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A MODIFIED BENEDICT-WEBB-RUBIN EQUATION OF STATE FOR PARAHYDROGEN-II

H. M. Roder
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Final Report

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SYMBOLS

A = parameters for equation 1
B = parameters for vapor pressure equation
C_p = specific heat at constant pressure
C_v = specific heat at constant volume
G = parameters for equation for saturation densities
N or G = parameters for equation of state
n = index of refraction
P = pressure
R = gas constant
r = parameters for index of refraction equation
T = temperature, T_{68} the International Practical Temperature Scale
x = reduced temperature
β = scaling law parameter
Φ = energy derivative
θ = specific heat input
ρ = density

Subscripts:

c = critical point
g = gaseous phase
ℓ = liquid phase
t = triple point

UNITS

The primary variables in the computer programs are

Pressure in atmospheres

Density in moles/liter, and

Temperature in Kelvin.

Conversions to other SI units and units normally used in applied problems are given in appendix C.

A MODIFIED BENEDICT-WEBB-RUBIN EQUATION OF STATE FOR PARAHYDROGEN - II

Hans M. Roder and Robert D. McCarty

A 32 term modified Benedict-Webb-Rubin equation of state has been applied to data for parahydrogen. The adjustable parameters in the equation of state were determined using 2665 points including very recent measurements at low temperatures and high pressures. The new values extend the range of the PVT data sufficiently to warrant a refitting of the equation of state. Temperatures for the data range from the triple point to about 700 K with pressures reaching 3000 atmospheres near ambient temperatures. The PVT data were adjusted to the T_{68} scale. In addition, extensive modifications have been made to the previously accepted PVT surface in the region near the critical point. These adjustments have been made on the basis of more recent refractive index data and the application of scaling law equations. Detailed comparisons between experimental and calculated values are given for density. Corresponding comparisons are made for enthalpy and the specific heat at constant pressure.

Key words: Critical point; density; enthalpy; equation of state; hydrogen; index of refraction PVT; saturation properties; scaling laws; specific heat.

1. Introduction

Almost all engineering problems requiring thermodynamic data for the cryogenic fluids are most easily solved by using an equation of state to describe the PVT surface of the gas, and to calculate values of such variables as enthalpy and specific heat. Quite often some modification of the Benedict-Webb-Rubin (1940) equation of state (hereafter referred to as MBWR) is preferred, because equations of this type are relatively easy to handle on a computer.

This report describes an accurate wide-range MBWR equation of state for parahydrogen[*]. The study of the equation of state was actually completed in two phases. The first phase was sponsored by the NASA-Lewis Research Center (P.O. C-32369-C) and is summarized in a report by McCarty (1974). The earlier work gives a review of the adjustments made to achieve the International Practical Temperature Scale, T_{68}, as defined in Metrologia (1969). Changes were made in the PVT data, in the vapor pressure curve, in the critical parameters, and in the two phase envelope near the critical point. Discussed briefly is the selection of the equation of state, 32 terms rather than 19, a description of the fitting program, and the results of a preliminary fit using the data available at that time. To provide a complete record, much of the earlier material is included into the present report.

The second, and present phase of the study is sponsored by NASA-Johnson Space Center (P.O. T-6570C). The main thrust is that new experimental PVT measurements at

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[*] Parahydrogen is the nuclear spin modification which is stable at low temperatures.

low temperatures and high pressures are now available (Weber, 1975). These values extend the range of the existing PVT data (Goodwin, et al., 1963 and Michels, et al., 1959a) sufficiently to warrant a refitting of the equation of state. The refit now includes the actual experimental PVT data, adjusted to the T_{68} scale, and calculated values of C_v, adjusted from normal* to parahydrogen, for the high temperature source (Michels, et al., 1959b). The representation of the PVT surface and derived thermodynamic functions is greatly improved over previous versions. This fact is shown clearly, and for the first time by detailed comparisons between experimental and calculated values of density, and by corresponding intercomparisons for enthalpy and specific heat at constant pressure, C_p.

2. The Sources of Data

The major sources from which experimental or calculated values are taken originate in the laboratories of NBS and of the University of Amsterdam. A description of these basic references follows. Weber, et al. (1962) measured vapor pressures, Roder, et al. (1963) present critical parameters and densities along the two phase envelope. The bulk of the PVT data is given in Goodwin, et al. (1963), while experimental heat capacity data is found in the papers of Younglove and Diller (1962a, b). These papers cover pressures from 0 to 340 atmospheres with temperatures from the triple point to 100 K, and they are smoothed and combined to yield calculated thermodynamic functions by Roder, et al. (1965). The very recent measurements by Weber (1975) extend coverage to pressures up to 800 atmospheres with temperatures up to 300 K. The second extensive set of PVT data is presented by Michels, et al. (1959a), and these values are used to calculate thermodynamic properties in Michels, et al. (1959b).

A number of other references on hydrogen exist, see for example the survey by Woolley, et al. (1948). We have omitted these sets of data because they do not cover a large range of pressure and temperature, because the various sets are mutually inconsistent, and because the experimental errors are estimated to be larger than the sources chosen. Indirectly these sources are included because they were used by McCarty and Weber (1972) in deriving parameters for the 17 term equation of state described in that paper. We use 40 points generated from that equation in the fitting of the present equation. These generated points insure that the present equation is not subject to undue oscillations for temperatures from 423 to 2200 K with pressures up to 680 atmospheres.

The input to the fitting program, the "data" is taken from these sources as shown in table 1. It is clear from the table that in addition to using PVT data the fitting procedure uses higher order thermodynamic data such as C_v and the Gibbs constraint, in other words the technique of simultaneous or multiproperty fitting.

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* Normal hydrogen is the equilibrium mixture at room temperature, 75% ortho, 25% para.

Table 1. Data Used to Determine the Parameters of the Equation of State

Type of data	number of points	source		comments
PVT	1218	Goodwin, et al.	(1963)	
	377	Weber	(1975)	
	18	Roder, et al.	(1965)	extrapolated beyond the melting line
	482	Michels, et al.	(1959a)	
	40	McCarty and Weber	(1972)	calculated, temperatures above 423 K
	38	Roder, et al.	(1963)	saturated liquid, saturated vapor adjusted by McCarty (1974)
C_v	163	Younglove and Diller	(1962)	
	15	Roder, et al.	(1965)	calculated values
	295	Michels, et al.	(1959b)	calculated values
Gibbs constraint	19	Roder, et al.	(1965)	saturated liquid - saturated vapor
Total Points:	2665			

3. Adjustment and Modification of the Data

Adjustment of the raw data was necessary for two reasons. First, international agreement on a practical low temperature scale which is very close to the thermodynamic scale was reached in 1968 (T_{68} Metrologia 1969). Second, an index of refraction experiment by Diller (1968) indicated that the definition of the PVT surface given by Roder, et al. (1965) is in error as much as 7% in density in the region near the critical point. The fact that the two-phase envelope might be in error was pointed out as early as 1963, [see for example figure 4 in Roder, et al. (1963)], through analysis of errors in the intersection temperatures of isochores - experimental runs - and the vapor pressure curve.

As a result, McCarty (1974) made adjustments in both temperature scale and density in the region near the critical point. The changes are most noticeable in the critical parameters, the vapor pressure curve, and the saturated liquid and vapor densities. The sequence adopted was to first find values for the densities of saturated liquid and vapor from the index of refraction experiment; next to estimate new critical parameters from these densities using values close to the critical point and a mathematical representation based on the scaling laws. The results were checked by looking at the rectilinear diameter. Finally, the newly defined saturation boundaries near the critical point and densities at lower temperatures were represented with empirical equations which include scaling law terms. PVT values generated from these equations were finally used as "data" for the equation of state, see line 6, table 1.

3.1 Temperature Scale Changes

The NBS 55 temperature scale was used to determine the PVT data of Goodwin, et al. (1963), the heat capacity data of Younglove and Diller (1962a, b), and the PVT data of Weber (1975). For these references the conversion of the experimental temperatures to the T_{68} scale was straightforward.

Conversion of the temperature scale used by the University of Amsterdam is based on a similar adjustment made for the PVT data of Argon (see Gosman, et al., 1969). The assumption is made that the same thermometer and scale was used for hydrogen as was used for argon. The temperatures given by Michels, et al. (1959a, b) and the ones chosen for the present fitting are contrasted in table 2. Two bits of evidence indicate that the assignment of temperatures for this set of data are reasonable. First, the authors' experimental temperature scale (Levelt-Sengers, 1966) included a calibration point at the temperature of sublimating CO_2. Thus the experimental temperature scale except for the three lowest and for the very highest temperatures is remarkably close to the T_{68} scale as subsequently defined. This is of course exactly what the authors were trying to achieve; to make the measurements as nearly on the thermodynamic scale as possible. Second, a separate analysis also indicated that the temperatures shown in table 2 are the most likely set. The analysis consisted of fitting a surface to this set of PVT data, first with the temperatures adjusted from IPTS 48 to T_{68}, and then by assuming that the temperatures were measured on a local scale (Levelt-Sengers, 1966) with subsequent corrections to IPTS 48 and then to T_{68}. A comparison of the sum of the residuals of the two fittings favors the second procedure.

Table 2. Temperatures Assigned to the PVT Data of Michels, et al.

Reference, °C	T_{68}, K this paper	Reference, °C	T_{68}, K this paper
-175	98.1835	- 25	248.147
-170	103.1835	0	273.15
-160	113.173	25	298.142
-150	123.1625	50	323.140
-135	138.1585	75	348.143
-120	153.161	100	373.15
-100	173.166	125	398.1595
- 75	198.165	150	423.170
- 50	223.1555		

3.2 Adjustment of Saturated Liquid and Vapor PVT Near the Critical Point

In addition to the temperature scale change, an adjustment was made in densities on the basis of an index of refraction experiment by Diller (1968). Diller measured the index of refraction, temperature, and pressure. He obtained densities from the PVT surface defined by Roder, et al. (1965) which on the saturation boundaries is identical to Roder, et al. (1963). The salient graph from Diller's paper is reproduced in figure 1, where it is seen that the saturation boundaries fall on two separate legs which do not meet at the critical density. The Lorentz-Lorenz function of the saturation boundaries should have the same general shape as do the isotherms. In particular, for temperatures between 28 K and critical the two-phase envelope should be very close to the 35 K isotherm. The two legs of two-phase envelope are ascribed to incorrect densities in the critical region. More precisely, as indicated earlier, the errors stem from the intersection temperatures of experimental runs and the vapor pressure curve, which near the critical point are nearly co-linear.

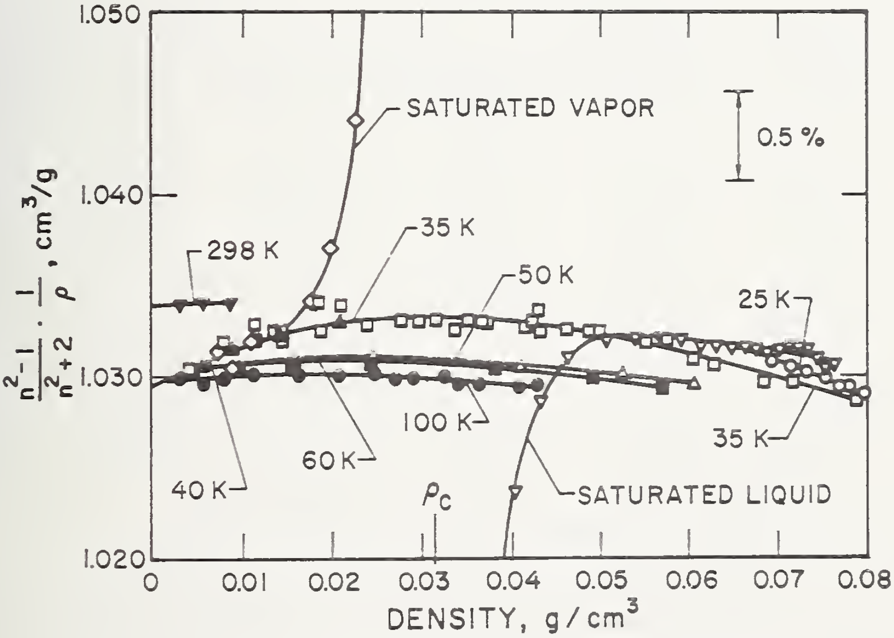


Figure 1. The Lorentz-Lorenz Function for Hydrogen

To adjust the saturation densities in the critical region the function

$$\rho = \sum_{K=1}^{N} A_K n^{K-1}, \qquad (1)$$

was fit to the 35 K isotherm, where ρ is density in g/cm^3 and n is the index of refraction.

Equation (1) was fit to 24 experimental index of refraction points with densities ranging from 0.003969 to 0.078833 g/cm^3. It is important that the data not be "overfit." Since statistical significance of the coefficients to eq (1) was lost when more than 4 terms were used the 4 term equation was chosen. The coefficients obtained for eq (1) are given in table 3.

Table 3. Least Squares Estimates of the Coefficients for Equation (1)

A_1 = -1.0880215243
A_2 = 1.8280271481
A_3 = -1.0378774469
A_4 = 0.29788205862

The measured index of refraction along the saturated liquid and vapor was then used to calculate the adjusted densities using eq (1). The densities given by Roder, et al. (1963) and the adjusted densities are contrasted in table 4.

Table 4. Adjusted Saturation Densities Near the Critical Point

Temp,K		Density of Liquid, g/cm^3			Density of Vapor, g/cm^3		
NBS-55	T_{68}	Index of Refraction	Roder et al. (1963)	Eq (1)	Index of Refraction	Roder et al. (1963)	Eq (1)
28.0	28.0071	1.092881	.058966	.058998	1.011312	.007298	.007299
29.0	29.0073	1.089174	.056646	.056674	1.013767	.008887	.008876
30.0	30.0076	1.084824	.053930	.053944	1.016892	.010882	.010881
31.0	31.0080	1.079479	.050589	.050586	1.021040	.013541	.013539
31.6	31.6082	1.075401	.048057	.048021			
32.0	32.0084	1.072075	.045993	.045927	1.027273	.017498	.017525
32.4	32.4086	1.067671	.043320	.043152	1.031177	.019934	.020017
32.7	32.7088	1.062766	.040412	.040057	1.035711	.022664	.022906
32.9	32.9089	1.055690	.036941	.035586	1.042271	.025490	.027074

3.3 Estimation of Critical Density and Temperature

Extrapolation of the rectilinear diameter yields the best estimate for the critical density. A plot of $(\rho_\ell + \rho_g)/2$ against temperature, as shown in figure 2, limits the critical density to a value between 0.03122 and 0.03142 g/cm^3. The value of the critical density is seen to depend only slightly on temperature. Therefore, the next step is to extrapolate the rectilinear diameter numerically.

To achieve this the equation given in the next section, eq (5) which describes the saturation boundaries is used. The equation is truncated to 4 terms resulting in

$$\rho_g + \rho_\ell = 2\rho_c + (G_{1g} + G_{1\ell})(\Delta T)^{\beta} + (G_{2g} + G_{2\ell})(\Delta T)^{1-\alpha} + (G_{3g} + G_{3\ell})(\Delta T), \quad (2)$$

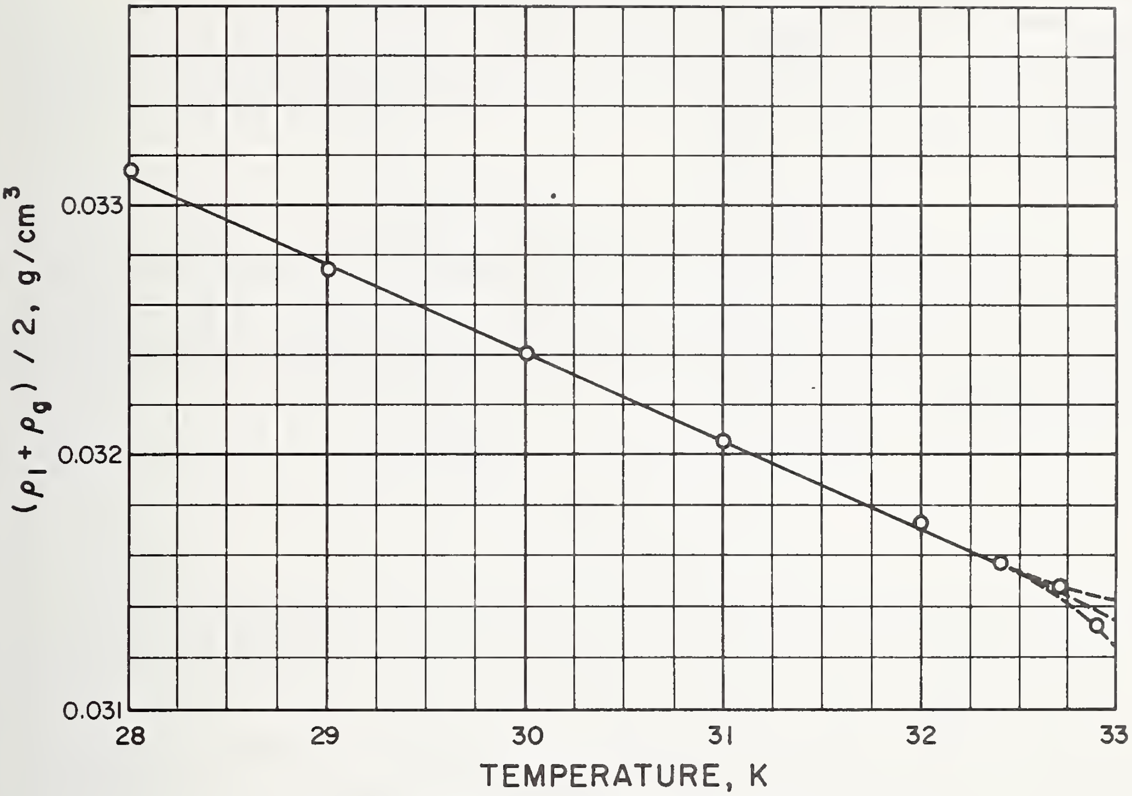


Figure 2. The Rectilinear Diameter for Parahydrogen

where $\Delta T = (T_c - T)/T_c$. Note that the exponents of the last two terms are $1-\alpha$ and 1 rather than 1 and 4/3. $G_{1\ell}$ is usually assumed to be equal to $-G_{1g}$ and the second term of eq (2) vanishes. There is some doubt about the validity of this assumption, but in this particular case at least, the assumption cannot be disproved on the basis of the available data. Thus the problem of estimating β is eliminated. A least squares fit of the eight pairs of liquid-vapor data in table 4 resulted in a critical density of 0.03136 g/cm^3 for values of $\alpha = 0.1$ and $T_c = 32.933$ K. The fit was repeated several times with values of α and T_c ranging from $\alpha = 0.1$ to $\alpha = 0.25$ and $T_c = 32.938$ to $T_c = 32.95$. The resulting estimates of ρ_c did not vary significantly (i.e., maximum variation was less than ± .00001 g/cm^3).

The next step is to estimate the critical temperature. In this case eq (5) is truncated to two terms, that is to the terms originating from the scaling laws. The resulting equation, eq (3),

$$\rho_{sat} = \rho_c + G_1 (\Delta T)^\beta \qquad (3)$$

is obviously valid only for densities very close to critical. With some trial and error temperatures between 31.9 and 32.8 were found to be applicable. A value for ρ_c is at hand, a value for T_c can be estimated from the equation if pairs of ρ_{sat} and T_{sat} are available. Since very few of the experimental densities are at temperatures between 31.9 and 32.8 K, a parametric interpolation function for n was used to provide the necessary input to eq (1). The function

$$n = r_1 + r_2 (\Delta T)^{r_3} , \qquad (4)$$

was fit to the index of refraction data of the saturation boundary (liquid and vapor) between 28 and 32.9 K. In eq (4) n is the index of refraction, and $\Delta T = (T_c - T)/T_c$. The coefficients used in eq (4) are given in table 5. By combining equations (4) and (1) densities could be calculated

Table 5. Coefficients for equation (4)

r_1 = 1.0509586594
T_c = 32.93313976
r_2 = 0.091463402563
r_3 = 0.41043983745

every 0.1 K between 31.9 and 32.8 K. The data so interpolated were finally used in a fit of eq (3) with $\rho_c = 0.03136$ g/cm^3, establishing the critical temperature T_c as 32.938 K, and also $\beta_{gas} = 0.3483$, $\beta_{liquid} = 0.3478$.

The values of the β's are quite close to the 0.35 predicted by the scaling laws. The value of the critical temperature is virtually the same as that calculated previously by Weber from index of refraction data (unpublished but cited by Goodwin, 1970, page 226).

