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in the Range 75—300 K and 2—20 kbar**

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DERIVED THERMODYNAMIC PROPERTIES FOR FLUID $n\text{-T}_2$

IN THE RANGE 75-300 K AND 2-20 kbar

by

D. H. Liebenberg, R. L. Mills, and J. C. Bronson

ABSTRACT

The tritium equation of state, extended from measurements of the lighter hydrogen isotopes, is used to derive thermodynamic properties of tritium fluid. Tabular values are given at rounded kbar pressures and 25 K temperature intervals in the range 75-300 K and 2-20 kbar. Included are the isobaric thermal expansion coefficient α_p , the molar heat capacity at constant pressure C_p , adiabatic compressibility coefficient χ_s , heat capacity ratio γ , and molar entropy S . Computer-drawn graphs of these variables vs pressure along five isotherms are shown.

I. INTRODUCTION

Tritium, the heavy radioactive isotope of hydrogen, is an important fuel component in fusion schemes. Compressing tritium in a fusion system from its natural gaseous state requires accurate knowledge of the equation of state (EOS) of this material. As with other hydrogen isotopes, embrittlement of high-strength steels has, together with the natural radioactivity of tritium, limited experimental studies. At Los Alamos we have developed techniques for extending hydrogen¹ and deuterium² measurements up to 20 kbar at 300 K. We use these data together with suitable extrapolations to determine P-V-T and sound velocity in tritium. An EOS for these derived data is calculated and used to derive other thermodynamic properties in the same manner as we have described for $n\text{-H}_2$ ⁴ and $n\text{-D}_2$ ⁵ fluids.

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II. EQUATION-OF-STATE DEVELOPMENT

There are no experimental data available for tritium molar volumes or sound velocities in the range 2-20 kbar and 75-300 K. We have deduced the molar volume and sound velocity in tritium from our measured values in hydrogen and deuterium in Ref. 3. In this case the scaling laws were used after correction for quantum effects.

These data, $V(P,T)$ and $v_s(P,T)$, were then fit to a volume-explicit EOS as discussed in Refs. 4 and 5. A Benedict⁶ form of the general EOS is given as

$$V = (AT^{-1/2} + B + CT)P^{-1/3} + (D + ET)P^{-2/3} + (FT^{-1} + GT^{-1/2} + H + JT)P^{-1} \quad (1)$$

In order to use the P - V - T and v_s data in a double-process least-squares fit of Eq. (1) the heat capacity at constant pressure must be known at some normalizing pressure over the full temperature range. Since $C_p(T)$ is dependent on the nuclear spins of the component molecules and Eq. (1) is sensitive to the details of $C_p(T)$, there was no possibility of obtaining an EOS for tritium by scaling the coefficients in Eq. (1). We did scale $C_p(T)$ values using earlier data for n -H₂ and n -D₂ and the reduced de Broglie wavelength as a quantum parameter, $\Lambda^* = h/\sigma (M\epsilon)^{1/2}$, where σ and ϵ are constants in the Lennard-Jones 6-12 potential. The resultant equation at 2 kbar pressure is

$$C_{p=2}(T) = -0.30565T + 19.875T^{1/2} - 434.56 + 4610.1T^{-1/2} - 15645T^{-1} \quad (2)$$

[J/mole-K].

The quantum parameter Λ^* was also used to readjust the critical volumes for use in a classical law of corresponding states to scale T_2 volumes³ from the D₂ data. These volumes were in good agreement with those found from a virial equation, also corrected for quantum effects.

Derived values of the sound velocity were obtained by kinetic theory scaling so that $v_s(T_2) = v_s(D_2)[M(D_2)/M(T_2)]^{1/2}$. From our measurements in hydrogen and deuterium, $v_s(H_2)/v_s(D_2)$ was observed to be well fit by the kinetic theory scaling except at the lowest pressures and temperatures where this ratio increased slightly. The application of the quantum parameter to these data was used in the scaling to correct the lower pressure and temperature data.

In Table I we give the values of the constants in Eq. (1) as derived from a fit of the corrected tritium data. This EOS fits the derived data with an average deviation of less than 0.1%.

III. DERIVED THERMODYNAMIC PROPERTIES

We have previously described⁴ the thermodynamic relations used together with the volume-explicit EOS to determine the isobaric expansion coefficient α_p , the heat capacity at constant pressure C_p , the adiabatic compressibility χ_s , the specific heat ratio γ , and the molar entropy s .

From Ref. 3 a value of the entropy that is thermodynamically consistent with the heat capacity is determined using $C_{p=2} = T(\partial S/\partial T)_{p=2}$ and gives

$$S_{p=2} = -0.30565T + 39.750T^{1/2} - 434.56 \ln T - 9220.2T^{-1/2} + 15645T^{-1} + 2447.96 \text{ [J/mole-K]}, \quad (3)$$

where the last value is a fitted constant of integration.

