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THERMODYNAMIC PROPERTIES OF PHOSGENE

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ABSTRACT

Thermodynamic properties of phosgene have been evaluated up to a temperature of 600°K and a pressure of 150 atmospheres using Martin and Hou equation of state. The results are presented in tabular form and as an entropy-temperature diagram.

INTRODUCTION

Phosgene is used in chemical warfare. It is also used as an intermediate, capable of producing a wide variety of new products in very many fields ranging from solvents to plastics. However, thermodynamic data needed for the purposes of design are completely lacking. Hence it is desirable to know the thermodynamic properties of phosgene.

SURVEY OF EXISTING DATA

1. *Molecular weight and critical data:*

The available data on the critical constants of phosgene are presented in Table I.

TABLE I
Molecular weight and critical constants of phosgene
Molecular weight of Phosgene=98.924

Year	Investigator	T_c , °K	P_c , atm.	d_c , gm./c.c.	Method*	Reference
1919	Hackspill and Mathieu ...	456.31	a	8
1926	Germann and Taylor ...	455.16	56.0	0.52	a, b	4
Values selected :		455.16	56.0	0.52		

a : Disappearance meniscus.
b : Law of rectilinear diameters.

Hackspill and Mathieu⁸ fractionally distilled the industrial phosgene to remove contaminants consisting of sulfur compounds and removed chlorine by contact with mercury for 24 hours.

For obtaining a relatively pure sample, Germann and Taylor⁴ repeatedly fractionated commercial phosgene. However, these investigators could not condense the sample completely at constant pressure. The temperatures of disappearance and reappearance of the meniscus were found to be 454.96°K and 454.76°K respectively. The critical pressure found by observation was 55.3 atmospheres where as by extrapolation of vapour pressure curve, it was found to be 55.6 atmospheres. The value reported by these investigators namely 455.16°K for the critical temperature has been accepted for this investigation.

Vapour pressure equation as given by these investigators⁴ predict a pressure of 56.0 atmospheres at the accepted critical temperature. Hence a pressure of 56.0 atmospheres for the critical pressure was accepted for this investigation.

Critical density was determined by using the law of rectilinear diameters by making use of the density data of Paterno and Mazzuchelli¹¹, by Germann and Taylor.

For this investigation, the critical data of Germann and Taylor⁴ have been used. Thus the critical constants used for this work are :

$$T_c = 455.16^\circ K$$

$$P_c = 56.0 \text{ atm.}$$

$$d_c = 0.52 \text{ gm./c.c.}$$

2. Vapour pressure:

The vapour pressure data of phosgene has been experimentally determined by Atkinson *et al.*¹, Paterno and Mazzucchelli¹¹, Germann and Taylor⁴ and Giauque and Jones⁵. Vapour pressure data is also presented in the International Critical Tables⁹. Table 2 gives the available data along with the range of availability.

The method adopted by Germann and Taylor⁴ for the purification of the sample used is mentioned earlier. The vapour pressure data are stated to be accurate to 0.1 atm. The sample used by Giauque and Jones⁵ is stated to be 99.993 mole % pure. However, the accuracy of the vapour pressure data are not reported. Paterno and Mazzucchelli¹¹ have not reported the accuracy of the data. Germann and Taylor⁴ determined vapour pressure of phosgene over two temperature regions, namely 273.16 – 301.06 °K and 426.26 – 455.16 °K. These authors fitted their data to the equation:

$$\log P = 4.4659 - (1207.9/T) + (13297/T^2) \quad [1]$$

where T is in °K and P is in atmospheres.

TABLE 2
Vapour pressure of phosgene

Year	Investigator	Range of Temperature, °K	Range of Pressure, atm.	Reference
1920	Atkinson <i>et al.</i>	193.16-373.16	0.00-16.07	1
1920	Paterno and Mazzucchelli	249.74-294.29	0.25-1.75	11
1926	Germann and Taylor	273.16-455.16	0.75-56.00	4
1928	International Critical Tables	281.11-455.16	1.00-56.00	9
1948	Giauque and Jones	215.48-281.10	0.03-1.02	5

The vapour pressure data was calculated using Equation [1] and was found to be in very good agreement with that presented in International Critical Tables.

For this investigation, the vapour pressure data above 1 atm. has been taken from the International Critical Tables. Below 1 atm., the data of Giauque and Jones⁵ has been used.