3.4 Revised Saturation Boundary Equations

The equation used to represent the saturation boundaries is based in part on the scaling laws but is otherwise empirical. The equation is

$$\rho_{Sat} = \rho_c + G_1 (\Delta T)^{\beta} + \sum_{I=1}^{8} G_{(I+1)} (\Delta T)^{[1 + (I-1)/3]} \qquad (5)$$

using the values established in the previous section for T_c, ρ_c and the betas, eq (5) is used to represent the saturation boundaries. Input for the fitting are the saturated liquid and vapor values of Roder, et al. (1963) with temperatures adjusted to the T_{68} scale, except that for temperatures of 28 K and above the adjusted densities given in table 4 are used, and that for the vapor a few generated values were added to balance numbers between liquid and vapor. The coefficients for eq (5) are given in table 6. Table 7 gives the deviations between calculated and input densities.

Table 6. Coefficients for Equation (5)

	Vapor	Liquid
ρ_c	0.03136 g/cm^3	0.03136 g/cm^3
β	0.3483	0.3479
G_1	-0.047501571529	0.048645813003
G_2	$3.4871213005\text{x}10^{-2}$	$-3.4779278186\text{x}10^{-2}$
G_3	$-4.1221290925\text{x}10^{-1}$	$4.0776538192\text{x}10^{-1}$
G_4	1.5666598550	-1.1719787304
G_5	-2.8061427339	1.62139244
G_6	2.7105455626	-1.1531096683
G_7	-1.3074773595	0.33825492039
G_8	0.22921285922	0.0

3.5 Revised Vapor Pressure Equation

The vapor pressure data of Weber, et al. (1962) was converted to the T_{68} scale and refit to the nonanalytical vapor pressure equation of Goodwin (1969). That equation is

$$\ell n\ (P/P_t) = B_1 X + B_2 X^2 + B_3 X^3 + B_4 X\ (1-X)^{B_5}\ , \qquad (6)$$

where $X = (1-T_t/T)/(1-T_t/T_c)$, T is in kelvins. The coefficients to eq (6) are given in table 8. The two data points given by Weber, et al. (1962) for T = 22 and 23 K were omitted from the fit because their inclusion seriously degraded the representation of the rest of the data. The T_{68} triple point temperature of hydrogen, 13.81 K, could not be used because it also degraded the fit. Similarly the boiling point of parahydrogen could not be constrained to the T_{68} value of 20.280 K, but is rather 20.277 K. Since Goodwin's equation is sensitive to the values chosen at the triple point and has been sucessfully used to force thermodynamic consistency for several other gases, we interpret the departure at the triple point and at the normal boiling point to indicate some remaining low level inconsistency in the defined temperature scale, T_{68}. Table 9 gives the vapor pressures from Weber, et al. (1962), the adjusted temperatures, and the deviations between the experimental and calculated data points. The critical pressure is obtained by inserting the critical temperature into eq (6).

Table 8. Coefficients for equation (6)

T_t = 13.8 K
T_c = 32.938 K
P_t = 0.0695 atm
B_1 = 3.05300134164
B_2 = 2.80810925813
B_3 = -0.655461216567
B_4 = 1.59514439374
B_5 = 1.5814454428

Table 7. Saturation Densities and Deviations from Equation (5)

Saturated Liquid				Saturated Vapor			
Temp, K T-68 Scale	Density, Eq(5) g/cm^3	Percent Diff.	Density, Exp. g/cm^3	Temp, K T-68 Scale	Density, Eq(5) g/cm^3	Percent Diff.	Density, Exp. g/cm^3
32.9089	.035571	0.04	.035586	32.8300	.024883	0.01	.024886
32.7088	.040071	-0.03	.040057	32.8400	.025100	0.01	.025102
32.4086	.043161	-0.02	.043152	32.8500	.025332	0.01	.025333
32.0084	.045911	0.04	.045927	32.8600	.025581	0.00	.025582
31.6082	.048023	-0.01	.048021	32.8700	.025852	0.00	.025852
31.0080	.050580	0.01	.050586	32.8800	.026150	-0.00	.026149
30.0076	.053945	-0.00	.053944	32.8900	.026483	-0.00	.026483
29.0073	.056664	0.02	.056674	32.9000	.026865	0.01	.026866
28.0071	.058980	0.03	.058998	32.9100	.027319	0.03	.027328
32.8300	.038028	-0.03	.038018	32.9000	.026865	0.01	.026866
32.8400	.037803	-0.02	.037796	32.7088	.022921	-0.06	.022906
32.8500	.037564	-0.01	.037559	32.4086	.020015	0.01	.020017
32.8600	.037307	-0.00	.037305	32.0084	.017522	0.02	.017525
32.8700	.037027	0.01	.037029	31.0080	.013537	0.02	.013539
32.8800	.036720	0.02	.036726	30.0076	.010883	-0.01	.010881
32.8900	.036377	0.03	.036387	29.0073	.008884	-0.09	.008876
32.9000	.035983	0.04	.035998	28.0071	.007297	0.02	.007299
32.9100	.035516	0.04	.035531	28.0071	.007297	0.02	.007299
13.8030	.077026	0.01	.077032	13.8030	.000126	-0.08	.000126
13.9977	.076861	-0.01	.076856	13.9977	.000139	0.05	.000139
15.0020	.075995	-0.01	.075987	15.0020	.000223	-0.05	.000223
16.0051	.075101	0.01	.075110	16.0051	.000339	-0.05	.000339
17.0071	.074171	-0.00	.074170	17.0071	.000492	0.00	.000492
18.0084	.073197	0.00	.073200	18.0084	.000690	0.06	.000690
19.0088	.072173	0.01	.072178	19.0088	.000938	0.11	.000939
20.0090	.071091	-0.01	.071084	20.0090	.001246	0.13	.001247
20.2770	.070791	-0.01	.070784	20.2770	.001339	-0.10	.001338
21.0089	.069944	0.01	.069949	21.0089	.001620	-0.10	.001619
22.0088	.068721	-0.02	.068710	22.0088	.002072	-0.05	.002071
23.0086	.067414	0.01	.067423	23.0086	.002612	-0.01	.002612
24.0083	.066009	0.00	.066010	24.0083	.003254	0.01	.003255
25.0078	.064490	-0.00	.064489	25.0078	.004016	0.01	.004017
26.0073	.062835	0.01	.062841	26.0073	.004921	0.01	.004921
27.0071	.061014	0.00	.061015	27.0071	.005999	0.01	.006000
28.0071	.058980	-0.03	.058963	28.0071	.007297	0.01	.007298
29.0073	.056664	-0.04	.056643	29.0073	.008884	0.03	.008887

Table 9. Vapor Pressures and Deviations

Pressure, atm Experimental	T_{68}, K	Pressure, atm Eq (6)	Percent Diff.
1.6124	22.0088	1.6143	-0.12*
2.0688	23.0086	2.0712	-0.11*
1.0000	20.2770	1.0000	-0.00
3.2462	25.0078	3.2469	-0.02
3.9826	26.0073	3.9822	0.01
4.8285	27.0071	4.8275	0.02
5.7920	28.0071	5.7918	0.00
6.8863	29.0073	6.8847	0.02
8.1162	30.0076	8.1169	-0.01
8.1169	30.0076	8.1169	-0.00
8.1171	30.0076	8.1169	0.00
8.7873	30.5078	8.7891	-0.02
8.7885	30.5078	8.7891	-0.01
8.7886	30.5078	8.7891	-0.01
9.5029	31.0080	9.5010	0.02
9.5023	31.0080	9.5010	0.01
9.5005	31.0080	9.5010	-0.01
9.5003	31.0080	9.5010	-0.01
10.2525	31.5082	10.2546	-0.02
10.2535	31.5082	10.2546	-0.01
10.2539	31.5082	10.2546	-0.01
11.0502	32.0084	11.0528	-0.02
11.0516	32.0084	11.0528	-0.01
11.0522	32.0084	11.0528	-0.01
11.8988	32.5087	11.8992	-0.00
11.8976	32.5087	11.8992	-0.01
11.8989	32.5087	11.8992	-0.00
12.0749	32.6087	12.0748	0.00
12.0742	32.6087	12.0748	-0.00
12.0751	32.6087	12.0748	0.00
12.2526	32.7088	12.2527	-0.00
12.2520	32.7088	12.2527	-0.01
12.2536	32.7088	12.2527	0.01
12.4326	32.8089	12.4330	-0.00
12.4330	32.8089	12.4330	0.00
12.4352	32.8089	12.4330	0.02
12.6168	32.9089	12.6160	0.01
12.6187	32.9089	12.6160	0.02
12.6183	32.9089	12.6160	0.02
0.0778	13.9977	0.0778	-0.03
0.1327	15.0020	0.1327	0.01
0.2129	16.0051	0.2129	0.01
0.3250	17.0071	0.3250	0.01
0.4759	18.0084	0.4759	-0.00
0.6726	19.0088	0.6727	-0.00
0.9228	20.0090	0.9229	-0.02
0.0695	13.8000	0.0695	-0.00
	32.9380	12.6698**	

* Points omitted from the least squares fit.

** Critical pressure

4. The Equation of State for Hydrogen

Since the major modification of the Benedict-Webb-Rugin (1940) equation of state by Strobridge (1962), there have been many more. Each author claims his particular modification to be the best of several he has tried for the particular fluid being correlated. In some cases a given form was chosen because it worked well for a number of fluids. Several of the MBWR's have been applied to hydrogen. Strobridge's equation (16 terms) was applied by Roder and Goodwin (1961) to parahydrogen. It was found that two sets of coefficients, one for liquid and one for gas, were required to reproduce the experimental PVT surface. In 1967 (see Roder, et al., 1972) a 17 term equation was applied to values above 50 K, thus omitting the two-phase region entirely. In this fit major discrepancies remained at the junction of the two sets of experimental data near 100 K, and in addition the enthalpies around ambient temperatures showed statistically significant deviations. A subsequent refit of this equation by McCarty and Weber (1972) included values of C_v in the data set. While the enthalpies near 300 K were improved the departures in PVT at 100 K remained substantial (see figure 4h this report, the line labelled TN 617).

In phase I of this work McCarty (1974) studied both the 19 term version by Bender (1970) and the 32 term version by Jacobsen (1972). He selected the 32 term equation as being superior, and that equation of state is used here. Actually, if the term ρRT is counted there are 33 terms, and if the coefficient of the exponential term γ is counted there are 33 parameters. The equation of state is:

$$\begin{aligned}
P = \rho RT &+ \rho^2 (N_1 T + N_2 T^{1/2} + N_3 + N_4/T + N_5/T^2) \\
&+ \rho^3 (N_6 T + N_7 + N_8/T + N_9/T^2) \\
&+ \rho^4 (N_{10} T + N_{11} + N_{12}/T) + \rho_5 (N_{13}) \\
&+ \rho^6 (N_{14}/T + N_{15}/T^2) + \rho^7 (N_{16}/T) \\
&+ \rho^8 (N_{17}/T + N_{18}/T^2) + \rho^9 (N_{19}/T^2) \\
&+ \rho^3 (N_{20}/T^2 + N_{21}/T^3) \exp(-\gamma\rho^2) \\
&+ \rho^5 (N_{22}/T^2 + N_{23}/T^4) \exp(-\gamma\rho^2) \\
&+ \rho^7 (N_{24}/T^2 + N_{25}/T^3) \exp(-\gamma\rho^2) \\
&+ \rho^9 (N_{26}/T^2 + N_{27}/T^4) \exp(-\gamma\rho^2) \\
&+ \rho^{11} (N_{28}/T^2 + N_{29}/T^3) \exp(-\gamma\rho^2) \\
&+ \rho^{13} (N_{30}/T^2 + N_{31}/T^3 + N_{32}/T^4) \exp(-\gamma\rho^2)
\end{aligned} \tag{7}$$

The coefficients for the equation of state were estimated from a least squares fit using the data set indicated in table 1 with ρ in moles/liter, P in atmospheres, and T in kelvins. For these units the values of R and γ are given below.

Table 10. Coefficients for the Equation of State (7)

R = 0.08205616 ℓ.atm/mol.K. γ = -0.0041

```
G( 1)   = 4.61438775565437326033D-04
G( 2)   = 4.23318455608677043440D-02
G( 3)   =-5.09655622650373332157D-01
G( 4)   = 2.92305973826958605346D+00
G( 5)   =-2.98760914721136029049D+01
G( 6)   = 1.88314860141070378866D-05
G( 7)   =-1.32225695463922652067D-03
G( 8)   = 3.01650443170189249291D-01
G( 9)   = 5.09370556085174282592D+01
G(10)   = 1.97382832491904714077D-07
G(11)   = 2.85849203982822717063D-04
G(12)   =-2.22827923912348057045D-02
G(13)   =-2.25748113676430406972D-06
G(14)   = 2.41427236974667590421D-05
G(15)   =-1.69571339858841047013D-03
G(16)   =-5.39367639127519319151D-07
G(17)   = 3.99895524432808380862D-09
G(18)   = 1.14245756127449354105D-06
G(19)   =-1.25256622589605274123D-08
G(20)   =-4.91786193488263988296D+01
G(21)   =-1.58566601736867779697D+02
G(22)   =-1.90160294627218554366D-01
G(23)   = 9.19802086250050278199D+00
G(24)   =-3.18045551881044498741D-04
G(25)   = 1.19105779192652709183D-03
G(26)   =-3.79135277322599176132D-07
G(27)   =-3.98337769909539545092D-05
G(28)   =-1.23451085468897290708D-10
G(29)   = 1.95026629349906989681D-09
G(30)   =-2.38034391710916984687D-13
G(31)   =-4.07357660819289386618D-13
G(32)   = 8.80135493077762486716D-12
```

Several comments on the final fit of the equation of state are appropriate. The critical point was constrained to the value P = 12.670 atm, ρ = 15.556 moles per liter, T = 32.938 K and the derivatives to $\partial P/\partial\rho = \partial^2 P/\partial\rho^2 = 0$. The thermodynamic conditions for phase equilibrium for the coexisting liquid and vapor phases have been included as data in the least squares estimating procedure. The fitting of the equation of state was attempted with several combinations of the available data. Representation of the data improved in steps as the data set was changed. Initially we added Weber's (1975) new measurements. Next, we replaced all but 40 points of the data generated from the PVT surface of McCarty and Weber (1972) with the experimental PVT data of Michels, et al. (1959a). A significant improvement occurred when we added the calculated values of C_v by Michels, et al. (1959b). A final improvement resulted when we added 15 calculated values of C_v along the saturated vapor line, and 18 generated PVT points near the melting curve. In both locations the definition of C_p was improved considerably.

5. The Properties Deck

The "properties deck" is a collection of subroutines and functions designed to return a wide variety of state variables, thermodynamic properties and derivatives. A listing of the deck is given in appendix A, a test program and sample results in appendix B. For the user we classify the programs into initialization, basic programs, and second level programs.

Initialization. The first step in a using program would be to call the data subroutine DATAPH2. This routine is normally called only once to set the coefficients of the equation of state, the vapor pressure curve, etc. It will be evident from the program listings given in appendix A that an index N can be associated with this routine and certain of the ideal gas functions. N identifies the species of hydrogen under consideration, and for the purposes of this report is always assumed to be = 1, i.e., we are considering only parahydrogen.

Basic programs. In most problems two of the variables in the set of pressure-density-temperature are known, and the requirement is to find the third variable. Accordingly the three possibilities are

1) density and temperature known, find pressure → subroutine PRESS(PR, D, T),
2) pressure and temperature known, find density → function FINDD(P, T), and
3) pressure and density known, find temperature → function FINDT(P, D)

Since the equation of state is explicit in pressure the subroutine PRESS is straightforward. However, both FINDD and FINDT have to be based on an iterative solution of the equation of state using some initial guess and appropriate derivatives of the PVT surface.

Second level programs. The common denominator for the second level programs is that they require as input some combination of pressure, density, and temperature. More often than not a basic program has to be called before a second level program can be used. All of the remaining subroutines and functions are included in this grouping, that is all phase boundaries, all derivatives and integrals of the equation of state, all thermodynamic functions, and all other properties such as transport properties or dielectric constant.

Flow chart and table of programs. The schematic flow chart, figure 3, presents the logic a user has to apply to any given problem. Approximately 30 programs combining about 50 possible entry points comprise the spagetti bowl which is loosely labelled "properties deck." Each of the entry points corresponds to a single result, answer, output, property returned. These 50 or so possible end points are shown in table 11, which is arranged according to the input these programs require. It is evident from table 11 that density is the input most often required.

One peculiarity in the structure of the properties deck should be noted. The sub-

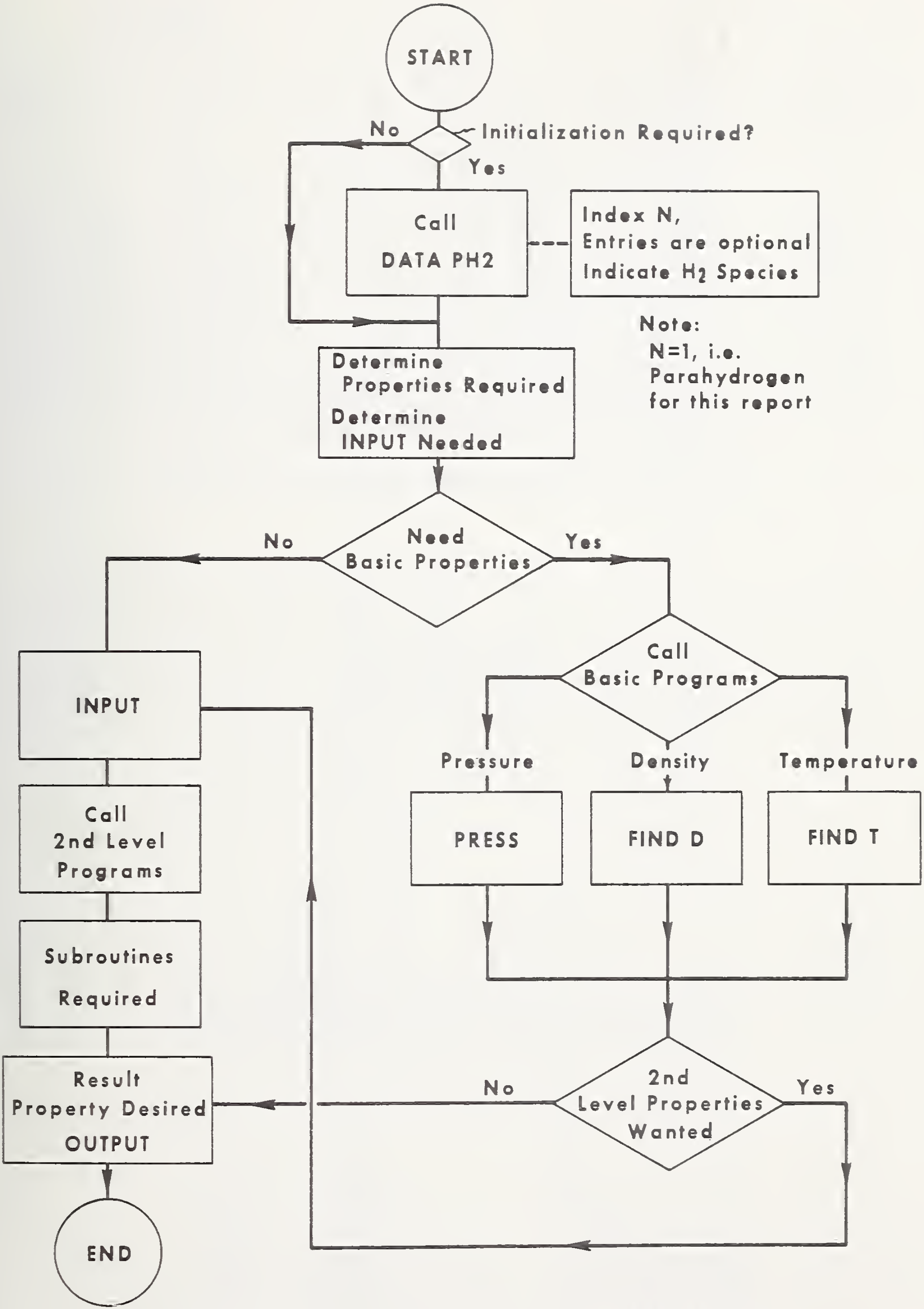


Figure 3. Schematic Flow Chart for Properties Deck

Table 11. Listing of Subroutines, Functions, and Entry Points of the Properties Deck

INPUT	program/ entry points	other programs required	RESULT, i.e. Property Calculated	END
Pressure	FINDTV(P)	VPN, DPDTVP	temperature corresponding to vapor pressure	
	PMELT (P)	PRESSM	temperature corresponding to melting pressure	
Density	DIE (D)		dielectric constant	
Temperature	VPN(T)		vapor pressure	
	DPDTVP (T)	VPN	derivative of the vapor pressure curve dP/dT at T	
	PRESSM (T)		melting pressure	
	DSATV (T)/DSATL (T)		density of saturated vapor or liquid	
	CPI(T)/SI(T)/HI(T)	CPO, CPOS, CPOH	ideal gas specific heat, entropy, and enthalpy	
	DILV (T)/DILT (T)		zero density limit of viscosity and thermal conductivity	
Temperature, N	CPO (T, N)	CPOH, ATKINT*	ideal gas specific heat	hydrogen species according to index N
	CPOH (T, N)	ATKINT*	ideal gas enthalpy	
	CPOS (T, N)	ATKINT*	ideal gas entropy	
Pressure, Density	FINDT (P, D)	PRESS, DPDT , T1	temperature	
Pressure, Temperature	FINDD (P, T)	RHO1, PRESS, DPDD	density	
Density, Temperature	PROPS (PR, D, T)		None	
	/PRESS (PR, D, T)		pressure	the return is made through the dummy variable PR
	/DPDD (PR, D, T)		the derivative $\left(\frac{\partial P}{\partial \rho}\right)_T$	
	/DP DT (PR, D, T)		the derivative $\left(\frac{\partial P}{\partial T}\right)_\rho$	
	/DSDN (PR, D, T)		the derivative of entropy with respect to the EQS coefficients	
	/DUDN (PR, D, T)		the derivative of internal energy with respect to the EQS coefficients	
	/TDSDT (PR, D, T)		the derivative of C_v with respect to the EQS coefficients	
	/DP2D2(PR, D, T)		the derivative $(\partial^2 P/\partial D^2)_T$.	

