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Interim Report

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This is an interim report. The final report will appear in the *Journal of Physical and Chemical Reference Data*.

This report is to be superseded by a future publication which will receive general distribution and should be cited as a reference. Please consult the NBS Office of Technical Information and Publications to obtain the proper citation.

Prepared for
The Office of Standard Reference Data
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The Equation of State for Ammonia

by

Lester Haar and John Gallagher

1. Introduction.

In this report, we present an outline of the basic results of an extensive correlation of the thermodynamic properties of ammonia¹. The purpose of this report is to present an early working version of that correlation for the convenience of those workers with an immediate need for such results and to which they can refer in an unambiguous manner. This report has been prepared in answer to several urgent requests for such a version.

We present the basic equations used for the description of the properties of ammonia and listings of computer programs from which all the thermodynamic properties for ammonia can be calculated for the temperature range including the triple point temperature to about 5/3 the critical temperature and for the pressure range including the dilute gas to about 8000 bars. The reference state for all properties is the ideal gas at zero kelvin. The physical constants used are consistent with those recommended by Cohen and Taylor². The mass of a mole of ammonia was taken to be 17.03026 grams³.

2. The derivation of the thermodynamic surface.

In this section, we describe the results of a fit of selected P, ρ, T data schematically represented in figure 1 to an analytic equation of state in the least squares sense. A detailed discussion of the process of data selection and of the selection of parts of the analytic equation is contained in reference 1. The equation so obtained contains the pressure as a 44 term double power series function of temperature and density. This equation can then be used to

reproduce all the available P, ρ, T experimental data as well as to produce limited extrapolations (based on thermodynamic arguments) of the surface into important regions where data are sparse. The range of the equation is bounded at low temperatures by the triple point temperature (195.48K) and the melting curve for the liquid, and at high temperatures by the isotherm at 750K (which is approximately 5/3 the critical temperature). The pressure range extends to 8,000 bar. No mathematical constraints were imposed on the equation, and only P, ρ, T data were used in the least squares fit.

Following Keenan et al. the Helmholtz free energy function was represented in reference 1 as the sum of two terms: the first is the contribution from the equation of state; the second is a function of temperature only and refers to the properties of the ideal gas. Thus the Helmholtz free energy was expressed,

$$A(\rho, T) = \bar{A}(\rho, T) + A^0(T), \quad (1)$$

where $A^0(T)$ is the contribution of the ideal gas. T is the absolute temperature in Kelvin and ρ is the density in grams per cm^3 . A quantity $Q(\rho, T)$ was defined by

$$\bar{A}(\rho, T) \equiv RT [\ln \rho + \rho Q(\rho, T)] \quad (2)$$

Since $P = \rho^2 \partial A / \partial \rho$,

Eqs. (1) and (2) yield,

$$P = \rho RT [1 + \rho Q + \rho^2 \partial Q / \partial \rho] . \quad (3)$$

We note that

$$Q(\rho=0) = B_2, \quad (3a)$$

where B_2 is the second virial coefficient. The form chosen for Q was

$$Q = \sum_{i=1}^9 \sum_{j=1}^6 a_{ij} \rho^{i-1} (\tau - \tau_c)^{j-1}, \quad (4)$$

where $\tau = \frac{500}{T}$, $\tau_c = 1.2333498$ and R is the gas constant. Equation 3 for the pressure was fitted in the least squares sense to the experimental P, ρ, T data. The results of this fit are values for the constants a_{ij} listed in table 1. ($a_{ij} = 0$ for all ij not listed in table 1). By differentiation of eq (1) we obtain for the entropy,

$$S(\rho, T) = R[\ln \rho + \rho Q - \rho \tau \partial Q / \partial \tau] + S^0(T), \quad (5)$$

the internal energy,

$$E(\rho, T) = R \rho T \tau \partial Q / \partial \tau + E^0(T), \quad (6)$$

the constant volume heat capacity,

$$C_v(\rho, T) = -R \rho \tau^2 \partial^2 Q / \partial \tau^2 + C_v^0, \quad (7)$$

Table 1

i	j	a_{ij}
1	1	-6.4690439557
1	2	-13.295625875
1	3	-8.1211770915
1	4	-6.9690043553
1	5	-9.7365802349
1	6	3.4816642617
2	1	8.8100445762
2	2	-5.0789548707
2	3	-68.261583422
2	4	-74.727156949
2	5	49.751854179
2	6	-14.487156374
3	1	-10.467902857
3	2	361.91907645
3	3	1327.8270222
3	4	1484.2843304
3	5	-82.229122939
3	6	20.170856719
4	1	75.049574001
4	2	-2103.9451938
4	3	-7576.1007937
4	4	-8334.8746422
4	5	43.998475959
4	6	-9.2773376718
5	1	-409.02964153
5	2	6212.2822515
5	3	22341.800329
5	4	23618.791735
6	1	1072.479955
6	2	-10816.10642
6	3	-38259.344112
6	4	-38233.534003
7	1	-1471.4013145
7	2	11195.138723
7	3	38544.628190
7	4	35887.294649
8	1	1046.2341301
8	2	-6365.7466698
8	3	-21314.815310
8	4	-18162.094974
9	1	-305.80081169
9	2	1532.0616045
9	3	5021.6962092
9	4	3812.3691534

