. ,4. ,8. ,16. ,. 1,. 05,. 005,. 0005,. 00005  LTEOS
     1 ,1. ,2. /                                                           LTEOS
      DIMENSION COLDP(12)                                                  29AP72
      DATA COLDP/. 9524,. 96154,. 97087,. 98039,. 990991,1. 0000,1. 0417,1. 087,  29AP72
     1 1. 1364,1. 1905,1. 250,1. 66666/                                    29AP72
C                                                                          29AP72
C     MAIN SUBROUTINE - IT CALCULATES (IN THIS ORDER) THE T=0 CURVE, THE   29AP72
C     CRITICAL POINT, THE MIXED PHASE REGION AND THE ISOTHERM PRESSURES    29AP72
C     AND ENERGIES                                                         29AP72
C                                                                          29AP72
```

```
C***** SETS UP T=0 CALCULATION ****************************************      29AP72
  200  READ (10,1) ATMNO,ATMWT,R0,S,C0,P0,U,H4                              LTEOS
    1  FORMAT(8E10.3)                                                       LTEOS
       IF(ATMNO .GT. 25. .AND. ATMNO .LT. 27.) GO TO 990                    LTEOS
       IF(ATMWT .EQ. 0) GO TO 1001                                          LTEOS
       B = 125.*R0                                                          LTEOS
       CALL EOS(0,B,.01,PUPPER,EUPPER)                                      LTEOS
       PUPPER = PUPPER*PSI(125.,.01)                                        21AP72
       CALL COLCOF(S,C0,PUPPER,U)                                           LTEOS
       PRINT 4,ATMNO,R0,ATMWT,RCOLD,S,U,C0,P0,PUPPER,H4                     4APR72
    4  FORMAT(1H1,28X,*INPUT PARAMETERS*//*  ATOMIC NUMBER    = *,1PE12.5,  LTEOS
     1 *   NORMAL DENSITY(GM/CM3)  = *,E12.5,/*  ATOMIC WEIGHT    = *,     LTEOS
     2 E12.5,*   COLD DENSITY(GM/CM3)     = *,E12.5/*  HUGONIOT S        = * 4APR72
     3 ,E12.5,*   COHESIVE ENERGY(EV)      = *,E12.5/*  HUGONIOT C0       =  LTEOS
     4 *,E12.5,*   TENSILE STRENGTH(MBARS) = *,E12.5 /32X,*   PRESSURE(ET   LTEOS
     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                           LTEOS
    8  FORMAT(1H0,/*-------------------------------------------------------  EXPLA
     6 */     22X,*T = 0 ISOTHERM CALCULATIONS*//*  GRUNEISEN GAMMA = *,    EXPLA
     1 1PE12.5,/*  MINIMUM PRESSURE LOCATION(ETA) = D1 = *,E12.5//*          EXPLA
     2 EQUATION CONSTANTS*/*  ETA LESS THAN D1-------K = *,E12.5//*  ETA     EXPLA
     3 BETWEEN D1 AND 1.-C1 = *,E12.5/24X,*C2 = *,E12.5/24X,*C3 = *,E12.5     EXPLA
     4 /24X,*C4 = *,E12.5/24X,*C5 = *,E12.5//*  ETA GREATER THAN 1.----A     EXPLA
     5 = *,E12.5/24X,*BR = *,E12.5/24X,*BA = *,E12.5)                        EXPLA
C*************** START OF CRITICAL POINT SEARCH SECTION ***************      LTEOS
       T0 = .05                                                             LTEOS
       ESTART = AK*D1/(AK + 1.) + .11*D1                                    LTEOS
       EREF = 0.                                                            LTEOS
       TREF = 0.                                                            LTEOS
       DELT = 1.                                                            LTEOS
       ITEMP = 8                                                            LTEOS
       IRHO = 8                                                             LTEOS
       DELRHO = GEN(IRHO)                                                   LTEOS
    3  S8 = 1.                                                              LTEOS
       CALL PDPCAL(T0,ESTART,PRES,PRESP,S0,1)                               29AP72
       SREF = S0                                                            LTEOS
       IF(S8*SREF .GT. 0) GO TO 6                                           LTEOS
       ESTART = 1.                                                          LTEOS
       PRINT 5                                                              LTEOS
    5  FORMAT(1X,*AM RESTARTING ETA AT 1.*)                                 LTEOS
       GO TO 3                                                              LTEOS
    6  ESTART = ESTART*(1. - DELRHO)                                        LTEOS
       CALL PDPCAL(T0,ESTART,PRES,PRESP,S0,1)                               29AP72
       IF(S8*S0 .LT. 0) GO TO 10                                            LTEOS
       SREF = S0                                                            LTEOS
       IF(ESTART .GT. .05) GO TO 6                                          LTEOS
       PRINT 7,ESTART                                                       LTEOS
