CONFIGURATIONAL PROPERTIES OF LIQUIDS

A Thesis

Presented to

the Faculty of the Department of Chemical Engineering

University of Houston

In Partial Fulfillment

of the Requirements for the Degree

Master of Science in Chemical Engineering

---

by

Kenneth Earl Bush

May, 1971

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ABSTRACT

A program has been underway in the Chemical Engineering Department to investigate properties of liquids and solutions; the work presented in this thesis is one part of the program. The objective was to determine the configurational thermodynamic properties of certain substances as a function of liquid density and molecular size and shape, which could be used later in theoretical molecular models for, 1) the configurational properties of pure components as a function of density, and 2) the excess thermodynamic functions for species in solution.

Fifteen nonpolar and polar substances were chosen covering a wide range of molecular weights and acentric factors:

Hydrocarbons: methane, cis-pentene-2, cyclohexane, benzene, n-hexane, 2,3 dimethylbutane, 2,2,4 trimethylpentane, n-octane, n-decane.

Hydrogen bonded substances: water, methyl alcohol, isopropyl alcohol.

Others: argon, nitrogen, carbon tetrachloride.

Using the approach of molecular statistical thermodynamics, a "sum of contributions" method was employed, involving translation, external rotation, internal vibration plus rotation, and intermolecular configuration; also the total property can be visualized as made up of two parts: one temperature dependent and the other density dependent.

The results obtained for the configurational energy indicate a very decided effect of molecular size and shape for all classes of substances, and similarly for the configurational entropy; however for the latter, the trends are somewhat obscured, and not as apparent as for the energy.

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CHAPTER I

INTRODUCTION AND PURPOSE OF THE WORK

Methods of calculating or correlating the thermodynamic properties of liquids based on theory are not as highly developed as for gases. Empirical methods for estimating some properties, particularly heat capacity, are in existence (6, 33), and these methods serve the purpose of supplying reasonably accurate numbers which are satisfactory for many design requirements. Few of these methods, however, can be applied on a general basis with predictable accuracy. At the present time if accurate numbers are required it is necessary to rely upon experimental data.

For several years a program has been underway in the Chemical Engineering Department of the University of Houston under the direction of Dr. Prengle to investigate properties of liquids and solutions. The work presented in this thesis is one part of the program.

Hildebrand and Scott (16) state, "....in order to calculate the thermodynamic properties of a system by statistical mechanical methods, we must be able to evaluate a partition function for the system. The success of any theoretical treatment of the liquid state will depend upon the validity of the simplifying assumptions made. ....two assumptions are fairly general and common to most theories of liquids, a) the translational degrees of freedom of the molecules are essentially classical, and b) the internal degrees of freedom are the same in the liquid as in the gas." The work of Davies and Matheson (9) and others indicates that these

assumptions should be amended to include, 1) free rotation in the liquid for many molecules and 2) a much less (cf. perfect gas) translational entropy contribution for the liquid. As a general proposition the total liquid phase partition function can be presented as,*

$$Q_L = q_{TR}\, q_{ER}\, q_I\, q_C \tag{I-1}$$

giving for the classical thermodynamic properties,

$$E_L = E_{TR} + E_{ER} + E_I + E_c \tag{I-2}$$

$$S_L = S_{TR} + S_{ER} + S_I + S_c \tag{I-3}$$

This "sum of contributions" method also leads to visualizing the total property as made up of two parts: one temperature dependent and the other density dependent; e.g.

$$E_L(T,\rho) = E(T) + E_c(\rho) \tag{I-4}$$

Using this approach the most difficult parts to evaluate theoretically are the translational and configurational partition functions. Prengle and Mauk (30) proposed that the configurational contributions could be evaluated by a combination of perfect gas state calculations, to get q_I and q_{ER}, and PVT data.

The overall purpose of this work was to determine the configurational thermodynamic properties of certain substances as a function of liquid density and the size and shape of the molecule, which can be used later in theoretical molecular models for, 1) the configurational properties of pure components as a function of density, and 2) the pure component parameters for species in solution. Fifteen substances listed in Table I were chosen

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*Nomenclature presented on p 124.

covering a wide range of molecular weights and acentric factor, ω.

More specifically the following were the objectives of this work:

1.-To prepare a generalized computer program to calculate the perfect gas state thermodynamic properties, including corrections for hindered rotation, of pure components.

2.-To prepare a general computer program to calculate the configurational thermodynamic properties of pure components.

3.-To calculate the configurational thermodynamic properties of each of the fifteen substances.

4.-To attempt preliminary empirical correlation of the configurational energy and entropy.

TABLE I-PURE COMPONENTS CONSIDERED

	Component		MW	T_{TP} (°K)	ρ_{TP} (g./ml.)	NBP °K	T_c (°K)	P_c (atm)	ρ_c (g./ml.)	Z_c	ω	μ (D)
1.	Argon	Ar	39.948	83.96	1.4113	87.46	150.86	48.34	0.535	0.290	≃0	0
2.	Methane	CH_4	16.042	90.68	0.4528	111.7	190.7	45.8	0.1620	0.290	0.013	0
3.	Nitrogen	N_2	28.016	63.19	0.8694	77.35	126.2	33.5	0.3110	0.291	0.040	0
4.	Cyclohexane	C_6H_{12}	84.156	279.83	0.7915	353.9	553.67	40.0	0.2730	0.271	0.186	0
5.	Carbon tetrachloride	CCl_4	153.823	250.6	1.6809	349.7	556.4	45.0	0.5570	0.271	0.202	0
6.	Benzene	C_6H_6	78.11	278.69	0.8948	353.3	562.1	48.6	0.3000	0.274	0.215	0
7.	2,3 Dimethylbutane	C_6H_{14}	86.17	145.19	0.7907	331.2	499.9	30.9	0.2410	0.270	0.257	0
8.	Cis-pentene-2	C_5H_{10}	70.13	121 .80	0.8029	310.10	475.56	40.4	0.237	0.266	0.280	≃0.20
9.	N-hexane	C_6H_{14}	86.172	177.84	0.7579	341.90	507.90	29.92	0.2340	0.264	0.290	0
10.	2,2,4 Trimethylpentane	C_8H_{18}	114.220	165.78	0.7945	372.4	543.6	25.4	0.2370	0.274	0.310	0
11.	Water	H_2O	18.02	273.16	1.0719	373.16	647.0	218.3	0.3220	0.230	0.348	1.82
12.	N-octane	C_8H_{18}	114.220	216.38	0.7642	398.83	569.4	24.6	0.2350	0.256	0.408	0
13.	Methyl alcohol	CH_3OH	32.040	175.48	0.8939	337.8	512.28	78.7	0.2720	0.224	0.556	1.71
14.	N-decane	$C_{10}H_{22}$	142.28	243.51	0.7650	447.3	617.6	20.8	0.2360	0.247	0.586	0
15.	Isopropyl alcohol	C_3H_7OH	60.097	185.20	0.8693	355.39	508.32	53.0	0.2730	0.248	0.773	1.68

CHAPTER II

THEORY OF CALCULATION OF CONFIGURATIONAL PROPERTIES

The liquid energies and entropies can be calculated from perfect gas state and PVT properties by, refer to Figure 1,

$$E_L = E^\circ - \Delta E\Big|_o^{sv} - \Delta E^v - \Delta E_{\Delta v} \tag{II-1a}$$

$$S_L = S^\circ - \Delta S\Big|_o^{sv} - \Delta S^v - \Delta S_{\Delta v} \tag{II-1b}$$

and for the liquid at saturation pressure,

$$E_L = E^\circ - \Delta E\Big|_o^{sv} - \Delta E^v \tag{II-2a}$$

$$S_L = S^\circ - \Delta S\Big|_o^{sv} - \Delta S^v \tag{II-2b}$$

The configurational energy can be calculated by

$$E_c = E_L - (E_{TR} + E_{ER} + E_I)_L \tag{II-3a}$$

and if we assume that the translational, external rotational, and internal (vibrational + rotational) energies are the same in the liquid as in the perfect gas, then

$$E_c = E_L - E^\circ_{TR} - E^\circ_{ER} - E^\circ_I \tag{II-3b}$$

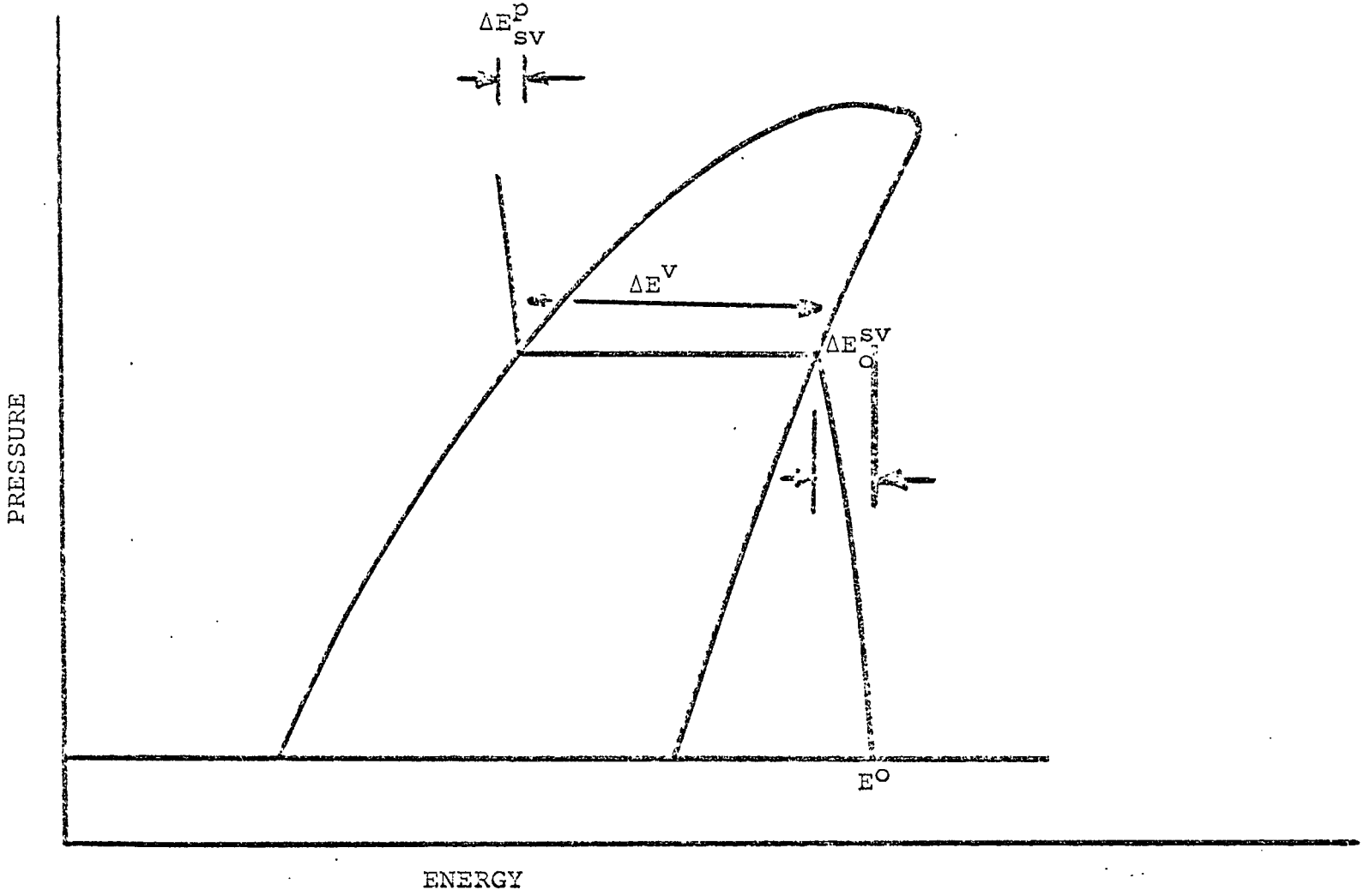
$$= \left[E^\circ - \Delta E\Big|_o^{sv} - \Delta E^v\right] - E^\circ_{TR} - E^\circ_{ER} - E^\circ_I$$

$$= \left[(E^\circ_{TR} + E^\circ_{ER} + E^\circ_I) - \Delta E\Big|_o^{sv} - \Delta E^v\right] - E^\circ_{TR} - E^\circ_{ER} - E^\circ_I$$

$$E_c = -\Delta E\Big|_o^{sv} - \Delta E^v \tag{II-4}$$

FIGURE 1

PRESSURE ENERGY DIAGRAM



When considering the entropy, an important difference is that $S_{TR}(liq) \neq S^{\circ}_{TR}$, because the "free volume" for translational motion is not known, and cannot be calculated with any degree of certainty. However, as discussed in Appendix D, a configurational entropy can be defined and calculated by,

$$S^{*}_{c} = S_{L} - (S^{\circ}_{TR} - R \ln \frac{RT/p^{\circ}}{V_{L}}) - S^{\circ}_{ER} - S^{\circ}_{I} \qquad \text{(II-5)}$$

$$= \left[S^{\circ} - \Delta S\Big|_{o}^{sv} - \Delta S^{v}\right] - (S^{\circ}_{TR} - R \ln \frac{RT/p^{\circ}}{V_{L}}) - S^{\circ}_{ER} - S^{\circ}_{I}$$

$$= \left[(S^{\circ}_{TR} + S^{\circ}_{ER} + S^{\circ}_{I}) - \Delta S\Big|_{o}^{sv} - \Delta S^{v}\right] - (S^{\circ}_{TR} - R \ln \frac{RT/p^{\circ}}{V_{L}}) - S^{\circ}_{ER} - S^{\circ}_{I}$$

$$S^{*}_{c} = -\Delta S\Big|_{o}^{sv} - \Delta S^{v} + R \ln \frac{RT/p^{\circ}}{V_{L}} \qquad \text{(II-6)}$$

The methods of calculation to determine the perfect gas properties, the corrections from perfect gas state to the saturated vapor state, and the properties of vaporization are discussed as subsequent parts of this thesis.

A. Ideal Gas Properties

The perfect gas state properties and the contribution of each mode were calculated by methods of statistical thermodynamics. The theory and equations necessary to make these statistical calculations have been developed by others (1, 4, 5, 25,26,27,28). Computer Program No. 1 used in this work combines these equations together into a general program.

Generally speaking there are five different modes of energy which contribute to the total energy of a perfect gas.

$$E^{o} = E^{o}_{TR} + E^{o}_{ER} + E^{o}_{IR} + E^{o}_{VIB} + E^{o}_{EL} \qquad (II-7)$$

A particular substance will not necessarily have contributions from all of these modes.