Table 11. Listing of Subroutines, Functions, and Entry Points of the Properties Deck (continued)

INPUT	program/ entry points	other programs required	RESULT, i.e. Property Calculated	END
Density, Temperature (continued)	CP (D, T)	CV, DPDT, DPDD	specific heat at constant pressure	
	CV (D, T)	TDSDT, CPI	specific heat at constant volume	
	ENTROP (D, T)	DSDN, SI	entropy	
	VISC (D, T)	DILV, FDCV, EXCESV	viscosity	
	FDCV (D, T)/FDCT (D, T)		first density correction of viscosity/thermal conductivity	
	EXCESV (D, T)/EXCEST (D, T)		change in viscosity/thermal conductivity with density	
	THER M (D, T)	DILT, FDCT, EXCEST, CRITC	thermal conductivity	
	CRITC (D, T)	DPDT, DPDD, VISC	enhancement of thermal conductivity in the critical region	
	SOUND (D, T)	CP, CV, DPDD	speed of sound	
	THETA (D, T)	CP, DPDD, DPOT	specific heat input	
	PHI (D, T)	CV, DPDT	energy derivative	
Pressure, Density, and Temperature	ENTHAL (P, D, T)	DSDN, DUDN, HI	enthalpy	
	RHO1(P,D,T)/TI(P,D,T)	VPN, DSATL	an approximate density, first guess in D/ an approximate temperature, first guess in T	

* ATKINT is a general purpose interpolation routine.

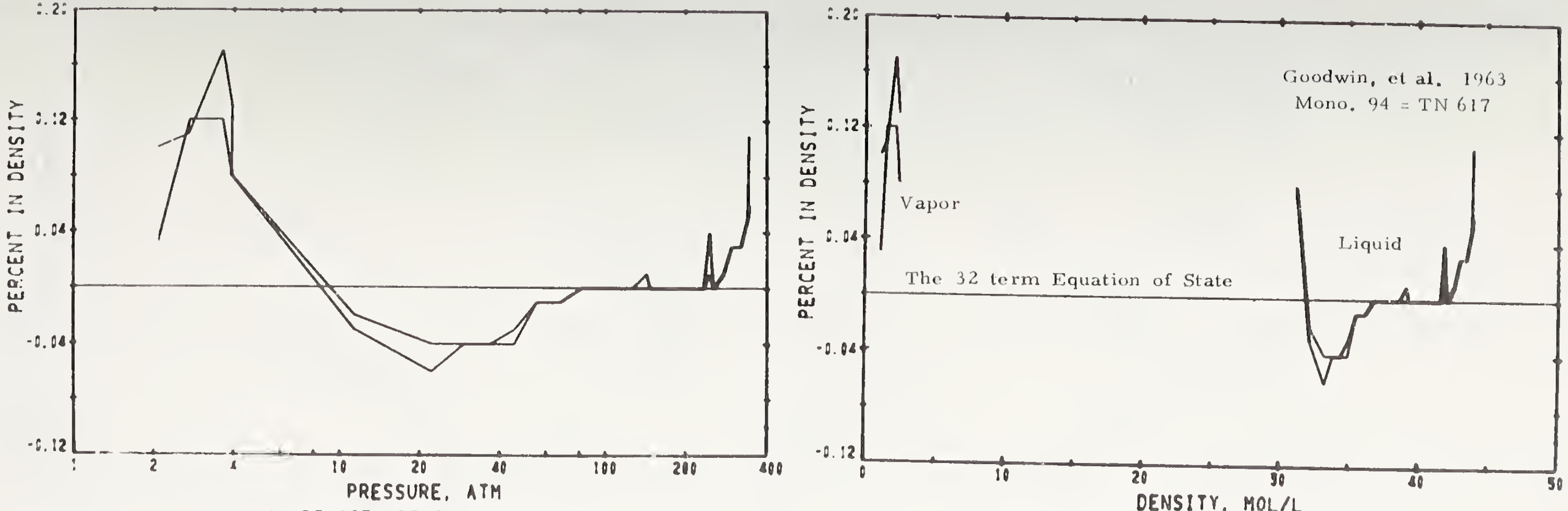
routine PROPS is a multiple entry routine designed to reduce the number of operations involving the coefficients and terms of the equation of state. Included in closed form are derivatives and integrals of the equation of state which are required to obtain enthalpy and entropy.

6. Discussion, Intercomparisons and Errors

Hydrogen may be the first, and perhaps the only case where we can determine, with reasonable assurance, what the errors in the PVT surface and in the derived properties actually are. This fortunate circumstance arises because for hydrogen there is a wealth of data available which can be used both as input to the equation of state and to check the quality of the MBWR. We show the results of extensive comparisons in two different ways. The first set of graphs might be called "standard," because it is the conventional way of plotting density deviations for a set of selected isotherms. The second set of graphs gives an overview of density, enthalpy, and C_p errors in the P-T plane. In the last part of this section we look at the MBWR extrapolation to high densities.

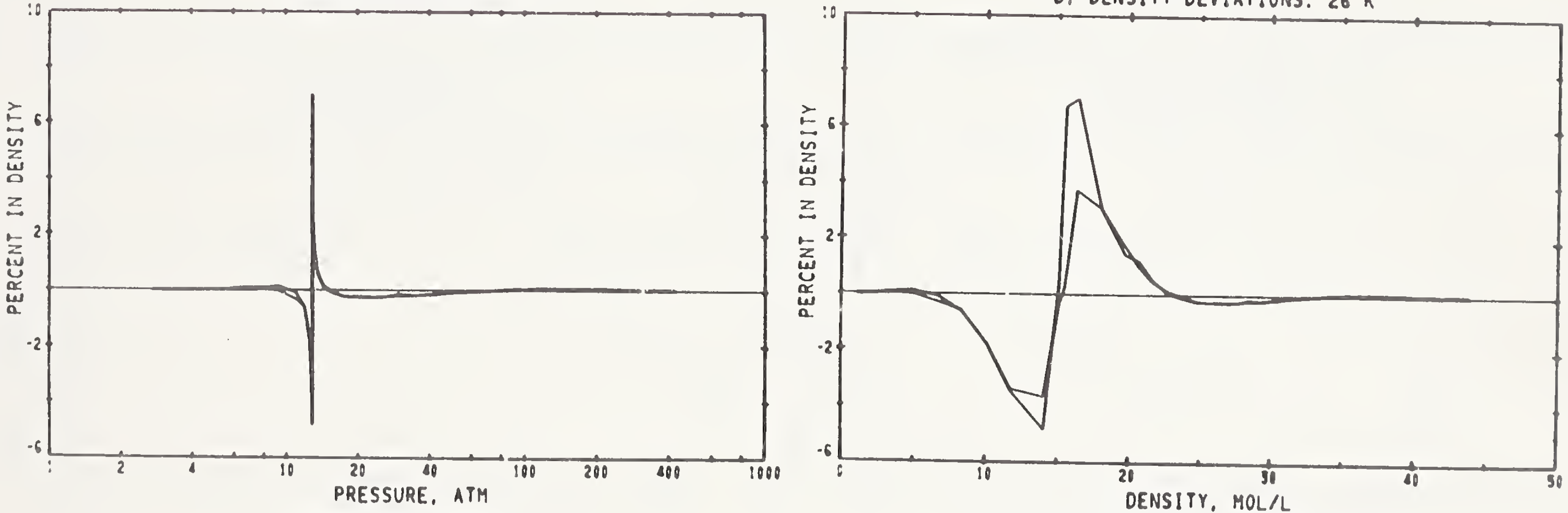
6.1 Density Deviations Along Isotherms

Density deviations are plotted in 16 segments of figure 4 for isotherms of 26, 33, 60, 98/100, 150/153, 198/200, 298/300 and 423 K. The deviations, expressed in percent, are the differences between values predicted by the MBWR on the one hand and the PVT data of Goodwin, et al. (1963), Weber (1975), and Michels, et al. (1959a) and one prior correlation by McCarty and Weber (NBS Technical Note 617, 1972) on the other hand. In these graphs the 32 term MBWR is the zero or reference line, and the departures for each isotherm are plotted against both pressure and density. One of the reasons for plotting against both variables is evident for the 26 K isotherm, figure 4a and 4b. The plot against pressure is continuous, the plot against density shows both vapor and liquid segments of the isotherm. Figure 4 illustrates that the differences between the data of Goodwin and the correlation of TN 617 — a polynomial smoothing of the surface — are negligible. The plot against pressure in figure 4c is typical of temperatures near critical. This plot shows the inability of an analytic equation of state, the MBWR, to accurately represent a PVT surface near the critical point. In the corresponding plot 4d it is seen that these departures extend over quite a large range in density, and also that there is some difference between the experimental data (Goodwin, et al., 1963) and the polynomial smoothing (Roder, et al., 1965). The lowest temperature at which we are able to intercompare all sources is 98/100 K, figure 4h. We note that the rather sharp change between Goodwin, et al. (1963) and Weber (1975) first seen at 60 K is also evident at 100 K. At low densities Goodwin and Michels disagree, at higher densities the agreement between Weber and Michels is very satisfactory. We note the large deviation of TN 617. We are forced to conclude that the 17