    7  FORMAT(1X,*CAN NOT FIND NEG. SEC. DERV. DOWN TO ETA = *,1PE12.5)     LTEOS
       GO TO 1000                                                           LTEOS
   10  IF(ABS(S0) .LT. 1.E-5) GO TO 15                                      LTEOS
       ESTART = ESTART*(1. + DELRHO*(1. - ABS(SREF/(SREF-S0))))             LTEOS
       CALL PDPCAL(T0,ESTART,PRES,PRESP,S0,1)                               29AP72
       SREF = S0                                                            LTEOS
```

```
      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
```

```
   41  FORMAT(1H0,/*-------------------------------------------------- EXPLA
     1 */22X,*CRITICAL POINT RESULTS*//*  T-CRIT(EV)     = *,1PE15.7/*  P- EXPLA
     2 CRIT(MBARS) = *,E15.7/*  ETA-CRIT        = *,E15.7)             EXPLA
       TCRIT = T0                                                     LTEOS
       ETACRT = ESTART                                                LTEOS
C                                                                     LTEOS
C***** START OF MIXED PHASE BOUNDARY CALCULATION **********************LTEOS
C                                                                     LTEOS
       ETA1(1) = ETACRT                                               LTEOS
       ETA2(1) = ETACRT                                               LTEOS
       PRESS1(1) = PCRIT                                              LTEOS
       PRESS2(1) = PCRIT                                              LTEOS
       ENERG1(1) = ECRIT                                              LTEOS
       ENERG2(1) = ECRIT                                              LTEOS
       TSTORE(1) = TCRIT                                              LTEOS
       ITEMP = 2                                                      LTEOS
       PRINT 42                                                       LTEOS
   42  FORMAT(1H1,1X,*MIXED PHASE BOUNDARY PARAMATERS*//3X,*TEMPERATURE*, EXPLA
     1 8X,*ETA*,9X,*PRESSURE*,7X,*ENERGY*,5X,*GIBBS ENERGY*/7X,*(EV)*,24X EXPLA
     2 ,*(MBAR)*,5X,*(MBAR-CC/GM)*//)                                 EXPLA
       ICYCLE = 1                                                     LTEOS
       DELTP = .05                                                    LTEOS
       DELT = .1                                                      LTEOS
       IF(T0 .LE. 1.) DELT = .05                                      29AP72
       MTEMP = 10.*T0                                                 LTEOS
       TEM = MTEMP                                                    LTEOS
       T0 = TEM/10.                                                   LTEOS
       IF(TCRIT - T0 .LT. DELT) T0 = T0 - DELT                        LTEOS
       E = ESTART - .15                                               LTEOS
       IF(E .LT. 0.) E = .01                                          LTEOS
       CALL PGCAL(0,E,T0,PTO,PPTOT,ETOT,GTOT,GPTOT)                   4APR72
       DO 45 I = 1,100                                                LTEOS
       E = E + .01                                                    LTEOS
       CALL PGCAL(0,E,T0,PNEW,PPTOT,ETOT,GTOT,GPTOT)                  4APR72
       IF (PNEW .GT. PTO ) GO TO 45                                   LTEOS
       SAVE(1) = E - .06                                              LTEOS
       ELOW = E + .01                                                 18APR72
       GO TO 46                                                       LTEOS
   45  PTO = PNEW                                                     LTEOS
       PRINT 43                                                       LTEOS
   43  FORMAT(* FAILED TO FIND STARTING POINT FOR CRITICAL BOUNDARY*) LTEOS
   46  PTO = PNEW                                                     LTEOS
       DO 48 I = 1,100                                                LTEOS
       E = E + .01                                                    LTEOS
       CALL PGCAL(0,E,T0,PNEW,PPTOT,ETOT,GTOT,GPTOT)                  4APR72
       IF(PNEW .LT. PTO ) GO TO 48                                    LTEOS
       SAVE(2) = E + .03                                              LTEOS
       EHIGH = E - .01                                                18APR72
       GO TO 50                                                       LTEOS
   48  PTO = PNEW                                                     LTEOS
   50  CONTINUE                                                       LTEOS
       DO 60 I = 1,50                                                 LTEOS
       S8 = 1.                                                        LTEOS