1. The Translational energy is that due to the translational motion of the molecules. The only information required to calculate this contribution is the molecular weight and the temperature.

2. The External Rotational energy is that due to the rotation or tumbling of the molecule about three mutually perpendicular axis. A monoatomic molecule will have no external rotational contribution since the mass is located at the origin.

In order to calculate this contribution it is necessary to have the external moments of inertia and the number of equivalent positions of the molecule. For simple molecules such as ethane or propane this data is available in the literature (26). However, for most substances it is necessary to calculate these quantities. To calculate the moments of inertia about each axis it is necessary to know, the atomic masses, the bond angles, and the bond lengths. For complex molecules the procedure is complicated; large molecules sometimes have several possible configurations making the moments of inertia somewhat arbitrary. However, by choosing the most convenient configurations and calculating the moment about each of the three axis an average value will be obtained which is satisfactory (26).

The number of equivalent positions of a molecule, σ , is determined by rotating the molecule about each of its three axis and finding the number of positions that are equivalent to other positions.

3. The Internal Rotational energy contribution is due to the rotation about the bonds between atoms. Monoatomic molecules such as argon or diatomic molecules such as nitrogen have no internal rotational contribution. Some polyatomic molecules such as methane will have no internal rotational contribution; others like ethane and propane have rotation of the methyl groups about the carbon - carbon bonds.

Early workers in the field of statistical thermodynamics obtained unsatisfactory results, however, when they assumed completely free rotation about these bonds. Pitzer (26) extended their early methods to allow for a sinusoidal potential barrier restricting rotation. The potential barrier cannot be obtained by direct means, however, and is determined from experimental entropy values (27). This parameter, therefore, absorbs all the inaccuracies and approximations in the method of calculation.

The data required to calculate the energy contribution for internal rotation of a particular group is the reduced moment of inertia, I_R, the height of potential barrier, V_o; and the number of maximi in the barrier. Typical values for the height and number of maximi of the barrier for certain rotating groups have been published, (26, 27) however, as pointed out previously, sometimes the barrier height must be adjusted to agree with experimental data. Aston and Fritz (4) present a method of calculation for the internal reduced moment of ertia of a rotating group.

4. The Vibrational energy contribution is that due to vibration (stretching, bending, etc.) of the atomic masses in the molecule. All molecules except monoatomic molecules have one or more vibrational contributions to the energy. Numerous vibrations are present in the more complex molecules. For instance, in an ethane molecule the hydrogen atoms vibrate in three different ways: (1) stretching of the C-H bonds, (2) bending of the H-C-H bonds, and (3) bending of the C-C-H bonds. Also present is the contribution from the stretching of the C - C bond. These vibrations all take place at different frequencies and contribute to the total engery in different magnitudes.

Pitzer has presented a good method for determining the frequencies and the number of contributions (multiplicity or degeneracy) of the various vibrations (14). This data can also be obtained from an infrared spectrogram of the substance in question. The relative magnitude of the vibrational contribution to the total energy is such that small errors in assigning frequencies will make only slight differencies in the total energy; consequently, similar vibrations can be assigned average frequencies and calculated together.

5. The Electronic contribution to the total energy of a molecule is that due to the excited states of electrons within the atoms. This contribution is significant only at very high temperatures and consequently was not considered in this work.

B. Ideal Gas to Real Gas Correction

The thermodynamic property changes which take place as each substance goes from the perfect gas state to the saturated vapor state were

calculated by the methods of Lyderson, Greenkorn, and Hougen (32). These calculations were made by hand and were part of the input data to Computer Program No. 2; "Configurational Energy, Ethalpy, and Entropy at Saturation Pressure."

C. Property Change Due to Vaporization

Computer Program No. 2 takes as input data information calculated by Computer Program No. 1, along with the property differences between the ideal gas and the saturated vapor. Using this information Program No. 2 calculates vapor pressures, liquid densities, property changes due to vaporization, and the configurational thermodynamic properties of the substance.

Two Antoine equations were necessary to calculate the vapor pressures from the triple point up to two atmospheres. Since most of the Antoine equation constants given in the literature (e.g. API Project 44, Ref. 1) cover the range 10mm to 1500mm H_g, it was necessary also to have suitable constants applicable down to the triple point. A second set of constants (A, B, NC) was obtained by use of the Third Law Entropy, and assuming that A and B did not change, and solving for a new C-Value, called NC, at the triple point, in the following manner:

$$S^{SV} = S_L + \Delta S^V \tag{II-8}$$

and,

$$S^{SV} = S^O - (S^O - S^{SV}) = S^O - R \ln P^V \tag{II-9}$$

Now

$$\Delta S^V = z RT \left(\frac{d \ln P}{dT}\right) = z RT \frac{2.30259\, B}{(NC-273.16 + T)^2} \tag{II-10}$$

$$\ln P^{SV}\ (atm) = 2.30259A - \ln 760 - \frac{2.30259B}{(NC-273.16+T)} \qquad (II-11)$$

Equating (II-9) and (II-10) and substituting (II-11) and II-12) gives,

$$\left[\frac{(S^{o} - S_{L}^{TP})}{R} + \ln 760 - 2.30259A\right] X^{2} + 2.30259B\ X - 2.30259B\ z\ T_{TP} = 0 \qquad (II-12)$$

which can be solved for X, then,

$$NC = X + 273.16 - T_{TP}$$

Above two atmospheres Gamson - Watson Constants were developed from experimental data obtained from various literature sources (1, 8, 22, 23, 24). A computer program developed by Tseng and Prengle (38) was used to obtain the Gamson - Watson Constants.

Liquid densities were calculated by the Francis Equation, using constants obtained by correlating experimental data from the literature and a computer program developed by Tseng and Prengle (37).

The Clapeyron Equation was used to calculate property changes due to vaporization, using vapor pressures and liquid densities calculated by the same program.

CHAPTER III

METHODS OF CALCULATION

In order to calculate the configurational thermodynamic properties for each of the fifteen substances described in this thesis the following steps were taken.

1. - The perfect gas thermodynamic properties were calculated for the substances using Computer Program No. 1, "Perfect Gas State Thermodynamic Properties by Statistical Thermodynamic Methods Including Hindered Internal Rotation Correction by Pitzer."
2. - Using vapor pressure data obtained from various literature sources as input data Gamson - Watson Constants were calculated using the computer program "Evaluation of Gamson - Watson Constants for Experimental Vapor Pressure or Bubble Point Data" which was developed by Tseng and Prengle.
3. - Using liquid density data also obtained from literature as input data Francis Constants were calculated using the Computer program "Saturated Liquid Densities and Mole Volumes by Francis Equation" developed by Tseng and Prengle.

4. - Using the methods of Lyderson, Greenkorn, and Hougen as given in tables in Reid and Sherwood (32) the differences between saturated vapor and perfect gas thermodynamic properties at constant temperature were calculated by hand. Compressibility factors for each saturated vapor at the various temperatures were also calculated by this method.

5. - Data generated from all the above sources were fed as input data into Computer Program No. 2, "Configurational Energy, Enthalpy, and Entropy at Saturation" which calculated values of E_L, S_L, E_c, S_c^*, E_c/RT and S_c^*/R.

A. Perfect Gas Properties

The first phase of the work described by this thesis was to develop a general computer program to calculate the perfect gas thermodynamic properties of a substance using statistical thermodynamic methods. The necessary equations have all been developed previously (1, 4, 5, 25, 26, 28, 29).

1. Translation - The following are the equations necessary to calculate the translational mode contribution to the overall thermodynamic properties:

$$\text{Ln } Q = 2.5 \text{ Ln } T + 1.5 \text{ Ln } M - 1.336 \qquad \text{(III-1)}$$

$$H^\circ - H_o^\circ = 2.5\ RT;\quad E^\circ - E_o^\circ = 1.5\ RT \qquad \text{(III-2)}$$

$$C_p^\circ = 2.5\ R \qquad \text{(III-3)}$$

$$S^\circ = 2.9841 \text{ Ln } M + 2.31498 + 4.9735 \text{ Ln } T \quad \text{(III-4)}$$

$$F^\circ - H_o^\circ = T\left[-2.9841 \text{ Ln } M + 7.28295 - 4.9735 \text{ Ln } T\right] \quad \text{(III-5)}$$

2. External Rotation - The equations required to calculate the thermodynamic property contribution due to the external rotation mode for a substance having a molecule composed of two identical atoms are as follows.

$$\text{Ln } Q = 1.5 \text{ Ln } (T \times I \times 10^{39}) - \text{Ln } \sigma + 88.408 \quad \text{(III-6)}$$

$$H^\circ - H_o^\circ = E^\circ - E_o^\circ = RT \quad \text{(III-7)}$$

$$C_p^\circ = R \quad \text{(III-8)}$$

$$S^\circ = 1.9894 \text{ Ln } (I \times 10^{39}) - 2.15787 + 1.9894 \text{ Ln } T \quad \text{(III-9)}$$

$$F^\circ - H_o^\circ = T\left[-1.9894 \text{ Ln } (I \times 10^{39}) + 4.14506 - 1.9894 \text{ Ln } T\right] \quad \text{(III-10)}$$

For a substance having a molecule composed of two different atoms the following two equations apply; the other quantities are the same as those for the molecule with two identical atoms.

$$S^\circ = 1.9894 \text{ Ln } (I \times 10^{39}) - 0.78045 + 1.9894 \text{ Ln } T \quad \text{(III-11)}$$

$$F^\circ - H_o^\circ = T\left[-1.9894 \text{ Ln } (I \times 10^{39}) + 2.76764 - 1.9894 \text{ Ln } T\right] \quad \text{(III-12)}$$

For a substance having a non-linear molecule the equations are

$$\text{Ln } Q = 1.5 \text{ Ln } T + 0.5 \text{ Ln } (I_X \times 10^{39}) + 0.5 \text{ Ln } (I_Y \times 10^{39}) + 0.5 \text{ Ln } (I_Z \times 10^{39}) - \text{Ln } \sigma + 133.186 \quad \text{(III-13)}$$

$$H^\circ - H_o^\circ = E^\circ - E_o^\circ = 1.5 RT \quad \text{(III-14)}$$

$$C_p^o = 1.5\ R \qquad \text{(III-15)}$$

$$S^o = 0.9947 \left[\text{Ln}\,(I_X \times 10^{39}) + \text{Ln}\,(I_Y \times 10^{39}) + \text{Ln}\,(I_Z \times 10^{39}) \right] - 1.9894\ \text{Ln}\,\sigma - 0.3329 + 2.9841\ \text{Ln}\,T \qquad \text{(III-16)}$$

$$F^o - H_o^o = T \left[-0.9947 \left(\text{Ln}\,(I_X \times 10^{39}) + \text{Ln}\,(I_Y \times 10^{39}) + \text{Ln}\,(I_Z \times 10^{39}) \right) + 1.9894\ \text{Ln}\,\sigma + 3.01407 - 2.9841\ \text{Ln}\,T \right] \qquad \text{(III-17)}$$

The number of equivalent positions, σ , of most polyatomic molecules is equal to one, and is the number of possible positions of the molecule which are indistinguishable from other positions. Molecules which are symmetrical and equivalent about each of three axis are known as spherical tops. The number of equivalent positions is 12 and the moments of inertia I_X, I_Y, and I_Z are equal.

3. Internal Rotation - Some early workers in statistical thermodynamics made calculations for internal rotation based on the assumption of free rotation about single bonds (25). Pitzer later extended their methods to allow for a sinusoidal potential barrier, V, restricting internal rotation (28), and published tables of corrected values of C_p^o, H^o/T, S^o, $S_f - S^o$, $-F^o/T$, $(F^o - F_f)/T$ as a function of V/RT and Q allowing for the restricted rotation.

For the statistical thermodynamic properties Program No. 1 each of Pitzer's six tables were read into the program as arrays of data. The computer calculates values for V/RT and I/Q and performs a search procedure to find the corresponding values of C_p^o and H^o/T. For values

of $I/Q \geq 0.25$ this same procedure was repeated for S° and $-F^\circ/T$. For I/Q values < 0.25 a different procedure is necessary to find S° and $-F^\circ/T$ since the entropy and free energy approach infinity as I/Q approaches zero. The computer calculates values for S_F and F_f/T assuming free rotation, and correction factors are read from data tables as described above.

The input data required by this calculation are; I_r, the reduced moment of inertia of the rotating group; V, the height of the sinusoidal potential barrier; n, the number of maxima of the potential barrier per 360°.

The required equations are:

$$Q = 2.7935 \left[(I_r \times 10^{38})\ T \right]^{1/2} / n \qquad \text{(III-18)}$$

$$S_f = 0.5\ R\ \text{Ln}\ T + 0.5\ \text{Ln}\ (I_r \times 10^{40}) - \text{Ln}\ n - 0.775 \qquad \text{(III-19)}$$

$$F_f = -R\ T \left[2.5\ \text{Ln}\ T - 0.5\ \text{Ln}\ (I_r \times 10^{40}) - \text{Ln}\ n - 1.275 \right] \qquad \text{(III-20)}$$

The routine described above to determine the internal rotational contribution to the total thermodynamic properties must be repeated for each rotating group in the molecules. Among the 15 substances studied in this work the number of rotating groups varied from zero for argon, nitrogen, methane, water, carbon tetrachloride, cyclohexane and benzene, to nine rotating groups for n-decane.

4. Vibration - The equations necessary to calculate the vibrational contributions to the thermodynamic properties are listed below.

$$Y = 1.4387\ \nu/T \tag{III-21}$$

$$C_P^o = R\ \ Y^2\ \ e^Y / \ (e^Y - 1)^2 \tag{III-22}$$

$$H^o - H_o^o = E^o - E_o^o = \frac{R\ \ T\ \ Y}{e^Y - 1} \tag{III-23}$$

$$S^o = \frac{R\ \ Y}{e^Y - 1} - R\ \mathrm{Ln}\ (1 - e^{-Y}) \tag{III-24}$$

$$F^o - H_o^o = H^o - TS^o \tag{III-25}$$

$$\mathrm{Ln}\ Q = 1\ -\ (F^o - H_o^o) \tag{III-26}$$

Pitzer described an excellent method for determining the frequencies and number of vibrations for hydrocarbons (25). Although this is an approximate method its accuracy is sufficient for these purposes. To determine the total vibrational contributions of the molecule the following procedure can be used,

a. Take the number of atoms in the molecule as N.

b. The total number of degrees of freedom of the molecule is then 3N.

c. The degrees of freedom due to translation, N_{TR}, is always three.

d. The degrees of freedom due to external rotation, N_{ER}, is either zero, two, or three depending upon whether the molecule is monoatomic, linear, or nonlinear.

e. The degrees of freedom due to internal rotation, N_{IR}, is equal to the number of rotating groups in the molecule.

f. The degrees of freedom due to vibration, N_{VIB}, is thus equal to

$$3N - N_{TR} - N_{ER} - N_{IR}$$

5. Total Quantities - The total thermodynamic properties are the summation of the contributions of all the modes. The computer print out of the results for each of the 15 substances included in this study is included in Appendix C.