A, DENSITY DEVIATIONS, 26 K

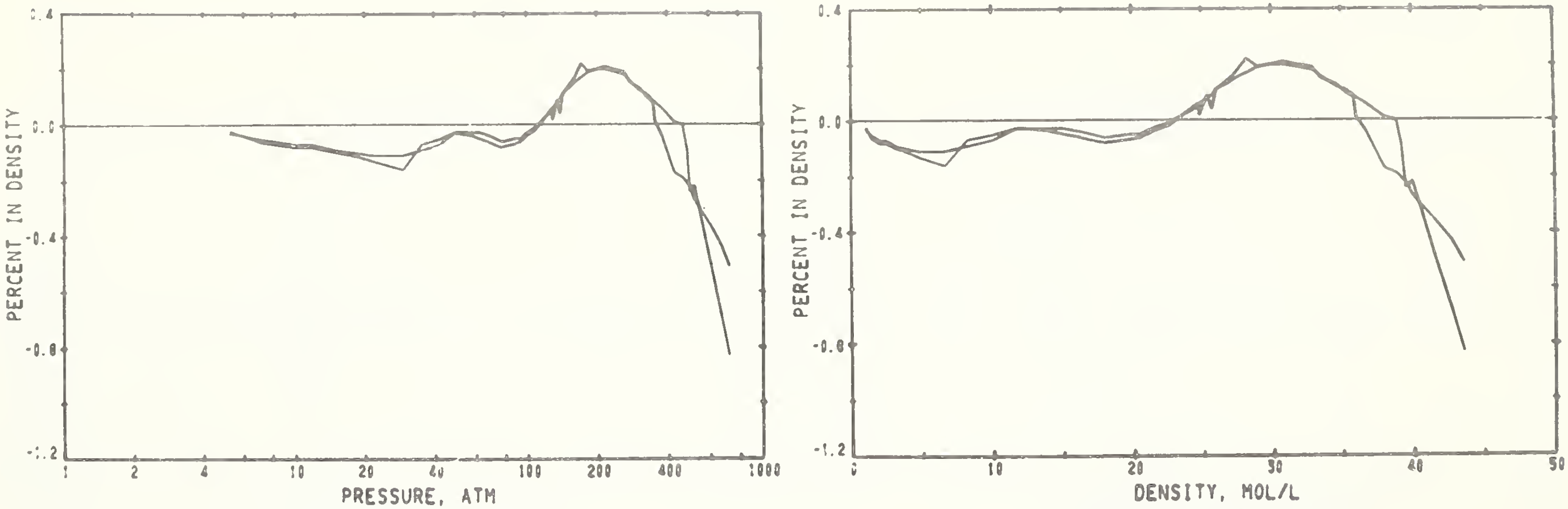
B, DENSITY DEVIATIONS, 26 K



C, DENSITY DEVIATIONS, 33 K

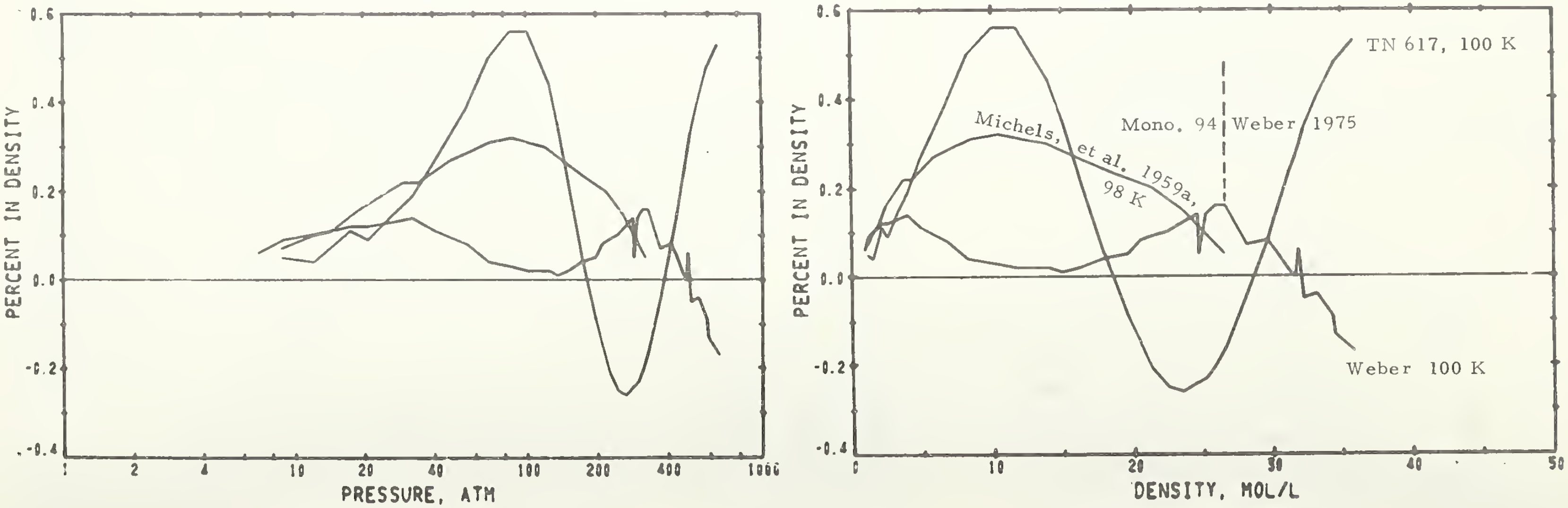
D, DENSITY DEVIATIONS, 33 K

Figure 4. Density Deviations along Isotherms



E, DENSITY DEVIATIONS, 60 K

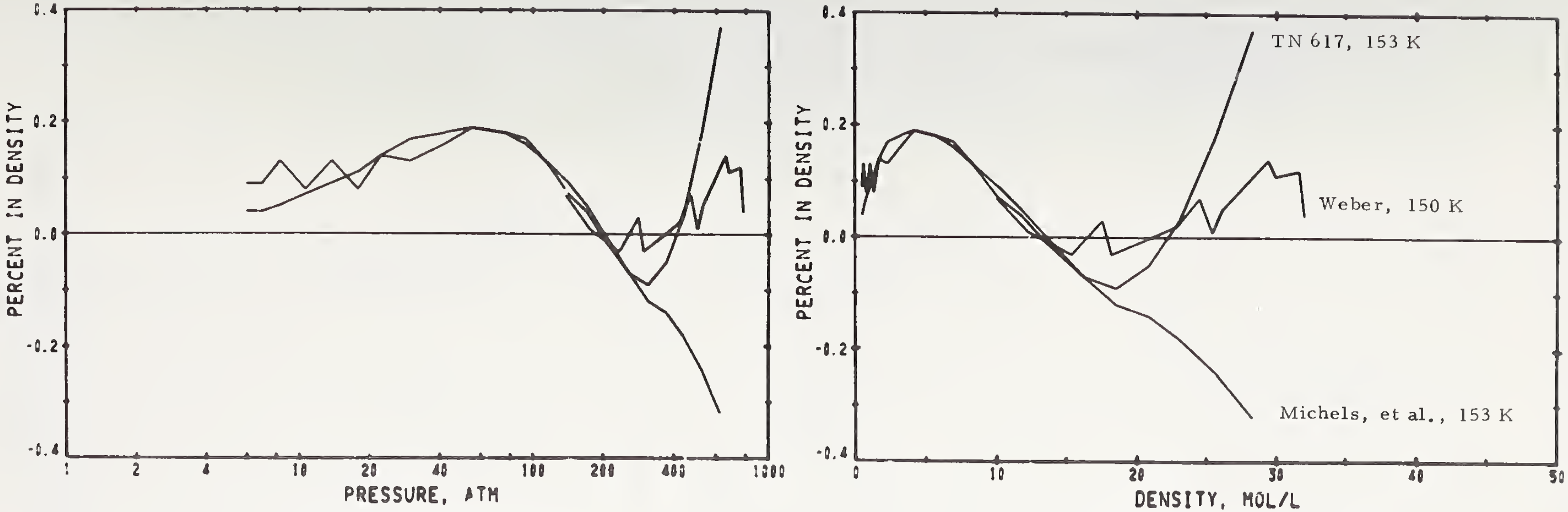
F, DENSITY DEVIATIONS, 60 K



G, DENSITY DEVIATIONS, 100 K

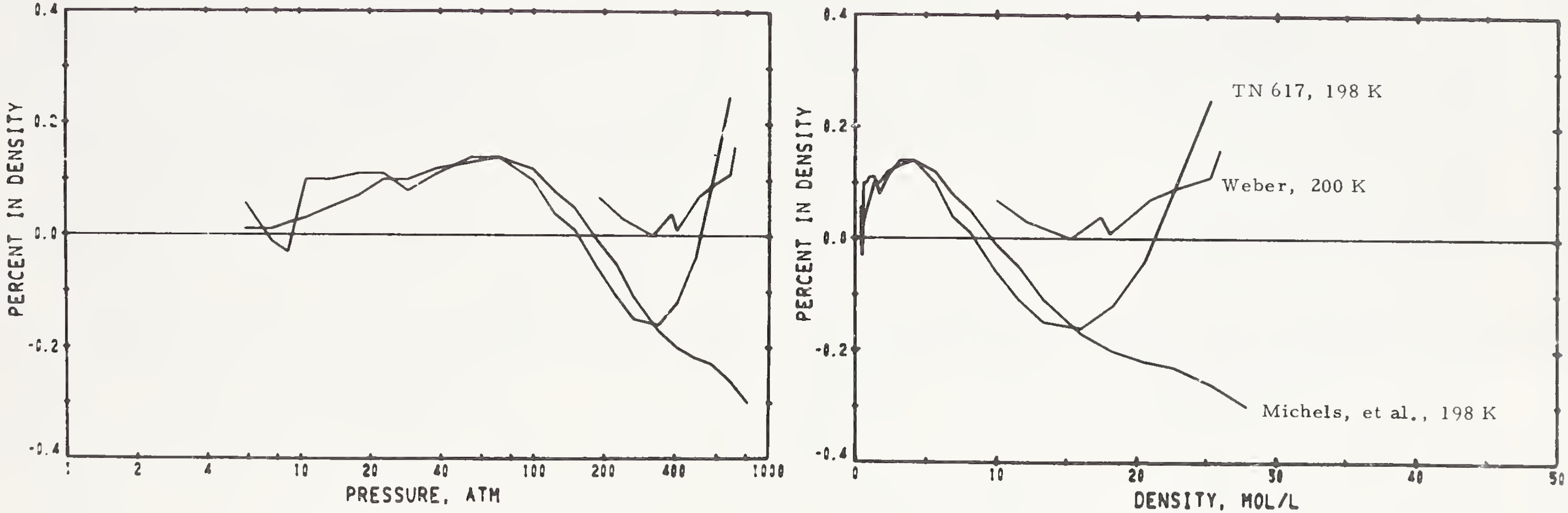
H, DENSITY DEVIATIONS, 100 K

Figure 4. - Continued



I. DENSITY DEVIATIONS, 150 K

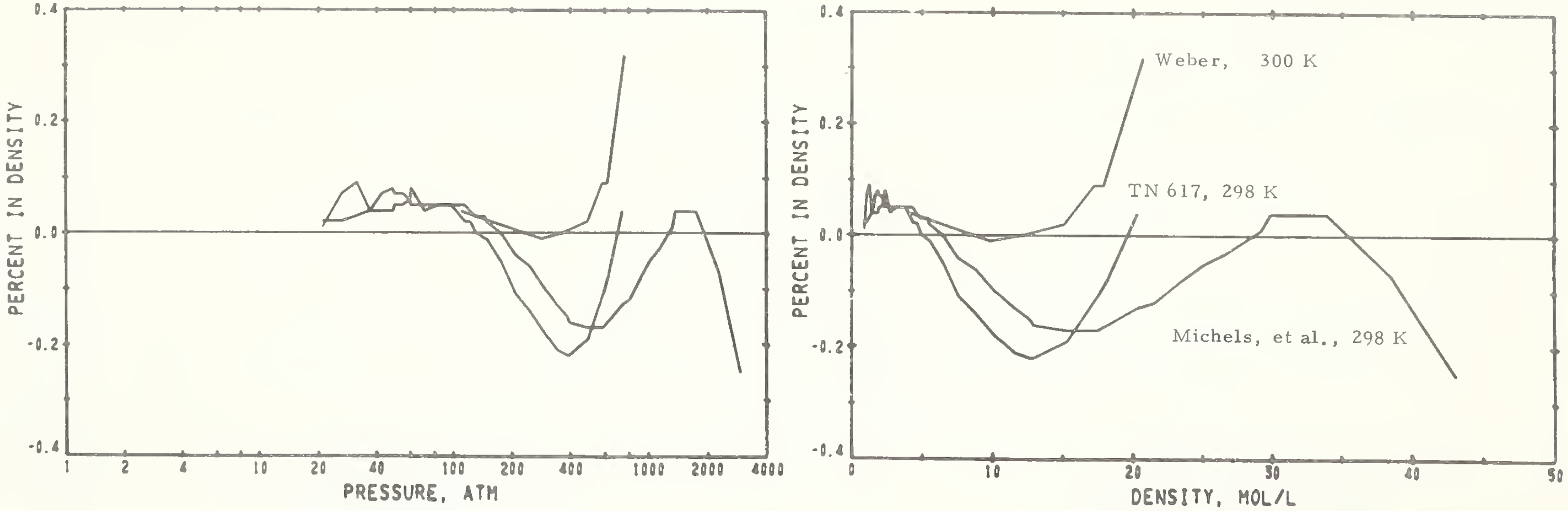
J. DENSITY DEVIATIONS, 150 K



K. DENSITY DEVIATIONS, 200 K

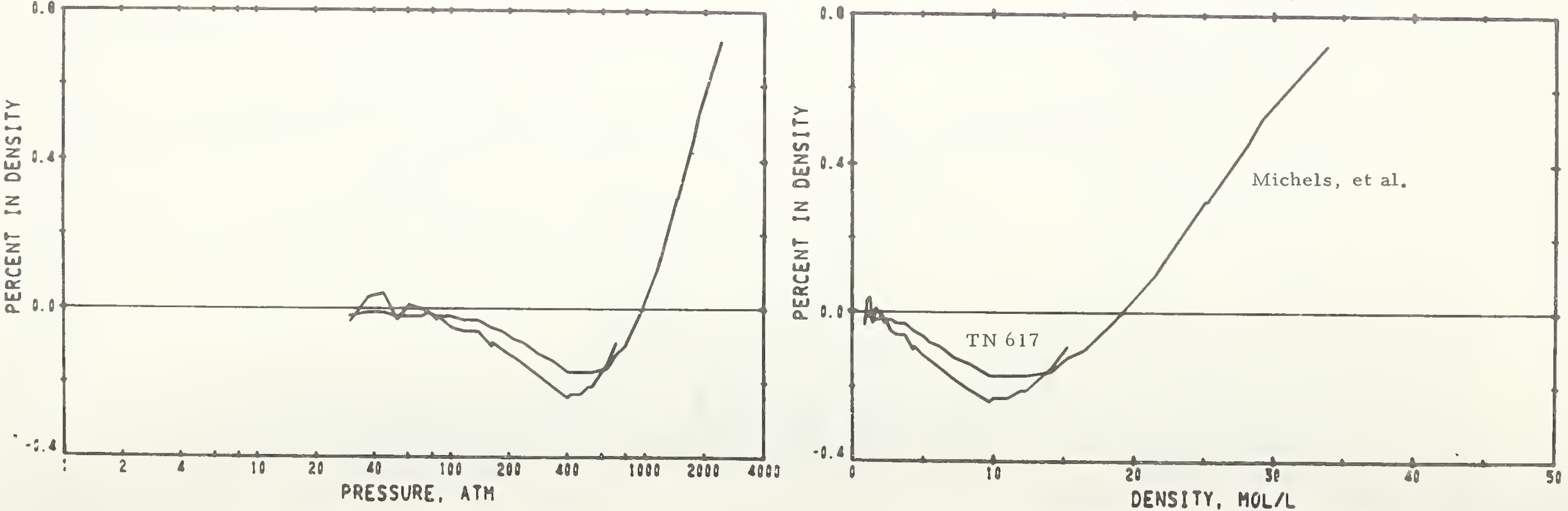
L. DENSITY DEVIATIONS, 200 K

Figure 4. - Continued



M, DENSITY DEVIATIONS, 300 K

N, DENSITY DEVIATIONS, 300 K



O, DENSITY DEVIATIONS, 423 K

P, DENSITY DEVIATIONS, 423 K

Figure 4. - Continued

term MBWR used in TN 617 does not offer sufficient flexibility to represent an entire PVT surface.

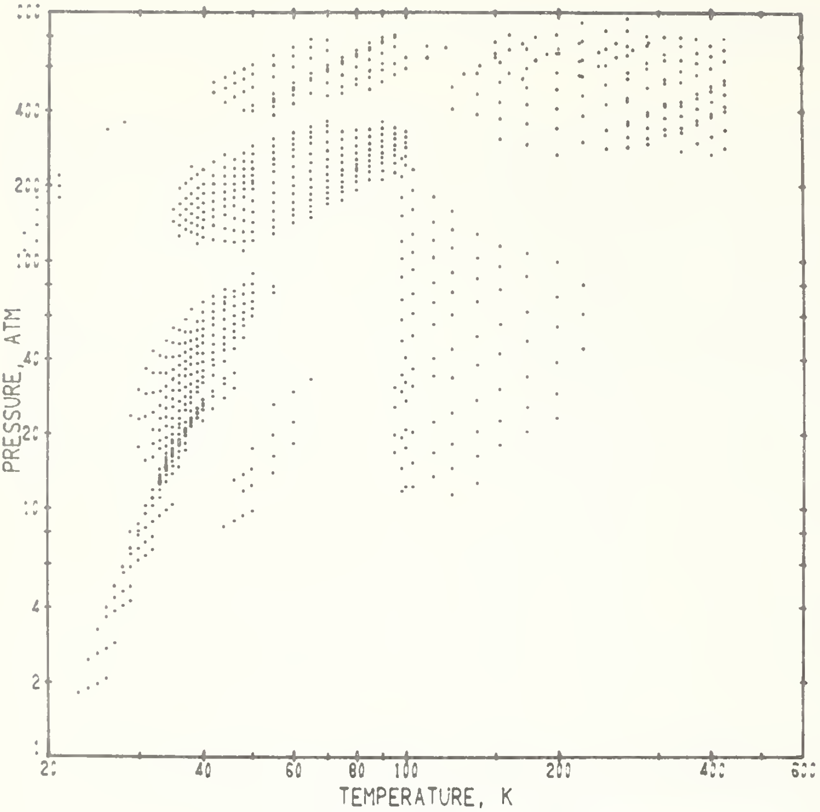
Of the remaining plots figure 4n is particularly interesting. The general progression of Michels' and Weber's data is quite similar up to a density of 30 mol/l. Can the difference be ascribed to different assumptions about the stretching of the PVT pipet? The drastic change in Michels' data at densities above 30 mol/l is not understood, particularly in view of figure 4p. Could the change be a one-time nonelastic stretching of the pipet? The behavior of the 17 term MBWR (TN 617) is also of interest in figure 4n. At low densities this surface follows Michels' data,at higher densities it switches to represent the extrapolation isochores of Goodwin, et al. (1963). The latter can now be seen to be qualitatively similar to the new measurements of Weber (1975).

6.2 Departures in the P-T Plane

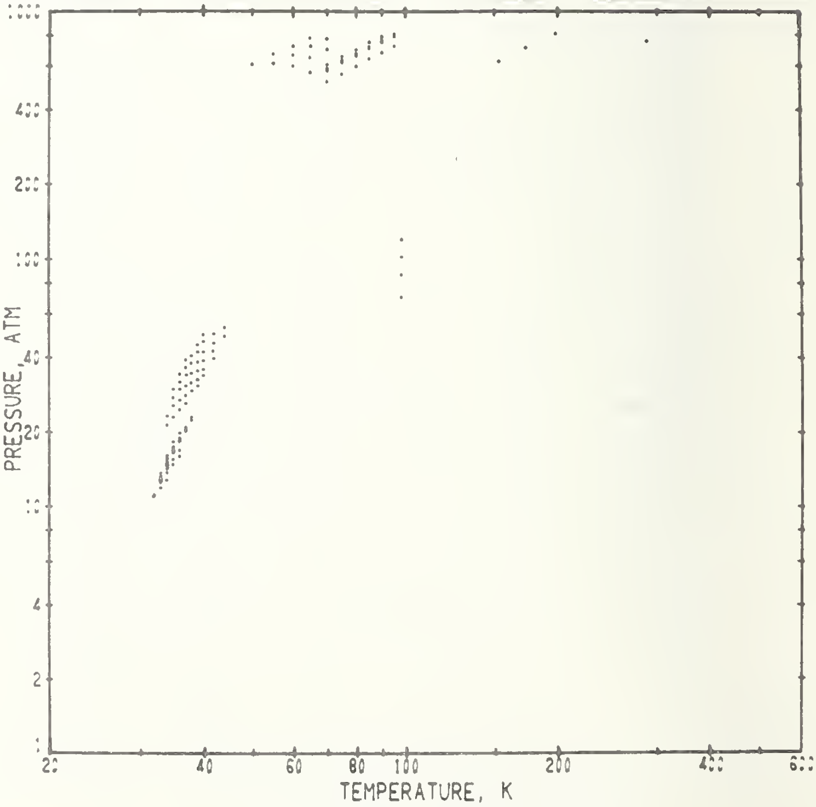
These deviation plots involve density because density is the most basic variable (see table 11), and enthalpy as well as C_p because these are the most important properties for the engineer. The graphs are assembled in three sets of four plots each. The three sets should be considered together since they are interdependent. Each set is obtained by plotting the P-T locus of successively larger errors of the variable under consideration. From these sets it is quite clear that the region near the critical point is the only area which is really troublesome.

The error plots for density, figure 5, are in percent without regard to sign, and are taken directly against the two major sources of experimental data, NBS and Michels. The average deviation in density is 0.14%. This is slightly larger than the average experimental uncertainty, and is about the best one could possibly expect.

The error plots for enthalpy, figure 6, are in J/mol for the simple reason that the enthalpy values go through zero, from about -600 to 15000 J/mol. The comparison is between different methods of calculation, values are compared at the experimental points of PVT. Values calculated with the 32-term equation are compared with those calculated by Roder, et al. (1965), by Weber (1975) and by Michels, et al. (1959b). The graphs illustrate clearly that given a density deviation there will be a corresponding departure in enthalpy. At first sight departures of up to 30 J/mol at the higher temperatures, 300 - 423 K, are startling. A little reflection shows these errors to be almost negligible. We recall that what is plotted are differences in enthalpy, not percent. A specific example concerns the ideal gas value at 300 K which is about 8400 J/mol and the enthalpy value at 2200 atm and 300 K which is 11600 J/mol. Given these values a difference of 30 J/mol for the isothermal increment of about 3200 J/mol is not severe. From figure 6 we estimate the average enthalpy deviation to be around 3 J/mol.



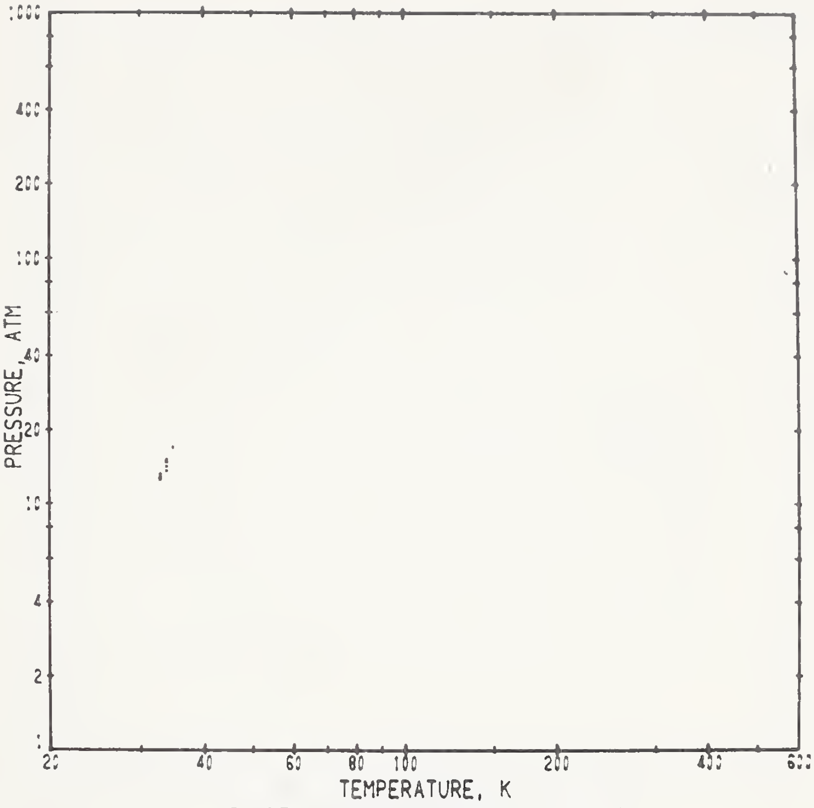
A, DEV. GREATER THAN 0.1 PERCENT



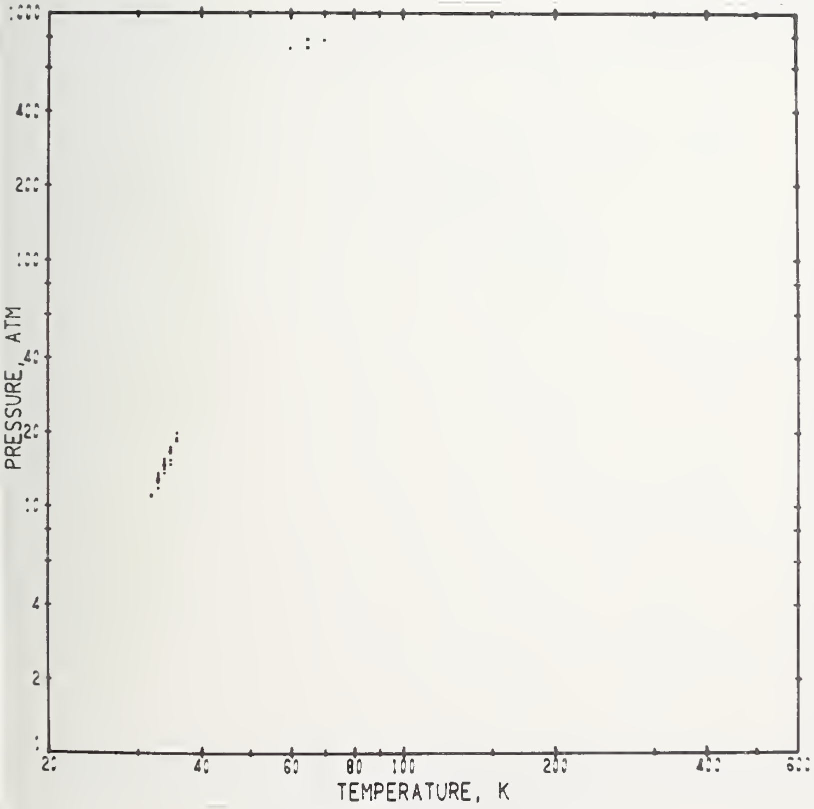
B, DEV. GREATER THAN 0.3 PERCENT

Figure 5.

Density Deviations in the P-T Plane



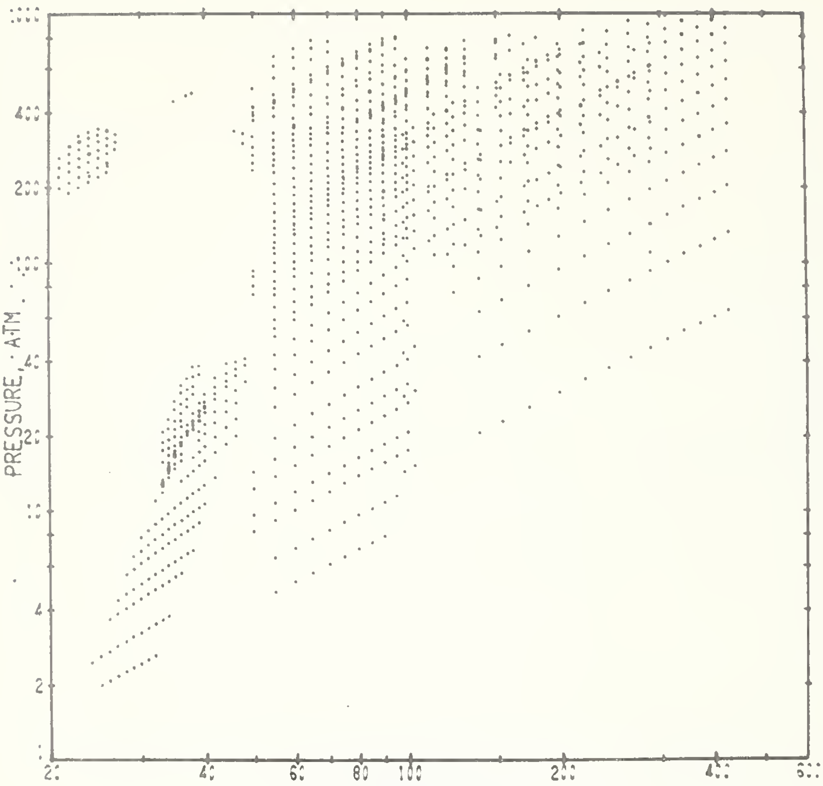
D, DEV. GREATER THAN 1.0 PERCENT



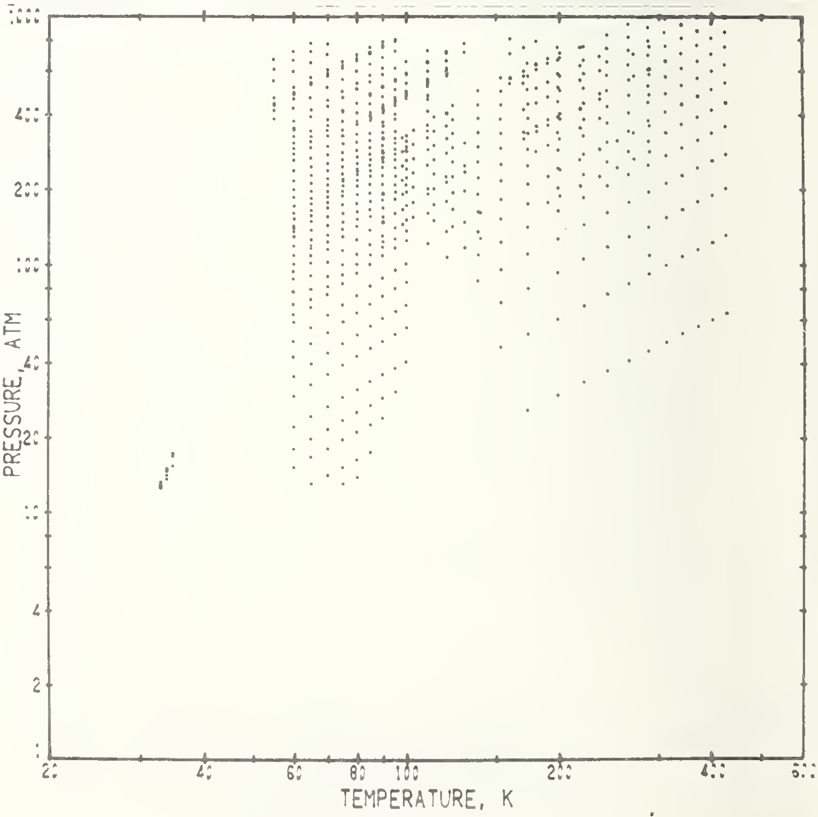
C, DEV. GREATER THAN 0.5 PERCENT

Figure 5.