Giauque and Jones⁵ fitted their data to the equation:

$$\log P = 7.7994 - (1690.3/T) - (7.8981 \times 10^{-3}T) + (5.5847 \times 10^{-6}T^2) \quad [2]$$

where, P is in atmospheres and T is in °K.

Equation [2] predicts the vapour pressure data with a maximum deviation of 0.1%.

In the present work, the vapour pressure data above 1 atm. was fitted to the equation,

$$\log P = A + (B/T) + C \log T + DT \quad [3]$$

where, $A = 3.7349229$

$B = -1290.8709$

$C = 0.41355479$

$D = -5.5134925 \times 10^{-6}$

This equation predicts vapour pressure data⁹ with average absolute and maximum deviations of 0.1% and 0.23% respectively.

For this work Equations [2] and [3] have been used.

3. Saturated Liquid and Vapour Densities :

Saturated Liquid and Vapour Densities of phosgene have been determined over a temperature range of 163 to 323 °K by Atkinson *et al*¹ and over a temperature range of 258 to 455 °K by Paterno and Mazzucchelli¹¹.

Both the investigators did not mention the purity of the sample used and the accuracy of the data. Vapour density of phosgene has been determined by Paterno and Mazzucchelli¹¹ over a temperature range of 333-455 °K.

Liquid and vapour density data over a temperature range of 281 to 455 °K are presented in the International Critical Tables⁹. For this investigation all the available data on the densities of saturated liquid and vapour were combined and smoothened. Smoothened data have been used for this investigation. The smoothened data agree with the raw data within a maximum deviation of 1%.

4. Heat Capacity from Calorimetric Data :

Heat capacity of phosgene over a temperature range of 15 °K to 280 °K has been determined by Giaque and Jones⁵. As stated earlier, the sample used by these investigators was very pure. Later, in a careful study Giaque and Ott⁶ found, that the data of Giaque and Jones⁵ below a temperature of 118.3 °K was applicable to pure solid II and above this temperature, to solid I. These authors have presented heat capacity data for solid I, which is the most stable state and also for solid II. The accuracy of the data are not reported. The entropy evaluated using the heat capacity data of solid I at 280.71 °K (normal boiling point) is in very good agreement with their entropy calculated using spectroscopic data.

5. Heat Capacity of Ideal Gas :

Heat capacity of phosgene in the ideal gaseous state have been evaluated by Thompson¹³, Gordon and Goland⁷ and by Giaque and Ott⁶. Giaque and Ott used the constant recommended by Rossini *et al.*¹² and Dumond and Cohen³. The data of Gordon and Goland⁷ deviates by about 5% with the data of Giaque and Ott⁶.

For this investigation, the data of Giaque and Ott has been used. The heat capacity data of Giaque and Ott was fitted by the method of least squares to the equation :

$$C_p^* = a + bT + cT^2 + dT^3 \quad [4]$$

where, $a = 3.3388$

$$b = 5.6707 \times 10^{-2}$$

$$c = -8.8784 \times 10^{-5}$$

$$d = 5.4200 \times 10^{-8}$$

Equation [4] predicts heat capacity data with maximum and average absolute deviations of 0.03% and 0.02% respectively. For the calculation of thermodynamic properties, Equation [4] has been used.

6. Heat of Vaporization :

Heat of vaporization of phosgene has been experimentally determined by Giaque and Jones⁵. No other data is available on the heat of vaporization of phosgene.

As already mentioned, Giaque and Jones⁵ used very pure sample of phosgene. They claim an accuracy of 99.9%.

Heat of vaporization was calculated using Clausius-Clapeyron equation,

$$\text{viz.,} \quad \Delta H_v = (dP/dT)T \cdot (V_g - V_l) \quad [5]$$

by making use of the experimental specific volumes. The heat of vaporization calculated at the normal boiling point agrees within 2% with the experimental data of Giaque and Jones⁵.

CALCULATION OF THERMODYNAMIC PROPERTIES

For the calculation of thermodynamic properties Martin and Hsu (MH) equation of state:

$$P = \frac{RT}{(V-b_0)} + \frac{A_2 + B_2T + C_2 \exp. (-KT/T_c)}{(V-b_0)^2} + \frac{A_3 + B_3T + C_3 \exp. (-KT/T_c)}{(V-b_0)^3} + \frac{A_4}{(V-b_0)^4} + \frac{B_5T + C_5 \exp. (-KT/T_c)}{(V-b_0)^5} \quad [6]$$

with $K = 5.475$ has been used.