The properties were calculated at various temperatures between the triple point and the critical point including the normal boiling point. In addition to those properties previously discussed the print out also includes the value for RT and the total value of $E^o - E_o^o$.

$$E^o - E_o^o = (H^o - H_o^o) - RT \qquad \text{(III-27)}$$

B. Gamson - Watson Constants

To calculate vapor pressures of the various substances two Antoine Equations were used below two atmospheres as described previously and the Gamson - Watson Equation above two atmospheres. Antoine Constants for each of the substances were available from API Project 44 Tables (1), "MCA-Selected Values of Properties of Chemical Compounds," (22) or elsewhere. Gamson - Watsons Constants were not as readily available, but were calculated using a computer program by Tseng and Prengle (38) and vapor pressure data. The vapor pressure data were available from API Project 44 Tables (1), "Selected Values of Properties of Chemical Compounds," (22) Chemical Engineers Handbook, (24) or other sources.

C. Francis Constants

The Francis Equations (11) were used to calculate the liquid densities of each of the substances. In order to obtain Francis Constants for the substances another computer program developed by Tseng and Prengle was used; liquid density data were obtained from various literature sources.

The Francis Equation was found to give a poor fit for water liquid density data. In this case the Smith - Keyes Equation (35) was used to obtain a satisfactory fit.

D. Property Change from Ideal Gas to Saturated Vapor

As indicated previously the difference in the respective properties between the perfect gas state and the real saturated vapor must be calculated. Tables developed by Lyderson, Greenkorn, and Hougen, given in Reid and Sherwood, (32) were used to make these calculations. These tables list values for $H^o - H/Tc$, f/p, and Z as functions of critical compressibility factor, reduced temperature, and reduced pressure. Using the values obtained from the tables the information required was calculated using the equations,

$$\frac{E^o - E^{SV}}{RT_c} = \frac{H^o - H^{SV}}{RT_c} + T_r (Z-1) \qquad \text{(III-28)}$$

$$\frac{S^o - S^{SV}}{R} = \frac{H^o - H^{SV}}{RT} + \text{Ln } f/p + \text{Ln } P \qquad \text{(III-29)}$$

E. Configurational Energy, Enthalpy, and Entropy at Saturation

The data generated by calculations and computations to this point were used as input to the computer program "Configurational Energy, Enthalpy and Entropy at Saturation." Listed below is the input data to this program

for each of the 15 substances under study.

1. $E^{o} - E^{sv}$
2. $E^{o} - E^{o}_{o}$
3. S^{o}
4. Z (vapor)
5. $S^{o} - S^{sv}$
6. S^{ER}
7. Antoine constants
8. Gamson - Watson Constants
9. Francis Constants

Using the above information the computer calculates and prints out values for the following properties at the desired temperatures for each substance.

1. Vapor pressure
2. d (Ln P)/d T
3. Liquid volume
4. Vapor volume
5. $P (V_G - V_L)$
6. Energy of vaporization
7. Enthalpy of vaporization
8. Entropy of vaporization
9. Liquid density

10. Energy due to external rotation

11. Energy of the liquid, E_L

12. Configurational energy of the liquid E_c

13. Entropy of the liquid, S_L

14. E_c/RT

15. S_c^*/R

The liquid density was calculated by the Francis Equations (11). The following equation is used from the triple point up to near the critical temperature.

$$\rho = A - B\,T - C/(E - T) \qquad \text{(III-30)}$$

Near the critical temperature it is necessary to use the following equation.

$$(\rho - \rho_c)^H = G\,(T_c - T) \qquad \text{(III-31)}$$

Two Antoine Equations were used to calculate vapor pressures from the triple point up to a vapor pressure of two atmospheres.

$$\text{Log } P = A - B/(NC - 273.16 + T); \quad P < 10\text{mm} \qquad \text{(III-32a)}$$

$$\text{Log } P = A - B/(C - 273.16 + T); \quad 10\text{mm} < P < 2\text{ atm} \qquad \text{(III-32b)}$$

Above two atmospheres the Gamson - Watson Equation is used to calculate the vapor pressure.

$$\text{Log } P = A\,T_c/T + B - e^{-20\,(T/T_c - b)^2} \qquad \text{(III-33)}$$

The value of d Ln P /dT is calculated at each temperature by using a differentiation of either the Antoine Equation or the Gamson - Watson

Equation. A value for d (Ln P)/dT is required to calculate the energy of vaporization of a substance using the Clapeyron Equation:

$$\Delta E^V = P\,(V_G - V_L)\left[T\ d\ \mathrm{Ln}\ P/\ dT - 1.0\right]\ 24.21 \qquad \text{(III-34)}$$

The enthalpy and entropy of vaporization is calculated from the following equations

$$\Delta H^V = \Delta E^V + P\ (V_G - V_L)\ 24.21 \qquad \text{(III-35)}$$

$$\Delta S^V = \Delta H^V / T \qquad \text{(III-36)}$$

The configurational properties and the saturated liquid properties are then calculated.

$$E_c = -\ \Delta E\big|_o^{SV} - \Delta E^V \qquad \text{(III-37)}$$

$$S_c^* = -\ \Delta S\big|_o^{SV} - \Delta S^V + R\ \mathrm{ln}\ \frac{RT/P}{V_L} \qquad \text{(III-38)}$$

$$E_L = E^o - \Delta E\big|_o^{SV} - \Delta E^V \qquad \text{(III-39)}$$

$$S_L = S^o - \Delta S\big|_o^{SV} - \Delta S^V \qquad \text{(III-40)}$$

In order to smooth out some irregularities in the properties of some substances in the range between the triple point and 10 mm Hg vapor pressure the following steps were taken. A straight line interpolation between the triple point and 10 mm Hg for the energy of vaporization was made. From these values of ΔE^V a NC value was calculated at each temperature. This NC value is a new C constant for the Antoine Equation and is discussed in Chapter II. From the NC value the properties of the substance are calculated in the range between the triple point and 10mm Hg.

CHAPTER IV

RESULTS OF THE CALCULATIONS

In order to indicate the agreement between Third Law Entropy values and our configurational and perfect gas states properties, Tables IIA to XVIA are presented. Also summaries of the densities and configurational properties, as a function of temperature, tabulated in Appendix C, are presented as Tables IIB through XVIB. In addition, empirical least squares fits of the configurational energy and entropy functions, of the form,

$$(E_c/E_{cTP}) = 1 + A\,(1-\rho/\rho_{TP}) + B\,(1-\rho/\rho_{TP})^2 + C\,(1+\rho/\rho_{TP})^3 \quad \text{(IV-1)}$$

and

$$(S_c^*/S_{cTP}) = 1 + A\,(1-\rho/\rho_{TP}) + B\,(1-\rho/\rho_{TP})^2 + C\,(1+\rho/\rho_{TP})^3 \quad \text{(IV-2)}$$

along with the Francis equations for the density as a function of the temperature were made and are included for each substance.

Figure 2 is a plot of the entropy as a function of the temperature and graphically shows the relationship between S (solid), S (saturated liquid), S^o and S (saturated vapor): also a breakdown of S_L into S_{TR}, S_l and S_C.

Figure 3 is a similar plot for the energy, $(E-E_o^o)$ - values. These plots very strikingly indicate that for,

$P <$ 1atm, $(E^{SV} - E^o) = 0$

$P <$ 1 atm, $(S^{SV} - S^o) = R \ln P^{SV} \neq 0$

TABLE IIA - ARGON, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(83.96, 87.46, 150.86° K)		Clusius & Frank (7)		Our Work
1. S (0 → 10° K, extrapolation)		0.303		
2. ΔS (10 → 83.96° K, crys)		8.815		
3. ΔS^f (83.96)		3.352		
	S_L (83.96)	12.470	ΔS^*_{TR}	12.70 0.16
4. ΔS (83.96 → 87.46 liq)		0.413	ΔS_{ER-I} ΔS^*_C	- 0 - 0.06
	S_L (87.46)	12.883		12.92
5. ΔS^V (87.46)		17.84		17.85
6. (S^o - S), (87.46)		0.13		0.16
	$S^o_{87.46}$	30.85		30.93
7. ΔS^o (87.46 298.15)		6.104		6.10
	$S^o_{298.16}$	36.95 ± 0.2		37.03
	presently accepted value	36.99 $(\frac{cals}{g\ mol,\ K})$		

(7) Clusius, K., Frank, A., Ztschr. Electrochem. 49, 308 (1943).

TABLE IIB

PROPERTIES OF ARGON

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	K cals/mole	cals/mole °K
83.96	1.4113	1.413	7.10
87.46	1.3895	1.397	7.04
90.00	1.3733	1.386	6.94
100.00	1.3067	1.357	6.57
103.16	1.2844	1.343	6.47
113.16	1.2084	1.260	5.83
123.16	1.1198	1.164	5.04
133.16	1.0076	0.998	3.92
138.16	0.9351	0.925	3.54
143.16	0.8430	0.837	3.07
148.16	0.7690	0.742	2.56
150.86	0.5356	0.603	2.16

$$\rho = 1.9309 - 0.4768 \times 10^{-2} T - 10/(167.83 - T), \quad T \leq 146.33$$

$$(\rho - .5356)^{2.39} = .01144\,(150.86 - T), \quad T > 146.33$$

	A	B	C
E_c/E_{CTP}	-0.3863	-3.0314	3.4992
S_c/S_{CTP}	-1.0243	-2.9068	4.4109

TABLE IIIA - METHANE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(90.6, 111.7, 190.7°K)	Kelley (21)		Our Work
1. $S(90.6\ ^{\circ}K)$	13.63		
2. $\Delta S^{f}(90.6)$	2.47		
$S^{L}_{90.6}$	16.10		16.03
3. ΔS (90.6 → 111.7 liq)	2.70	ΔS^{*}_{TR}	0.75
		ΔS_{ER-I}	0.63
		ΔS^{*}_{c}	1.45
$S^{L}_{111.7}$	18.81		18.86
4. $\Delta S^{V}(111.7) = 19.55/111.7$	17.50		17.50
5. $(S^{\circ} - S\ ), (111.7)$	0.22		0.22
$S^{\circ}_{111.7}$	36.53		36.58
6. ΔS° (111.7 → 298.16)	7.98		7.98
$S^{\circ}_{298.16}$	44.51 ± 0.20		44.56
presently accepted value (1)	$\underline{\underline{44.50}}$ $\left(\frac{cals}{g\ mol\ K}\right)$		

(21) Kelley, K. K., Bureau of Mines Bulletin No. 350 (1932).

TABLE IIIB

PROPERTIES OF METHANE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/Mole °K
90.68	0.4528	1.921	8.26
93.16	0.4496	1.904	8.09
100.00	0.4407	1.856	7.54
103.16	0.4364	1.831	7.30
110.00	0.4269	1.768	6.72
111.70	0.4245	1.754	6.81
113.16	0.4225	1.742	6.97
120.00	0.4124	1.689	6.39
123.16	0.4076	1.685	6.50
130.00	0.3968	1.643	6.02
133.16	0.3916	1.616	5.85
140.00	0.3799	1.549	5.43
143.16	0.3742	1.528	5.27
150.00	0.3611	1.458	4.90
153.16	0.3547	1.428	4.72
160.00	0.3398	1.368	4.38
163.16	0.3324	1.340	4.28
170.00	0.3137	1.250	3.82
173.16	0.3047	1.208	3.61
180.00	0.2810	1.097	3.14
183.16	0.2666	1.038	2.91
190.00	0.2057	0.870	2.39
190.70	0.1620	0.762	2.16

$$\rho = 0.5925 - 0.8749 \times 10^{-3} T - 9/(239.84 - T) \qquad T \leq 163.16$$

$$(\rho - .1620)^{2.72} = .2859 \times 10^{-3} (190.70 - T), \qquad T > 163.16$$

	A	B	C
E_c/E_{CTP}	-1.1800	-0.0336	0.6593
S_c/S_{CTP}	-2.3680	2.3901	-0.6982

TABLE IVA - NITROGEN, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(63.19, 77.35, 126.2 °K)	Giaugue & Clayton (13)		Our Work
1. S (0 → 10 °K)	0.46		
2. ΔS (10 → 35.61, cry II)	6.03		
3. ΔS^T (35.61) = 54.71/35.61	1.54		
4. ΔS (35.61 → 63.19 cry I)	5.59		
5. ΔS^f (63.14) = 172.3 / 63.19	2.73		
$S^L_{63.19}$	16.36		16.
6. ΔS (63.14 → 77.35 liq)	2.73	ΔS^*_{TR}	0.75
		ΔS_{ER-I}	0.40
		ΔS^*_c	1.14
$S^L_{77.32}$	19.07		18.96
7. ΔS^V (77.35) = (1333 /77.35)	17.24		17.23
8. (S^o-S) 77.35	0.22		0.22
$S^o_{77.35}$	36.53		36.41
9. ΔS^o (77.35 298.16)	9.24		9.40
$S^o_{298.16}$	45.77 ± 0.1 (API)		45.81

(13) Giaugue, W. F., Clayton, J.O; J. AM. Chem. Soc. 55, 4875 (1933).

TABLE IVB

PROPERTIES OF NITROGEN

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
63.19	0.8694	1.295	8.24
75.00	0.8184	1.229	7.27
77.35	0.8077	1.200	7.10
100.00	0.6905	0.990	5.02
125.00	0.4211	0.615	2.54
126.20	0.3110	0.504	2.12

$$\rho = 1.1510 - 0.3318 \times 10^{-2} T - 6/(146.62-T) \quad , \quad T \leq 120.0$$

$$(\rho - 0.3110)^{3.36} = 0.5030 \times 10^{-3} (126.20-T), \quad T > 120$$

	A	B	C
E_c/E_{CTP}	-1.1550	-0.0721	0.5857
S_c/S_{CTP}	-2.2844	1.9914	-0.3825

TABLE VA - CYCLOHEXANE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(279.83, 353.90, 553.67°K)		Ruehrivein & Huffman (33)		Our Work
1. S (0 → 13°K)		0.201		
2. ΔS (13 → 186.1 K, cry II)		23.887		
3. ΔS^T (186.1) = 1610.8/186.1		8.655		
4. ΔS (186.1 → 279.82, cry I)		11.478		
5. ΔS^f (279.82) = 639.8/279.82		2.286		
	$S^L_{279.82}$	46.507		46.35
6. ΔS (279.82 → 298.16 liq)		2.330	ΔS^*_{TR}	0.24
			ΔS_{ER-I}	1.24
			ΔS^*_c	1.00
	$S^L_{298.16}$	48.84± 0.10		48.83
7. $(S^\circ - S^{SV})$, 298.16		-4.079		(-4.08)
8. ΔS^V (298.16) = 7,895/298.16		26.48		(26.48)
	$S^\circ_{298.16}$	71.24		(71.23)
9. ΔS (298.16 353.90, liq.)			ΔS^*_{TR}	0.65
			ΔS_{ER-I}	4.00
			ΔS^*_c	2.12
	$S^L_{353.90}$	-		55.60
10. ΔS° (298.16 → 353.90)		4.84		-
11. ΔS^V (353.40)		-		20.32
12. $(S^\circ - S)$ 353.90		-		0.16
	$S^\circ_{353.90}$	76.08		76.07

(33) Ruehrivein, R. A., Huffman, H. M., J. Am. Chem. Soc. 65, 1620 (1943).