the enthalpy function,

$$H(\rho, T) = RT[\rho Q + \rho^2 \partial Q / \partial \rho + \rho \tau \partial Q / \partial \tau + 1] + E^{\circ}(T), \quad (8)$$

the constant pressure heat capacity,

$$C_p(\rho, T) = C_v + R \cdot \frac{\alpha}{\beta}, \quad (8a)$$

where,

$$\alpha = 1 + \rho Q + \rho^2 \partial Q / \partial \rho - \rho \tau \partial Q / \partial \tau - \rho^2 \tau \partial^2 Q / \partial \tau \partial \rho,$$

and

$$\beta = 1 + 2 \rho Q + 4 \rho^2 \partial Q / \partial \rho + \rho \partial^2 Q / \partial \rho^2,$$

the heat capacity for the saturated fluid,

$$C_s = C_p - \frac{T}{\rho^2} \frac{(\partial P / \partial T)_{\rho}}{(\partial P / \partial \rho)_T} \cdot \frac{dP_s}{dT}, \quad (9)$$

where P_s is the vapor pressure of the liquid.

S° , E° and C_v° are the corresponding contributions obtained from $A^{\circ}(T)$:

$$A^{\circ}(T) = (G^{\circ} - E_0^{\circ}) - RT(1 + \ln 4.8180 T),$$

$$S^{\circ} = - \frac{d}{dT} A^{\circ}(T),$$

$$E^{\circ} = A^{\circ}(T) - T \frac{dA^{\circ}(T)}{dT}, \quad (10)$$

$$C_v^{\circ} = - T d^2 A^{\circ}(T) / dT^2,$$

where G° is an analytic representation of the results reported by Haar⁵ for the properties of the ideal gas state,

$$\frac{G^\circ - E_0^\circ}{RT} = a_1 \ln T + \sum_{i=2}^{11} a_i T^{i-3}, \quad (10a)$$

where E_0° is the energy for the ideal gas at 0 K. The coefficients a_i are listed in table 2.

Table 2

a_1	=	-3.872727
a_2	=	.64463724
a_3	=	3.2238759
a_4	=	-.0021376925
a_5	=	.86890833x10 ⁻⁵
a_6	=	-.24085149x10 ⁻⁷
a_7	=	.36893175x10 ⁻¹⁰
a_8	=	-.35034664x10 ⁻¹³
a_9	=	.2056303x10 ⁻¹⁶
a_{10}	=	.6853420x10 ⁻²⁰
a_{11}	=	.9939243x10 ⁻²⁴

The heat capacity values and the other thermodynamic functions calculated from eq (10a) for the temperature range $100 \text{ K} \leq T \leq 1000 \text{ K}$ agree with those tabulated in reference 5 to within the accuracy of those values.

Though equations (1-10a) are complete, it is necessary to introduce the Gibbs phase conditions in order to calculate the properties for the coexisting phases. However, it was shown by Haar and Gallagher¹, that almost negligible error results if an explicit relation is used for P_g fitted separately to the saturated vapor pressure data of Cragoe⁶ for the range from the triple point to 373K and of the mean of the data of Beattie and Lawrence⁷ and Keyes⁸ above 373K. The equation so obtained is

$$\log_e P_s = \frac{A}{T} + B + CT + DT^2 + ET^3$$

T in kelvin (IPTS68), P in atm.

- A = -3684.7798
- B = 20.428787 (10b)
- C = -.02893289
- D = 3.4798128x10⁻⁵
- E = -9.2219845x10⁻⁹ .

Equation (10b) and eq (3) define the coexisting phases for this report and all properties over the temperature-pressure range of the thermodynamic surface, subject to the low temperature boundary of the melting solid. The thermodynamic surface is consistent with the following values for the parameters at the triple point,

$$T_t = 195.48 \text{ K}$$

$$P_t = .06063 \text{ bar}$$

$$\rho_t^g = .00006382 \text{ g/c}^3, \rho_t^l = .73374 \text{ g/c}^3,$$

and at the critical point,

$$T_c = 405.4 \text{ K}$$

$$P_c = 113.04 \text{ bar}$$

$$\rho_c = .2350 \text{ g/c}^3$$

The relationship between the pressure and temperature of the melting solid was calculated by means of the Clapyron equation, using the latent heat of fusion and the specific volumes for the saturated liquid and solid. For the latent heat, the value reported by Overstreet and Giauque⁹ was used; for the specific volume for the solid at the normal melting point, the value reported by McKelvey and Taylor¹⁰ was used, and for the corresponding specific

volume of the liquid the value reported by Cragoe and Harper¹¹ was used.