The output data at rounded kbar increments to 22 kbar or up to the freezing pressure and along isotherms from 75 to 300 K at 25 K intervals are available in Table II. Values of χ_T , the isothermal compressibility and C_v , the heat capacity at constant volume, can be found from χ_s and C_p , respectively, and $\gamma \equiv C_p/C_v = \chi_T/\chi_s$.

Variations of these thermodynamic quantities with pressure along five isotherms from 100-300 K at 50 K intervals are shown as Figs. 1-9 drawn with computer graphics from the EOS.

IV. DISCUSSION

A comparison of molar volumes with earlier derivations is given in Ref. 3. There are no sound velocity measurements in our temperature and pressure range.

G. Kerley⁷ has modified the deuterium EOS calculations and provided densities and sound velocities for tritium vs pressure along several isotherms that we have compared with our EOS calculations in Table II. In Figs. 10 and 11 the comparison data are shown. Agreement between densities averages about 2% over the pressure and temperature range. Sound velocities are in agreement to about 1.1% on the average. This agreement is considered quite good particularly since the EOS of Kerley is designed for accuracy at higher temperatures and pressures.

Fig. 1.
Molar volume of fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 2.
Sound velocity in fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 3.
Isobaric thermal expansion coefficient of fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 4.
Heat capacity at constant pressure for fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 5.
Heat capacity at constant volume for fluid $n\text{-T}_2$ as a function of pressure along five isotherms² computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 6.
Isothermal compressibility coefficient of fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 7.
Adiabatic compressibility coefficient for fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 8.
Heat capacity ratio, C_p/C_v , for fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 9.

Molar entropy for fluid $n\text{-T}_2$ as a function of pressure along five isotherms computed from Eqs. (1) and (3) using the constants in Table I. Solid line, 300 K; dotted line, 250 K; dashed line, 200 K; short-dash line, 150 K; dash-dot line, 100 K.

Fig. 10.

Log pressure for fluid $n\text{-T}_2$ vs density. The points are from Table II where $\circ$, $T=300$ K; ∇ , $T=200$ K, and $\times$, $T=100$ K. The solid curves are from calculations by Kerley⁷ along these isotherms.

Fig. 11.

Sound velocity for fluid $n\text{-T}_2$ vs pressure along two isotherms. The points are from Table II where $\circ$, $T=300$ K and $\times$, $T=100$ K and the solid curves from calculations by Kerley⁷ along these isotherms.

TABLE I

CONSTANTS OF EQ. (1) AS DETERMINED BY A DOUBLE-PROCESS LEAST-SQUARES FIT TO THE SMOOTH-DATA SET DERIVED IN REF. 3

A	34.3418
B	0.000265155
C	14.3171
D	-27.5059
E	0.0175803
F	24.2685
G	0.0501453
H	-280.186
J	1161.07

TABLE II
CALCULATED VALUES FROM EOS FOR $n\text{-T}_2$

CALCULATED VALUES FROM EOS FOR $T(2)$ AT 300.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	27.479	1.571	1.539E-03	32.004	1.330	1.844E-01	85.94
2.50	24.708	1.709	1.392E-03	32.252	1.318	1.403E-01	84.04
3.00	22.757	1.831	1.278E-03	32.444	1.305	1.125E-01	82.46
3.50	21.290	1.941	1.185E-03	32.600	1.294	9.363E-02	81.11
4.00	20.136	2.042	1.109E-03	32.729	1.283	8.004E-02	79.92
4.50	19.197	2.135	1.044E-03	32.837	1.274	6.982E-02	78.86
5.00	18.413	2.221	9.884E-04	32.929	1.265	6.187E-02	77.91
5.50	17.746	2.301	9.401E-04	33.009	1.257	5.553E-02	77.04
6.00	17.167	2.377	8.976E-04	33.079	1.249	5.036E-02	76.24
6.50	16.660	2.448	8.595E-04	33.140	1.242	4.607E-02	75.49
7.00	16.210	2.516	8.262E-04	33.193	1.236	4.245E-02	74.80
7.50	15.807	2.580	7.958E-04	33.241	1.230	3.935E-02	74.15
8.00	15.443	2.642	7.681E-04	33.283	1.224	3.668E-02	73.54
8.50	15.112	2.700	7.430E-04	33.320	1.219	3.435E-02	72.96
9.00	14.809	2.757	7.199E-04	33.354	1.214	3.230E-02	72.42
9.50	14.530	2.811	6.986E-04	33.384	1.209	3.048E-02	71.90
10.00	14.273	2.863	6.789E-04	33.410	1.205	2.886E-02	71.40
10.50	14.033	2.913	6.607E-04	33.434	1.201	2.740E-02	70.93
11.00	13.810	2.962	6.437E-04	33.455	1.197	2.609E-02	70.47
11.50	13.602	3.009	6.278E-04	33.474	1.193	2.489E-02	70.04
12.00	13.408	3.055	6.130E-04	33.491	1.190	2.381E-02	69.62
12.50	13.222	3.099	5.990E-04	33.506	1.186	2.281E-02	69.22
13.00	13.048	3.142	5.859E-04	33.519	1.183	2.190E-02	68.83
13.50	12.883	3.184	5.735E-04	33.530	1.180	2.106E-02	68.45
14.00	12.727	3.225	5.618E-04	33.540	1.177	2.028E-02	68.09
14.50	12.579	3.265	5.507E-04	33.549	1.174	1.955E-02	67.74
15.00	12.438	3.304	5.402E-04	33.556	1.172	1.888E-02	67.40
15.50	12.304	3.342	5.302E-04	33.563	1.169	1.826E-02	67.06
16.00	12.176	3.379	5.206E-04	33.568	1.167	1.767E-02	66.74
16.50	12.053	3.416	5.116E-04	33.572	1.165	1.712E-02	66.43
17.00	11.935	3.451	5.029E-04	33.575	1.162	1.661E-02	66.13
17.50	11.822	3.486	4.946E-04	33.578	1.160	1.612E-02	65.83