TABLE V B

PROPERTIES OF CYCLOHEXANE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
279.83	0.7915	7.609	12.64
290.00	0.7818	7.434	12.05
298.16	0.7741	7.308	11.64
300.00	0.7723	7.272	11.52
310.00	0.7627	7.120	11.05
323.16	0.7499	6.927	10.48
330.00	0.7432	6.855	10.21
348.16	0.7251	6.628	9.57
353.90	0.7193	6.557	9.52
373.16	0.6994	6.314	8.96
383.16	0.6889	6.125	8.42
393.16	0.6781	5.993	8.10
400.00	0.6705	5.912	7.96
403.16	0.6670	5.866	7.84
423.16	0.6439	5.618	7.30
433.16	0.6318	5.489	7.01
448.16	0.6127	5.279	6.61
458.16	0.5991	5.146	6.33
473.16	0.5771	4.933	5.96
498.16	0.5353	4.569	5.34
500.00	0.5319	4.549	5.30
523.16	0.4810	3.999	4.42
548.16	0.3801	3.116	3.17
553.67	0.2730	2.399	2.36

$$\rho = 1.0584 - 0.8395 \times 10^{-3} T - 10/(592.03-T) \quad , T \leq 473.16$$

$$(\rho - 0.2730)^{2.58} = 0.5701 \times 10^{-3} (553.67 - T) \quad , \quad T > 473.16$$

	A	B	C
E_c/E_{CTP}	-1.5835	1.2933	-0.7131
S_c/S_{CTP}	-2.9082	4.5091	-2.9601

TABLE VIA - CARBON TETRACHLORIDE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(250.3, 349.7, 556.4°K)		Hicks, Hooley Stephenson(16)		Our Work
1. S (0 → 18°K)		1.39		
2. ΔS (18 → 225.35, cry II)		34.12		
3. ΔS^T (225.35) = 1095/225.35		4.86		
4. ΔS (225.35 → 250.3, cry I)		3.01		
5. ΔS^f 250.3 = 601/250.3		2.40		
	$S^L_{250.3}$	45.78		45.92
6. ΔS (250.3 → 298.16 liq)		5.48	ΔS^*_{TR}	0.64
			ΔS_{ER-I}	2.50
			ΔS^*_c	2.89
	$S^L_{298.16}$	51.26 ± 0.2		51.95
7. $(S^\circ - S^{SV})$, 298.16		-3.76		(-3.76)
8. ΔS^V(298.16)				(25.86)
	$S^\circ_{298.16}$	74.04	MCA	(74.05)
9. ΔS (298.16 → 349.7 liq)		-	ΔS^*_{TR}	0.61
			ΔS_{ER-I}	2.49
			ΔS^*_c	1.68
	$S^L_{349.7}$	-		56.73
10. ΔS° (298.16 → 349.7)		3.28		-
11. ΔS^V (349.7)		-		20.46
12. $(S^\circ - S)$ (349.7)		-		0.14
	$S^\circ_{349.7}$	77.32		77.33

(16) Hicks, J.F.G., Hooley, J. G., Stephenson, C.C., J. AM. Chem. Soc. 66, 1064 (1944).

TABLE VIB

PROPERTIES OF CARBON TETRACHLORIDE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	K cals/mole	cals/mole °K
250.30	1.6815	8.037	14.00
298.16	1.5861	7.124	11.11
300.00	1.5823	7.096	11.02
349.70	1.4806	6.504	9.43
350.00	1.4800	6.497	9.38
373.16	1.4312	6.313	8.93
398.16	1.3769	5.854	7.81
400.00	1.3728	5.832	7.77
423.16	1.3202	5.569	7.14
448.16	1.2595	5.239	6.47
473.16	1.1918	4.920	5.88
498.16	1.1100	4.579	5.29
500.00	1.1030	4.550	5.23
523.16	0.9920	4.028	4.42
548.16	0.8319	3.306	3.36
556.40	0.5570	2.410	2.35

$$\rho = 2.1832 - 0.1880 \times 10^{-2}T - 10/(571.32-T) \quad , \quad T \leq 523.16$$

$$(\rho - 0.5570)^{3.27} = 0.1780 \times 10^{-2} (556.40-T) \quad , \quad T > 523.16$$

	A	B	C
E_c/E_{CTP}	-1.6366	1.4192	-0.7688
S_c/S_{CTP}	-3.0229	4.6606	-2.9208

TABLE VIIA - BENZENE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(278.69, 353.3, 562.1°K)		Ahlberg, Blanchard Lundberg(2)		Our Work
1. S (0 → 20°K)		0.73		
2. ΔS (20 → 90°K, cry)		10.16		
3. ΔS (90 → 278.6 cry)		20.02		
4. ΔS^f(278.6)= 2345./278.6		8.43		
	$S^L_{278.69}$	39.34		38.94
5. ΔS (278.69 → 298.16 liq)		2.15	ΔS^*_{TR}	0.24
			ΔS_{ER-I}	0.94
			ΔS^*_c	1.15
	$S^L_{298.16}$	41.49		41.27
6. $(S^\circ - S^{SV})$, 298.16		-4.13		(-4.13)
7. ΔS^V ,(298.16)		27.13		(27.13)
	$S^\circ_{298.16}$	64.45		(64.28)
8. ΔS (298.16 → 353.3, liq)		-	ΔS^*_{TR}	0.65
			ΔS_{ER-I}	2.83
			ΔS^*_c	2.25
	$S^L_{353.3}$	-		47.00
9. ΔS° (298.16 → 353.3)		3.67		-
10. ΔS^V (353.3)		-		20.83
11. $(S^\circ - S)$, (353.3)		-		0.12
	$S^\circ_{353.3}$	68.01		67.95

(2) Ahlberg, J. E., Blanchard, E. R., Lundberg, W. D., J. Chem. Phys. 5, 539 (1937).

TABLE VIIB

PROPERTIES OF BENZENE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	K cals/mole	cals/mole °K
278.69	0.8948	7.845	13.00
293.16	0.8795	7.595	12.16
298.16	0.8741	7.501	11.85
300.00	0.8722	7.463	11.72
323.16	0.8472	7.112	10.62
348.16	0.8196	6.773	9.63
353.30	0.8139	6.726	9.60
373.16	0.7913	6.438	8.90
398.16	0.7619	6.093	8.10
400.00	0.7597	6.085	8.10
423.16	0.7309	5.786	7.48
448.16	0.6976	5.450	6.76
473.16	0.6606	5.095	6.10
500.00	0.6135	4.717	5.46
523.16	0.5609	4.229	4.65
548.16	0.4726	3.860	4.25
562.10	0.3000	2.401	2.40

$$\rho = 1.1928 - 0.9575 \times 10^{-3} T - 10/(599.49 - T), \quad T \leq 553.16$$

$$(\rho - .3000)^{2.70} = 0.6250 \times 10^{-3} (562.10 - T), \quad T > 553.16$$

	A	B	C
E_c/E_{CTP}	-1.8013	2.2663	-1.6828
S_c/S_{CTP}	-3.2125	5.7827	-4.1531

TABLE VIIIA - 2, 3 DIMETHYLBUTANE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

	(145.19, 331.30, 499.90 °K)		Douslin & Huffman (10)		Our Work
1.	S (0 → 13°K)		0.318		
2.	ΔS (13 → 136.07, cry II)		23.326		
3.	ΔS^T (136.07) = 1552/136.07		11.406		
4.	ΔS (136.07 → 145.19, cry I)		2.127		
5.	ΔS^f (145.19) = 191.42/145.19		1.318		
		$S^L_{145.19}$	38.495		38.48
6.	ΔS(145.19 → 298.16 liq)		27.833	ΔS^*_{TR}	2.52
				ΔS_{ER-I}	15.04
				ΔS^*_c	10.47
		$S^L_{298.16}$	66.36		66.50
7.	$(S^\circ - S^{SV})$, 298.16		-2.28		(-2.34)
8.	ΔS^V,(298.16)		23.34		(23.32)
		$S^\circ_{298.16}$	87.42		(87.48)
9.	$\underline{\Delta}S$ (298.16 → 331.20 liq)		-	ΔS^*_{TR}	0.41
				ΔS_{ER-I}	2.28
				ΔS^*_c	1.21
		$S^L_{331.20}$	-		70.41
10.	ΔS° (298.16 → 331.20)		2.81		-
11.	ΔS^V(331.2)		-		19.70
12.	$(S^\circ - S)$ 331.2		-		0.18
		$S^\circ_{331.20}$	90.23		90.29

(10) Douslin, D.R., Huffman, H.M., J. Am. Chem. Soc. 68, 1704 (1946).

TABLE VIIIB

PROPERTIES OF 2.3 DIMETHYLBUTANE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
145.19	0.7907	8.086	21.06
160.00	0.7783	7.962	19.39
180.00	0.7613	7.793	17.56
200.00	0.7442	7.625	16.08
220.00	0.7269	7.457	14.87
240.00	0.7094	7.274	13.81
260.00	0.6917	6.970	12.65
273.16	0.6798	6.796	12.03
280.00	0.6735	6.683	11.61
298.16	0.6568	6.381	10.59
300.00	0.6550	6.361	10.50
323.16	0.6329	6.034	9.51
331.20	0.6251	5.939	9.38
348.16	0.6080	5.679	8.68
373.16	0.5816	5.363	7.96
393.16	0.5588	5.103	7.33
400.00	0.5505	5.002	7.09
423.16	0.5203	4.678	6.36
448.16	0.4814	4.303	5.69
458.16	0.4546	4.092	5.30
473.16	0.4245	3.700	4.59
498.16	0.3132	2.671	2.98
499.90	0.2410	2.175	2.36

$$\rho = 0.9283 - 0.7774 \times 10^{-3}T - 10/(549.70 - T), \quad T \leq 448.16$$

$$(\rho - 0.2410)^{2.93} = 0.2600 \times 10^{-3}\,(499.90-T), \quad T > 448.16$$

	A	B	C
E_c/E_{CTP}	-1.3088	-0.0795	0.6148
S_c/S_{CTP}	-3.7542	6.7063	-4.4921

TABLE IXA - CIS-PENTENE- 2, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

	(121.8, 310.10, 475.56)		API(1)		Our Work
1.	$S^{L}_{121.8}$		32.79		32.81
2.	ΔS (121.8 → 298,16 liq)			ΔS^{*}_{TR}	3.21
				ΔS_{ER-I}	12.71
				ΔS^{*}_{c}	12.91
3.		$S^{L}_{298.16}$	61.81		61.54
4.	$(S^{o}-S^{SV})$ 298.16		-0.85		(-0.85)
5.	ΔS^{V} (298.16)		(21.88)		(21.88)
6.		$S^{o}_{298.16}$	82.76		(82.57)
7.	ΔS (298.16 → 310.10 liq)		-	ΔS^{*}_{TR}	0.15
				ΔS_{ER-I}	0.65
				ΔS^{*}_{c}	0.36
8.		$S^{L}_{310.10}$	-		62.70
9.	ΔS^{o} (298.16 → 310.10)		0.83		-
10.	ΔS^{V}, (310.10)		-		20.55
11.	$(S^{o} - S)$, 310.10		-		0.16
12.		$S^{o}_{310.10}$	83.59		83.40

(36) Todd, S.S., Oliver, G. D., Huffman, H.M., J. AM. Chem. Soc. 69, 1519, (1947).

TABLE IXB

PROPERTIES OF CIS-PENTENE - 2

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	K cals/mole	cals/mole °K
121.80	0.8029	7.755	23.18
125.00	0.8002	7.731	22.68
150.00	0.7787	7.546	19.51
200.00	0.7349	7.175	15.48
250.00	0.6894	6.584	12.48
273.16	0.6675	6.268	11.34
298.16	0.6429	5.960	10.27
300.00	0.6410	5.945	10.19
310.10	0.6306	5.811	9.91
323.16	0.6167	5.629	9.36
348.16	0.5880	5.423	8.76
350.00	0.5857	5.388	8.67
373.16	0.5541	4.983	7.80
398.16	0.5254	4.558	6.95
400.00	0.5231	4.520	6.89
423.16	0.4897	4.102	6.06
448.16	0.4398	3.453	4.77
450.00	0.4351	3.405	4.64
473.16	0.3259	2.465	2.93
475.56	0.2370	2.136	2.78

$$\rho = 0.9184 - 0.8060 \times 10^{-3} T - 6/(468.57 - T) \quad , \quad T \leq 353.16$$

$$(\rho - 0.2370)^{2.95} = 0.3299 \times 10^{-3}(475.56 - T) \quad , \quad T > 353.16$$

	A	B	C
E_c/E_{CTP}	-0.8517	-1.7554	2.1287
S_c/S_{CTP}	-3.7174	6.4078	-4.1025

TABLE XA - H-HEXANE, THIRD LAW ENTROPY &
LIQUID PHASE CONFIGURATIONAL VALUES

(177.84, 341.90, 507.90°K)		Douslin & Huffman (10)		Our Work
1. $S\ (0 \rightarrow 13)$		0.299		
2. $\Delta S\ (13 \rightarrow 177.84)$		30.838		
3. $\Delta S^f(177.84) = 3126.1/177.84$		17.579		
	$S^L_{177.84}$	48.72		48.74
4. $\Delta S\ (177.84 \rightarrow 298.16\ liq)$		22.045	ΔS^*_{TR}	1.84
			ΔS_{ER-I}	12.87
			ΔS^*_c	7.37
	$S^L_{298.16}$	70.76		70.82
5. $(S^o - S^{SV}),\ (298.16)$		-3.22		(-3.21)
6. $\Delta S^V,\ (298.16)$		25.29		(25.29)
	$S^o_{298.16}$	92.83(API)		(92.89)
7. $\Delta S(298.16 \rightarrow 341.90\ liq)$		-	ΔS^*_{TR}	0.54
			ΔS_{ER-I}	4.28
			ΔS^*_c	1.88
	$S^L_{341.90}$	-		77.51
8. $\Delta S^o\ (298.16 \rightarrow 341.90)$		4.96		-
9. $\Delta S^V(341.90)$		-		20.71
10. $(S^o - S)\ 341.90$		-		0.18
	$S^o_{341.90}$	97.79		97.86

(10) Douslin, D.R., Huffman, H.M., J. Am. Chem. Soc., 68, 1704 (1946).