The constants in Equation (6), evaluated following the procedures outlined by the authors¹⁰ are:

$$b_0 = 0.04516972$$

$$A_2 = -16.059997$$

$$B_2 = 1.2038081 \times 10^{-2}$$

$$C_2 = 142.96485$$

$$A_3 = 2.0331332$$

$$B_3 = -1.3197412 \times 10^{-3}$$

$$C_3 = -22.568742$$

$$A_4 = -9.005015 \times 10^{-2}$$

$$B_5 = 5.0038055 \times 10^{-6}$$

$$C_5 = 3.849143 \times 10^{-2}$$

Using the available experimental specific volumes of saturated vapour in Equation [6], pressures were computed. For 21 points tested, the average absolute and maximum deviations were found to be 1.23% and 3.08% respectively. Such a comparison is shown in Table 3. Comparison could not be made in the superheated vapour region because of lack of data.

Specific volumes of saturated and superheated vapour were calculated using Equation [6] by making use of Newton-Raphson iterative method on IBM 1620 digital computer, for various temperatures and pressures.

Entropy and Enthalpy of the Superheated Vapour:

Considering the entropy and enthalpy to be function of volume temperature, we have,

$$dS = (\partial S / \partial T)_V dT + (\partial S / \partial V)_T dV \quad [7]$$

TABLE 3
Comparison of Calculated Pressures

T, °K	P, atms	PCOM, atms.	% Deviation
340.0	6.295	6.0908	3.244
350.0	8.100	7.9941	1.308
360.0	10.21	10.1397	0.688
370.0	12.72	12.6762	0.344
380.0	15.70	15.4213	1.775
385.0	17.40	17.009	2.247
390.0	19.15	18.673	2.491
395.0	21.10	20.449	3.085
400.0	23.00	22.384	2.677
405.0	25.15	24.592	2.219
410.0	27.50	26.98	1.892
415.0	30.05	29.626	1.410
420.0	32.55	32.456	0.281
425.0	35.50	35.208	0.822
430.0	38.45	38.278	0.448
435.0	41.50	41.551	-0.124
440.0	44.80	44.881	-0.180
445.0	48.15	48.317	-0.347
450.0	51.95	52.013	-0.121
455.0	55.95	55.883	0.119
455.16	56.00	56.000	0.000

% Deviation = $(P - \text{PCOM})/P \times 100$

Using Maxwell's relations, we obtain,

$$dS = (C_v^* / T) dT + (\partial P / \partial T)_v dV \quad [8]$$

Using $dH = TdS + VdP$ in Equation [8] we obtain

$$\begin{aligned} dH &= C_v^* dT + T(\partial P / \partial T)_v dV + VdP \\ &= C_p^* dT + d(PV) - PdV + T(\partial P / \partial T)_v dV \end{aligned} \quad [9]$$

From Equation [6] we have

$$\begin{aligned} (dP/dT)_V = & \frac{R}{(V-b_0)} + \frac{B_2 - (K/T_c) C_2 \exp. (-KT/T_c)}{(V-b_0)^2} \\ & + \frac{B_3 - (K/T_c) C_3 \exp. (-KT/T_c)}{(V-b_0)^3} + \frac{B_5 + C_5 (K/T_c) \exp. (-KT/T_c)}{(V-b_0)^5} \end{aligned} \quad [10]$$

Using Equations [8] and [9],

$$S = \int (C_v^*/T) dT + \int (\partial P/\partial T)_V dV \quad [11]$$

and

$$H = \int (C_p^*) dT + \int T(\partial P/\partial T)_V dV - \int PdV + PV \quad [12]$$