TABLE II (contd)

16.00	11.714	3.520	4.867E-04	33.579	1.158	1.567E-02	65.54
18.50	11.610	3.553	4.791E-04	33.580	1.156	1.524E-02	65.26
19.00	11.509	3.586	4.718E-04	33.580	1.154	1.483E-02	64.98
19.50	11.412	3.619	4.649E-04	33.579	1.153	1.444E-02	64.72
20.00	11.319	3.650	4.581E-04	33.578	1.151	1.408E-02	64.45
20.50	11.229	3.681	4.517E-04	33.576	1.149	1.373E-02	64.20
21.00	11.142	3.712	4.454E-04	33.574	1.147	1.340E-02	63.95
21.50	11.058	3.742	4.394E-04	33.571	1.146	1.309E-02	63.70
22.00	10.976	3.772	4.337E-04	33.568	1.144	1.279E-02	63.46
22.50	10.897	3.801	4.281E-04	33.564	1.143	1.250E-02	63.23

CALCULATED VALUES FROM E O S FOR T(2) AT 275.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	26.416	1.571	1.620E-03	32.084	1.335	1.774E-01	83.15
2.50	23.843	1.711	1.459E-03	32.337	1.320	1.350E-01	81.23
3.00	22.026	1.835	1.334E-03	32.533	1.306	1.084E-01	79.63
3.50	20.656	1.946	1.234E-03	32.690	1.293	9.036E-02	78.27
4.00	19.576	2.048	1.151E-03	32.819	1.281	7.736E-02	77.07
4.50	18.694	2.141	1.081E-03	32.927	1.270	6.758E-02	76.00
5.00	17.956	2.227	1.022E-03	33.019	1.260	5.998E-02	75.04
5.50	17.327	2.308	9.702E-04	33.097	1.251	5.390E-02	74.16
6.00	16.781	2.384	9.250E-04	33.165	1.243	4.894E-02	73.35
6.50	16.301	2.455	8.849E-04	33.224	1.236	4.482E-02	72.61
7.00	15.874	2.523	8.491E-04	33.275	1.229	4.134E-02	71.91
7.50	15.492	2.587	8.168E-04	33.320	1.222	3.837E-02	71.26
8.00	15.146	2.648	7.877E-04	33.360	1.216	3.579E-02	70.64
8.50	14.831	2.707	7.611E-04	33.395	1.211	3.355E-02	70.06
9.00	14.542	2.763	7.367E-04	33.425	1.206	3.157E-02	69.51
9.50	14.276	2.817	7.143E-04	33.452	1.201	2.982E-02	68.99
10.00	14.030	2.869	6.936E-04	33.476	1.196	2.825E-02	68.49
10.50	13.801	2.919	6.744E-04	33.497	1.192	2.684E-02	68.02
11.00	13.588	2.968	6.566E-04	33.515	1.188	2.557E-02	67.56
11.50	13.388	3.015	6.400E-04	33.530	1.184	2.442E-02	67.12
12.00	13.200	3.060	6.244E-04	33.544	1.181	2.336E-02	66.70
12.50	13.023	3.104	6.098E-04	33.555	1.177	2.240E-02	66.30
13.00	12.856	3.147	5.960E-04	33.565	1.174	2.151E-02	65.91
13.50	12.698	3.189	5.831E-04	33.573	1.171	2.069E-02	65.53
14.00	12.549	3.230	5.709E-04	33.580	1.168	1.994E-02	65.17
14.50	12.406	3.269	5.593E-04	33.585	1.165	1.924E-02	64.82
15.00	12.270	3.308	5.483E-04	33.589	1.163	1.858E-02	64.47
15.50	12.141	3.346	5.379E-04	33.592	1.160	1.797E-02	64.14
16.00	12.017	3.383	5.280E-04	33.594	1.158	1.740E-02	63.82
16.50	11.898	3.419	5.185E-04	33.595	1.155	1.687E-02	63.51
17.00	11.785	3.454	5.095E-04	33.595	1.153	1.637E-02	63.20
17.50	11.676	3.489	5.009E-04	33.593	1.151	1.590E-02	62.91
18.00	11.571	3.523	4.926E-04	33.592	1.149	1.545E-02	62.62
18.50	11.470	3.556	4.847E-04	33.589	1.147	1.503E-02	62.34
19.00	11.373	3.589	4.772E-04	33.585	1.145	1.464E-02	62.06
19.50	11.280	3.621	4.699E-04	33.581	1.143	1.426E-02	61.79
20.00	11.190	3.652	4.629E-04	33.577	1.141	1.390E-02	61.53
20.50	11.102	3.683	4.562E-04	33.571	1.140	1.356E-02	61.28
21.00	11.018	3.714	4.498E-04	33.566	1.138	1.324E-02	61.03
21.50	10.936	3.744	4.436E-04	33.559	1.136	1.293E-02	60.78
22.00	10.857	3.773	4.376E-04	33.552	1.135	1.264E-02	60.54
22.50	10.780	3.802	4.318E-04	33.545	1.133	1.236E-02	60.31