Continued



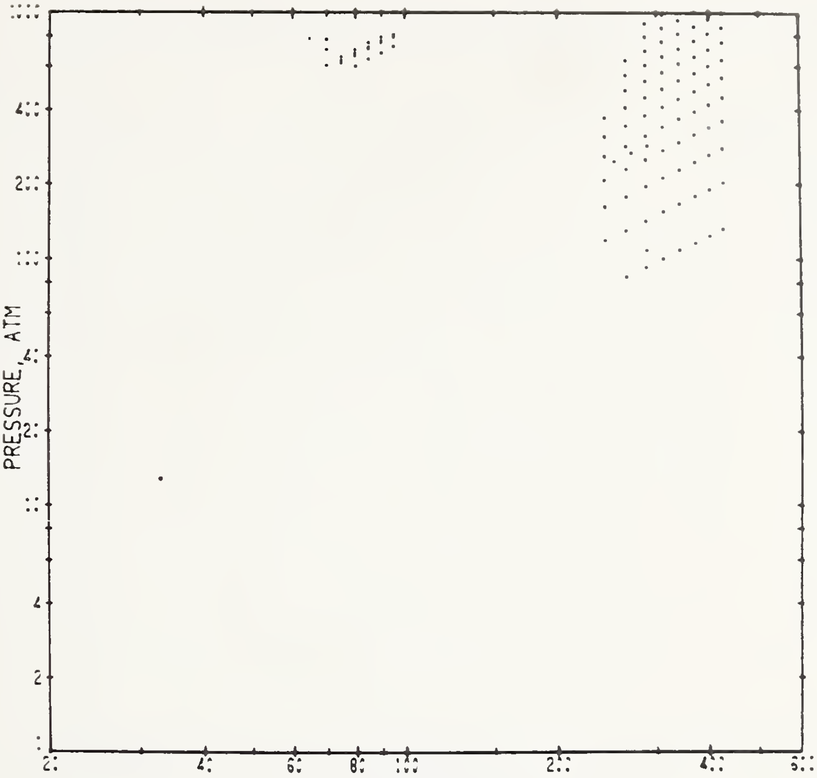
A, DEV. GREATER THAN 1.0 J/MOL



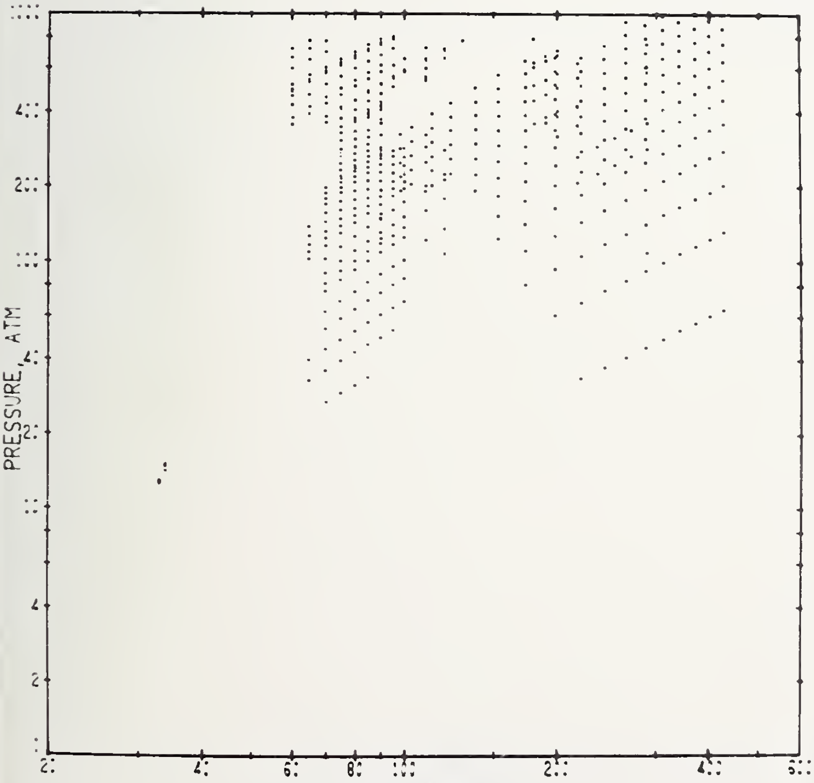
B, DEV. GREATER THAN 3.0 J/MOL

Figure 6.

Enthalpy Deviations in the
P-T Plane



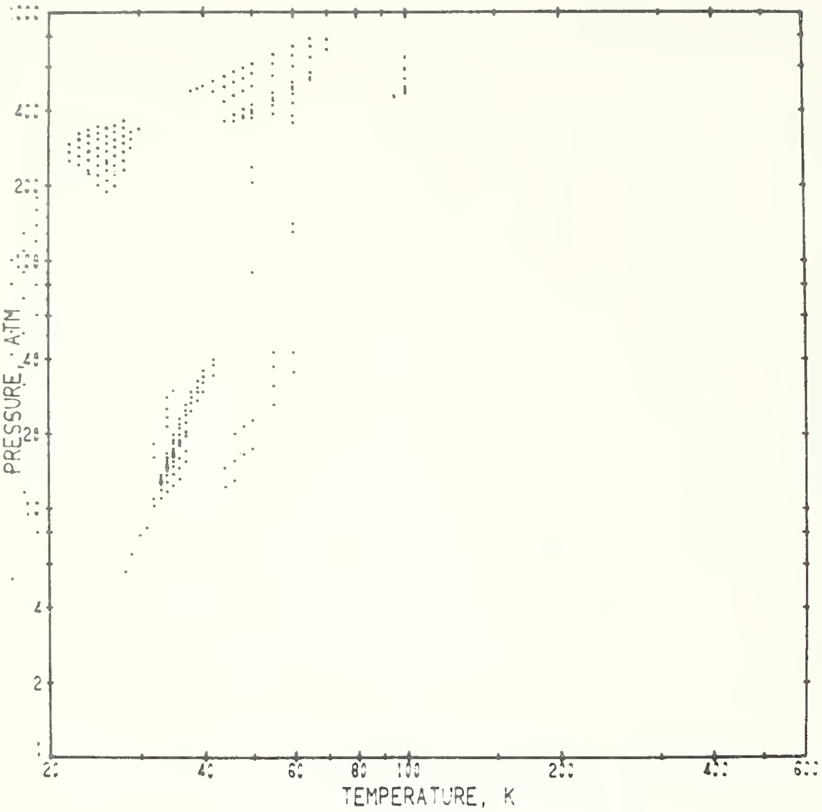
C, DEV. GREATER THAN 10. J/MOL



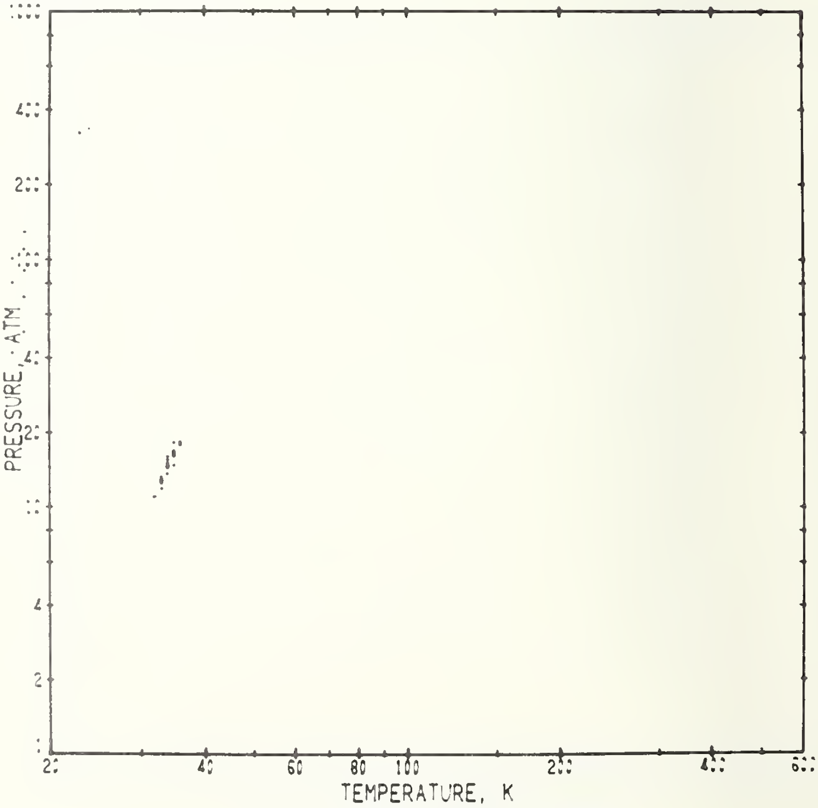
C, DEV. GREATER THAN 5.0 J/MOL

Figure 6.

Continued



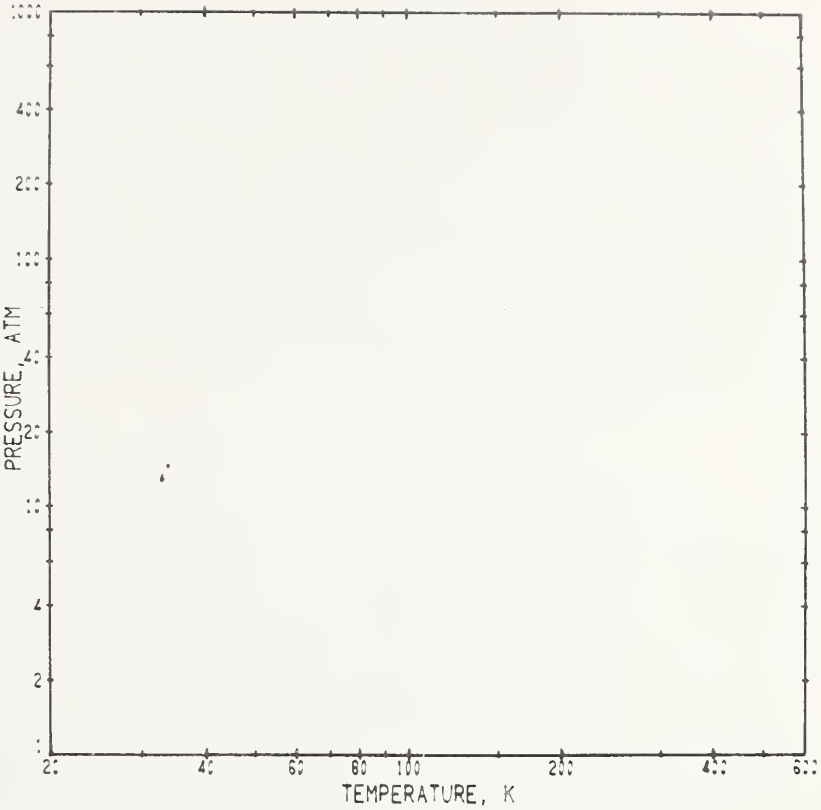
A, DEV. GREATER THAN 1.0 PERCENT



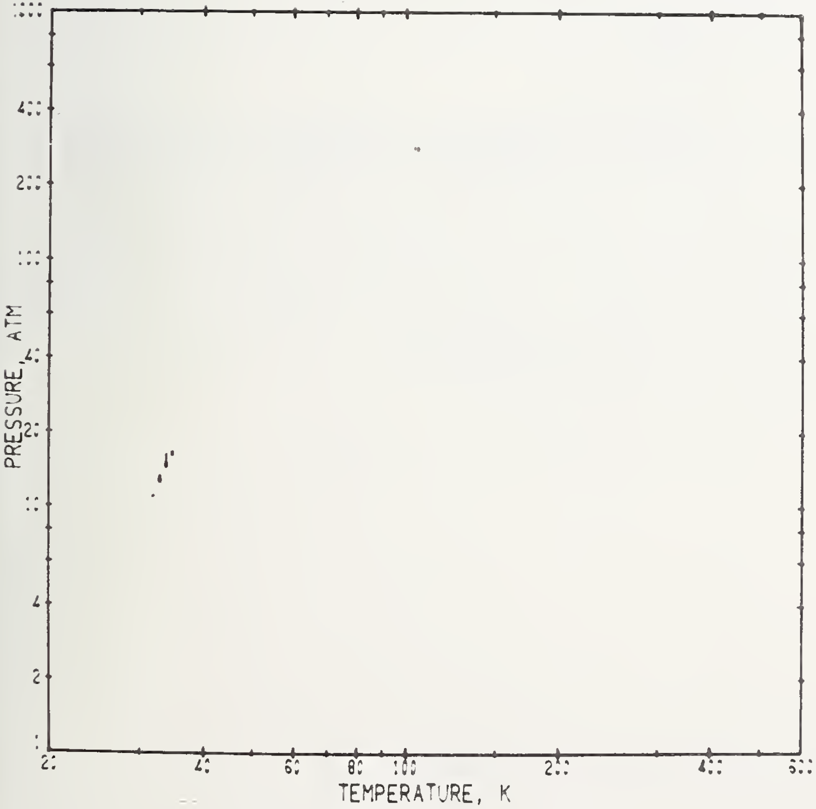
B, DEV. GREATER THAN 3.0 PERCENT

Figure 7.

Cp Deviations in the P-T Plane



D, DEV. GREATER THAN 10. PERCENT



C, DEV. GREATER THAN 5.0 PERCENT

Figure 7.

Continued

The C_p plots figure 7, which are in percent, show that the departures at the higher temperatures are negligible, just as the enthalpy departures would be had we expressed them in percent. The effect of adding C_v data along the saturated vapor line (line 8, table 1) is to reduce departures in C_p from several percent to less than 1 percent. Similarly the addition of extrapolated PVT data (line 3, table 1) improves the errors in C_p near the melting line from greater than 10 percent to 3 percent or less. In addition, an inconsistency in C_p noted in the earlier correlation (see isotherm 140°R, figure 5) of McCarty and Weber (1972) is removed. From figure 7 we estimate the average departure in C_p to be somewhat less than 3 percent.

6.3 The MBWR Extrapolated to High Densities

One of the peculiarities of the MBWR is that occasionally the iteration to find density yields an invalid result*. The situation can be understood by considering figure 8 where an isotherm of the MBWR is extrapolated to high densities. The range of valid PVT data is normally somewhere to the left of the maximum in pressure. It is easy to visualize an iteration using the slope $(\partial P/\partial \rho)_T$ of the surface and an initial density of $\rho = 0$ yielding a density to the right of the maximum in pressure, i.e., an invalid result. A case in point is the addition of extrapolated PVT data (line 3, table 1) mentioned in section 6.2. Adding these 15 generated points shifts the maximum in pressure for the 23 K isotherm from ~ 380 atm to ~ 1000 atm. It is the change in slope $(\partial P/\partial \rho)_T$ near the melting line ~ 200 to 350 atm that results in the desired change in C_p.

The present equation of state yields only negative pressures for densities beyond the cutoff shown in figure 8. We note that this behavior is diametrically opposed to what one might anticipate. In general one would expect pressure to increase as the density increases unless a phase transition is encountered. At the possible phase transitions liquid/solid and molecular/atomic the pressure would remain constant for the associated change in density. Several attempts to force the 32 term MBWR to return positive pressures at very high densities have not been sucessful.

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* Occasionally described as "the equation of state blows up."

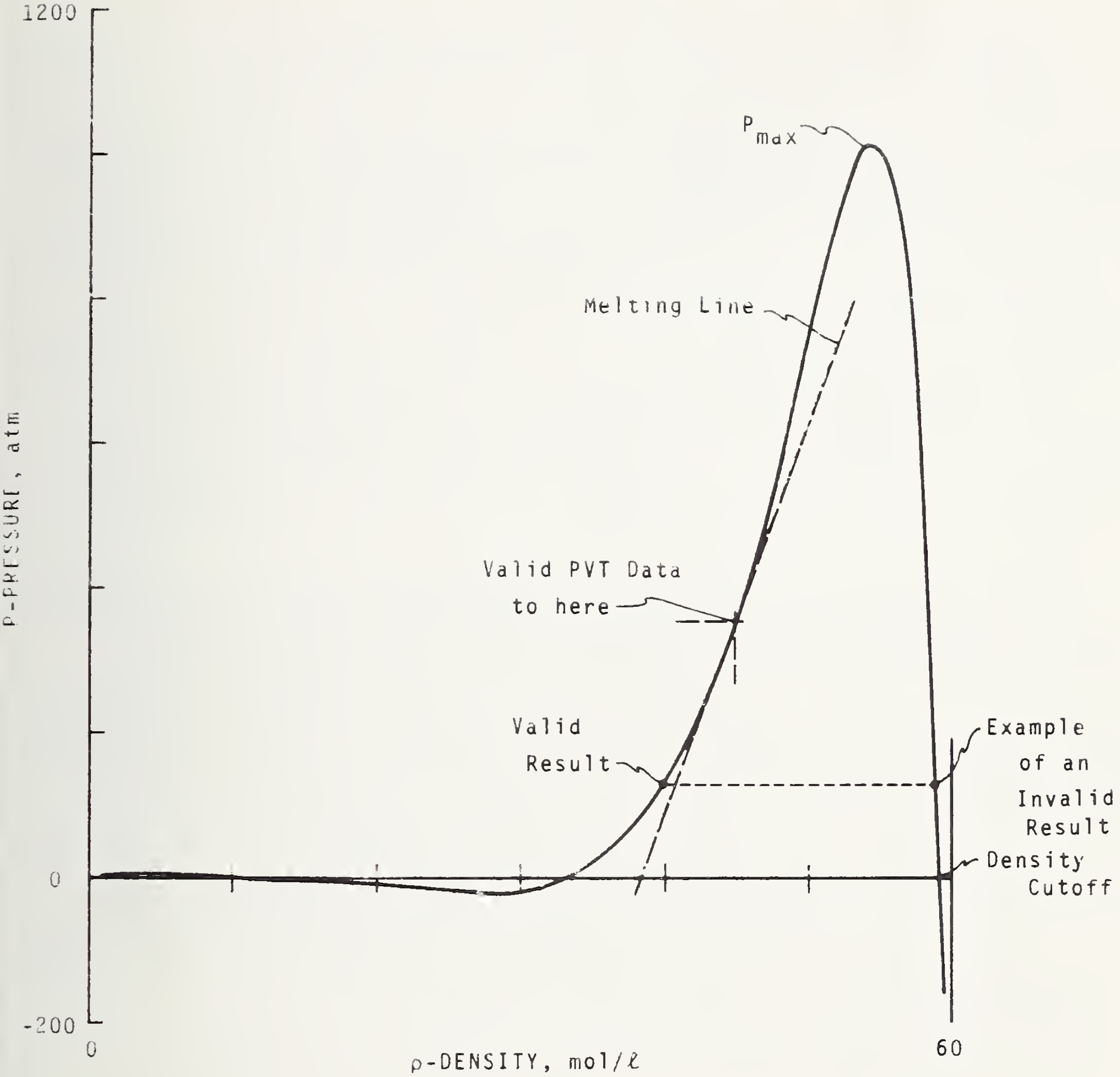

Figure 8. The MBWR at High Densities

7. Summary

To obtain the desired equation of state 2665 points were used including very recent measurements at low temperatures and high pressures. All PVT and C_v data had to be changed to the T_{68} scale, a non-analytical equation was applied to the vapor pressure, and the results of an index of refraction experiment were applied to the critical parameters and the two phase envelope near the critical point. Multi-property fitting of PVT and C_v data and the imposition of Gibbs phase constraints insured a substantially improved representation of the various thermodynamic quantities.