Using Equations [4] and [10] in the above equations and carrying out the integration, we obtain expressions for entropy and enthalpy as:

$$\begin{aligned} S = & (a-R) \ln T + bT + (c/2)T^2 + (d/3)T^3 + R \ln (V-b_0) \\ & - \frac{B_2}{(V-b_0)} - \frac{B_3}{2(V-b_0)^2} - \frac{B_5}{4(V-b_0)^4} \\ & + \left[\frac{C_2}{(V-b_0)} + \frac{C_3}{2(V-b_0)^2} + \frac{C_5}{4(V-b_0)^4} \right] (K/T_c) \exp. (-KT/T_c) + C_5 \end{aligned} \quad [13]$$

and

$$\begin{aligned} H = & (a-R)T + (b/2)T^2 + (c/3)T^3 + (d/4)T^4 \\ & + \frac{A_2 + (1+KT/T_c)C_2 \exp. (-KT/T_c)}{(V-b_0)} + \frac{A_3 + (1+KT/T_c)C_3 \exp. (-KT/T_c)}{(V-b_0)^2} \\ & + \frac{A_4}{3(V-b_0)^3} + \frac{(1-KT/T_c)C_5 \exp. (-KT/T_c)}{4(V-b_0)^4} + PV - RT \cdot C_H \end{aligned} \quad [14]$$

where C_v and C_H are the constants of integration.

Reference State :

The reference state chosen depends upon the available data. The reference state chosen should facilitate easy comparison and utilization of the tabulated data. The reference state $H=0$ and $S=R$ in $P=0$ for elements² is applicable for pure substances and also for pure substances that undergo a chemical reaction.

In the present work the reference state as given above has been used.

Entropy value at the normal boiling point was evaluated using the ideal gas thermodynamic properties and the Berthelot correction. Enthalpy at the normal boiling point was evaluated by making use of the heat of formation at $0^\circ H$, the ideal gas thermodynamic properties and the Berthelot correction for enthalpy. The integration constants C_S and C_H were evaluated using the values of entropy and enthalpy at the normal boiling point.

Entropy and enthalpy of saturated vapour were evaluated by using the experimental specific volumes in Equations [13] and [14]. Wherever the experimental data were not available these were calculated using Equation [6] and were used.

Entropy and Enthalpy of the Saturated Liquid :

The entropy of vaporization is related to the heat of vaporization by the relation

$$\Delta H_v = T \Delta S_v \quad [15]$$

The entropy and enthalpy of the saturated liquid were calculated using the equations

$$S_l = S_g - \Delta S_v \quad [16]$$

$$H_l = H_g - \Delta H_v \quad [17]$$

The properties of saturated and superheated phosgene are presented in the graphical form as Fig. 1.

Internal Consistency of the Tabulated Results :

The relation $dH = TdS + VdP$ may be used to check the internal consistency of the entropy and enthalpy values.

At constant pressure,

$$dH = TdS \quad [18]$$

Hence, $dH = d(TS) - SdT$ from which

$$H_2^2 = T_2 S_2 - T_1 S_1 - \int_1^2 SdT \quad [19]$$

Internal consistency checks were made for superheated region by using Equation [19]. The definite integral in Equation [19] was evaluated by Simpson's rule. Table 4a gives the comparison of calculated and tabulated values of changes of enthalpy ΔH for 5 isobars.

TEMPERATURE, °K

450.0
500.0
550.0
600.0
650.0
700.0
750.0
800.0
850.0
900.0
950.0
1000.0

TEMPERATURE-ENTHALPY
DIAGRAM FOR
PROSENE

PREPARED BY: S. HACHIDAI, WASHINGTON, D.C.
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P = PRESSURE, ATMOSPHERES
H = ENTHALPY, CALORIES/GRAM-MOLE
V = VOLUME, LITRES/GRAM-MOLE
X = WEIGHT FRACTION
REFERENCE STATE C (GRAPHITE) O₂(G) AND
H₂O AND S-RIND-0