CALCULATED VALUES FROM E O S FOR T(2) AT 250.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	25.339	1.574	1.710E-03	32.267	1.339	1.696E-01	80.09
2.50	22.969	1.716	1.533E-03	32.520	1.321	1.293E-01	78.14
3.00	21.288	1.841	1.396E-03	32.714	1.305	1.040E-01	76.52
3.50	20.016	1.954	1.286E-03	32.869	1.290	8.689E-02	75.14
4.00	19.010	2.056	1.197E-03	32.995	1.277	7.453E-02	73.93
4.50	18.186	2.150	1.122E-03	33.099	1.265	6.523E-02	72.86
5.00	17.496	2.236	1.058E-03	33.187	1.254	5.799E-02	71.89
5.50	16.905	2.317	1.002E-03	33.261	1.245	5.219E-02	71.00
6.00	16.391	2.392	9.541E-04	33.324	1.236	4.746E-02	70.19
6.50	15.939	2.464	9.113E-04	33.378	1.228	4.352E-02	69.43
7.00	15.536	2.531	8.732E-04	33.425	1.220	4.019E-02	68.73
7.50	15.174	2.595	8.389E-04	33.465	1.214	3.734E-02	68.07
8.00	14.847	2.656	8.080E-04	33.499	1.207	3.487E-02	67.46
8.50	14.548	2.715	7.798E-04	33.529	1.202	3.272E-02	66.87

TABLE II (contd)

9.00	14.273	2.771	7.541E-04	33.554	1.196	3.082E-02	66.32
9.50	14.021	2.824	7.304E-04	33.576	1.191	2.913E-02	65.80
10.00	13.786	2.876	7.086E-04	33.594	1.186	2.762E-02	65.30
10.50	13.568	2.926	6.884E-04	33.610	1.182	2.627E-02	64.82
11.00	13.364	2.974	6.696E-04	33.622	1.178	2.504E-02	64.36
11.50	13.173	3.021	6.521E-04	33.633	1.174	2.392E-02	63.92
12.00	12.994	3.066	6.358E-04	33.641	1.170	2.291E-02	63.50
12.50	12.825	3.110	6.204E-04	33.647	1.167	2.197E-02	63.10
13.00	12.665	3.153	6.060E-04	33.652	1.164	2.112E-02	62.71
13.50	12.513	3.194	5.925E-04	33.655	1.161	2.032E-02	62.33
14.00	12.369	3.235	5.797E-04	33.656	1.158	1.959E-02	61.96
14.50	12.232	3.274	5.675E-04	33.656	1.155	1.891E-02	61.61
15.00	12.102	3.313	5.561E-04	33.655	1.152	1.828E-02	61.27
15.50	11.977	3.350	5.452E-04	33.653	1.150	1.769E-02	60.94
16.00	11.858	3.387	5.348E-04	33.649	1.147	1.713E-02	60.62
16.50	11.744	3.423	5.250E-04	33.645	1.145	1.661E-02	60.30
17.00	11.635	3.458	5.156E-04	33.639	1.143	1.613E-02	60.00
17.50	11.530	3.492	5.066E-04	33.633	1.140	1.567E-02	59.70
18.00	11.429	3.526	4.980E-04	33.626	1.138	1.523E-02	59.42
18.50	11.332	3.559	4.898E-04	33.618	1.136	1.482E-02	59.13
19.00	11.238	3.592	4.819E-04	33.610	1.134	1.444E-02	58.86
19.50	11.147	3.624	4.743E-04	33.601	1.133	1.407E-02	58.59
20.00	11.060	3.655	4.671E-04	33.591	1.131	1.372E-02	58.33
20.50	10.976	3.686	4.601E-04	33.580	1.129	1.339E-02	58.08
21.00	10.894	3.716	4.534E-04	33.569	1.128	1.308E-02	57.83
21.50	10.815	3.746	4.469E-04	33.558	1.126	1.278E-02	57.58
22.00	10.739	3.775	4.407E-04	33.546	1.124	1.249E-02	57.34
22.50	10.664	3.804	4.347E-04	33.534	1.123	1.222E-02	57.11