The resulting equation of state is valid for temperatures from the triple point, 13.8 K, to the onset of dissociation ~ 1500 K; it includes pressures gradually increasing from 700 atmospheres at the melting line to 3000 atmospheres at room temperature. In practical terms pressures up to 12000 psia are included, and the equation can be used for temperatures up to 5000°R if appropriate arrangement is made for dissociation.

Two characteristics of this equation of state must be kept in mind. First, the equation is analytic in nature, this means the critical region cannot be represented accurately. Second, the limiting behavior at high densities does not correspond to our a priori expectations, this means care has to be exercised to stay within the valid range of the equation.

The equation developed here sets a standard of what can be achieved in the fitting of an equation of this type. The high quality of the surface, illustrated in extensive deviation plots, is possible because ample data over a wide range of temperatures and pressures with inherently high precision is available as input. The PVT surface defined by the equation needs no further numerical treatment unless new experimental data become available, or the international temperature scale is redefined.

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```
      SUBROUTINE DATA P H2
      DIMENSION G(32),VP(8),GI(11)
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(4)
      COMMON/CPID/GI
      COMMON/CRIT/ EM, EOK, RM, TC, DC, X , PC, SIG
      COMMON/DATA/G,R,GAMMA,VP,DTP
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      TYPE DOUBLEG,R,GAMMA
      COMMON/PARA/PERCEN
      COMMON/ISP/N
      N=1
      GO TO 1
      ENTRY N H2
      N=2
      GO TO 1
      ENTRY O H2
      N=3
      GO TO 1
      ENTRY E H2
      N=4
      GO TO 1
      ENTRY F H2
      N=5
    1 CONTINUE
      EM=2.01594
      GAMMA=-.0041
      R=.08205616
      G( 1)   = 4.61438775565437326033D-04
      G( 2)   = 4.23318455608677043440D-02
      G( 3)   =-5.09655622650373332157D-01
      G( 4)   = 2.92305973826958605346D+00
      G( 5)   =-2.98760914721136029049D+01
      G( 6)   = 1.88314860141070378866D-05
      G( 7)   =-1.32225695463922652067D-03
      G( 8)   = 3.01650443170189249291D-01
      G( 9)   = 5.09370556085174282592D+01
      G(10)   = 1.97382832491904714077D-07
      G(11)   = 2.85849203982822717063D-04
      G(12)   =-2.22827923912348057045D-02
      G(13)   =-2.25748113576430406972D-06
      G(14)   = 2.41427236974667590421D-05
      G(15)   =-1.63571339858841047013D-03
      G(16)   =-5.39367639127519319151D-07
      G(17)   = 3.99895524432808380862D-09
      G(18)   = 1.14245756127449354105D-06
      G(19)   =-1.25256622589605274123D-08
      G(20)   =-4.91786193488253988296D+01
      G(21)   =-1.58566601736857779697D+02
      G(22)   =-1.90160294627218554366D-01
      G(23)   = 9.19802086250050278199D+00
      G(24)   =-3.18045551881044498741D-04
      G(25)   = 1.19105779192652709183D-03
      G(26)   =-3.79135277322539176132D-07
      G(27)   =-3.98337769909539545092D-05
      G(28)   =-1.23451085468897290708D-10
      G(29)   = 1.95026629349906989681D-09
      G(30)   =-2.38034391710916984687D-13
      G(31)   =-4.07357660819289386618D-13
      G(32)   = 8.80135493077752486716D-12
      VP(1)=3.05300134164
      VP(2)=2.80810925813
      VP(3)=-0.555461216567
      VP(4)=1.53514439374
      VP(5)=1.53144544428
      VP(7)=13.8
      VP(6)=0.0695
      VP(8)=32.938
      DTP=1./26.17*1000.
      RETURN
      END
```

```
      FUNCTION FINDTV(POBS)
C     CHANGED TO WORK FOR HYDROGEN, STARTS AT T-CRITICAL
      COMMON/DATA/G,R,GAMMA,VP,DTP
      DIMENSION G(32),VP(8)
      TYPE DOUBLEG,R,GAMMA
      T=VP(8)
      DO 7 I=1,30
      P=VPN(T)
      IF(ABS (P-POBS)-.000001*POBS)8,8,6
    6 CONTINUE
      CORR=(POBS-P)/DPDTVP(T)
    7 T=T+CORR
    8 CONTINUE
      FINDTV=T
      RETURN
      END

      FUNCTION PMELT(P)
C     FINDS TEMPERATURE FOR AN INPUT MELTING PRESSURE
    2 DIMENSION PP(77),TT(77)
      DATA(NTR=1)
    4 IF(NTR.EQ.2)  GO TO 12
    5 NTR=2
    6 T=14.000
    7 DO 11 I=1,77
    9 PP(I)=PRESSM(T)
   10 TT(I)=T
   11 T=T+0.120
   12 DO 14 I=1,77
   13 IF(PP(I)-P)14,15,15
   14 CONTINUE
   15 TAPP=TT(I)
   16 DO 23 I=1,10
   17 T=TAPP
   18 PM=PRESSM(T)
   19 FUNC=PM-P
   20 T=TAPP+0.001
   21 PM=PRESSM(T)
   22 FUNCP=(PM-FUNC-P)/0.001
   23 TAPP=TAPP-FUNC/FUNCP
   24 PMELT=TAPP
   25 RETURN
      END

      FUNCTION DIE(DP)
      DI=DP
      CM=.99575-0.09069*DI+1.1227*DI**2
      CM=1./CM
      DICM=DI*CM
      EP=-(1.+2.*DICM)/(DICM-1.)
      DIE=EP
      RETURN
      END

      FUNCTION VPN(TT)
      COMMON/DATA/G,R,GAMMA,VP
      DIMENSION G(32),VP(8)
      TYPE DOUBLE G,R,GAMMA
      T=TT
      X=(1.-VP(7)/T)/(1.-VP(7)/VP(8))
      VPN=VP(6)*EXP (VP(1)*X+VP(2)*X*X+VP(3)*X**3+VP(4)*X*(1.-X)**VP(5))
      RETURN
      END

      FUNCTION DPDTVP(TT)
      COMMON/DATA/G,R,GAMMA,VP
      DIMENSION G(32),VP(8)
      TYPE DOUBLE G,R,GAMMA
      T=TT
      IF(TT.GT.VP(8))GO TO 1
      X=(1.-VP(7)/T)/(1.-VP(7)/VP(8))
      DXDT=(VP(7)/T**2)/(1.-VP(7)/VP(8))
      DPDT=VP(1)*DXDT+2.*VP(2)*X*DXDT+VP(3)*3.*X**2*DXDT+VP(4)*
     1((1.-X)**VP(5))*DXDT+VP(4)*X*((1.-X)**(VP(5)-1.))*VP(5)*(-DXDT)
      DPDT=DPDT*VPN(T)
      DPDTVP=DPDT
      RETURN
    1 DPDTVP=0
      RETURN
      END
```

```
      FUNCTION PRESSM(T)
C     CALCULATES MELTING PRESSURE FROM AN INPUT TEMPERATURE
   21 PS=.0695+(T-13.803)*30.3312*EXP (-5.693/T)+(T-13.803)*2.0*T/3.0
   19 PRESSM=PS
      RETURN
      END

      FUNCTION DSATV(T)
      DIMENSION GV(8),GL(7)
      DATA(GL=0.04864581300З,-3.4779278186E-2,4.0776538192E-1,
     1-1.1719787304,1.62139244,-1.1531096683,0.33825492039)
      DATA(RHOC=0.03136),(BETAL=.34786027325),(TC=32.938)
      DATA(GV=-0.047501571529,3.4871213005E-2,-4.1221290925E-1,
     11.566659855,-2.8061427339,2.7105455626,-1.307477359,
     20.22921285922),(BETAV=.34831237625),(FACT=496.04651)
      A=(TC-T)/TC
      DV=RHOC+GV(1)*A**BETAV
      DO 1 I=1,7
    1 DV=DV+GV(I+1)*A**(1.+(I-1)/3.)
      DV=DV*FACT
      DSATV=DV
      RETURN
      ENTRY DSATL
      A=(TC-T)/TC
      DV=RHOC+GL(1)*A**BETAL
      DO 2 I=1,6
    2 DV=DV+GL(I+1)*A**(1.+(I-1)/3.)
      DV=DV*FACT
      DSATV=DV
      RETURN
      END

      FUNCTION CPI(T)
      COMMON/CPID/G(11)
      COMMON/ISP/N
      IF(N.NE.0)GO TO 5
      K=1
    1 U=G(9)/T
      EU=EXP (U)
      TS=1./T**4
      GO TO (2,3,4),K
    2 CPI=G(8)*U*U*EU/(EU-1.)**2
      DO 10 I=1,7
      TS=TS*T
   10 CPI=CPI+G(I)*TS
      CPI=CPI*8.31434
      RETURN
    5 CPI=CPO(T,N)
      RETURN
      ENTRY SI
      IF(N.NE.0)GO TO 6
      K=2
      GO TO 1
    3 CPI=G(8)*(U/(EU-1.)-ALOG(1.-1./EU))
     1-G(1)*TS*T/3.-G(2)*TS*T*T/2.-G(3)/T+G(4)*ALOG(T)+G(5)*T+G(6)*T*T/2
     2.+G(7)*T**3/3.
      CPI=CPI*8.31434+G (11)
      RETURN
    6 CPI=CPOS(T,N)
      RETURN
      ENTRY HI
      IF(N.NE.0)GO TO 7
      K=3
      GO TO 1
    4 CPI=G(8)*U*T/(EU-1.)-G(1)/(2.*T*T)-G(2)/T+G(3)*ALOG(T)+G(4)*T
     1+G(5)*T*T/2.+G(6)*T**3/3.+G(7)*T**4/4.
      CPI=CPI*8.31434+G(10)
      RETURN
    7 CPI=CPOH(T,N)
      RETURN
      END

      FUNCTION DILV(T)
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(4)
      SUM=0
      TF=T**(1./3.)
      TFF=T**(-4./3.)
      DO 10 I=1,9
      TFF=TFF*TF
   10 SUM=SUM+GV(I)*TFF
      DILV=SUM*1000.
      RETURN
      ENTRY DILT
      TF=T**(1./3.)
```

```
      TFF=T**(-4./3.)
      SUM=0
      DO 20 I=1,9
      TFF=TFF*TF
   20 SUM=SUM+GT(I)*TFF
      DILV=SUM
      RETURN
      END

      FUNCTION CPO(TI,N)
      DIMENSION T(58),CPP(58),CPN(58),CPO(58),CPE(58)
      COMMON/PARA/ PERCEN
C     CALCULATES IDESL GAS SPECIFIC HEAT FOR H2 BY INTERPOLATING
C     DATA TAKEN FROM RP 1932, UNITS OF THE TABLES ARE  CAL/MOL DEG 5.
C     UNITS OF OJTPUT ARE JOULES/MOL DEG K.  THE INDEX N DETERMINES THE
C     SPECIES,FOR N=1,PARAHYDROGEN,N=2 NORMAL, N=3 ORTHO, N=4 EQUILIB
C     N=5,SOME ORTHO-PARA MIXTURE SPECIFIED BY COMMON /PARA/,PERCENT
C     RANGE OF TEMP IS FROM 10 TO 5000K.
      DATA(T=
     1 10.0, 12.0, 14.0, 16.0, 18.0, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0,
     2 50.0, 55.0, 60.0, 65.0, 70.0, 75.0, 80.0, 85.0, 90.0, 95.0,100.0,
     3105.0,110.0,115.0,120.0,125.0,130.0,135.0,140.0,145.0,150.0,160.0,
     4170.0,180.0,190.0,200.0,210.0,220.0,230.0,240.0,250.0,260.0,270.0,
     5280.0,290.0,300.0,350.0,400.0,500.0,600.,700.,1000.,1500.,2000.,
     63000.,4000.,5000.)
      DATA((CPE(I),I=1,58)=4.968   ,4.96884,4.97647,5.01153,5.07451,5.208
     11,5.83508,6.81282,7.87989,8.60613,9.00231,9.08005,8.93278,8.65894,
     28.33603,8.01207,7.71009,7.4416,7.21109,7.01858,6.85857,6.72957,6.6
     32055,6.53555,6.46904,6.42003,6.38403,6.36151,6.34602,6.33753,6.340
     401,6.34577,6.37276,6.413,6.45925,6.50975,6.5605,6.6095,6.65724,
     7                                         6.692,6.734,6.771,6.804,6.832,
     56.856,6.877,6.895,6.950,6.974,6.993,7.009,7.036,7.219,7.720,8.195,
     68.859,9.342,9.748)
      DATA(CPO=
     14.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,
     24.968,4.968,4.968,4.969,4.972,4.975,4.981,4.990,5.002,5.018,5.039,
     35.064,5.094,5.129,5.169,5.213,5.261,5.313,5.369,5.427,5.487,5.612,
     45.741,5.868,5.992,6.109,6.219,6.320,6.411,6.493,6.566,6.629,6.684,
     56.732,6.773,6.808,6.917,6.962,6.993,7.009,7.036,7.219,7.720,8.195,
     68.859,9.342,9.748)
      DATA(CPP=
     14.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,4.969,4.972,4.983,
     25.006,5.048,5.114,5.207,5.328,5.475,5.646,5.835,6.036,6.245,6.454,
     36.659,6.854,7.037,7.203,7.351,7.480,7.590,7.681,7.753,7.807,7.870,
     47.883,7.858,7.808,7.742,7.667,7.591,7.516,7.445,7.380,7.322,7.270,
     57.225,7.186,7.152,7.050,7.010,6.998,7.010,7.037,7.219,7.720,8.159,
     68.859,9.342,9.748)
      DATA(CPN=
     14.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,4.968,4.969,4.972,
     24.977,4.988,5.005,5.029,5.061,5.100,5.147,5.201,5.261,5.325,5.393,
     35.463,5.534,5.606,5.677,5.748,5.816,5.882,5.947,6.008,6.067,6.177,
     46.276,6.366,6.446,6.517,6.581,6.638,6.687,6.731,6.769,6.802,6.831,
     56.855,6.876,6.894,6.950,6.974,6.993,7.009,7.036,7.219,7.720,8.195,
     68.859,9.342,9.748)
      GO TO(1,2,3,4,5),N
    1 CPO=ATKINT(TI,CPP,T,58, 6,NES,.01)*4.184
      RETURN
    2 CPO=ATKINT(TI,CPN,T,58, 6,NES,.01)*4.184
      RETURN
    3 CPO=ATKINT(TI,CPO,T,58, 5,NES,.01)*4.184
      RETURN
    4 CPO=ATKINT(TI,CPE,T,58, 6,NES,.01)*4.184
      RETURN
    5 TUP=TI+.5
      TDN=TI-.5
      HUP=CPOH(TJP,5)
      HDN=CPOH(TDN,5)
      CPO=(HUP-HDN)
      RETURN
      END

      FUNCTION CPOH(TI,N)
      DIMENSION T(58),HP(58),HN(58),HO(58),HE(58)
      COMMON/PARA/ PERCEN
C     CALCULATES THE ENTHALPY OF THE IDEAL GAS FOR H2 BY INTERPOLATION
C     DATA TAKEN FROM RP 1932, UNITS OF TABLES ARE CAL/MOL
C     UNITS OF OJTPUT ARE JOULE/MOL.  THE INDEX N DETERMINES THE SPECIES
C     SPECIES,FOR N=1,PARAHYDROGEN,N=2 NORMAL, N=3 ORTHO, N=4 EQUILIB
C     N=5,SOME ORTHO-PARA MIXTURE SPECIFIED BY COMMON /PARA/,PERCENT
C     RANGE OF TEMP IS FROM 10 TO 5000K.
      DATA(T=
     1 10.0, 12.0, 14.0, 16.0, 18.0, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0,
     2 50.0, 55.0, 60.0, 65.0, 70.0, 75.0, 80.0, 85.0, 90.0, 95.0,100.0,
     3105.0,110.0,115.0,120.0,125.0,130.0,135.0,140.0,145.0,150.0,160.0,
     4170.0,180.0,190.0,200.0,210.0,220.0,230.0,240.0,250.0,260.0,270.0,
```

```
5280.0,290.0,300.0,350.0,400.0,500.0,600.,700.,1000.,1500.,2000.,
63000.,4000.,5000.)
 DATA(HN=
1 303.67, 313.60, 323.54, 333.48, 343.41, 353.35, 378.19, 403.03,
1 427.86, 452.71, 477.56, 502.43, 527.34, 552.32, 577.40, 602.62,
3 628.02, 653.64, 679.51, 705.66, 732.13, 758.92, 786.06, 813.55,
4 841.40, 869.61, 898.17, 927.08, 956.33, 985.91,1015.80,1045.99,
51107.22,1169.49,1232.71,1296.78,1361.60,1427.10,1493.20,1559.84,
61626.93,1694.44,1762.30,1830.48,1898.91,1967.57,2036.43,2382.74,
72730.94,3429.46,4129.51,4831.66,6966.23,10697.2,14679.2,
823230.9,32345.,41895.)
 DATA(HP=
1  49.68,  59.61,  69.55,  79.49,  89.42,  99.36, 124.20, 149.04,
2 173.88, 198.73, 223.61, 248.58, 273.71, 299.11, 324.90, 351.22,
3 378.22, 406.01, 434.71, 464.38, 495.09, 526.84, 559.62, 593.41,
4 628.14, 663.75, 700.14, 737.23, 774.92, 813.10, 851.69, 890.60,
5 969.04,1047.84,1126.58,1204.93,1282.69,1359.74,1436.03,1511.56,
61586.36,1660.49,1733.99,1805.95,1879.42,1951.47,2023.15,2377.83,
72729.17,3429.24,4129.48,4831.65,6966.23,10697.2,14679.2,
823230.9,32345.,41895.)
 DATA(HO=
1 388.33, 398.27, 408.20, 418.14, 428.07, 438.01, 462.85, 487.69,
2 512.53, 537.37, 562.21, 587.05, 611.89, 636.73, 661.57, 686.42,
3 711.29, 736.18, 761.11, 786.09, 811.14, 836.28, 861.54, 886.93,
4 912.49, 938.23, 964.18, 990.37,1016.80,1043.51,1070.50,1097.78,
51153.27,1210.04,1268.09,1327.39,1387.91,1449.56,1512.26,1575.93,
61640.46,1705.76,1771.74,1838.32,1905.41,1972.94,2040.86,2384.38,
72731.52,3429.53,4129.52,4831.66,6966.23,10697.2,14679.2,
823230.9,32345.,41895.)
 DATA(HE=
1  49.68,  59.62,  69.57,  79.56,  89.66,  99.96, 127.50, 159.12,
2 195.77, 236.90, 280.97, 326.24, 371.33, 415.35, 457.86, 498.74,
3 538.05, 575.93, 612.56, 648.13, 682.82, 716.78, 750.14, 783.03,
4 815.54, 847.76, 879.77, 911.63, 943.40, 975.11,1006.80,1038.52,
51102.11,1166.03,1230.39,1295.23,1360.58,1426.43,1492.76,1559.55,
61626.75,1694.32,1762.23,1830.43,1898.88,1967.55,2036.42,2382.74,
72730.94,3429.46,4129.51,4831.66,6966.23,10697.2,14679.2,
823230.9,32345.,41895.)
 GO TO(1,2,3,4,5) ,N
1 CPOH=ATKINT(TI,HP,T,58, 6,NES,.01)*4.184
  RETURN
2 CPOH=ATKINT(TI,HN,T,58, 6,NES,.01)*4.184
  RETURN
3 CPOH=ATKINT(TI,HO,T,58, 6,NES,.01)*4.184
  RETURN
4 CPOH=ATKINT(TI,HE,T,58,6 ,NES,.01)*4.184
  RETURN
5 PERCENT=PERCEN /100.
  CPOH=(ATKINT(TI,HO,T,58,6,NES,.01)*(1.-PERCENT)+
 1ATKINT(TI,HP,T,58,6,NES,.01)*PERCENT)*4.184
  RETURN
  END