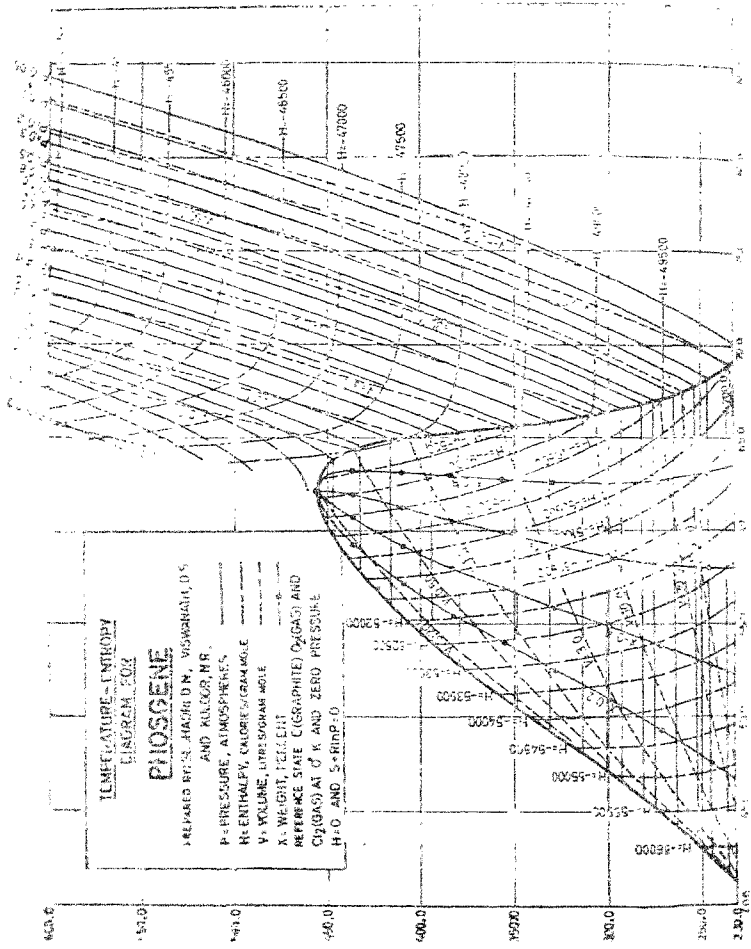


TABLE 4a
Comparison of the values of ΔH

Isobar atm.	Range of temp. °K.	$\Delta H_{calc.}$	ΔH_{tables}	% Deviation
0.10	240 - 600	5500.0	5501	0.02
0.00	300 - 600	4706.0	4704	0.04
10.00	380 - 600	3584.0	3583	0.03
50.00	460 - 600	2760.2	2760	0.01
100.00	540 - 600	1466.7	1465	0.08

NOMENCLATURE

A, B, C, D	Constants in Equation [3]
a, b, c, d	Constants in Equation (4)
$b_0, A_2, B_2, C_2,$ $A_3, B_3, C_3, A_4,$ B_4, C_4, K	} Constants in Equation [6]
C_p	
C_v	Heat capacity at constant volume, cal./gram mole °K
C_S, C_H	Constants of integration in Equations [13] and [14]
H	Enthalpy, cal./gram mole
P	Pressure, atmospheres
R	Gas constant
S	Entropy, cal./gram mole °K
T	Temperature, °K
V	Specific volume, litres/gram mole
ΔH_V	Enthalpy of vaporization, cal./gram mole
ΔS_V	Entropy of vaporization, cal./gram mole °K

Superscript

* Properties at zero pressure or ideal gaseous state

Subscripts

c	Critical point
g	Gas or vapour
l	Liquid
p	Pressure
T	Temperature
v	Volume

PHOSGENE

 TABLE 4
 Properties of Saturated Liquid and Vapour

T°K	P. Atm.	V_l	V_f	S_l	ΔS_b	S_g	H_l	ΔH_b	H_g
230.0	0.0850	0.06477	221.8	41.27	27.90	69.17	-56439	6417	-50422
240.0	0.1534	0.06557	128.2	42.18	26.46	68.64	-56247	6350	-49897
250.0	0.2585	0.06661	79.07	43.04	25.02	68.06	-56021	6255	-49766
260.0	0.4180	0.06770	50.77	43.89	23.69	67.58	-55800	6159	-49641
270.0	0.6517	0.06887	33.71	44.80	22.39	67.19	-55500	6045	-49535
280.0	0.9640	0.07008	23.54	45.54	21.36	66.90	-55360	5980	-49380
290.0	1.390	0.07138	22.74	46.33	20.31	66.64	-55138	5890	-49248
300.0	1.965	0.07267	16.82	47.09	19.33	66.42	-54917	5800	-49117
310.0	2.693	0.07553	9.39	47.84	18.40	66.24	-54702	5705	-48997
320.0	3.650	0.07704	6.896	48.55	17.51	66.06	-54461	5603	-48858
330.0	4.845	0.07874	5.302	49.27	16.71	65.96	-54247	5514	-48733
340.0	6.295	0.08045	4.148	49.98	15.88	65.86	-53986	5399	-48587
350.0	8.100	0.08231	3.257	50.70	15.00	65.70	-53733	5250	-48483
360.0	10.21	0.08439	2.601	51.38	14.20	65.58	-53488	5112	-48376
370.0	12.72	0.08658	2.099	52.16	13.32	65.48	-53202	4928	-48274
380.0	15.70	0.08780	1.705	52.91	12.51	65.42	-52919	4753	-48166

TABLE 4—(concl'd.)