The Clapeyron equation is the relation

$$\frac{dT}{T} = \frac{u' - u}{L} dP, \quad (11)$$

where the quantities u' and u refer to the specific volumes of the liquid and solid, respectively, and L refers to the latent heat of fusion. From the above data, the quantity $\frac{u' - u}{L} \approx 4 \times 10^{-5} \text{ atm}^{-1}$; and Eq (11) can be integrated to yield

$$T = T_s \exp[4 \times 10^{-5} (P - P_s)], \quad (12)$$

where T_s and P_s are the triple point values. (The differences between the triple point values and those of the normal melting point are negligible.) Also, since P_s at the triple point is very small, the relationship can be simplified to

$$T = 195.48 \exp \{4 \times 10^{-5} P (\text{atm})\}. \quad (13)$$

3. Computer programs.

The properties calculated from the equations presented in this report have been compared with the various thermodynamic measurements reported for ammonia in the comprehensive review in reference 1. In almost all cases the agreement is within the experimental accuracy of the data. Comparisons of results with P, ρ, T data are given here in figures 2 and 3. It was established in reference 1 that for most of the vapor phase and for the coexisting phases, the calculated enthalpies are accurate to within 0.1%.

To facilitate the application of these results we present in Appendices I and II computer programs with which the various properties of ammonia can be calculated. Two such programs are included:

Computer program I in Appendix I refers only to certain properties for the coexisting phases, including the latent heat of vaporization, the vapor pressure of the saturated liquid, the densities of the saturated vapor and the saturated liquid. The dependent variable for these is either the temperature or the corresponding pressure of the saturated liquid.

Computer program II in Appendix II is a general program for all the thermodynamic properties discussed in section 2 of this report. The dependent variables are either pressure and temperature or density and temperature.

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Figure Caption

Fig. 1. P-T Schematic of the data included in this correlation. The various polygons represent the range of the individual sets. The numbers refer to references in this report for the sources of the various data sets.

Figs. 2,3. Comparisons of calculated values with P, ρ ,T data. The results are presented as fractional differences in percent vs pressure in atmospheres. The numbers to the left of the various plots refer to data references in the text. Figure 2 refers to pressure deviations for densities less than 1.5 times the critical density. Figure 3 refers to density deviations for values of density greater than 1.5 times the critical density.