TABLE XB

PROPERTIES OF N-HEXANE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
177.84	0.7579	8.322	19.07
180.00	0.7561	8.307	18.89
190.00	0.7478	8.234	18.10
200.00	0.7395	8.161	17.38
210.00	0.7312	8.088	16.73
220.00	0.7228	8.015	16.13
230.00	0.7143	7.942	15.59
240.00	0.7058	7.869	15.09
250.00	0.6972	7.768	14.55
260.00	0.6885	7.573	13.80
273.16	0.6770	7.331	12.93
298.16	0.6545	6.957	11.70
300.00	0.6528	6.926	11.60
323.16	0.6312	6.538	10.42
341.90	0.6131	6.270	9.82
348.16	0.6068	6.189	9.55
373.16	0.5808	5.778	8.44
398.16	0.5522	5.476	8.09
400.00	0.5500	5.467	8.15
423.16	0.5196	5.061	7.17
473.16	0.4259	4.060	5.20
498.16	0.3572	3.090	3.07
500.00	0.3476	3.059	3.03
507.90	0.2340	2.300	2.48

$$\rho = 0.9183 - 0.7492 \times 10^{-3} T - 10/(545.67-T), \quad T \leq 473.16$$

$$(\rho - 0.2340)^{2.57} = 0.4726 \times 10^{-3} (507.90-T), \quad T > 473.16$$

	A	B	C
E_c/E_{CTP}	-1.2463	0.5059	1.1107
S_c/S_{CTP}	-3.2443	4.7014	-2.6617

TABLE XIA - 2, 2, 4 TRIMETHYLPENTANE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

	(165.78, 372.40, 543.60°K)	Pitzer(27)		Our Work
1.	S (0 → 14.13)	0.683		
2.	ΔS (14.13 → 165.78, cry)	35.309		
3.	ΔS^f (165.78) = 2201.6/165.78	13.279		
	$S^L_{165.78}$	49.27		49.28
4.	ΔS (165.78 → 298.16 liq)	29.132	ΔS^*_{TR}	2.04
			ΔS_{ER-I}	17.91
			ΔS^*_c	9.31
	$S^L_{298.16}$	78.40± 0.20		78.54
5.	$(S^\circ - S^{SV})$ 298.16	-5.41		(-5.43)
6.	ΔS^V(298.16)	28.16		(28.16)
	$S^\circ_{298.16}$	101.15		(101.27)
7.	ΔS (298.16 → 372.40 liq)	-	ΔS^*_{TR}	0.86
			ΔS_{ER-I}	8.80
			ΔS^*_c	2.81
	$S^L_{372.40}$	-		91.02
8.	ΔS°(298.16 → 372.40)	9.90		-
9.	ΔS^V (372.40)	-		19.90
10.	$(S^\circ - S)$ (372.40)	-		0.26
	$S^\circ_{372.40}$	111.06		111.18

(27) Pitzer, K. S., J. Am. Chem. Soc. 62, 1224 (1940).

TABLE XIB

PROPERTIES OF 2, 2, 4 TRIMETHYLPENTANE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
165.78	0.7945	9.298	22.11
180.00	0.7835	9.167	20.59
200.00	0.7679	8.981	18.80
220.00	0.7522	8.796	17.32
240.00	0.7362	8.611	16.09
273.16	0.7094	8.251	14.29
298.16	0.6887	7.808	12.80
300.00	0.6872	7.778	12.70
323.16	0.6675	7.440	11.69
348.16	0.6456	7.094	10.66
358.16	0.6366	6.969	10.28
372.40	0.6234	6.772	9.99
390.81	0.6058	6.559	9.52
393.16	0.6035	6.431	9.16
400.00	0.5966	6.369	8.99
423.16	0.5723	6.066	8.32
448.16	0.5432	5.654	7.46
458.16	0.5303	5.503	7.14
473.16	0.5090	5.244	6.68
498.16	0.4646	4.764	5.84
500.00	0.4611	4.701	5.77
523.16	0.4059	3.939	4.50
533.16	0.3685	3.526	3.89
543.60	0.2370	2.323	2.34

$$\rho = 0.9371 - 0.7162 \times 10^{-3} T - 10/(585.25-T), \quad T \leq 493.16$$

$$(\rho - 0.2370)^{2.68} = 0.4167 \times 10^{-3} (543.60-T), \quad T > 493.16$$

	A	B	C
E_c/E_{CTP}	-1.3233	0.0800	0.3747
S_c/S_{CTP}	-3.6008	6.2620	-4.1486

TABLE XIIA - WATER, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(273.16, 373.16, 647.0°K)		Giauque & Stout (14)		Our Work
1.	S (0 → 10°K)	0.02		
2.	ΔS (10 → 273.16, crys)	9.08		
3.	ΔS (randomness of H-bonds in ice crystals, R ln 6/4)	0.81		
4.	ΔS^f (273.16) = 1435.7/273.16	5.26		
5.	$S^L_{273.16}$	15.17		15.20
			ΔS^*_{TR}	0.27
			ΔS_{ER-I}	0.27
6.	ΔS (273.16 → 298.16, liq)	1.58	ΔS^*_c	0.97
7.	$S^L_{298.16}$	16.75 ± 0.03		16.70
8.	$(S^o - S^{SV})$, (298.16)	-6.89		(-6.82)
9.	ΔS^V (298.16)	35.26		(35.24)
10.	$S^o_{298.16}$	45.13		(45.12)
11.	ΔS^L (298.16 → 373.16)	-	ΔS^*_{TR}	0.75
			ΔS_{ER-I}	0.68
			ΔS^*_c	2.69
12.	$S^L_{373.16}$	-		20.83
13.	ΔS^o (298.16 → 373.16)	1.81		-
14.	ΔS^V, (373.16)	-		26.05
15.	$(S^o - S)$, (373.16)	-		0.04
16.	$S^o_{373.16}$	46.94		46.92

(14) Giauque, W. F., Stout, J. W., J. Am. Chem. Soc. 58, 1144 (1936).

TABLE XIIB

PROPERTIES OF WATER

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
273.16	0.9998	10.095	15.06
298.16	0.9968	9.915	14.09
300.00	0.9964	9.887	14.00
350.00	0.9738	9.247	12.03
373.16	0.9584	8.995	11.40
375.16	0.9571	8.981	11.33
398.16	0.9390	8.741	10.79
400.00	0.9375	8.727	10.76
423.16	0.9169	8.398	9.99
448.16	0.8922	8.098	9.32
473.16	0.8647	7.831	8.79
498.16	0.8339	7.564	8.31
500.00	0.8315	7.552	8.28
523.16	0.7992	7.279	7.82
548.16	0.7594	6.894	7.23
573.16	0.7125	6.410	6.44
598.16	0.6540	5.989	6.01
623.16	0.5668	5.349	5.10
635.00	0.5082	4.630	4.37
647.00	0.3220	3.844	3.67

$$\rho = \frac{1 + 0.1342489\,(647. - T)^{1/3} - 3.946263 \times 10^{-3}\,(647. - T)}{3.1975 - 0.3151548\,(647. - T)^{1/3} - 1.203374 \times 10^{-3}\,(647. - T) + 7.48908\,(647. - T)^4}$$

$$T \leq 600.$$

$$(\rho - .3220)^{2.51} = .1226 \times 10^{-2}\,(647. - T) \qquad T > 600.$$

	A	B	C
E_c/E_{CTP}	-1.6823	2.0683	-1.3123
S_c/S_{CTP}	-3.2551	6.5945	-4.8535

TABLE XIIIA - N-OCTANE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(216.38, 398.83, 569.40 °K)		API(1)		Our Work
1.	$S^{L}_{216.38}$	-		67.52
2.	ΔS (216.38 → 298.16 liq)		ΔS^{*}_{TR}	1.14
			ΔS_{ER-I}	11.27
			ΔS^{*}_{c}	6.37
	$S^{L}_{298.16}$	86.25		86.31
3.	$\Delta (S^{o} - S^{SV})$, 298.16	-7.95		(-7.94)
4.	ΔS^{V} (298.16)	33.25		(33.25)
	$S^{o}_{298.16}$	111.55		(111.62)
5.	ΔS^{V} (298.16 → 398.83 liq)	-	ΔS^{*}_{TR}	1.13
			ΔS_{ER-I}	12.86
			ΔS^{*}_{c}	4.64
	$S^{L}_{398.83}$	-		104.95
6.	ΔS^{o} (298.16 → 398.83)	14.01		-
7.	ΔS^{V} (398.83)	-		20.96
8.	$\Delta (S^{o} - S)$, (398.83)	-		0.02
	$S^{o}_{398.83}$	125.56		125.93

TABLE XIIIB

PROPERTIES OF N-OCTANE

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
216.38	0.7642	10.591	21.73
250.00	0.7377	10.109	20.35
298.16	0.6989	9.328	15.36
300.00	0.6974	9.286	15.22
323.16	0.6782	8.849	13.90
348.16	0.6569	8.440	12.66
373.16	0.6349	8.067	11.64
398.16	0.6120	7.711	10.73
398.83	0.6113	7.700	10.72
400.00	0.6102	7.673	10.64
423.16	0.5876	7.289	10.09
448.16	0.5613	6.880	9.17
473.16	0.5318	6.305	7.98
498.16	0.4971	5.913	7.30
500.00	0.4942	5.839	7.16
523.16	0.4576	5.324	6.29
548.16	0.4003	4.487	5.01
569.40	0.2350	2.750	2.73

$$\rho = 0.9446 - 0.7158 \times 10^{-3} T - 10/(608.12 - T), \quad T \leq 503.16$$

$$(\rho - 0.2350)^{2.61} = 0.4288 \times 10^{-3} (569.40 - T), \quad T > 503.16$$

	A	B	C
E_c/E_{CTP}	-1.5208	0.7034	-0.0825
S_c/S_{CTP}	-3.5020	6.1559	-4.1669

TABLE XIVA - METHYL ALCOHOL, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(175.48, 337.8, 512.28°K)		Kelley (20) MCA (10)		Our Work
1.	S (0 → 16.5 °K)	0.26		
2.	ΔS (16.5 → 157.4, cry II)	14.18		
3.	ΔS^T = (154.3/157.4)	0.98		
4.	ΔS (157.4 → 175.22, cry I)	1.24		
5.	ΔS^f = (757.0/175.22)	4.32		
	$S^L_{175.48}$	20.98		21.02
6.	ΔS (175.48 → 298.16. liq)	9.90	/ ΔS^*_{TR}	1.83
			ΔS_{ER-I}	1.39
			ΔS^*_c	6.64
	$S^L_{298.16}$	30.88 ± 0.2		30.88
7.	$(S^o - S^{SV})$, (298.16)	-3.59		(-3.59)
8.	ΔS^V, (298.16)	30.00		(30.00)
	$S^o_{298.16}$	57.29		(57.29)
9.	ΔS (298.16 → 337.8, liq)	-	ΔS^*_{TR}	0.47
			ΔS_{ER-I}	0.67
			ΔS^*_c	1.49
	$S^L_{337.8}$	-		33.52
10.	ΔS^o, (298.16 → 337.8)	1.31		-
11.	ΔS^V, (337.8)	-		24.96
12.	$(S^o - S)$, (337.8)	-		0.12
	$S^o_{337.8}$	58.60		58.60

(20) Kelley, K. K., J. Am. Chem. Soc. 51, 180 (1929).
(10) MCA Tables

TABLE XIVB

PROPERTIES OF METHYL ALCOHOL

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
175.48	0.8939	9.389	20.34
273.16	0.8099	8.823	15.16
298.16	0.7873	8.374	13.70
300.00	0.7856	8.334	13.57
323.16	0.7639	8.014	12.60
337.86	0.7495	7.838	12.21
348.16	0.7392	7.709	11.87
373.16	0.7127	7.343	11.01
398.16	0.6829	7.078	10.39
400.00	0.6805	7.061	10.40
423.16	0.6472	6.690	9.56
448.16	0.6022	6.169	8.52
473.16	0.5423	5.502	7.31
498.16	0.4509	4.591	5.77
500.00	0.4411	4.501	5.64
512.28	0.2720	3.207	3.92

$$\rho = 1.0493 - 0.7827 \times 10^{-3} T - 6/(507.77 - T), \quad T \leq 423.16$$

$$(\rho - 0.2720)^{2.47} = 0.1010 \times 10^{-2} (512.28 - T), \quad T > 423.16$$

	A	B	C
E_c/E_{CTP}	-0.9886	-0.5942	0.9140
S_c/S_{CTP}	-3.0302	4.8328	-3.0584

TABLE XVA - N-DECANE, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(243.51, 447.28, 617.6 °K)		API(1)		Our Work
1.	$S^{L}_{243.51}$	-		88.26
2.	ΔS (243.51→ 298.16 liq)		ΔS^{*}_{TR}	0.71
			ΔS_{ER-I}	9.43
			ΔS^{*}_{c}	4.37
	$S^{L}_{298.16}$	101.66		102.78
3.	$(S^{o} - S^{SV})$, 298.16	-12.66		(-12.19)
4.	ΔS^{V}, (298.16)	41.17		(39.95)
	$S^{o}_{298.16}$	130.17		(130.53)
5.	ΔS (298.16 → 447.28 liq)	-	ΔS^{*}_{TR}	1.57
			ΔS_{ER-I}	24.97
			ΔS^{*}_{c}	6.85
	$S^{L}_{447.28}$			136.16
6.	ΔS^{o} (298.16 → 447.28)	27.56		-
7.	ΔS^{V} (447.28)	-		21.00
8.	$(S^{o} - S)$, (447.28)	-		0.36
	$S^{o}_{447.28}$	157.73		157.52