CALCULATED VALUES FROM E O S FOR T(2) AT 225.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	24.248	1.579	1.813E-03	32.600	1.341	1.612E-01	76.67
2.50	22.083	1.724	1.615E-03	32.844	1.320	1.232E-01	74.70
3.00	20.541	1.851	1.464E-03	33.029	1.302	9.938E-02	73.06
3.50	19.369	1.964	1.344E-03	33.173	1.285	8.321E-02	71.66
4.00	18.438	2.067	1.246E-03	33.289	1.271	7.154E-02	70.44
4.50	17.674	2.160	1.165E-03	33.384	1.258	6.275E-02	69.36
5.00	17.031	2.247	1.096E-03	33.462	1.246	5.590E-02	68.38
5.50	16.480	2.328	1.036E-03	33.526	1.236	5.041E-02	67.48
6.00	15.999	2.403	9.846E-04	33.579	1.226	4.591E-02	66.66
6.50	15.575	2.474	9.388E-04	33.624	1.218	4.216E-02	65.90
7.00	15.196	2.541	8.981E-04	33.661	1.210	3.899E-02	65.20
7.50	14.855	2.605	8.616E-04	33.692	1.203	3.628E-02	64.56
8.00	14.546	2.666	8.287E-04	33.717	1.197	3.392E-02	63.92
8.50	14.263	2.724	7.988E-04	33.737	1.191	3.186E-02	63.33
9.00	14.004	2.780	7.715E-04	33.754	1.185	3.004E-02	62.78
9.50	13.764	2.833	7.464E-04	33.766	1.180	2.842E-02	62.25
10.00	13.542	2.884	7.234E-04	33.776	1.175	2.698E-02	61.75
10.50	13.334	2.934	7.020E-04	33.782	1.171	2.567E-02	61.27
11.00	13.140	2.982	6.822E-04	33.786	1.166	2.449E-02	60.81
11.50	12.958	3.028	6.638E-04	33.788	1.162	2.342E-02	60.37
12.00	12.787	3.073	6.466E-04	33.788	1.159	2.244E-02	59.95
12.50	12.626	3.117	6.305E-04	33.786	1.155	2.154E-02	59.54
13.00	12.473	3.159	6.153E-04	33.782	1.152	2.071E-02	59.15
13.50	12.328	3.201	6.011E-04	33.776	1.149	1.995E-02	58.78
14.00	12.190	3.241	5.876E-04	33.769	1.146	1.924E-02	58.41
14.50	12.059	3.280	5.749E-04	33.761	1.143	1.858E-02	58.06
15.00	11.934	3.318	5.629E-04	33.752	1.140	1.796E-02	57.72
15.50	11.814	3.355	5.515E-04	33.741	1.138	1.739E-02	57.39
16.00	11.700	3.392	5.407E-04	33.730	1.135	1.685E-02	57.07
16.50	11.590	3.428	5.303E-04	33.717	1.133	1.635E-02	56.76
17.00	11.485	3.462	5.205E-04	33.704	1.131	1.588E-02	56.45
17.50	11.384	3.497	5.111E-04	33.690	1.129	1.543E-02	56.16
18.00	11.287	3.530	5.022E-04	33.675	1.127	1.501E-02	55.87
18.50	11.193	3.563	4.936E-04	33.659	1.125	1.461E-02	55.59
19.00	11.103	3.595	4.854E-04	33.643	1.123	1.423E-02	55.32
19.50	11.016	3.627	4.775E-04	33.626	1.121	1.388E-02	55.05
20.00	10.931	3.658	4.699E-04	33.609	1.119	1.354E-02	54.79
20.50	10.850	3.689	4.627E-04	33.591	1.118	1.322E-02	54.54
21.00	10.771	3.719	4.557E-04	33.572	1.116	1.291E-02	54.29
21.50	10.695	3.748	4.490E-04	33.553	1.115	1.262E-02	54.05
22.00	10.621	3.777	4.425E-04	33.534	1.113	1.234E-02	53.81
22.50	10.549	3.806	4.362E-04	33.514	1.112	1.207E-02	53.58

TABLE II (contd)