  FUNCTION CPOS(TI,N)
  DIMENSION T(60),SP(60),SN(60),SO(60),SE(60)
  COMMON/PARA/ PERCEN
C CALCULATES  THE ENTROPY OF THE IDEAL GAS FOR H2 BY INTERPOLATING
C DAKEN FROM RP 1932, UNITS OF THE TABLES ARE CAL/MOL DEG K.  1
C UNITS OF OUTPUT ARE JOULES/MOL DEG K.  THE INDEX N DETERMINES THE
C SPECIES,FOR N=1,PARAHYDROGEN,N=2 NORMAL, N=3 ORTHO, N=4 EQUILIB
C N=5,SOME ORTHO-PARA MIXTURE SPECIFIED BY COMMON /PARA/,PERCENT
C RANGE OF TEMP IS FROM 10 TO 5000K.
  DATA(T=
 1 10.0, 12.0, 14.0, 16.0, 18.0, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0,
 2 50.0, 55.0, 60.0, 65.0, 70.0, 75.0, 80.0, 85.0, 90.0, 95.0,100.0,
 3105.0,110.0,115.0,120.0,125.0,130.0,135.0,140.0,145.0,150.0,160.0,
 4170.0,180.0,190.0,200.0,210.0,220.0,230.0,240.0,250.0,260.0,270.0,
 5280.0,290.0,300.0,350.0,400.0,450.0,500.0,550.0,600.0,700.,1000.,
 61500.,2000.,3000.,4000.,5000.)
  DATA(SP=
 U11.214,12.123,12.885,13.549,14.135,14.658,15.766,16.672,17.438,
 I18.102,18.688,19.214,19.693,20.135,20.548,20.938,21.310,21.669,
 022.017,22.356,22.688,23.014,23.334,23.648,23.957,24.260,24.557,
 424.848,25.132,25.410,25.681,25.945,26.451,26.929,27.379,27.802,
 528.201,28.577,28.932,29.268,29.586,29.889,30.177,30.452,30.716,
 630.969,31.212,32.305,33.244,34.069,34.806,35.473,36.082,37.165,
 739.701,42.720,45.007,51.221,53.839,55.969)
  DATA(SO=
 115.581,16.486,17.252,17.916,18.501,19.024,20.133,21.038,21.804,
 222.466,23.053,23.576,24.050,24.482,24.880,25.248,25.591,25.912,
 326.215,26.500,26.771,27.029,27.275,27.512,27.739,27.958,28.170,
 428.375,28.575,28.769,28.958,29.143,29.502,29.846,30.177,30.498,
 530.808,31.109,31.401,31.684,31.958,32.225,32.484,32.735,32.979,
 633.216,33.446,34.505,35.432,36.253,36.989,37.656,38.265,39.348,
 741.884,44.903,47.190,51.221,53.839,55.969)
```

```
      DATA(SN=
     115.607,16.512,17.278,17.941,18.527,19.050,20.159,21.064,21.830,
     222.494,23.079,23.603,24.078,24.513,24.914,25.288,25.638,25.969,
     326.283,26.582,26.868,27.143,27.407,27.663,27.911,28.151,28.384,
     428.611,28.832,29.047,29.256,29.461,29.856,30.234,30.595,30.942,
     531.274,31.594,31.901,32.197,32.483,32.758,33.025,33.282,33.531,
     733.772,34.005,35.073,36.003,36.825,37.561,38.228,38.836,39.920,
     742.455,45.475,47.762,51.221,53.839,55.969)
      DATA(SE=
     111.215,12.120,12.887,13.554,14.149,14.692,15.918,17.069,18.196,
     219.294,20.331,21.285,22.145,22.911,23.592,24.198,24.740,25.229,
     325.674,26.080,26.455,26.804,27.129,27.435,27.724,27.999,28.260,
     428.510,28.750,28.980,29.203,29.418,29.828,30.216,30.584,30.934,
     531.269,31.591,31.899,32.196,32.482,32.758,33.024,33.282,33.531,
     633.772,34.005,35.073,36.003,36.825,37.561,38.228,38.836,39.920,
     742.455,45.475,47.762,51.221,53.839,55.969)
      GO TO(1,2,3,4,5),N
    1 CPOS=ATKINT(TI,SP,T,60, 6,NES,.01)*4.184
      RETURN
    2 CPOS=ATKINT(TI,SN,T,60, 6,NES,.01)*4.184
      RETURN
    3 CPOS=ATKINT(TI,SO,T,60, 6,NES,.01)*4.184
      RETURN
    4 CPOS=ATKINT(TI,SE,T,60, 6,NES,.01)*4.184
      RETURN
    5 PERCENT=PERCEN /100. $ PER=1.-PERCENT
      CPOS=(ATKINT(TI,SO,T,60,6,NES,0.01)*PER+ATKINT(TI,SP,T,60,6,NES,.0
     11)*PERCENT)*4.184-(8.317*(PERCENT*ALOG(PERCENT)+PER*ALOG(PER)))
      RETURN
      END


      FUNCTION FIND T(P,D)
C     NEW FEB 1975
      COMMON/DATA/G,R,GAMMA,VP,DTP
      DIMENSION G(32),VP(8)
      TYPE DOUBLEG,R,GAMMA
      PP=P
      DD=D
C     USES A FIRST GUESS IN TEMPERATURE FROM T1
      CALL T1(PP,DD,TA)
      TT=TA
      DO 10 I=1,10
      CALL PRESS(PP,DD,TT)
      P2=PP
      IF(ABS (P-P2)-1.E-7*P)20,20,1
    1 CALL DPDT(PP,DD,TT)
      DP=PP
      CORR=(P2-P)/DP
      IF(ABS (CORR)-1.E-5  )20,20,10
   10 TT=TT-CORR
   20 FIND T=TT
      RETURN
      END


      FUNCTION FIND D(P,T)
C     CHANGED, TRIAL DENSITY VIA SUBROUTINE RHO1/T1, 24 FEB 1975
      COMMON/DATA/G,R,GAMMA,VP,DTP
      DIMENSION G(32),VP(8)
      TYPE DOUBLEG,R,GAMMA
      TT=T
      CALL RHO1(P,D,TT)
      DD=D
      DO 10 I=1,50
      CALL PRESS(PP,DD,TT)
      P2=PP
      IF(ABS (P-P2)-1.E-7*P)20,20,1
    1 CALL DPDD(PP,DD,TT)
      DP=PP
      CORR=(P2-P)/DP
      D=DD
      IF(ABS (CORR)-1.E-7*D)20,20,10
   10 DD=DD-CORR
   20 FIND D=DD
      RETURN
      END


      SUBROUTINE PROPS(PP,DD,TT)
      DIMENSION X(33)
      DIMENSION B(33),G(32)
      COMMON/DATA/G,R,GAMMA
      TYPE DOUBLE B,G          ,D,T,P,D2,D3,D4,D5,D6,D7,D8,D9,D10,D11,D12
     1,D13,TS,T2,T3,T4,T5,F ,F1,F21,F22,     F23,F24,F25,F26,GAMMA,R
      TYPE DOUBLE F212,F222,F232,F242,F252,F262
      TYPE DOUBLE G1,G2,G3,G4,G5,G6,X
```