       DO 55 J = 1,2                                                  LTEOS
```

```
      E = SAVE(J)                                                          LTEOS
      CALL PGCAL(1,E,T0,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(11)                                                 LTEOS
      PCHECK(I) = SAVE(12)                                                 LTEOS
      AP(1) = SAVE(13) - SAVE(11)                                          LTEOS
      AP(2) = SAVE(12) - SAVE(10)                                          LTEOS
      IF(ABS(AP(1)/SAVE(11)) .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(10)) .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(11)) .GT. 1.E-6) GO TO 89                          LTEOS
   64 IF(SAVE(10) .GT. 1.E-8) GO TO 89                                     LTEOS
      IPOS = 0                                                             LTEOS
      IF(SAVE(10) .LT. SAVE(12)) IPOS = 1                                  LTEOS
      SIG = ABS(SAVE(10) - SAVE(12))/(SAVE(10) - SAVE(12))                 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,T0,PTEMP,PPTOT,ETOT,GTEM,GPTOT)                     4APR72
      IPOSP = 0                                                            LTEOS
      IF(SAVE(10) .LT. PTEMP) IPOSP = 1                                    LTEOS
      IF(IPOS .NE. IPOSP) GO TO 62                                         LTEOS
      ITEM = ITEM + 1                                                      LTEOS
   76 CONTINUE                                                             LTEOS
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```
      PRINT 78,T0,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,T0,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 = T0                                                        29AP72
      T0 = T0 + .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) = T0                                                 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,T0,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) T0 = TCYCLE                                      4APR72
      ICYCLE = 1                                                         4APR72
  112 IF(T0 .LT. .11) DELTP = .025                                       LTEOS
      T0 = T0 - DELTP                                                    LTEOS
      IF(T0 .LT. .049) GO TO 150                                         4APR72
      EFAC = 2.                                                          LTEOS
      IF(T0 .LT. .2) EFAC = 1.                                           LTEOS
      SAVE(1) = SAVE(1)/EXP(TCRIT/(EFAC*T0))                             LTEOS
      SAVE(2) = ETA2(ITEMP-1)*1.20                                       LTEOS
      IF(ITEMP .GT. 6) SAVE(2) = 2.*ETA2(ITEMP-1) - ETA2(ITEMP-2)        LTEOS
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      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
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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
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```
      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/R0                                                       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)          LTEOS
      V5=(-A1*Z5*2.)*((1.-(1.+3.*R5)/R8**3)/6.)                           LTEOS
      V6=(Z5/2.)*R7**2+(2.*R6/3.)*(-1./R8**3)                             LTEOS
      V7=(Z5*.5)*(1.-R7**2)                                               LTEOS
      V8=.1-R7**2*(.5-.5*R7+.1*R7**3)                                     LTEOS
      VO=-Z**2*(V1+V2+V3+V4+V5+V6+V7)-FNZR2**2*V8                         LTEOS
      UO=(39.383*VO)/(R*A)*PS                                             21AP72
      IF(KKK.GT.0) GO TO 30                                               LTEOS
      U1=1.5*(P1/RO)+UO*.5                                                LTEOS
      IF(I5 .EQ. 1) GO TO 25                                              LTEOS
      P2 = P1                                                             LTEOS
      U = U1                                                              LTEOS
      GO TO 35                                                            LTEOS
   25 TO = .01                                                            LTEOS
      KKK=1                                                               LTEOS
      GO TO 15                                                            LTEOS
   30 U=1.5*(PO/RO)+UO*.5                                                 LTEOS