CALCULATED VALUES FROM E O S FOR T(2) AT 200.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	23.141	1.587	1.927E-03	33.143	1.341	1.522E-01	72.80
2.50	21.186	1.735	1.705E-03	33.360	1.317	1.167E-01	70.80
3.00	19.785	1.863	1.538E-03	33.520	1.296	9.444E-02	69.14
3.50	18.714	1.977	1.406E-03	33.641	1.277	7.932E-02	67.73
4.00	17.861	2.080	1.299E-03	33.735	1.261	6.840E-02	66.50
4.50	17.157	2.174	1.211E-03	33.809	1.247	6.015E-02	65.40
5.00	16.563	2.261	1.136E-03	33.867	1.235	5.371E-02	64.41
5.50	16.051	2.341	1.072E-03	33.912	1.224	4.854E-02	63.51
6.00	15.604	2.416	1.016E-03	33.947	1.214	4.430E-02	62.69
6.50	15.208	2.487	9.665E-04	33.973	1.205	4.076E-02	61.92
7.00	14.854	2.554	9.229E-04	33.993	1.197	3.775E-02	61.21
7.50	14.535	2.617	8.839E-04	34.007	1.190	3.518E-02	60.55
8.00	14.244	2.677	8.488E-04	34.015	1.183	3.294E-02	59.93
8.50	13.978	2.735	8.169E-04	34.020	1.177	3.097E-02	59.34
9.00	13.733	2.790	7.879E-04	34.020	1.171	2.924E-02	58.79
9.50	13.507	2.843	7.613E-04	34.017	1.166	2.769E-02	58.26
10.00	13.297	2.894	7.369E-04	34.011	1.161	2.631E-02	57.76
10.50	13.100	2.943	7.143E-04	34.003	1.157	2.506E-02	57.28
11.00	12.916	2.991	6.934E-04	33.992	1.153	2.393E-02	56.82
11.50	12.743	3.037	6.739E-04	33.980	1.149	2.290E-02	56.38
12.00	12.581	3.081	6.557E-04	33.965	1.145	2.196E-02	55.96
12.50	12.427	3.125	6.387E-04	33.949	1.142	2.109E-02	55.56
13.00	12.281	3.167	6.228E-04	33.931	1.138	2.029E-02	55.17
13.50	12.143	3.208	6.078E-04	33.912	1.135	1.956E-02	54.79
14.00	12.011	3.248	5.937E-04	33.892	1.132	1.887E-02	54.43
14.50	11.886	3.286	5.803E-04	33.870	1.130	1.824E-02	54.00
15.00	11.766	3.324	5.677E-04	33.848	1.127	1.764E-02	53.74
15.50	11.652	3.361	5.557E-04	33.825	1.125	1.709E-02	53.41
16.00	11.542	3.398	5.444E-04	33.800	1.122	1.57E-02	53.09
16.50	11.437	3.433	5.336E-04	33.775	1.120	1.608E-02	52.78
17.00	11.336	3.468	5.233E-04	33.749	1.118	1.562E-02	52.48
17.50	11.239	3.502	5.135E-04	33.723	1.116	1.519E-02	52.19
18.00	11.146	3.535	5.041E-04	33.696	1.114	1.478E-02	51.90
18.50	11.056	3.568	4.951E-04	33.668	1.112	1.440E-02	51.63
19.00	10.969	3.600	4.865E-04	33.640	1.110	1.403E-02	51.35
19.50	10.885	3.631	4.783E-04	33.611	1.108	1.368E-02	51.09
20.00	10.804	3.662	4.704E-04	33.582	1.107	1.335E-02	50.83
20.50	10.725	3.692	4.629E-04	33.552	1.105	1.304E-02	50.58
21.00	10.649	3.722	4.556E-04	33.522	1.104	1.274E-02	50.34
21.50	10.575	3.751	4.486E-04	33.492	1.102	1.245E-02	50.10
22.00	10.504	3.780	4.418E-04	33.461	1.101	1.218E-02	49.86
22.50	10.434	3.809	4.353E-04	33.430	1.099	1.192E-02	49.63

CALCULATED VALUES FROM E O S FOR T(2) AT 175.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	22.019	1.600	2.052E-03	33.964	1.335	1.425E-01	68.32
2.50	20.277	1.750	1.802E-03	34.119	1.308	1.097E-01	66.30
3.00	19.020	1.880	1.616E-03	34.225	1.285	8.921E-02	64.62
3.50	18.054	1.994	1.470E-03	34.298	1.265	7.523E-02	63.20
4.00	17.278	2.097	1.353E-03	34.347	1.247	6.510E-02	61.95
4.50	16.636	2.191	1.256E-03	34.380	1.233	5.744E-02	60.85
5.00	16.091	2.277	1.175E-03	34.399	1.220	5.143E-02	59.85
5.50	15.620	2.357	1.105E-03	34.407	1.208	4.660E-02	58.95
6.00	15.207	2.432	1.045E-03	34.407	1.198	4.263E-02	58.12
6.50	14.840	2.502	9.919E-04	34.401	1.189	3.930E-02	57.36
7.00	14.511	2.568	9.451E-04	34.388	1.181	3.647E-02	56.65
7.50	14.213	2.631	9.033E-04	34.371	1.173	3.404E-02	55.99
8.00	13.942	2.690	8.658E-04	34.350	1.167	3.192E-02	55.36
8.50	13.693	2.748	8.318E-04	34.326	1.161	3.006E-02	54.78
9.00	13.463	2.802	8.009E-04	34.298	1.155	2.841E-02	54.22
9.50	13.250	2.855	7.727E-04	34.268	1.150	2.694E-02	53.70
10.00	13.052	2.905	7.468E-04	34.236	1.145	2.563E-02	53.20
10.50	12.867	2.954	7.228E-04	34.202	1.141	2.444E-02	52.72
11.00	12.693	3.001	7.007E-04	34.166	1.137	2.335E-02	52.27
11.50	12.529	3.047	6.801E-04	34.129	1.133	2.237E-02	51.83
12.00	12.375	3.091	6.609E-04	34.090	1.129	2.147E-02	51.41
12.50	12.229	3.134	6.430E-04	34.051	1.126	2.064E-02	51.01
13.00	12.091	3.176	6.262E-04	34.010	1.123	1.987E-02	50.63
13.50	11.959	3.216	6.104E-04	33.968	1.120	1.916E-02	50.26
14.00	11.834	3.256	5.955E-04	33.925	1.117	1.850E-02	49.90
14.50	11.714	3.294	5.815E-04	33.882	1.114	1.789E-02	49.55