```
      EQUIVALENCE (B,X)
      DATA(ID=1)
      DATA(IZ=1)
C     PROPS FOR H2 USING THE STEWART-JACOBSEN EQUATION
    1 CONTINUE
      IF(IZ.LE.0)GO TO 2
      IZ=0
    2 CONTINUE
C     PROPS FOR METHANE USING STEWART-JACOBSEN EQUATION OF STATE
C     PRELIMINARY FIT - DENSE FLUID REGION EMPHASISED,MCCARTY,4/26/73
      D=DD
      P=PP
      T=TT
      GM=GAMMA
      D2=D*D
      D3=D2*D
      D4=D3*D
      D5=D4*D
      D6=D5*D
      D7=D6*D
      D8=D7*D
      D9=D8*D
      D10=D9*D
      D11=D10*D
      D12=D11*D
      D13=D12*D
      TS=DSQRT(T)
      T2=T*T
      T3=T2*T
      T4=T3*T
      T5=T4*T
      F=DEXP(GAMMA*D2)
      GO TO (100,200,300,400,500,600,700),K
      ENTRY PRESS
      K=1
      GO TO 1
  100 CONTINUE
      B( 1)=D2*T
      B( 2)=D2*TS
      B( 3)=D2
      B( 4)=D2/T
      B( 5)=D2/T2
      B( 6)=D3*T
      B( 7)=D3
      B( 8)=D3/T
      B( 9)=D3/T2
      B(10)=D4*T
      B(11)=D4
      B(12)=D4/T
      B(13)=D5
      B(14)=D6/T
      B(15)=D6/T2
      B(16)=D7/T
      B(17)=D8/T
      B(18)=D8/T2
      B(19)=D9/T2
      B(20)=D3*F/T2
      B(21)=D3*F/T3
      B(22)=D5*F/T2
      B(23)=D5*F/T4
      B(24)=D7*F/T2
      B(25)=D7*F/T3
      B(26)=D9*F/T2
      B(27)=D9*F/T4
      B(28)=D11*F/T2
      B(29)=D11*F/T3
      B(30)=D13*F/T2
      B(31)=D13*F/T3
      B(32)=D13*F/T4
      IF(ID.GT.0)GO TO 102
      B(33)=P-R*D*T
      RETURN
  102 P=0
      M=32
      DO 101 I=1,M
  101 P=P+B(I)*G(I)
      P=P+R*D*T
      PP=P
      RETURN
      ENTRY DPDD
      K=2
      GO TO 1
  200 CONTINUE
      F1=2.00*F*GM*D
      F21=3.000*F*D2 +F1*D3
      F22=5.000*F*D4 +F1*D5
      F23=7.000*F*D6 +F1*D7
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```
      F24=9.000*F*D8 +F1*D9
      F25=11.00*F*D10+F1*D11
      F26=13.00*F*D12+F1*D13
      B( 1)=2.00*D*T
      B( 2)=2.00*D*TS
      B( 3)=2.00*D
      B( 4)=2.00*D/T
      B( 5)=2.00*D/T2
      B( 6)=3.00*D2*T
      B( 7)=3.00*D2
      B( 8)=3.00*D2/T
      B( 9)=3.00*D2/T2
      B(10)=4.00*D3*T
      B(11)=4.00*D3
      B(12)=4.00*D3/T
      B(13)=5.00*D4
      B(14)=6.00*D5/T
      B(15)=6.00*D5/T2
      B(16)=7.00*D6/T
      B(17)=8.00*D7/T
      B(18)=8.00*D7/T2
      B(19)=9.00*D8/T2
      B(20)=F21/T2
      B(21)=F21/T3
      B(22)=F22/T2
      B(23)=F22/T4
      B(24)=F23/T2
      B(25)=F23/T3
      B(26)=F24/T2
      B(27)=F24/T4
      B(28)=F25/T2
      B(29)=F25/T3
      B(30)=F26/T2
      B(31)=F26/T3
      B(32)=F26/T4
      M=32
      IF(ID.GT.0)GO TO 202
      B(33)=P-R*T
      RETURN
202   P=0
      DO 201 I=1,M
201   P=P+B(I)*G(I)
      P=P+R*T
      PP=P
      RETURN
      ENTRY DPDT
      K=3
      GO TO 1
300   CONTINUE
      X( 1)=D2
      X( 2)=D2/(2.00*TS)
      X( 3)=0
      X( 4)=-D2/T2
      X( 5)=-2.00*D2/T3
      X( 6)=D3
      X( 7)=0
      X( 8)=-D3/T2
      X( 9)=-2.00*D3/T3
      X(10)=D4
      X(11)=0
      X(12)=-D4/T2
      X(13)=0
      X(14)=-D6/T2
      X(15)=-2.00*D6/T3
      X(16)=-D7/T2
      X(17)=-D8/T2
      X(18)=-2.00*D8/T3
      X(19)=-2.00*D9/T3
      X(20)=-2.00*D3*F/T3
      X(21)=-3.00*D3*F/T4
      X(22)=-2.00*D5*F/T3
      X(23)=-4.00*D5*F/T5
      X(24)=-2.00*D7*F/T3
      X(25)=-3.00*D7*F/T4
      X(26)=-2.00*D9*F/T3
      X(27)=-4.00*D9*F/T5
      X(28)=-2.00*D11*F/T3
      X(29)=-3.00*D11*F/T4
      X(30)=-2.00*D13*F/T3
      X(31)=-3.00*D13*F/T4
      X(32)=-4.00*D13*F/T5
      IF(ID.GT.0)GO TO 302
      X(33)=PP-R*D
      RETURN
302   P=0
      DO 301 I=1,32
301   P=P+G(I)*X(I)
```

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      PP=P+R*D
      RETURN
      ENTRY DSDN
      K=4
      GO TO 1
  400 CONTINUE
C     S=S0-R*ALOG(D*R*T/P0)+(DSDN(D)-DSDN(0))*101.325 +CPOS(T)
      G1=F/(2.00*GM)
      G2=(F*D2-2.00*G1)/(2.00*GM)
      G3=(F*D4-4.00*G2)/(2.00*GM)
      G4=(F*D6-6.00*G3)/(2.00*GM)
      G5=(F*D8-8.00*G4)/(2.00*GM)
      G6=(F*D10-10.00*G5)/(2.00*GM)
      X( 1)=-D
      X( 2)=-D/(2.00*TS)
      X( 3)=0.D0
      X( 4)=+D/T2
      X( 5)=2.00*D/T3
      X( 6)=-D2/2.00
      X( 7)=0.D0
      X( 8)=D2/(2.00*T2)
      X( 9)=D2/T3
      X(10)=-D3/3.00
      X(11)=0.D0
      X(12)=D3/(3.00*T2)
      X(13)=0.D0
      X(14)=D5/(5.00*T2)
      X(15)= 2.00*D5/(5.00*T3)
      X(16)=D6/(6.00*T2)
      X(17)=D7/(7.00*T2)
      X(18)=2.00*D7/(7.00*T3)
      X(19)=D8/(4.00*T3)
      X(20)=2.00*G1/T3
      X(21)=3.00*G1/T4
      X(22)=2.00*G2/T3
      X(23)=4.00*G2/T5
      X(24)=2.00*G3/T3
      X(25)=3.00*G3/T4
      X(26)=2.00*G4/T3
      X(27)=4.00*G4/T5
      X(28)=2.00*G5/T3
      X(29)=3.00*G5/T4
      X(30)=2.00*G6/T3
      X(31)=3.00*G6/T4
      X(32)=4.00*G6/T5
      IF(ID.GT.0)GO TO 402
      RETURN
  402 P=0
      DO 401 I=1,32
  401 P=P+G(I)*X(I)
      PP=P
      RETURN
      ENTRY DUDN
      K=5
      GO TO 1
  500 CONTINUE
C     H=H0+(T*DSDN(D)-DSDN(0))*101.325+(DUDN(D-DUDN(0))*101.325+CPOH(T)
C     +(P/D-R*T)*101.325
      G1=F/(2.00*GM)
      G2=(F*D2-2.00*G1)/(2.00*GM)
      G3=(F*D4-4.00*G2)/(2.00*GM)
      G4=(F*D6-6.00*G3)/(2.00*GM)
      G5=(F*D8-8.00*G4)/(2.00*GM)
      G6=(F*D10-10.00*G5)/(2.00*GM)
      X( 1)=D*T
      X( 2)=D*TS
      X( 3)=D
      X( 4)=D/T
      X( 5)=D/T2
      X( 6)=D2*T/2.00
      X( 7)=D2/2.00
      X( 8)=D2/(2.00*T)
      X( 9)=D2/(2.00*T2)
      X(10)=D3*T/3.00
      X(11)=D3/3.00
      X(12)=D3/(3.00*T)
      X(13)=D4/4.00
      X(14)=D5/(5.00*T)
      X(15)=D5/(5.00*T2)
      X(16)=D6/(6.00*T)
      X(17)=D7/(7.00*T)
      X(18)=D7/(7.00*T2)
      X(19)=D8/(8.00*T2)
      X(20)=G1/T2
      X(21)=G1/T3
      X(22)=G2/T2
      X(23)=G2/T4
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      X(24)=G3/T2
      X(25)=G3/T3
      X(26)=G4/T2
      X(27)=G4/T4
      X(28)=G5/T2
      X(29)=G5/T3
      X(30)=G6/T2
      X(31)=G6/T3
      X(32)=G6/T4
      IF(ID.GT.0)GO TO 502
      RETURN
  502 P=0
      DO 501 I=1,32
  501 P=P+G(I)*X(I)
      PP=P
      RETURN
      ENTRY TDSDT
      K=6
      GD TD 1
  600 CONTINUE
C     CV=CV0+(TDSDN(/)-TDSDN(D))*101.325
      G1=F/(2.00*GM)
      G2=(F*D2-2.00*G1)/(2.00*GM)
      G3=(F*D4-4.00*G2)/(2.00*GM)
      G4=(F*D6-6.00*G3)/(2.00*GM)
      G5=(F*D8-8.00*G4)/(2.00*GM)
      G6=(F*D10-10.00*G5)/(2.00*GM)
      X( 1)=0.D0
      X( 2)=-D/(4.00*TS)
      X( 3)=0.D0
      X( 4)=2.00*D/T2
      X( 5)=6.00*D/T3
      X( 6)=0.D0
      X( 7)=0.D0
      X( 8)=D2/T2
      X( 9)=3.00*D2/T3
      X(10)=0.D0
      X(11)=0.D0
      X(12)=(2.00*D3)/(3.00*T2)
      X(13)=0.D0
      X(14)=(2.00*D5)/(5.00*T2)
      X(15)=(6.00*D5)/(5.00*T3)
      X(16)=D6/(3.00*T2)
      X(17)=(2.00*D7)/(7.00*T2)
      X(18)=(6.00*D7)/(7.00*T3)
      X(19)=(3.00*D8)/(4.00*T3)
      X(20)=6.000*G1/T3
      X(21)=12.00*G1/T4
      X(22)=6.000*G2/T3
      X(23)=20.00*G2/T5
      X(24)=6.000*G3/T3
      X(25)=12.00*G3/T4
      X(26)=6.000*G4/T3
      X(27)=20.00*G4/T5
      X(28)=6.000*G5/T3
      X(29)=12.00*G5/T4
      X(30)=6.000*G6/T3
      X(31)=12.00*G6/T4
      X(32)=20.00*G6/T5
      IF(ID.GT.D)GO TO 602
      RETURN
  602 P=0
      DO 601 I=1,32
  601 P=P+G(I)*X(I)
      PP=P
      RETURN
      ENTRY DP2D2
      K=7
      GO TO 1
  700 CONTINUE
      F1=2.*F*GM*D
      F12=2.*F1*GM*D+2.*F*GM
      F212=3.*F1*D2+3.*2.*D*F+F12*D3+F1*3.*D2
      F222=5.*F1*D4 +5.*4.*D3*F+5.*D4*F1+F12*D5
      F232=7.*F1*D6+7.*6.*D5*F+7.*D6*F1+F12*D7
      F242=9.*F1*D8+9.*8.*D7*F+9.*D8*F1+F12*D9
      F252=11.*F1*D10+10.*11.*D9*F+11.*D10*F1+F12*D11
      F262=13.*F1*D12+13.*12.*D11*F+13.*D12*F1+F12*D13
      B(1)=2.*T   $B(2)=2.*TS   $  B(3)=2.
      B(4)=2./T   $  B(5)=2./T2   $  B(6)=6.*D*T
      B(7)=6.*D   $  B(8)=6.*D/T   $  B(9)=6.*D/T2
      B(10)=12.*D2*T   $  B(11)=12.*D2   $  B(12)=12.*D2/T
      B(13)=20.*D3   $  B(14)=30.*D4/T   $  B(15)=30.*D4/T2
      B(16)=42.*D5/T   $  B(17)=56.*D6/T   $  B(18)=56.*D6/T2
      B(19)=72.*D7/T2   $  B(20)=F212/T2   $  B(21)=F212/T3
      B(22)=F222/T2
      B(23)=F222/T4   $  B(24)=F232/T2   $  B(25)=F232/T3
```

```
      B(26)=F242/T2  $  B(27)=F242/T4   $  B(28)=F252/T2
      B(29)=F252/T3  $  B(30)=F262/T2   $  B(31)=F262/T3
      B(32)=F262/T4
      M=32
      IF(ID.GT.0)GO TO 702
      B(33)=PP
      RETURN
  702 P=0
      DO 701 I=1,M
  701 P=P+B(I)*G(I)
      PP=P
      RETURN
      END


      FUNCTION CP(D,T)
      CVEE=CV(D,T)
      CALL DPDT(DPT,D,T)
      CALL DPDD(DPD,D,T)
      CP=CVEE+(T/(D**2)*(DPT**2)/DPD)*101.325
      RETURN
      END


      FUNCTION CV(D,T)
      DATA(R=8.31434)
      DD=D
      TT=T
      CALL TDSDT(CD,DD,TT)
      DD=0
      CALL TDSDT(C0,DD,TT)
      CV=CPI(TT)+(C0-CD)*101.325
      CV=CV-R
      RETURN
      END


      FUNCTION ENTROP(D,T)
      R=.08205616
      DD=D
      TT=T
      CALL DSDN(SD,DD,TT)
      DD=0
      CALL DSDN(S0,DD,TT)
      ENTROP=(SD-S0)*101.325-R*ALOG(D*R*T)*101.325+SI(T)
      RETURN
      END


      FUNCTION VISC(DD,T)
      COMMON/CRIT/EM
      D=DD*EM/1000.
      VISC=DILV(T)+FDCV(D,T)+EXCESV(D,T)
      RETURN
      END


      FUNCTION FDCV(D,T)
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      DIMENSION GV(9),GT(9),FV(4),FT(4),EV(8),ET(4)
      FDCV=(FV(1)+FV(2)*(FV(3)-ALOG(T/FV(4)))**2)*D
      RETURN
      ENTRY FDCT
      FDCV=(FT(1)+FT(2)*(FT(3)-ALOG(T/FT(4)))**2)*D
      RETURN
      END


      FUNCTION EXCESV(D,T)
      COMMON/DATA1/GV,GT,FV,FT,EV,ET
      DIMENSION GV(9),GT(3),FV(4),FT(4),EV(8),ET(4)
      R2=D**(.5)*((D-EV(8))/EV(8))
      R=D**(.1)
      X=EV(1)+EV(2)*R2+EV(3)*R+EV(4)*R2/(T*T)+EV(5)*R/T**(1.5)+EV(6)/T
     1+EV(7)*R2/T
      X1=EV(1)+EV(6)/T
      EXCESV=EXP (X)-EXP (X1)
      RETURN
      ENTRY EXCEST
      R=D**(.1)
      X=ET(1)+ET(2)*R+ET(3)*R/T**(1.5)+ET(4)/T
      X1=ET(1)+ET(4)/T
      EXCESV=(EXP (X)-EXP (X1))/10.
      RETURN
      END
```

```
      FUNCTION THERM(DD,T)
      COMMON/CRIT/EM
      O=DD*EM/1000.
      THER=DILT(T)+FDCT(D,T)*100.+EXCEST(D,T)+CRITC(D,T)
       THERM=THER
      RETURN
      END


       FUNCTION CRITC(D,T)
      COMMON/CRIT/ EM, EOK, RM, TC, OC, X , PC, SIG
C D IN G/CM3 , T IN K
C  OJTPUT UNITS ARE MW/M.K
      AV=6.0225E+23 $ BK=1.38054E-16
C  CALCULATE DISTANCE PARAMETER
      R=(RM**2.5)*(D**0.5)*(AV/EM)**0.5
      R=R*(EOK**0.5)*X/(T**0.5)
C   GENERAL  EQUATION
      DX=D*1000.0/EM
C  DPDT  IN  ATS PER DEG.
      CALL DPDT(DPT,DX,T)
      DPT=DPT*1.01325E+6
C  DPDT NOW IN DYNES PRR DEG
C  DPDD UN ATS, MOL/L
      CALL DPDD(DPD,DX,T)
      DPD=DPD*1.01325E+6*(EM/1000.)
CDPDD NOW IN DYNES, GM/CM3
C   VISCOSITY IN GM/CM.S
      VIS=VISC(D,T)*(1.0E-06)
      COMPRES=1.0/(D*DPD)**0.5
      EX=BK*T**2*(DPT**2)*COMPRES
      EXB=R*((BK*T)**0.5)*(D**0.5)*((AV/EM)**0.5)
      CRIT=EX/(EXB*6.0*3.14159*VIS)
C   PUT IN DAMPING FACTOR
      BDD=((D-DC)/DC)**4
      BTT=((T-TC)/TC)**2
      FACT=EXP (-18.66*BTT - 4.25*BDO)
      OELC=CRIT*FACT/100.0
      CRITC=OELC
      RETURN
       ENO


      FUNCTION SOUND(D,T)
      COMMON/CRIT/W
      CALL DPOO(DP,D,T)
      SOUND=((CP(D,T)/CV(D,T))*DP*101325./W)**.5
      RETURN
      ENO


      FUNCTION PHI(D,T)
      CALL DPDT(DT,O,T)
      CSUBV=CV(D,T)
      PHI=DT/(CSUBV*D)
      RETURN
      END


      FUNCTION THETA(D,T)
      CALL DPDT(DT,D,T)
      CALL DPDD(DD,D,T)
      CSUBP=CP(D,T)
      THETA=D*CSUBP*DD/DT
      RETURN
      END


      FUNCTION ENTHAL(P,D,T)
      R=.08205615
      DD=D
      TT=T
      CALL DSDN(SD,DD,TT)
      CALL DUDN(UD,DD,TT)
      DD=0
      CALL DSDN(S0,DD,TT)
      CALL DUDN(U0,DD,TT)
      ENTHAL=T*(SD-S0)*101.325+(UD-U0)*101.325+HI(T)+(P/D-R*T)*101.325
      RETURN
      END

      SUBROUTINE RHO1(PP,DD,TT)
C     1ST CUT AT RHO FROM P=A+B*T
C     REALLY AN ITERATION, BUT IT MAY BE SMALL ENOUGH ANO FAST ENOUGH
C     P IN ATM, T IN K, RHO IN MOLES/LITER
      DIMENSION RHO(43),A(43),B(43)
```

```
      DATA((RHO(I),I=1,43)=1.,2.,3.,4.,5.,6.,7.,8.,9.,10.,11.,12.,13.,14
     1.,15.,16.,17.,18.,19.,20.,21.,22.,23.,24.,25.,26.,27.,28.,29.,30.,
     231.,32.,33.,34.,35.,36.,37.,38.,39.,40.,41.,42.,43.)
      DATA((A(I),I=1,43)=-.29599025741,-1.1388466175,-2.4851378102,-4.30
     141059317,-6.569655393,-9.2559185405,-12.336266965,-15.783961531,-1
     29.573370659,-23.681041295,-28.086458285,-32.772558951,-37.72660671
     39,-42.942371352,-48.424432541,-54.194465142,-60.287558106,-66.7267
     484771,-73.516518375,-80.643765419,-88.079905894,-95.781501825,-103
     5.68960091,-111.72777842,-119.79974172,-127.786579,-135.94257761,-1
     643.83339382,-151.26549964,-157.99608468,-163.7188857,-167.27870589
     7,-169.71922308,-169.76998914,-166.80726845,-160.22976454,-149.6001
     8063,-134.68300216,-116.11756401,-94.290117568,-67.824247269,-36.74
     92895824,-1.8295576977)
      DATA((B(I),I=1,43)=.085083208549,.17575158596,.27172674979,.372976
     118724,.47952911465,.59141276615,.70864366952,.83124684142,.9592844
     29114,1.0928802658,1.2322367731,1.3776455689,1.5294993198,1.6883212
     3266,1.8548249918,2.030005426,2.2151006109,2.4112674705,2.619508666
     45,2.8407043212,3.0756450876,3.325048554,3.5895525008,3.8696893541,
     54.1658593689,4.4782981944,4.8204022069,5.1840092761,5.569646053,5.
     69772524362,6.4057175531,6.8214242299,7.2780697825,7.7404616534,8.1
     7972575502,8.6358460465,9.0473286076,9.4260953807,9.8132635045,10.2
     822281363,10.63012984,11.05913828,11.565307194)
 10   P=PP
      T=TT
      IP=1
      PLO=0.
C     CHECK INPUT DATA FOR RANGE
C    INPUT RESTRICTIONS REMOVED
C     IF(P.GT.350.) GO TO 15
C     IF(T.GT.300.1) GO TO 15
C     GO TO 18
C 15  PRINT 16
C 16  FORMAT(24H INPUT DATA OUT OF RANGE)
C     DD=0.0
C     RETURN
C     CHECK MELTING LINE
 18   IF(T.GT.43.600) GO TO 23
      PS=.0695+(T-13.803)*30.3312*EXP (-5.693/T)+(T-13.803)*2.0*T/3.0
     1 +0.000001
      IF(P.LT.PS) GO TO 23
      PRINT 22
 22   FORMAT(26H INPUT CONDITIONS IN SOLID)
      DD=39.5
      RETURN
C     PHASEFINDER
 23   IF(T.LT.32.938) GO TO 27
      PPHASE=-50.6002+1.920888*T
      IF(P.GT.PPHASE) IP=15
      GO TO 36
 27   PVAP=VPN(T)
      IF(P-PVAP)36,32,35
 32   PRINT 33
 33   FORMAT(53H INPUT PLACES YOU EXACTLY ON THE VAPOR PRESSURE CURVE)
      DD=DSATL(T)
      RETURN
 35   DENL=DSATL(T)
      IP=DENL
C     START TABLE LOOKUP HERE
 36   CONTINUE
      DO 40 I=IP,43
      PCALC=A(I)+B(I)*T
      IF(P.LT.PCALC) GO TO 41
      PLO=PCALC
 40   CONTINUE
      IF(P.LT.PCALC) I=43
      IF(P.LT.PCALC) GO TO 41
C     PRINT 47
C 47  FORMAT(35H HIGH DENSITY, OUT OF RANGE FOR NOW)
      DD=44.
      RETURN
 41   CONTINUE
      DO 54 J=1,10
      RHOF=J
      RHOF=RHOF/10.
      IF(I.EQ.1) GO TO 50
      AA=A(I-1)+(A(I)-A(I-1))*RHOF
      BB=B(I-1)+(B(I)-B(I-1))*RHOF
      GO TO 52
 50   AA=A(I)*RHOF
      BB=B(I)*RHOF
 52   PCALC=AA+BB*T
      IF(P.LT.PCALC) GO TO 55
 54   PLO=PCALC
 55   FRAC=(P-PLO)/(PCALC-PLO)/10.
      DD   =I-1
      DD   =DD  +RHOF-0.1+FRAC
      RETURN
```

```
      ENTRY T1
C     FIRST GUESS FOR TEMPERATURE ITERATION OF FINDT
      P=PP
      D=DD
      DO 60 I=1,43
      IF(D.LT.RHO(I)) GO TO 61
   60 CONTINUE
      I=43
   61 FRAC=D-RHO(I-1)
      IF(I.EQ.1) GO TO 63
      AA=A(I-1)+(A(I)-A(I-1))*FRAC
      BB=B(I-1)+(B(I)-B(I-1))*FRAC
      GO TO 62
   63 FRAC=D
      AA=A(I)*FRAC
      BB=B(I)*FRAC
   62 TT=(P-AA)/BB
      END

      FUNCTION ATKINT(X,YMAT,XMAT,NELMTS,NMAX,NESSY,ACRCY)
C     THIS PROGRAM HAS BEEN CHANGED SO THAT THE OSCILLATING NATURE OF
C     THE MATRIX TO BE INTERPOLATED EXISTS ONLY AT THE UPPER END OF THE
C     TABLE
C     THIS ROUTINE WILL TAKE INPUT MATRICES OF UP TO 999 ELEMENTS EACH,
C     ARRANGED SO THAT THE X MATRIX(XMAT) IS IN EITHER ASCENDING OR
C     DESCENDING ORDER,SELECT NMAX OF THESE POINTS,CHOSEN SO THAT
C     SUCESSIVE X VALUES OSCILATE ABOUT THE VALUE OF THE ARGUMENT X
C     UNLESS THE ENDS OF THE XMATRIX INTERFERE (IN THIS CASE THE
C     OSCILATORY NATURE IS LOST BUT THE PROGRAM WILL STILL PERFORM AN
C     INTERPOLATION), INTERPOLATE ON THESE NMAX PAIRS OF DATA BY
C     AN OSCILATING VARIABLE POINT AITKEN INTERPOLATION ALGORITHM
C     EITHER UNTIL THE PERCENTAGE CHANGE IN THE INTERPOLANT IS LESS
C     THAN THE ACRCY ARGUMENT(THE ARGUMENT NESSY INDICATES THE
C     NUMBER OF THE POINT JUST BEFORE THE LAST ONE CHECKED) OR UNTIL
C     THE NMAX POINTS ARE ALL USED.  IT IS SUGGESTED THAT NMAX
C     BE LESS THAN 10, AND OF COURSE LESS THAN NELMTS.  NELMTS
C     INDICATES THE NUMBER OF ELEMENTS IN XMAT OR YMAT.
C     IF NESSY IS ZERO IT INDICATES THAT THE INTERPOLATION REQUIREMENT
C     HAS NOT BEEN SATISFIED.  IF NESSY IS 1 IT MEANS THAT THE VALUE OF
C     X LIES OUT SIDE THE RANGE OF XMAT.
      DIMENSION YMAT(999), XMAT(999),A(21,20)
  100 FORMAT(42HINTERPOLATION REQUIREMENT NOT SATISFIED(X=,E16.8,1H)/33H
     1LAST 2 APPROXIMATIONS OF Y ARE(Y=,E16.8,1H,,E16.8,1H))
  200 FORMAT(55HTHIS REPRESENTS AN EXTRAPOLATION OF THE  XMAT MATRIX(X=,
     1E16.8,1H)/33HNO CALCULATION HAS BEEN PERFORMED)
  300 FORMAT(24HNELMTS IS LESS THAN NMAX)
  400 FORMAT(22HNMAX IS LARGER THAN 20)
      IF(NMAX-20)71,71,69
   69 PRINT 400
      ATKINT=0.0
      RETURN
   71 IF(NMAX-NELMTS)75,75,73
   73 PRINT 300
      ATKINT=0.0
      RETURN
   75 CONTINUE
C     FIRST TWO SUCCESSIVE VALUES OF THE XMATRIX THAT STRADDLE THE
C     VALUE X WILL BE SOUGHT
      JJ1=NELMTS-1
      DO 20 I=1,JJ1
      DIF1=X-XMAT(I)
      DIF2=XMAT(I+1)-X
      IF(DIF1)16,15,16
   15 ATKINT=YMAT(I)
      NESSY =NMAX
      RETURN
   16 IF(DIF2)18,17,18
   17 ATKINT=YMAT(I+1)
      NESSY =NMAX
      RETURN
   18 RATIO=DIF1/ DIF2
      IF(RATIO)20,20,19
   19 IMID=I
      GO TO 32
   20 CONTINUE
C     AT THIS POINT ONE COULD PRINT THE FOLLOWING STATEMENT
C     WRITE OUTPUT TAPE 6,200,X
      NESSY=1
      ATKINT=0.0
      RETURN
   32 CONTINUE
C     NOTE THAT RATIO IS POSITIVE IF THE TWO POINTS STRADDLE X
C     REGARDLESS WHICH IS LARGER
      JJJ=IMID
      JUP=IMID
      JDN=IMID
```

```
      IF(JJJ+NMAX-NELMTS+1)98,98,102
   98 DO 201  J=1,NMAX
      JJJ=IMID+J-1
      A(1,J)=XMAT(JJJ)
  201 A(2,J)=YMAT(JJJ)
      GO TO 203
  102 DO 41  J=1,NMAX
      JJ=J/2
      JOE=J-2*JJ
C     JOE IS 0 IF J IS EVEN AND 1 IF J IS ODD
      IF(J-1)33,40,33
   33 IF(JDN-1)34,36,34
   34 IF(JUP-NELMTS)35,37,35
   35 IF(JOE)37,36,37
   36 JUP=JUP+1
      JJJ=JUP
      GO TO 40
   37 JDN=JDN-1
      JJJ=JDN
      GO TO 40
   40 A(1,J)=XMAT(JJJ)
      A(2,J)=YMAT(JJJ)
   41 CONTINUE
  203 NNN=NMAX+1
      DO 6  J=3,NNN
      L=J-1
      DO 5  K=L,NMAX
C     J IS THE COLUMN NUMBER
C     K IS THE ROW NUMBER
     0A(J,K)=(A(J-1,K)-A(J-1,J-2))*(X-A(1,J-2))/(A(1,K)-A(1,J-2))
     1       +A(J-1,J-2)
      IF(K-L)3,2,3
    2 IF(ABS  ((A(J,L)-A(J-1,L-1))/A(J,L))-ACRCY/100.0)7,7,3
    3 CONTINUE
    5 CONTINUE
    6 CONTINUE
      NESSY=0
C     AT THIS POINT ONE COULD PRINT OUT THE FOLLOWING STATEMENT.
C     WRITE OUTPUT TAPE 6,100,X,A(NNN,NMAX),A(NNN-1,NMAX-1)
      ATKINT=A(NNN,NMAX)
      RETURN
    7 NESSY=J-1
      ATKINT=A(J,L)
      RETURN
      END
```

Appendix B. Test Program and Sample Results

```
      PROGRAM VALUES
C     A SAMPLE PROGRAM TO CHECK RUNNING AT OTHER INSTALLATIONS.
C     CALCULATES THERMOFUNCTIONS OF PARA-H2 FROM THE 32 TERM MBWR.
C     INPUT IS READ FROM CARDS: P IN ATM, T IN DEG K.
C     OUTPUT: HEADING, UNITS, AND VALUES ARE PRINTED. HOWEVER, ONLY
C     A LIMITED NUMBER OF THE VARIABLES ARE CHECKED BY THIS SAMPLE DECK.
C     REQUIRED: ALL SUBROUTINES / FUNCTIONS LISTED IN NBSIR 75-814.
C     THE PROPERTIES DECK WAS LAST REVISED ON 75/06/17

      CALL DATAPH2
      PRINT 20
   20 FORMAT(82H1     P            T           RHO                 H           S
     1   C-V        C-P        VEL/82H     ATM           KELVIN       MOL/L
     2   J/MOL     J/MOL-K    J/MOL-K    J/MOL-K  M/SEC/1H )
      DO 19 I=1,4
    4 READ 5,P,T
    5 FORMAT(F6.3,F7.3)
      DEN=FINDD(P,T)
      H  =ENTHAL(P,DEN,T)
      S  =ENTROP(DEN,T)
      CVE=CV(DEN,T)
      CPE=CP(DEN,T)
      VEL=SOUND(DEN,T)
   12 PRINT 13,P,T,DEN,H,S,CVE,CPE,VEL
   13 FORMAT(F10.4,F12.5,F10.6,F12.1,3F10.2,F8.0)
   19 CONTINUE
      END
```

```
    P           T         RHO             H          S         C-V        C-P      VEL
   ATM        KELVIN     MOL/L          J/MOL     J/MOL-K    J/MOL-K    J/MOL-K  M/SEC

   1.0000    20.00000 35.279160        -521.9      15.84      11.33      19.11    1111
   1.0000    30.00000  0.420408         602.5      69.33      12.57      21.79     447
  15.0000    34.00000 17.424046          63.1      34.59      16.10     301.40     425
  70.0000    25.00000 36.713628        -289.9      17.53      12.30      19.52    1306
```

Appendix C. Conversion Factors

Temperature	1.8 R = 1 K
Pressure	14.695949 psia = 1 atm = 1.01325 x 10^5 N/m^2
Specific Volume	0.00794590 ft^3/lb_m = 1 cm^3/mol (1 cm^3 = 0.001 liter = 10^{-6} m^3)
Internal Energy, Enthalpy	0.213405 BTU/lb_m = 1 J/mol
Entropy, Specific Heat	0.118558 BTU/lb_mR = 1 J/mol-K
Thermal Conductivity	0.0578176 BTU/ft-hr-R = 1 mW/cm-K
Viscosity	0.067196897 lb_m/ft-s = 1 g/cm-s
Speed of Sound	3.2808 ft/s = 1 m/s
Molecular Weight	2.01594*
Surface Tension	0.5710147 x 10^{-5} lb_f/in = 1 dyn/cm (1 dyn = 10^{-5} N)

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* On the C^{12} = 12.000 scale

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

A 32 term modified Benedict-Webb-Rubin equation of state has been applied to data for parahydrogen. The adjustable parameters in the equation of state were determined using 2665 points including very recent measurements at low temperatures and high pressures. The new values extend the range of the PVT data sufficiently to warrant a refitting of the equation of state. Temperatures for the data range from the triple point to about 700 K with pressures reaching 3000 atmospheres near ambient temperatures. The PVT data were adjusted to the T_{68} scale. In addition, extensive modifications have been made to the previously accepted PVT surface in the region near the critical point. These adjustments have been made on the basis of more recent refractive index data and the application of scaling law equations. Detailed comparisons between experimental and calculated values are given for density. Corresponding comparisons are made for enthalpy and the specific heat at constant pressure.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

Critical point; density; enthalpy; equation of state; hydrogen; index of refraction PVT; saturation properties; scaling laws; specific heat

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