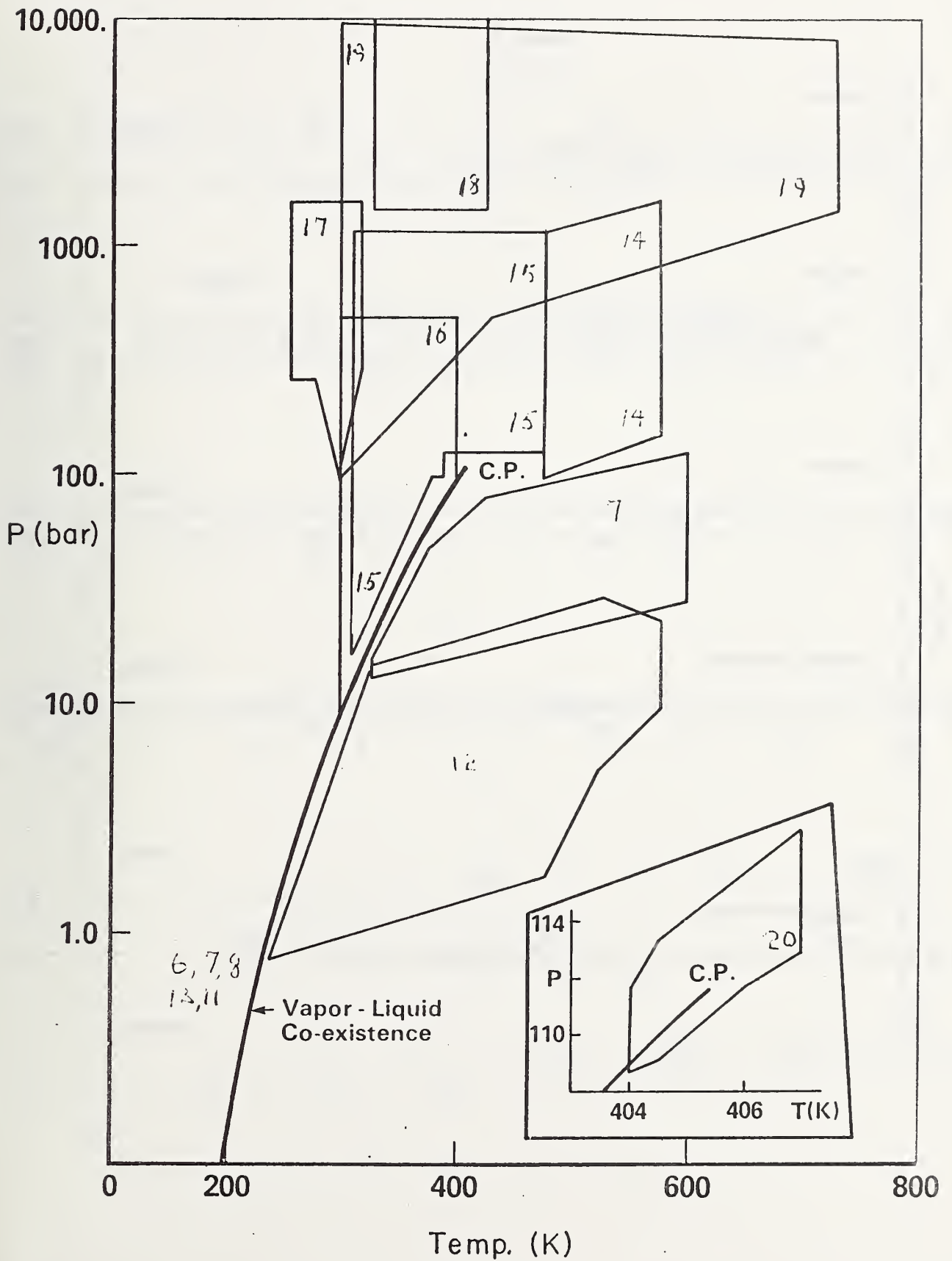


FIG. I

Figure 2

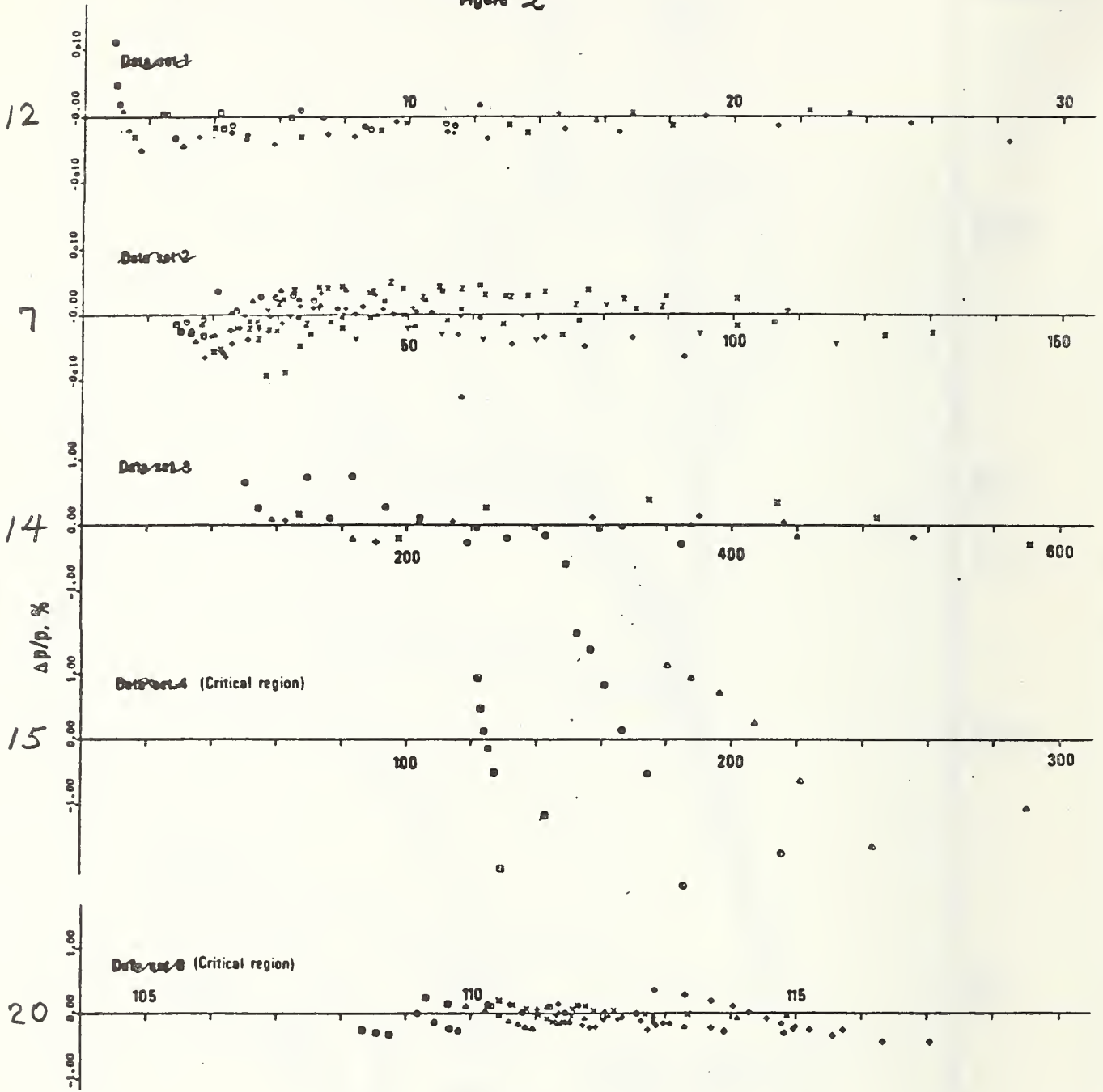
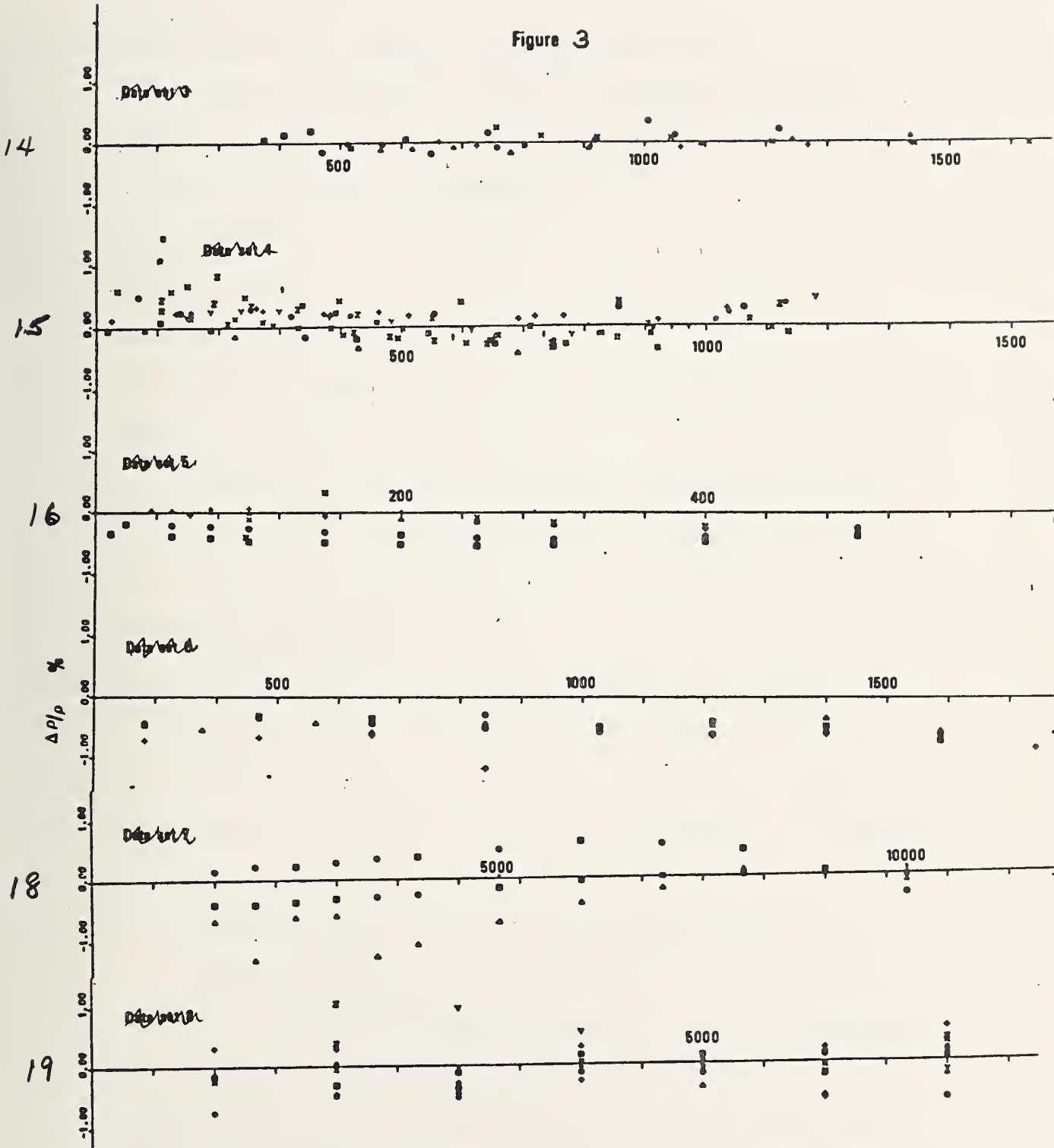


Figure 3



Listing of Fortran program I:

Temperatures, Pressures and Densities along Saturation Curve.

- A. The saturation pressure as a function of temperature and the saturation temperature as a function of pressure; where T is in degrees K, and p in atmospheres.

Function PS(T)

Function TS(P)

Function DPSDT(T)

- B. The saturation liquid and vapor densities as a function of Temperature: (densities in gram/cm^3).