      P2=P1-PO                                                            LTEOS
      U=U1-U                                                              LTEOS
   35 RETURN                                                              21AP72
C                                                                         LTEOS
10    FORMAT (*  LOW TEMP.  LOW DENSITY-ACCURACY*)                        LTEOS
11    FORMAT (*  DISCONTINUOUS POTENTIAL POSSIBLE*)                       LTEOS
12    FORMAT (* NO UNIQUE SOL.  CAN BE FOUND*)                            LTEOS
13    FORMAT (* SEE LINE 214*)                                            LTEOS
      END                                                                 LTEOS
      FUNCTION FNI (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 INNER JOIN RADIUS OF ELECTRONIC POTENTIAL                EXPLA
C                                                                         EXPLA
      X1 = S/R                                                            EXPLA
      A1=(Z/FNZR2)*(R/R2/(1.+AO*R2)**2)-R/R2+1.5                          LTEOS
      FNI=27.2*Z/R                                                        LTEOS
      FNI=FNI*(1./X1)*(1./(1.+AO*R*X1)**2)                                LTEOS
      FNI=FNI+27.2*FNZR2*(X1**2/2.-A1)/R                                  LTEOS
      RETURN                                                              LTEOS
      END                                                                 LTEOS
      SUBROUTINE SUB600                                                   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 1/2                    EXPLA
C                                                                         EXPLA
      IF(X .LE. 4.) GO TO 2                                               EXPLA
      Y=.666667*SQRT(X)*X                                                 LTEOS
      Y1=(1.+1.2337/X**2+1.06541/X**4)                                    LTEOS
      IF (X.GT.1.E+6) GO TO 1                                             LTEOS
      Y1=Y1+9.70152/X**6                                                  LTEOS
1     Y=Y*Y1                                                              LTEOS
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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
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      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
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      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                                       EXPLA
      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
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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
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      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))/          LTEOS
     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.)      LTEOS
     1  - 2.)/(D1*AK))/R0                                                    LTEOS
   50 RETURN                                                                 LTEOS
      END                                                                    LTEOS
   50 RETURN                                                                 LTEOS
      END                                                                    LTEOS
      SUBROUTINE PDPCAL(T0,E,PRES,PRESP,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(T0 .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,T0,AP(I1),ETOT)                                           21AP72
    2 I1 = I1 + 1                                                            LTEOS
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```
    3  RP(I) = (AP(I1-1) - AP(I1-2))/(.001*EP)                          LTEOS
       CALL MATINV(P,3,3,IROW,TEMP)                                     LTEOS
       CALL MATMPY(3,3,1,P,3,RP,3,D,3)                                  LTEOS
    5  DO 6 I = 1,3                                                     LTEOS
       AI = I                                                           LTEOS
       EP = E*(1. + .0005*(AI-2.))                                      LTEOS
       CALL PTHERM(EP,T0,PT,PTP,ET,ETP,ST,STP,SI)                       LTEOS
       CALL COLD(EP,PCOLD,PPCOLD,ECOLD,EPCOLD)                          LTEOS
       AP(I) = PTP + PPCOLD                                             LTEOS
       B = EP*R0                                                        29AP72
       CALL EOS(1,B,T0,AP(17+I),DELEE)                                  29AP72
    6  AP(I+3) = PT + PCOLD + AP(17+I)                                  29AP72