T°K	P. atm.	V_l	V_g	S_l	ΔS_b	S_g	H_l	ΔH_b	H_g
390.0	19.15	0.08921	1.399	53.68	11.64	65.32	-52613	4540	-48073
400.0	23.00	0.09208	1.149	54.54	10.69	65.23	-52271	4276	-47995
410.0	27.50	0.09569	0.9463	55.46	9.63	65.09	-51895	3948	-47947
420.0	32.55	0.1005	0.7342	56.44	8.43	64.87	-51476	3541	-47935
425.0	35.50	0.1034	0.6595	57.06	7.71	64.77	-51204	3277	-47927
430.0	38.45	0.1068	0.5854	57.63	7.01	64.64	-50953	3014	-47939
435.0	41.50	0.1111	0.5152	58.19	6.29	64.48	-50704	2736	-47968
440.0	44.80	0.1161	0.4517	58.82	5.47	64.29	-50417	2407	-48010
445.0	48.15	0.1226	0.3910	59.55	4.52	64.07	-50088	2011	-48077
450.0	51.95	0.1226	0.3243	60.31	3.39	63.70	-49733	1525	-48208
455.0	55.95	0.1667	0.2096	61.70	0.82	62.52	-49092	373.1	-48719
455.16	56.00	0.1902	0.1902	62.19	0.00	62.19	-48880	0.0	-48880

Thermodynamic Properties of Phosgene

165

TABLE 5—(contd.)

Temp, °K.	P, Atms.	Pressure Range: 0.05 to 3.00 atm.									
		0.05	0.10	0.20	0.30	0.50	0.80	1.00	1.50	2.00	3.00
360.0	V	590.5	295.1	147.4	98.18	58.79	36.63	29.25	19.40	14.48	9.551
	H	-48247	-48248	-48249	-48250	-48252	-48256	-48258	-48264	-48271	-48283
	S	76.30	74.93	73.55	72.74	71.72	70.79	70.34	69.53	68.95	68.13
380.0	V	623.3	311.5	155.6	103.7	62.08	38.70	30.90	20.51	15.31	10.11
	H	-47949	-47950	-47951	-47952	-47955	-47958	-47961	-47968	-47974	-47987
	S	77.11	75.73	74.35	73.55	72.53	71.59	71.14	70.33	69.75	68.93
400.0	V	656.2	328.0	163.8	109.1	65.38	40.76	32.56	21.62	16.15	10.67
	H	-47646	-47646	-47648	-47649	-47652	-47656	-47658	-47665	-47672	-47685
	S	77.89	76.51	75.13	74.32	73.31	72.37	71.92	71.11	70.53	69.70
420.0	V	689.0	344.4	172.1	114.6	68.68	42.83	34.21	22.73	16.98	11.24
	H	-47338	-47338	-47340	-47341	-47344	-47348	-47350	-47357	-47364	-47378
	S	78.64	77.26	75.88	75.08	74.06	73.12	72.67	71.86	71.28	70.45
440.0	V	721.8	360.8	180.3	120.1	71.97	44.89	35.87	23.83	17.82	11.80
	H	-47025	-47026	-47027	-47029	-47031	-47035	-47038	-47045	-47052	-47065
	S	79.37	77.99	76.61	75.80	74.78	73.85	73.40	72.58	72.00	71.18
460.0	V	754.7	377.2	188.5	125.6	75.27	46.96	37.52	24.94	18.65	12.36
	H	-46709	-46710	-46711	-46712	-46715	-46719	-46722	-46728	-46735	-46749
	S	80.07	78.69	77.31	76.51	75.49	74.55	74.10	73.29	72.71	71.88

TABLE 5---(cont'd)