1. SUBROUTINE DS(T,DL,DG) to calculate approximate densities from a simple polynomial to be used as initial guesses for the subroutine DFIND which will improve upon these by an iterative process.
2. SUBROUTINE DFIND(DOUT,P,DGUESS,T,DPDD) where P,T,DGUESS are inputs, DOUT and DPDD ($\partial P/\partial \rho$) are outputs and which also uses
3. Function PRES(D,T) which calculates the pressure in atmospheres at any point D and T

SUBROUTINE QQ(Q,L,K,T,D) which calculates "Q" or the derivatives $\frac{\partial^{L+K} Q}{\partial \rho^L \partial \tau^K}$ at any point T and D.

- C. SUBROUTINE HV(HH,T,DL,DG) which calculates the heat of vaporization as a function of T and the previously calculated liquid and vapor densities. The HV calculated here will be in dimensionless units, and to obtain results in joules per gram multiply by .4882 T or in BTU/lb. multiply by .210027 T (T in both cases in kelvins).

- D. Units and conversion factors: a package of subroutines is included which will convert Temp. in °F to K or K to °F, and P in PSIA to atm. or atm. to PSIA, and densities in lb/ft^3 to gm/c^3 or gm/c^3 to lb/ft^3 .


```

FUNCTION PS(T)
PL=-3684.7798/T+20.428787+T*(-.02693289+T*(3.4798128E-5-T*9.221984
15E-9))
PS=EXP(PL)
RETURN
END

```

```

FUNCTION TS(P)
Q=1./P
T=252.10703 + P*(5.6658636+P*(-.12457077+P*(.00135987-P*.000005319
142))) + Q*(-15.379678+Q*(1.528315-Q*.04906))
DTDP=1./DPSDT(T)
5 PX=PS(T)
IF(ABS(1.-P/PX).LT.1.E-5) GO TO 10
DT=(P-PX)*DTDP
T=T+DT
GO TO 5
10 TS=T
RETURN
END

```

```

FUNCTION DPSDT(T)
DF=-.02893289+3684.7798/T/T+6.9596256E-5*T-2.76659535E-8*T*T
DPSDT=DF*PS(T)
RETURN
END

```

```

SUBROUTINE DS(T,DL,DG)
DOUBLE PRECISION T,DL,DG
DC=.235
IF(T-405.4) 10,80,90
10 DT=1.-T/405.4
IF(T.LT.395.) GO TO 100
T1=DT**.25
T2=DT**.541
T3=T2*T2
T4=DT*.2653
DL=T4+T1*(2.117-1.4007*T2-.89802*T3)
DG=T4-T1*(2.117+1.1390*T2+.57253*T3)
DL=DC*(DL+1.)
DG=DC*(DG+1.)
RETURN
80 DL=DC
DG=DC
RETURN
90 DL=0.
DG=0.
RETURN
100 Q=DT
DL=.387131-.00096947/Q+Q*(1.1513875+Q*(-1.4943106+Q*1.1183325))
DG=.0828867+.00095867/Q+Q*(-.60039534+Q*(1.4434594
1 -Q*1.1678605))
RETURN
END

```

```

SUBROUTINE DFIND(DOUT,P,D,T,DPD)
COMMON /QQQQ/ Q0,Q1,Q2,Q10,Q20,Q11
DD=D
IF(T.LT.223.1 .AND. D.GT..01 .AND. D.LT..7) DD=.73
L=0
10 L=L+1
IF(DD.LE.0.) DD=1.E-8
IF(DD.GT..2) DD=.2
CALL QQ(Q0,0,0,T,DD)
CALL QQ(Q1,0,1,T,DD)
CALL QQ(Q2,0,2,T,DD)
DPD=DPDD(DD,T)
DPDX=DPD
IF(DPDX.LT.50.) DPDX=50.
PP=PRES(DD,T)
IF(ABS(1.-PP/P).LT.1.E-5) GO TO 20
X=(P-PP)/DPDX
DD=DD+X
IF(L.LE.20) GO TO 10
20 CONTINUE
30 DOUT=DD
RETURN
END