       IF(I5 .EQ. 0) GO TO 7                                            29AP72
       PRESPP = D(2) + 2.*E*D(3) + (AP(3) - AP(1))/(.001*E)             29AP72
    7  PRESP = AP(2) + (AP(20) - AP(18))/(.001*E)                       29AP72
       PRES = AP(5)                                                     29AP72
       RETURN                                                           LTEOS
       END                                                              LTEOS
       SUBROUTINE PTHERM(E,T0,PT,PTP,ET,ETP,ST,STP,SI)                  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
C                                                                       EXPLA
C    FOR INPUT TEMPERATURE AND DENSITY, CALCULATES THE THERMAL NUCLEAR  EXPLA
C    CONTRIBUTION TO THE PRESSURE AND ENERGY                            EXPLA
C                                                                       EXPLA
       IPRES = 0                                                        EXPLA
    2  B = .9653/ATMWT                                                  LTEOS
       IF(E .LT. 1.) GO TO 1                                            LTEOS
       GAMP = GAMMA/E + .6666667*((E-1.)/E)**2                          LTEOS
       GAMPP = -GAMMA/E**2 + 4.*(E-1.)/(3.*E**3)                        LTEOS
       DEBYE = H4*EXP((GAMMA/E - (3.*E-1.)/(3.*E**2))*(E-1.))*E**.6666667  LTEOS
       DEBYEP = 2.*DEBYE/(3.*E)+DEBYE*(GAMMA/E**2+2.*(1.-2.*E)/(3.*E**3))  LTEOS
       GO TO 10                                                         LTEOS
    1  IF(E .GT. 1.E-10) GO TO 5                                        LTEOS
       ET = 1.5*B*T0                                                    LTEOS
       ETP = 0.                                                         LTEOS
       PT = R0*E*B*T0                                                   LTEOS
       PTP = R0*B*T0                                                    LTEOS
       T = H4*EXP(1.5 - 2.*GAMMA)                                       LTEOS
       SI = .018596*(R0/ATMWT)**(2./3.)*T0*T/(ATMWT*E**(4./3.))         LTEOS
       ST = -B*(ALOG((.018596*T0/ATMWT)**1.5*R0*E/ATMWT/T0**3) - 2.5)*T0  LTEOS
       STP = -B/E*T0                                                    LTEOS
       GO TO 20                                                         LTEOS
    5  G5 = GAMMA - 1.                                                  LTEOS
       G6 = 1. - 2.*GAMMA                                               LTEOS
       GAMP = E*(G5 + G6*(E-1.))+1.                                     LTEOS
       GAMPP = G5 + G6*(2.*E - 1.)                                      LTEOS
       DEBYE = H4*E*EXP(((3.*GAMMA-2.)+.5*(1.-2.*GAMMA)*(E+1.))*(E-1.))  LTEOS
       DEBYEP = DEBYE/E + DEBYE*(3.*GAMMA-2. + E*(1.-2.*GAMMA))         LTEOS
   10  SI = .018596*(T0/DEBYE**2)*(E*R0/ATMWT)**.6666667/ATMWT          LTEOS
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```
      W = 2.*SI/(3.*E) - 2.*SI*DEBYEP/DEBYE                                  LTEOS
      ET = 1.5*B*T0*(2.+SI)/(1.+SI)                                          LTEOS
      ETP = -ET*W/((1.+SI)*(2.+SI))                                          LTEOS
      PT = R0*E*B*T0*(3.*GAMP + SI)/(1.+SI)                                  LTEOS
      PTP = PT/E-PT*W/(1.+SI)+PT*(3.*GAMPP+W)/(3.*GAMP+SI)                   LTEOS
      ST=-T0*B*(3.*ALOG(DEBYE/T0)- 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))*T0     LTEOS
   20 IF(IPRES .GT. 0) GO TO 30                                              LTEOS
      IPRES = IPRES + 1                                                      LTEOS
      S1 = SI                                                                LTEOS
      ET1 = ET                                                               LTEOS
      PT1 = PT                                                               LTEOS
      ST1 = ST                                                               LTEOS
      ETP1 = ETP                                                             LTEOS
      PTP1 = PTP                                                             LTEOS
      STP1 = STP                                                             LTEOS
      T1 = T0                                                                LTEOS
      T0 = .01                                                               LTEOS
      GO TO 2                                                                LTEOS
   30 T0 = T1                                                                LTEOS