TABLE II (contd)

15.00	11.600	3.332	5.682E-04	33.838	1.112	1.732E-02	49.22
15.50	11.491	3.368	5.557E-04	33.793	1.109	1.678E-02	48.89
16.00	11.386	3.404	5.438E-04	33.748	1.107	1.628E-02	48.58
16.50	11.286	3.440	5.324E-04	33.702	1.105	1.581E-02	48.27
17.00	11.189	3.474	5.217E-04	33.656	1.103	1.537E-02	47.98
17.50	11.096	3.508	5.114E-04	33.610	1.101	1.495E-02	47.69
18.00	11.006	3.541	5.016E-04	33.563	1.099	1.455E-02	47.41
18.50	10.920	3.573	4.922E-04	33.515	1.097	1.418E-02	47.14
19.00	10.836	3.605	4.832E-04	33.468	1.096	1.382E-02	46.87
19.50	10.756	3.636	4.747E-04	33.420	1.094	1.348E-02	46.61
20.00	10.678	3.667	4.664E-04	33.372	1.093	1.316E-02	46.36
20.50	10.602	3.697	4.585E-04	33.324	1.091	1.286E-02	46.11

CALCULATED VALUES FROM E O S FOR T(2) AT 150.0 °.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	20.884	1.618	2.182E-03	35.124	1.321	1.322E-01	63.00
2.50	19.360	1.770	1.899E-03	35.148	1.291	1.024E-01	60.96
3.00	18.250	1.901	1.691E-03	35.142	1.266	8.370E-02	59.28
3.50	17.389	2.016	1.529E-03	35.116	1.245	7.094E-02	57.85
4.00	16.693	2.118	1.400E-03	35.077	1.227	6.166E-02	56.60
4.50	16.113	2.211	1.295E-03	35.027	1.212	5.461E-02	55.50
5.00	15.619	2.297	1.206E-03	34.970	1.199	4.907E-02	54.51
5.50	15.189	2.376	1.131E-03	34.908	1.187	4.459E-02	53.61
6.00	14.811	2.450	1.066E-03	34.842	1.177	4.090E-02	52.78
6.50	14.473	2.519	1.009E-03	34.772	1.168	3.780E-02	52.02
7.00	14.169	2.585	9.588E-04	34.700	1.160	3.515E-02	51.32
7.50	13.894	2.647	9.141E-04	34.626	1.153	3.287E-02	50.66
8.00	13.642	2.706	8.741E-04	34.550	1.147	3.088E-02	50.05
8.50	13.410	2.762	8.379E-04	34.472	1.141	2.913E-02	49.47
9.00	13.195	2.816	8.051E-04	34.394	1.135	2.757E-02	48.92
9.50	12.996	2.868	7.751E-04	34.315	1.130	2.618E-02	48.41
10.00	12.810	2.918	7.477E-04	34.235	1.126	2.493E-02	47.92
10.50	12.636	2.967	7.223E-04	34.155	1.122	2.380E-02	47.45
11.00	12.473	3.013	6.989E-04	34.074	1.118	2.277E-02	47.00
11.50	12.318	3.058	6.772E-04	33.993	1.114	2.183E-02	46.58
12.00	12.173	3.102	6.570E-04	33.912	1.111	2.097E-02	46.17
12.50	12.035	3.144	6.381E-04	33.830	1.108	2.017E-02	45.78
13.00	11.904	3.186	6.205E-04	33.749	1.105	1.944E-02	45.40
13.50	11.779	3.226	6.039E-04	33.667	1.102	1.876E-02	45.04
14.00	11.660	3.265	5.883E-04	33.586	1.099	1.813E-02	44.69
14.50	11.546	3.303	5.736E-04	33.504	1.097	1.754E-02	44.35
15.00	11.438	3.340	5.597E-04	33.423	1.095	1.699E-02	44.02
15.50	11.333	3.377	5.466E-04	33.341	1.092	1.647E-02	43.71
16.00	11.234	3.412	5.341E-04	33.260	1.090	1.599E-02	43.40