TABLE XVB

PROPERTIES OF N-DECANE

T	ρ	$-E_c$	$-S_c$
°K	g/ml	k cals/mole	cals/mole °K
243.51	0.7650	12.229	22.54
250.00	0.7602	12.125	21.93
273.16	0.7431	11.741	19.94
298.16	0.7245	11.336	18.17
300.00	0.7231	11.300	18.02
323.16	0.7056	10.906	16.59
348.16	0.6864	10.387	15.09
373.16	0.6669	9.879	13.79
398.16	0.6468	9.458	12.77
400.00	0.6453	9.426	12.68
423.16	0.6259	9.047	11.81
447.28	0.6039	8.688	11.32
448.16	0.6031	8.652	11.25
473.16	0.5793	8.328	10.66
498.16	0.5531	7.740	9.62
500.00	0.5510	7.700	9.48
523.16	0.5234	7.055	8.44
548.16	0.4887	6.615	7.67
573.16	0.4457	5.814	6.53
598.16	0.3844	4.898	5.17
600.00	0.3783	4.809	5.02
617.60	0.2360	3.199	3.03

$$\rho = 0.9491 - 0.6899 \times 10^{-3} T - 6/(615.33 - T) \quad , \quad T \leq 443.16$$

$$(\rho - 0.2360)^{2.39} = 0.5379 \times 10^{-3} (617.60 - T) \quad , \quad T > 443.16$$

	A	B	C
E_c/E_{CTP}	-1.5316	0.6537	0.0146
S_c/S_{CTP}	-3.3240	5.6059	-3.7328

TABLE XVIA - ISOPROPYL ALCOHOL, THIRD LAW ENTROPY & LIQUID PHASE CONFIGURATIONAL VALUES

(185.20, 355.39, 508.32 °K)		Andon, et al(3) Green (15)		Our Work
1.	S (0 → 10 °K)	0.097		
2.	ΔS (10 → 185.20 °K)	21.95		
3.	ΔS^f (1293/185.20)	6.98		
4.	S_L (185.20)	29.03		28.77
5.	ΔS (185.20 → 298.15, liq)	14.12	ΔS^*_{TR}	1.63
			ΔS_{ER-I}	6.21
			ΔS^*_c	6.59
6.	S_L (298.15)	43.15		43.20
7.	$(S^\circ - S^{SV})$, 298.15	-5.64		(-5.67)
8.	ΔS^V	36.52		(36.45)
9.	$S^\circ_{298.16}$	74.03		(73.97)
10.	ΔS (298.15 → 355.39)	7.50	ΔS^*_{TR}	0.67
			ΔS_{ER-I}	2.80
			ΔS^*_c	3.56
11.	S_L (355.39)	50.65		50.22
12.	ΔS° (298.15 → 355.59)	(4.00)		
13.	ΔS^V,(355.39)	26.77		26.81
14.	$(S^\circ - S)$, 355.39	0.61		.61
	$S^\circ_{355.39}$	78.03		77.64

(3) Andon, R.J.L., Counsell, J.F., Martin, J.F., Trans. Faraday Soc. 59, 1555, (1963).
(15) Green, J.H.S., Trans. Faraday Soc., 59, 1559, (1963).

TABLE XVIB

PROPERTIES OF ISOPROPYL ALCOHOL

T	ρ	$-E_c$	$-S_c^*$
°K	g/ml	k cals/mole	cals/mole °K
185.20	0.8693	11.040	25.91
273.16	0.8019	10.740	20.99
298.16	0.7811	10.274	19.32
300.00	0.7795	10.138	18.85
324.56	0.7578	9.551	17.01
339.23	0.7440	9.156	15.84
355.39	0.7279	8.905	15.76
373.16	0.7085	8.494	14.24
398.16	0.6778	7.677	12.24
400.00	0.6754	7.527	11.86
423.16	0.6433	7.065	10.88
448.16	0.6013	6.547	9.86
473.16	0.5456	5.664	8.15
498.16	0.4504	4.232	5.61
500.00	0.4386	4.076	5.34
508.32	0.2730	2.546	3.19

$$\rho = 1.0171 - 0.6472 \times 10^{-3}\, T - 9/(507.39 - T) \quad , \quad T \leq 383.16$$

$$(\rho - 0.2730)^{2.89} = 0.6650 \times 10^{-3}\, (508.32 - T) \quad , \quad T > 383.16$$

	A	B	C
E_c/E_{CTP}	-1.3253	-0.9604	1.7289
S_c/S_{CTP}	-3.2643	4.4834	-2.3601

FIGURE 2

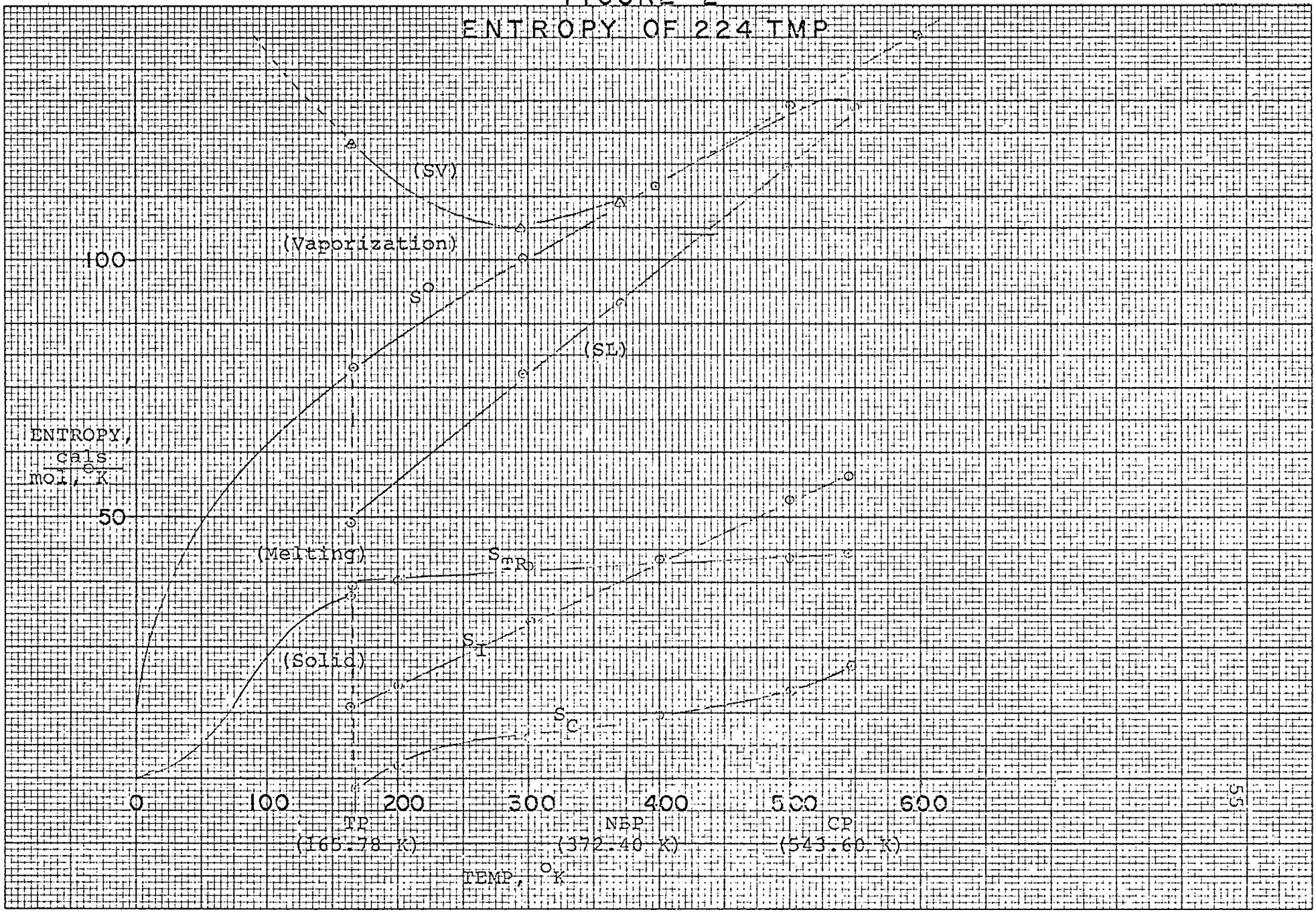

ENTROPY OF 224 TMP
(SV)
(Vaporization)
100
S°
(SL)
ENTROPY, cals/mol, °K
50
(Melting)
S_{TR}
S_I
(Solid)
S_C
0
100
200
300
400
500
600
TP
(165.78 K)
NBP
(372.40 K)
CP
(543.60 K)
TEMP, °K

FIGURE 3

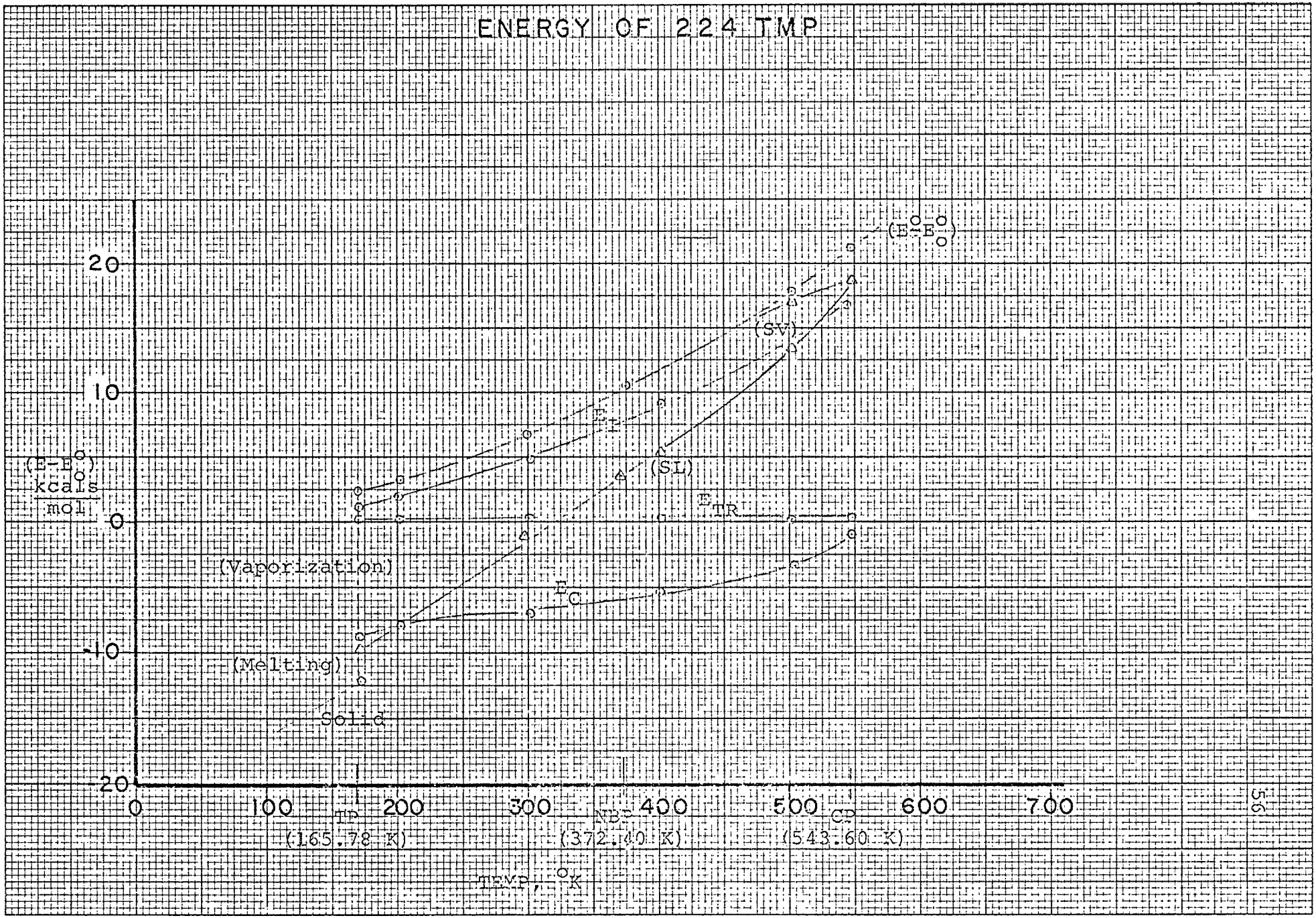

ENERGY OF 224 TMP
$(E-E_o^o)$
$(E-E_o^o)$ kcals/mol
20
10
0
-10
-20
(SV)
(SL)
E_{TR}
E_C
(Vaporization)
(Melting)
Solid
0
100
200
300
400
500
600
700
T_m
(165.78 K)
T_B
(372.40 K)
T_{CP}
(543.60 K)
TEMP, °K
56