T ^o K	P Atmos.	Pressure Range: 0.05 to 3.00 atm.									
		0.05	0.10	0.20	0.30	0.50	0.80	1.00	1.50	2.00	3.00
480.0	V	787.5	393.7	196.7	131.1	78.57	49.03	39.18	26.05	19.49	12.92
	H	46389	46390	46391	46392	46395	46399	46401	46408	46414	46428
	S	80.75	79.37	77.99	77.19	76.17	75.23	74.78	73.97	73.39	72.51
500.0	V	820.3	410.1	204.9	136.6	81.86	51.09	40.83	27.16	20.32	13.48
	H	46065	46066	46067	46068	46071	46075	46077	46084	46090	46103
	S	81.41	80.03	78.65	77.85	76.83	75.89	75.44	74.63	74.05	73.23
520.0	V	853.2	426.5	213.2	142.0	85.16	53.16	42.49	28.27	21.16	14.04
	H	45738	45739	45740	45741	45744	45747	45750	45756	45762	45775
	S	82.05	80.67	79.30	78.49	77.47	76.53	76.09	75.27	74.69	73.87
540.0	V	886.0	442.9	221.4	147.5	88.45	55.22	44.14	29.37	21.99	14.60
	H	45408	45408	45409	45411	45413	45417	45419	45425	45431	45443
	S	82.68	81.30	79.92	79.11	78.10	77.16	76.71	75.90	75.32	74.50
560.0	V	918.9	459.3	229.6	153.0	91.75	57.28	45.80	30.48	22.82	15.16
	H	45074	45074	45076	45077	45079	45083	45084	45091	45096	45108
	S	83.28	81.90	80.53	79.72	78.70	77.76	77.32	76.51	75.93	75.11
580.0	V	951.7	475.8	237.8	158.5	95.04	59.35	47.45	31.58	23.65	15.72
	H	44737	44737	44738	44740	44742	44745	44747	44753	44759	44770
	S	83.87	82.50	81.12	80.31	79.29	78.36	77.91	77.10	76.52	75.70
600.0	V	984.5	492.2	246.0	164.0	98.33	61.41	49.10	32.69	24.48	16.28
	H	44396	44397	44398	44399	44401	44404	44407	44412	44417	44428
	S	84.45	83.07	81.70	80.89	79.87	78.93	78.49	77.68	77.10	76.28

TABLE 5—(contd.)

T°K	P Atms.	Pressure Range: 5.0 to 150.0 atms.											
		5.0	8.0	10.0	15.0	20.0	30.0	50.0	80.0	100.0	150.0		
480.0	V	7.669	4.712	3.726	2.409	1.748	1.080	0.5212					
	H	-46455	-46.96	-46574	-46597	-46675	-46846	-47298					
	S	71.52	70.53	70.05	69.15	68.47	67.42	65.71					
500.0	V	8.011	4.932	3.905	2.534	1.847	1.155	0.5871	0.2415				
	H	-46129	-46169	-46196	-46267	-46340	-46500	-46892	-47844				
	S	72.18	71.20	70.72	69.82	69.15	68.13	66.54	64.07				
520.0	V	8.353	5.152	4.084	2.659	1.945	1.228	0.6457	0.3045	0.2079			
	H	-45800	-45839	-45865	-45932	-46002	-46152	-46502	-47225	-47738			
	S	72.83	71.84	71.37	70.48	69.81	68.81	67.31	65.29	64.07			
540.0	V	8.694	5.370	4.262	2.783	2.042	1.300	0.6998	0.3559	0.2493			
	H	-45467	-45505	-45530	-45594	-45661	-45801	-46119	-46717	-47156			
	S	73.45	72.48	72.00	71.11	70.46	69.47	68.03	66.25	65.17			
560.0	V	9.035	5.588	4.438	2.905	2.138	1.369	0.7509	0.4002	0.2882	0.1755		
	H	-45132	-45167	-45191	-45253	-45316	-45448	-45740	-46257	-46633	-47307		
	S	74.07	73.09	72.62	71.73	71.08	70.11	68.72	67.09	66.12	64.44		
580.0	V	9.375	5.805	4.614	3.027	2.233	1.438	0.7997	0.4401	0.3239	0.1951		
	H	-44792	-44827	-44850	-44908	-44969	-45093	-45364	-45822	-46149	-46809		
	S	74.66	73.69	73.22	72.34	71.69	70.74	69.38	67.85	66.97	65.32		
600.0	V	9.714	6.021	4.790	3.148	2.327	1.505	0.8467	0.4770	0.3569	0.2156		
	H	-44450	-44483	-44505	-44561	-44618	-44736	-44987	-45402	-45691	-46318		
	S	75.24	74.27	73.80	72.93	72.29	71.34	70.02	68.56	67.75	66.15		

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