```

```

FUNCTION TK(TF)
TK=(TF+450.67)*5./0.
RETURN
END

```

```

FUNCTION PATM(PSIA)
PATM=PSIA/14.696
RETURN
END

```

```

FUNCTION DGCC(DLRCE)
DGCC=DLRCE/62.428
RETURN
END

```

```

FUNCTION DLRCE(DGCC)
DLRCE=DGCC*62.428
RETURN
END

```

```

FUNCTION PSIA(PATM)
PSIA=PATM*14.696
RETURN
END

```

```

FUNCTION TF(TK)
TF=1.8*TK-450.67
RETURN
END

```

```
SUBROUTINE QQ(Q,L,K,T,L)
```

```
  DIMENSION P(5,5),DD(12),TT(7),A(44),TT(44),JJ(44),A1(22),A2(22)
```

```
  EQUIVALENCE (A1(1),A(1)),(A2(1),A(22))
```

```
  DATA TT/6*1,6*2,6*3,6*4,4*5,4*6,4*7,4*8,4*9/,N/44/
```

```
  DATA JJ/1,2,3,4,5,6,1,2,3,4,5,6,1,2,3,4,5,6,1,2,3,4,5,6,1,2,3,4,1,1,2,3,4,1,2,3,4,1,2,3,4/
```

```
  DATA P/2.,2.,3.,4.,5.,2.,4.,6.,12.,20.,3.,6.,12.,24.,60.,4.,12.,124.,48.,120.,5.,20.,60.,120.,240./
```

```
  DATA A1/-6.469043956 , -13.29562588 , -8.121177092 , -6.969004355 ,  
1 -9.736580235 , 3.481664262 , 8.810044576 , -5.078954571 , -68.2615834  
22 , -74.72715095 , 49.75105410 , -14.40715637 , -10.46790286 , 361.9190  
3765 , 1327.827022 , 1484.284330 , -82.22912294 , 20.17085672 ,
```

```
4 75.04957400 , -2103.945194 , -7576.100794 , -8334.874642 /
```

```
  DATA A2/43.97847596 , -9.277337672 , -409.0296415 , 6212.282252 ,  
122341.80033 , 23618.79174 , 1072.479955 , -10816.10642 , -38259.34411  
2, -38233.55400 , -1471.401315 , 11155.13872 , 38544.62017 , 35837.29465  
3 , 1046.234130 , -6365.758670 , -21314.81551 , -18162.09497 , -305.8008  
4117 , 1532.061605 , 5021.696209 , 3812.369153 /
```

```
  Q=0.
```

```
  IF(L+K) 12,14,18
```

```
12 RETURN
```

```
14 U=500./T
```

```
  C=U-1.23334077800
```

```
  IF(DABS(C).LT.1.D-8) C=1.D-8
```

```
  TT(1)=1.
```

```
  DO 15 I=2,7
```

```
15 TT(I)=TT(I-1)*C
```

```
  IF(D.LT.1.E-8) D=1.E-8
```

```
  DD(1)=1.
```

```
  DO 16 I=2,10
```

```
16 DD(I)=DD(I-1)*D
```

```
18 DO 200 M=1,N
```

```
  I=II(M)
```

```
  J=JJ(M)
```

```
  IF(J-L-1) 200,20,30
```

```
20 IF(L) 200,24,28
```

```
24 QT=1.
```

```
  GO TO 50
```

```
28 QT=P(L,L)/2.
```

```
  GO TO 50
```

```
30 IF(L) 200,32,40
```

```
32 QT=TT(J)
```

```
  GO TO 50
```

```
40 QT=P(L,J-1)*TT(J-L)
```

```
50 IF(K) 200,60,70
```

```
60 QT=QT*DD(I)
```

```
  GO TO 100
```

```
70 R=1.
```

```
  DO 72 MM=1,K
```

```
72 R=R*(1-MM)
```

```
  QT=QT*R*DD(I-K)
```

```
100 Q=Q+A(K)*QT
```

```
200 CONTINUE
```

```
  RETURN
```

```
  END
```

```

FUNCTION HV(T,DL,DG)
U=500./T
CALL QQ(Q0,0,0,T,DL)
CALL QQ(Q1,0,1,T,DL)
CALL QQ(Q2,1,0,T,DL)
CALL QQ(S0,0,0,T,DG)
CALL QQ(S1,0,1,T,DG)
CALL QQ(S2,1,0,T,DG)
HV=U*(DG*S2-DL*Q2) + DG*(S0+DG*S1) - DL*(Q0+DL*Q1)
RETURN
END

```

A SAMPLE PROGRAM TO CALCULATE, FOR INSTANCE, THE SATURATION TEMPERATURE IN DEG F, DENSITIES IN LB/CU FT AND HEAT OF VAPORIZATION IN BTU/LB AT A GIVEN PRESSURE IN PSIA COULD BE AS FOLLOWS -

```

READ 1,PSI
1 FORMAT(5F10.2)
P=PATM(PST)
T=TS(P)
CALL DS(T,XDL,XDG)
CALL DFIND(DL,P,XDL,T,DX)
CALL DFIND(DG,P,XDG,T,DY)
HH=HV(T,DL,DG)*.210027*T
DL=DLRCF(DL)
DG=DLRCF(DG)
T=TF(T)
PRINT 1, PSI,TT,DL,DG,HH
STOP
END

```

Listing of Fortran Program II:

Routines for calculating at any point on the thermodynamic surface.

Subroutine FZ(T,F,DF,DDF,DTF) which calculates for a given temperature T in deg K, the ideal gas functions for the free energy F, entropy DF, C_p , DDF, and internal energy DTF, all in dimensionless units.

Functions for calculating internal energy, enthalpy, entropy, C_p and C_v as functions of D,T and ideal gas functions, all in dimensionless units.

Phase finder: SUBROUTINE PHASE (P,T,DL,DG,K) which will, for any point P and T supplied, return a value of K as follows:

K=0 point is on sat. curve. guesses for DL and DG returned

K=1 $T < T_c$, vapor phase. guess for DG returned, DL set = DG

K=2 $T < T_c$, liquid phase. guess for DL returned, DG set = DL

K=3 $T > T_c$ DG=DL, guess returned.