      SI = S1                                                                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 ************************ LTEOS
      A = B0                                                             LTEOS
      B1 = 1.25*ALOG(A0/(3100.*B0))                                      LTEOS
      B2 = B1                                                            LTEOS
      DO 5 J = 1,100                                                     LTEOS
      P(1,1) = 3125.*EXP(.8*B1) - 25.*EXP(.8*B2)                         LTEOS
      P(2,1) = 1. + B1/3. - B2/3.                                        LTEOS
      P(3,1) = 1.333333 + TTHIRD*B1 + B1**2/9. - B2**2/9.                LTEOS
      RP(1) = A0 - P(1,1)*A                                              LTEOS
      RP(2) = B0 - P(2,1)*A                                              LTEOS
      RP(3) = D0 - P(3,1)*A                                              LTEOS
      IF (ABS(RP(1)/A0) .GT. .00001 ) GO TO 1                            LTEOS
      IF(ABS(RP(2)/B0) .GT. .00001) GO TO 1                              LTEOS
      IF(ABS(RP(3)/D0) .LE. .00001) GO TO 15                             LTEOS
    1 P(1,2) = 2500.*A*EXP(.8*B1)                                        LTEOS
      P(2,2) = A/3.                                                      LTEOS
      P(3,2) = A*(TTHIRD + 2.*B1/9.)                                     LTEOS
      P(1,3) = -20.*A*EXP(.8*B2)                                         LTEOS
      P(2,3) = -A/3.                                                     LTEOS
      P(3,3) = -2.*B2*A/9.                                               LTEOS
      CALL MATINV(P,3,3,IROW,TEMP)                                       LTEOS
      CALL MATMPY(3,3,1,P,3,RP,3,D,3)                                    LTEOS
      A = A + D(1)                                                       LTEOS
      B1 = B1 + D(2)                                                     LTEOS
    5 B2 = B2 + D(3)                                                     LTEOS
      WRITE (9,10)                                                       LTEOS
   10 FORMAT(3X,*HAVE DONE 100 ITERATIONS, CAN NOT CONVERGE*)            LTEOS
      GO TO 50                                                           LTEOS
   15 GAMMA = (D0 + TTHIRD*B0)/(2.*B0) - .3333333333                     LTEOS
      B = R0*D1                                                          4APR72
      CALL EOS(1,B,.02,DELPE,DELEE)                                      4APR72
      CALL PTHERM(D1,.02,PT,PTP,ET,ETP,ST,STP,SI)                        4APR72
      DELPEP = DELPE + PT                                                4APR72
      P0 = PSAVE - DELPEP                                                4APR72
      R0 = RSAVE                                                         4APR72
      CALL EOS(1,RSAVE,.02,DELPE,DELEE)                                  4APR72
      CALL PTHERM(1.,.02,PT,PTP,ET,ETP,ST,STP,SI)                        4APR72
      DELPEP = DELPE + PT                                                4APR72
      R0 = RCOLD                                                         4APR72
C********** PRESSURE CALCULATION FOR S/(S+1) LT. ETA LT. 1 ************* LTEOS
      D2 = 1. - D1**THIRD                                                LTEOS
      C1 = -P0/(D1*D1**THIRD*D2)                                         LTEOS
      C2 = C1*(5.*D1**THIRD - 4.)/(D1**THIRD*D2)                         LTEOS
      C3 = (3.*B0 - C1 - C2*D2)/D2**2                                    LTEOS
      G1 = 9.*D0 - 6.*C1 - (2.+6.*D2)*C2 - (6.*D2**2+4.*D2)*C3           LTEOS
      C4 = G1/(2.*D2**2)                                                 LTEOS
      G1 = 20.*R0*U - 30.*C1-(30.*D2-20.)*C2-(15.-40.*D2+30.*D2**2)*C3   LTEOS
      C5 = (G1-(30.*D2-12.-20.*D2**2)*C4)/(10. -24.*D2+15.*D2**2)        LTEOS
C********** PRESSURE CALCULATION FOR ETA LT. S/(S+1) ******************* LTEOS
      IF(NTRY .GT. 1) GO TO 105                                          4APR72
      E = 1.                                                             4APR72
      NTRY = 2                                                           4APR72
      DO 100 I = 1,10                                                    4APR72
      CALL COLD(E,PTEST(I),PPCOLD,ECOLD,EPCOLD)                          4APR72
```

```
      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 PTHERM(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 MESG(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/,(MESG(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
```

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