FIGURE 4

RELATIONSHIP OF CONFIGURATIONAL ENERGY AND LIQUID DENSITY FOR SATURATED PARAFFINS

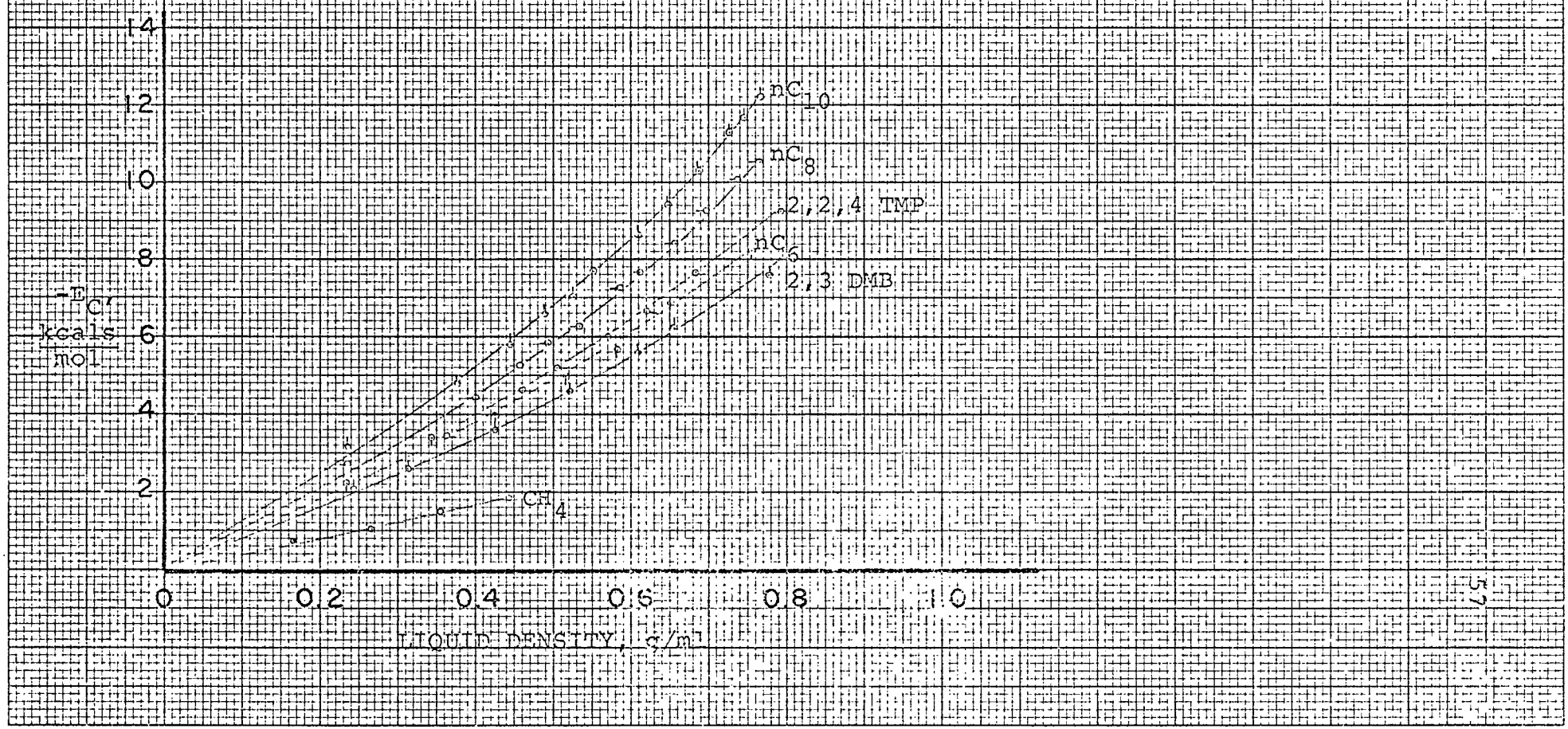


FIGURE 5

RELATIONSHIP OF CONFIGURATIONAL ENERGY AND LIQUID DENSITY FOR MISCELLANEOUS SUBSTANCES

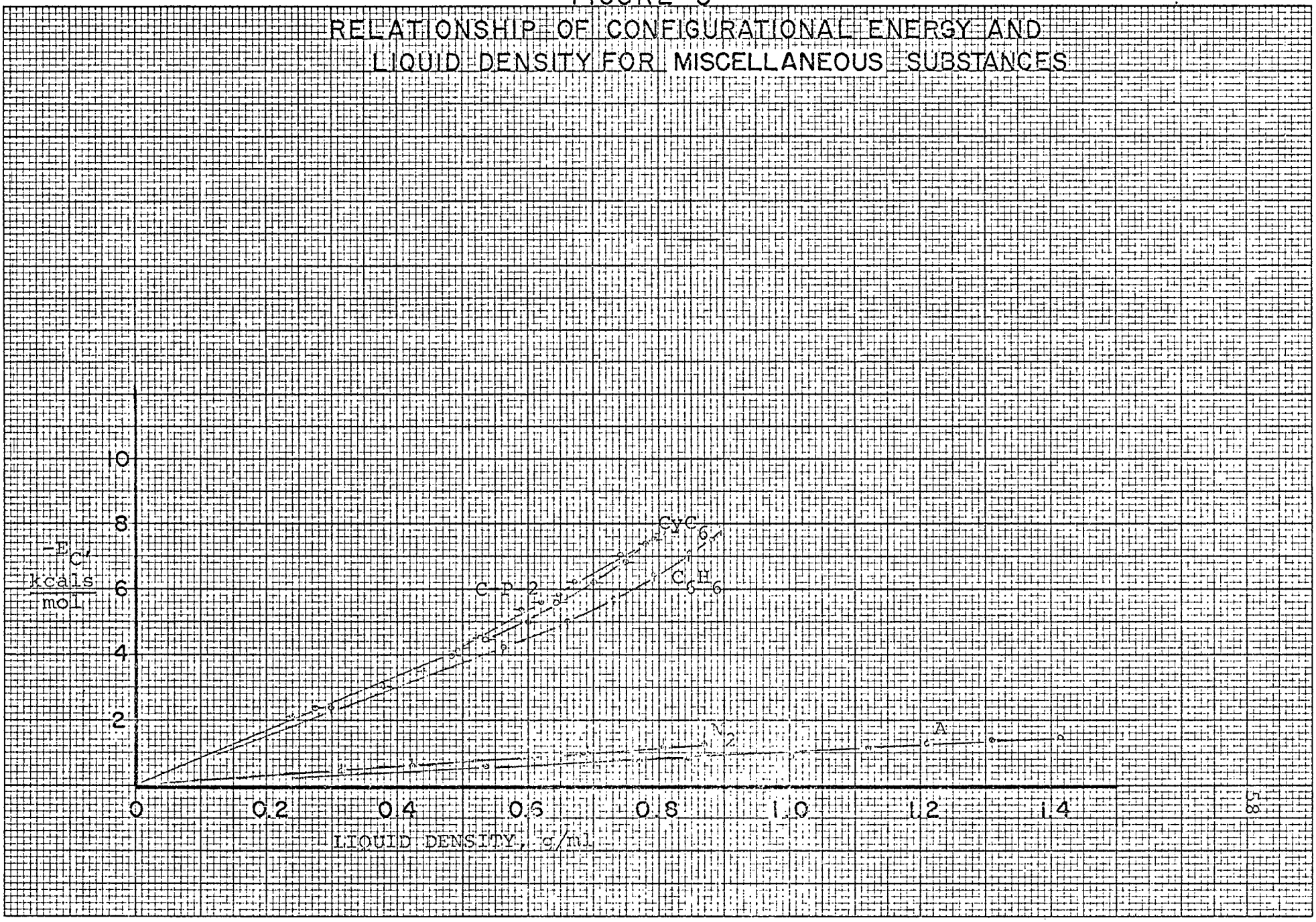


FIGURE 6

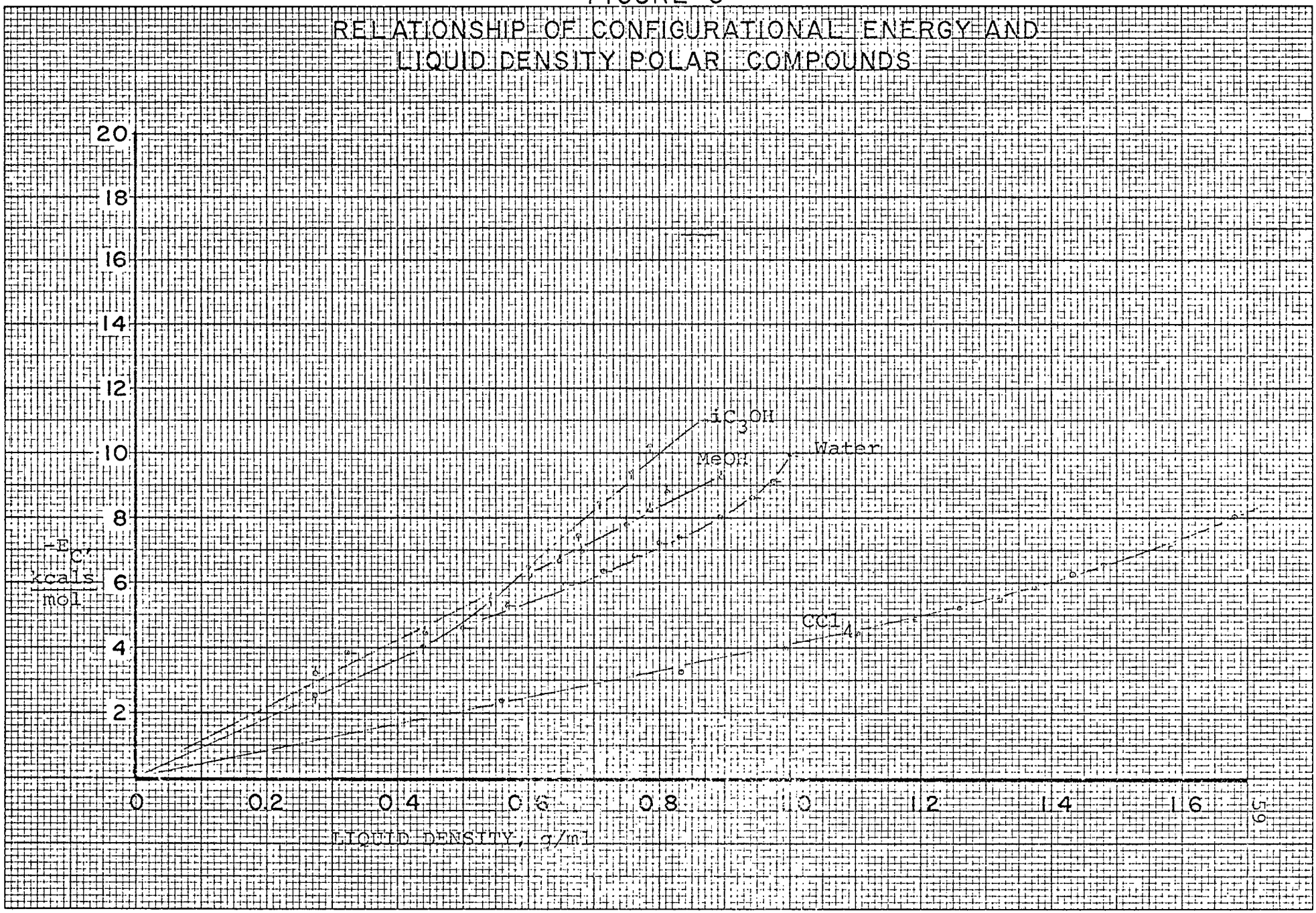

RELATIONSHIP OF CONFIGURATIONAL ENERGY AND LIQUID DENSITY POLAR COMPOUNDS
20
18
16
14
12
10
8
6
4
2
0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
-E'c kcals/mol
LIQUID DENSITY, g/ml
iC3OH
MeOH
Water
CCl4