K=-1 error return for $T \leq$ or $P \leq 0$. or for either P missing and $T > T_c$.

for $T < T_c$, and P missing or = 0., P_{sat} will be calculated, and the appropriate densities found. Similarly, for $P < P_c$ and T missing or = 0., T_{sat} will be calculated.

```

SUBROUTINE FZ(T,F,DF,DDF,DTF)
DOUBLE PRECISION T
DIMENSION A(12)
DATA A/-.3.872727,.64463724,.3.2238759,-.0021376925,.86890833E-5.
1 -.24085149E-7,.36893175E-10,-.35034664E-13,.20563027E-16,
2 -.685042E-20,.99392427E-24,0./
U=T
IF(T.LE.10.) U=10.
F=A(1)*ALOG(U)+A(2)/U+A(3)+A(4)*U+A(5)*U*U+A(6)*U**3+A(7)*U**4
1 +A(8)*U**5+A(9)*U**6+A(10)*U**7+A(11)*U**8
DF=A(1)*(ALOG(U)+1.)+A(3)+2.*A(4)*U+3.*A(5)*U*U+4.*A(6)*U
1**3+5.*A(7)*U**4+6.*A(8)*U**5+7.*A(9)*U**6+8.*A(10)*U**7
2 +9.*A(11)*U**8
DDF=A(1)/U+2.*A(4)+6.*A(5)*U+12.*A(6)*U*U+20.*A(7)*U**2+30.*A(8)*
1 U**4+42.*A(9)*U**5+56.*A(10)*U**6+72.*A(11)*U**7
DDF=-DDF*U
DF=-DF
DTF=DF+F-1.
RETURN
END

```

```

SUBROUTINE PHASE(P,T,DL,DG,K)
IF(P) 10,10,20
10 IF(T-105.) 00,12,12
12 IF(T-405.5) 14,00,00
14 P=PS(T)
16 CALL DS(T,DL,DG)
K=0
RETURN
20 IF(T) 22,22,30
22 IF(P-111.55) 24,24,00
24 IF(P-.06) 00,26,26
26 T=TS(P)
GO TO 16
30 IF(T-405.5) 32,50,50
32 PX=PS(T)
34 CALL DS(T,DL,DG)
IF(P-PX) 36,14,40
36 DG=DG*P/PX
DL=DG
K=1
RETURN
40 DG=DL
K=2
RETURN
50 D=P*(.0002107-5.19E-8*P-2.289E-7*T)-1.2823E-6*T
D=D+P/T/4.818
IF(D.LT.1.E-5) D=.00001
DL=D
DG=DL
K=3
RETURN
90 DL=0.
DG=0.
K=-1
RETURN
END

```

```

SUBROUTINE THERMF(D,T,CP,CV,F,H,S)
COMMON /QQQQ/ Q00,Q01,Q02,Q10,Q20,Q11
U=500./T
CALL QQQ(Q00,0,0,T,D)
CALL QQQ(Q01,0,1,T,D)
CALL QQQ(Q02,0,2,T,D)
CALL QQQ(Q10,1,0,T,D)
CALL QQQ(Q20,2,0,T,D)
CALL QQQ(Q11,1,1,T,D)
CALL FZ(T,FT,SIG,CPIG,FIG)
ENER=D*U*Q10 + FIG
ENTH=ENER + 1. + D*Q00 + D*D*Q01
FNTR=SIG+D*U*Q10-D*Q00-ALOG(4.818*D*T)
CV=CPIG-1.-D*U*U*Q20
CP=(1.+D*(Q00-U*Q10+D*(Q01-U*Q11)))**2/(1.+D*(2.*Q00+D*(4.*Q01+D*
1 Q02)))+CV
RETURN
END

```

THE FOLLOWING SAMPLE PROGRAM WILL CALCULATE THE DENSITY AND FIVE THERMODYNAMIC FUNCTIONS AT A POINT (P,T) SUPPLIED. P SUPPLIED IN BAR, T IN DEG C DENSITY IN GM/CC, CP,CV,S IN JOULES/GM DEG C, AND INTERNAL ENERGY, ENTHALPY IN JOULES/GM.

```

1 READ 2, PBAR,TC
2 FORMAT(2F10.3,F10.6,2F10.3,3F10.5)
P=PBAR/1.01325
IF(P.LE.0.) STOP
T=TC+273.15
CALL PHASE(P,T,DL,DG,K)
IF(K.EQ.-1) GO TO 1
CALL DFIND(D,P,DL,T,DX)
CALL THERMF(D,T,CP,CV,F,H,S)
CP=CP*.4882
CV=CV*.4882
S = S*.4882
H=H*.4882*T
E=F*.4882*T
PRINT 2, PBAR,TC,D,H,F,S,CP,CV
GO TO 1
END

```


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