CALCULATED VALUES FROM E O S FOR T(2) AT 125.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	19.746	1.641	2.291E-03	36.623	1.291	1.215E-01	56.46
2.50	18.444	1.795	1.972E-03	36.367	1.260	9.482E-02	54.44
3.00	17.482	1.926	1.740E-03	36.123	1.235	7.808E-02	52.78
3.50	16.728	2.041	1.563E-03	35.889	1.214	6.658E-02	51.37
4.00	16.113	2.142	1.423E-03	35.664	1.196	5.818E-02	50.14
4.50	15.596	2.235	1.308E-03	35.446	1.182	5.176E-02	49.06
5.00	15.152	2.319	1.213E-03	35.235	1.169	4.669E-02	48.09
5.50	14.764	2.397	1.132E-03	35.030	1.159	4.257E-02	47.22
6.00	14.421	2.470	1.062E-03	34.830	1.149	3.916E-02	46.42
6.50	14.113	2.539	1.002E-03	34.635	1.141	3.629E-02	45.68
7.00	13.835	2.603	9.488E-04	34.444	1.134	3.383E-02	45.00
7.50	13.581	2.665	9.015E-04	34.257	1.127	3.170E-02	44.37
8.00	13.348	2.723	8.592E-04	34.073	1.121	2.983E-02	43.78
8.50	13.134	2.779	8.212E-04	33.893	1.116	2.819E-02	43.22
9.00	12.934	2.832	7.867E-04	33.716	1.111	2.672E-02	42.70
9.50	12.749	2.883	7.552E-04	33.542	1.107	2.541E-02	42.20
10.00	12.575	2.933	7.265E-04	33.371	1.103	2.423E-02	41.73
10.50	12.413	2.981	7.000E-04	33.202	1.099	2.316E-02	41.29
11.00	12.259	3.027	6.755E-04	33.036	1.095	2.218E-02	40.86
11.50	12.114	3.071	6.529E-04	32.872	1.092	2.129E-02	40.46

TABLE II (contd)

CALCULATED VALUES FROM E O S FOR T(2) AT 100.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	18.640	1.666	2.287E-03	38.185	1.229	1.114E-01	48.10
2.50	17.556	1.821	1.942E-03	37.280	1.202	8.774E-02	46.20
3.00	16.741	1.952	1.694E-03	36.492	1.181	7.283E-02	44.65
3.50	16.093	2.065	1.507E-03	35.787	1.163	6.252E-02	43.34
4.00	15.558	2.166	1.359E-03	35.145	1.149	5.495E-02	42.21
4.50	15.103	2.257	1.240E-03	34.552	1.137	4.912E-02	41.21
5.00	14.709	2.341	1.142E-03	33.999	1.127	4.449E-02	40.33
5.50	14.362	2.418	1.058E-03	33.479	1.118	4.071E-02	39.53
6.00	14.052	2.490	9.872E-04	32.986	1.111	3.756E-02	38.80
6.50	13.774	2.558	9.255E-04	32.517	1.104	3.490E-02	38.14
7.00	13.520	2.621	8.713E-04	32.068	1.098	3.261E-02	37.52
7.50	13.288	2.682	8.233E-04	31.638	1.093	3.062E-02	36.96

CALCULATED VALUES FROM E O S FOR T(2) AT 75.0 K.

PRESS.	VOL.	V(S)	ALPHA	C(P)	GAMMA	CHI(S)	ENTROPY
KBAR	CC/MOLE	KM/S	/K	J/MOLE-K		/KBAR	J/MOLE-K
2.00	17.676	1.670	1.821E-03	38.367	1.109	1.050E-01	37.02
2.50	16.790	1.827	1.509E-03	35.740	1.096	8.340E-02	35.59
3.00	16.107	1.957	1.289E-03	33.518	1.086	6.967E-02	34.45
3.50	15.554	2.071	1.124E-03	31.581	1.078	6.011E-02	33.49
4.00	15.090	2.171	9.958E-04	29.854	1.071	5.304E-02	32.68
4.50	14.691	2.262	8.926E-04	28.296	1.065	4.757E-02	31.98

REFERENCES

1. R. L. Mills, D. H. Liebenberg, and J. C. Bronson, J. Chem. Phys. 66, 3076 (1977).
2. R. L. Mills, D. H. Liebenberg, and J. C. Bronson, J. Chem. Phys. (to be published).
3. R. L. Mills, D. H. Liebenberg, and J. C. Bronson, (to be published).
4. D. H. Liebenberg, R. L. Mills, and J. C. Bronson, "Thermodynamic Properties of Fluid n -H₂ in the Range 75-307 K and 2-20 kbar," Los Alamos Scientific Laboratory report LA-6645-MS (April 1977).
5. D. H. Liebenberg, R. L. Mills, and J. C. Bronson, "Thermodynamic Properties of Fluid n -D₂ in the 75 to 300 K and 2- to 20-kbar Range," Los Alamos Scientific Laboratory report LA-7007-MS (March 1978).
6. M. Benedict, J. Am. Chem. Soc. 59, 2233 (1937).
7. G. I. Kerley, "A Theoretical Equation of State for Deuterium," Los Alamos Scientific Laboratory report LA-4776 (January 1972); also private communication, 1978.