FIGURE 7

RELATIONSHIP OF CONFIGURATIONAL ENTROPY AND LIQUID DENSITY FOR SATURATED PARAFFINS

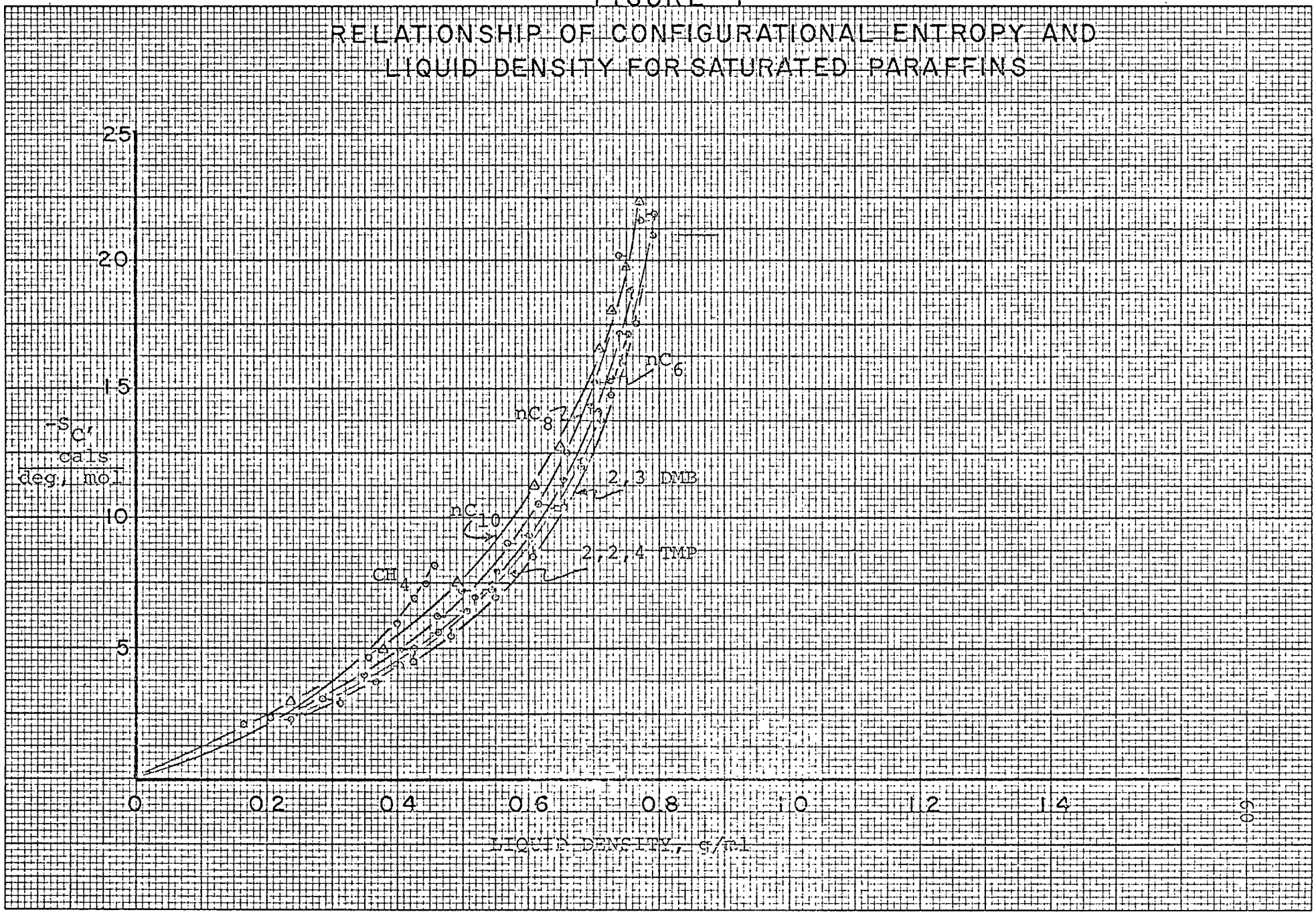


FIGURE 8

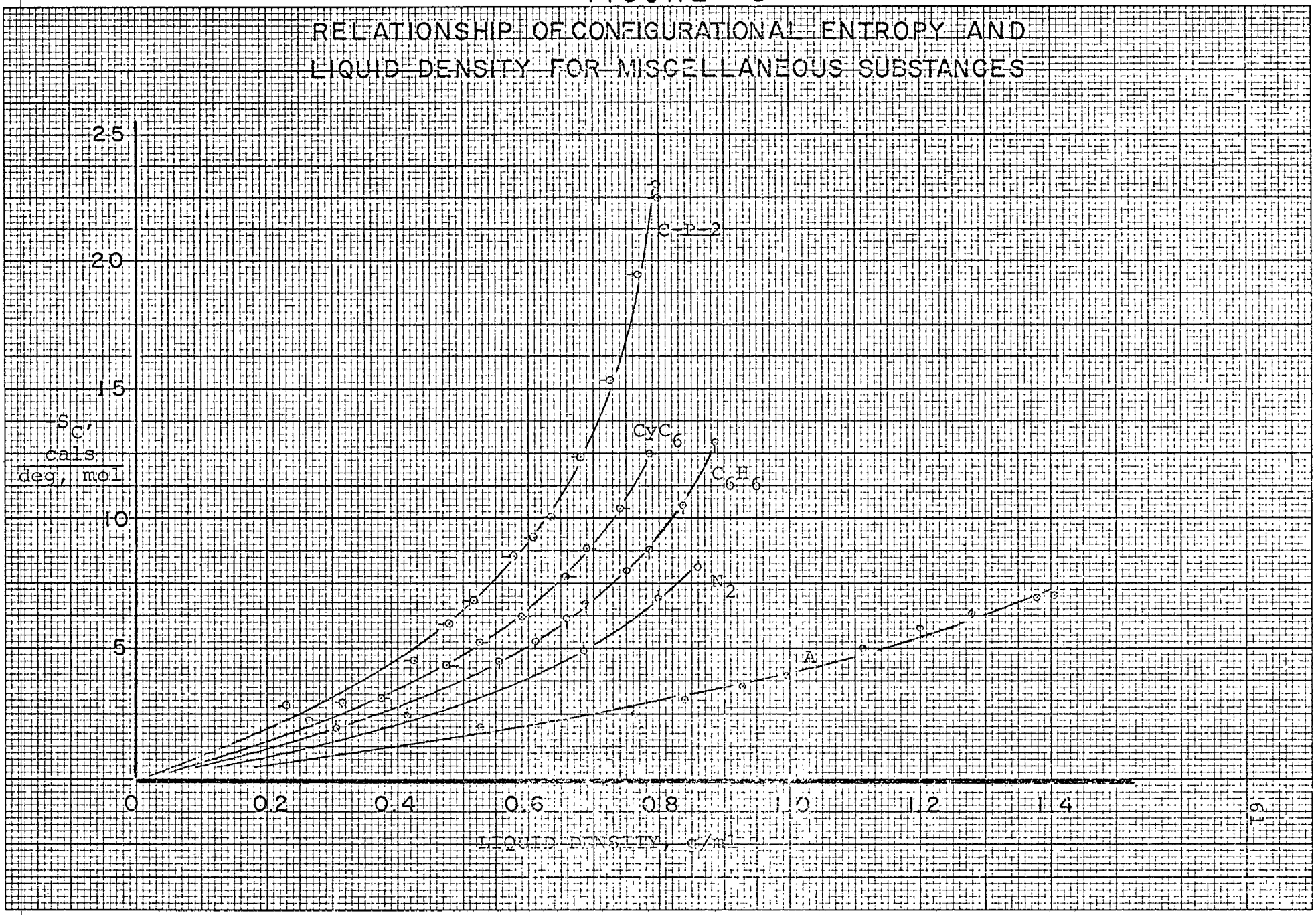
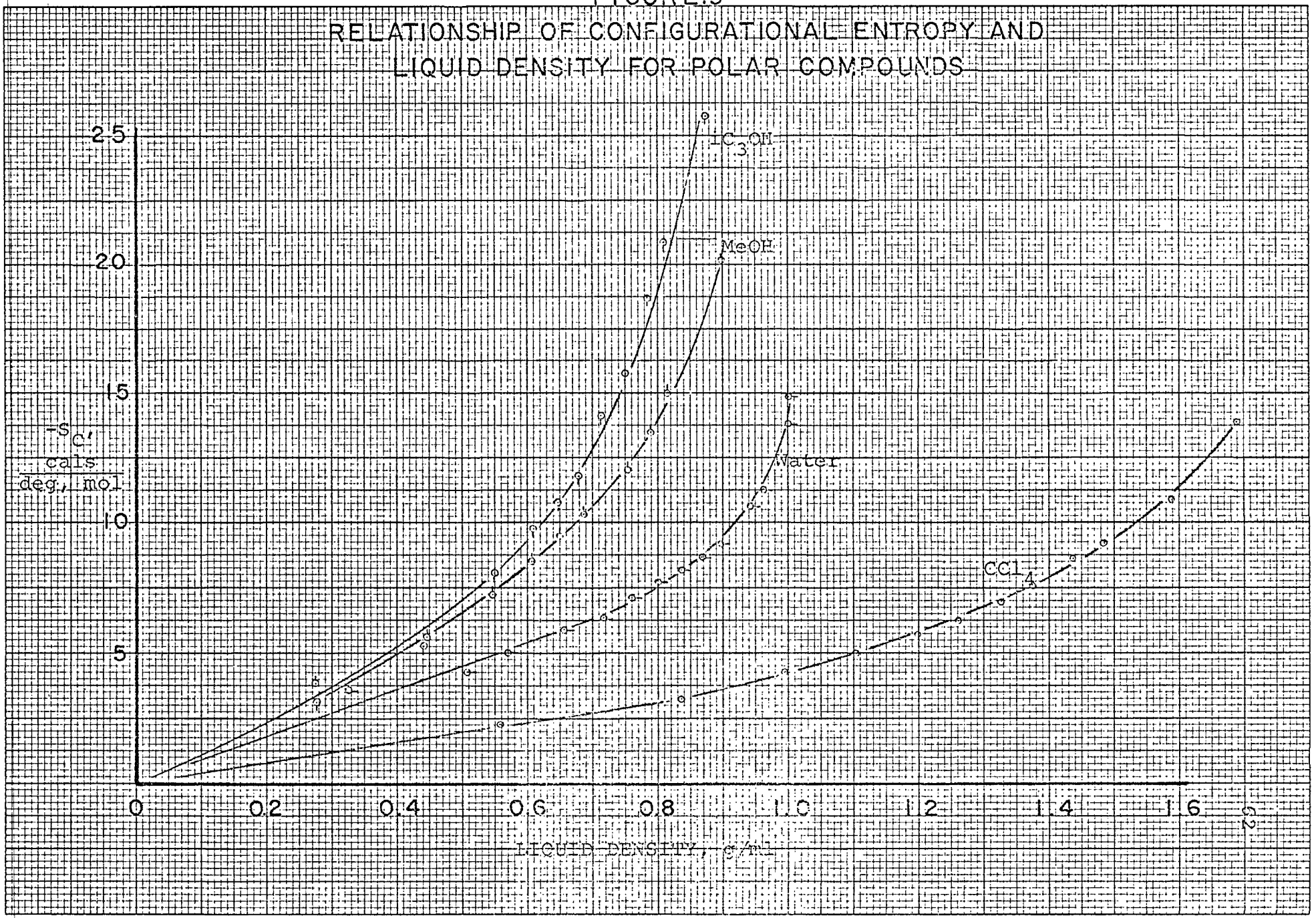

RELATIONSHIP OF CONFIGURATIONAL ENTROPY AND LIQUID DENSITY FOR MISCELLANEOUS SUBSTANCES
25
20
15
10
5
0
-S_C' cals/deg. mol
0.2
0.4
0.6
0.8
1.0
1.2
1.4
LIQUID DENSITY, g/ml
C-P-2
CyC6
C6H6
N2
A

FIGURE 9

RELATIONSHIP OF CONFIGURATIONAL ENTROPY AND LIQUID DENSITY FOR POLAR COMPOUNDS



CHAPTER V

CORRELATION OF CONFIGURATIONAL PROPERTIES

A. Configuration Energy

Figures 4, 5, and 6 show the relationship between the configurational energy and the liquid density for all the substances studied. The saturated paraffins studied are shown in Figure 4; the plot indicates that E_c is related directly to molecular weight and inversely to the amount of branching of the molecule.

The relationship between E_c and ρ for all the substances studied vary from the low slope straight line of argon to the steeper curve of n-decane. Note that the triple point values of $-E_c$ increase with molecular weight (molecular size) and decreases with branching (symmetry). Also note that $-E_c$ is larger for polar molecules than for nonpolar molecules of the same molecular weight.

$$-E_{CTP} \text{ (benzene)} = 7.845 \text{ (MW = 70.11)}$$

$$-E_{CTP} \text{ (isopropyl alcohol)} = 11.04 \text{ (MW = 60.097)}$$

B. Configurational Entropy Correlation

Figures 7, 8, and 9 show the relationship between the configurational entropy and the liquid density. The curves for the saturated paraffins studied, shown on Figure 7, indicates that $-S_c$ also increases with increasing molecular weight and decreases with branching of the molecule. However, the position of the curve for methane is not understood at this time.

C. Application of the Correlations

Correlation of the configurational properties E_c and S_c^* for a wide variety of substances will have several important applications.

1. Pure Component Liquids -

It has been suggested (31) that once the correlation of the configurational properties has been accomplished by an appropriate molecular model, then the calculation of the energy and entropy, E_L and S_L, of single component liquids, over the entire range from the triple point to the critical point, by a "sum of molecular contributions" method will be possible. That is, having the temperatures and densities of the triple, normal boiling and critical points, the calculations could be made at any temperature and density by,

$$E_L(T, \rho) = E^o_{TR}(T) + E^o_{ER}(T) + E^o_I(T) + E_c(\rho)$$
$$= E^o(T) + E_c(\rho) \qquad (V\text{-}1)$$

$$S_L(T, \rho) = S^o_{TR} - R \ln\left(\frac{\rho_L RT}{p^o}\right) + S^o_{ER} + S^o_I + S_c(\rho)$$
$$= S^o - R \ln\left(\frac{\rho_L RT}{p^o}\right) + S^*_c(\rho) \qquad (V\text{-}2)$$

The above approach is in contrast to the "Classical Thermodynamic" method,

$$E_L(T, \rho) = E^o(T) - E\Big|_o^{sv} - \Delta E^v + \int_{\rho_{SL}}^{\rho} \left(\frac{\partial E}{\partial \rho}\right)_T d\rho \qquad (V\text{-}3)$$

$$S_L(T, \rho) = S^o(T) - S\Big|_o^{sv} - \Delta S^v + \int_{\rho_{SL}}^{\rho} \left(\frac{\partial S}{\partial \rho}\right)_T d\rho \qquad (V\text{-}4)$$

which require a much greater knowledge of the liquid PVT relationships (integrals) in order to make the calculations.

(31) Prengle, H. W. Jr., private communication (Nov. 1970).

2. Liquid Solutions -

Once the molecular parameters have been deduced (interaction energies, coordination numbers, etc.) from the E_c and S_c^* values they can be used as a starting point in an appropriate model to predict the excess thermodynamic properties, including the activity coefficients, and hence the phase equilibria for the solutions.

CHAPTER VI

FUTURE WORK

It is obvious from the Figures in Chapter V that a correlation exists for the configurational properties of substances; further work along these lines is necessary to better define this relationship.

The first step in defining a general correlation would be to expand the study to include more substances with varying types of molecular structure. It is desirable to have a wide range of acentric factors and varying degrees of branching represented among the substances studied.

With a wider range of substances represented on plots similar to Figures 4 - 9 a series of empirical equations could be derived. These equations would most likely be a polynomial type equation with several constants. It is likely that some relationship will exist between these constants and the acentric factor or molecular structure of the substance.

A further extension of this work would be to investigate the relationship between the configurational energy and the liquid heat capacity. At present all methods of calculating liquid heat capacities are empirical. A theoretical method of calculating liquid heat capacities from configurational energies would be a very practical extension of the work done in this study.

BIBLIOGRAPHY

1. American Petroleum Institute Research Project 44, "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds," Carnegie Press, Pittsburgh, Pa., (1953).

2. Ahlberg, J. E., Blanchard, E. R., Lundberg, W. O., J. Am. Chem. Soc., 5, 539, (1937).

3. Andon, R.J. C., Counsell, J.F., Martin, J.F., Trans. Faraday Soc. 59, 1555, (1963).

4. Aston, J.G., Fritz, J.J., "Thermodynamics and Statistical Thermodynamics," John Wiley and Sons, Inc., New York, N.Y. , (1959).

5. Beckett, C. W., Pitzer, K., S., Spitzer, R., J. Am. Chem. Soc., 69, 2488, (1947).

6. Chow, W. M., Bright, J.N., Jr., CEP, 49, No. 4, 175, (1953).

7. Clusius, K., Frank, A., Ztschr. Electrochem, 49, 308, (1943).

8. Cook, G. A., "Argon, Helium, and the Rare Gases," Interscience Publishers, New York, N.Y., (1961).

9. Davies, D. B., Matheson, A.J., Disc. of Faraday Soc., No. 43, 216, (1967).

10. Douslin, D. R., Huffman, H. M., J. Am. Chem. Soc., 68, 1704, (1946).

11. Francis, A. W., I & EC, 49, No. 10, 1779, (1957).

12. Gambill, W. R., Chem. Engr., 64, 263, (1957).

13. Giaugue, W.F., Clayton, J.O., J. Am . Chem. Soc., 55, 4875, (1933).

14. Giaugue, W. F., Stout, J.W., J. Am. Chem. Soc., 58, 1144, (1936).

15. Green, J.H.S., Trans. Faraday Soc., 59, 1559, (1963).

16. Hicks, J.F.G., Hooley, J.G., Stephenson, C.C., J. Am. Chem. Soc., 66, 1064, (1944).

17. Hildebrand, J. H., Scott, R. L. "The Solubility of Nonelectrolytes," Third Edition, Dover Publications, Inc., New York, N.Y., (1964).

18. International Research Council and the National Academy of Sciences, "International Critical Tables of Numerical Data, Physics, Chemistry, and Technology," Vol. III, McGraw-Hill, New York, N.Y., (1928).

19. Johnson, A. I., Huang, Chen-Jung, Canadian Journal of Technology, 33, 421, (1955).

20. Kelley, K. K., J. Am. Chem. Soc., 51, 180, (1929).

21. Kelley, K. K., Bureau of Mines Bulletin No. 350, (1932).

22. Manufacturing Chemists Association Research Project, "Selected Values of Properties of Chemical Compounds," Department of Chemistry, Texas A&M University, College Station, Texas, (1968).

23. Michels, A., Levelt, J.M., DeGraaff, W., "Physics," 24, 669, (1958).

24. Perry, R.H., Chilton, C.H., Kirkpatrick, S.P., "Chemical Engineers' Handbook," Fourth Edition, McGraw-Hill, New York, N.Y., (1963).

25. Pitzer, K.S., J. Chem. Phys., 5, 473, (1937).

26. Pitzer, K. S., Chem. Review, 27, 39, (1940).

27. Pitzer, K. S., J. Am. Chem. Soc., 62, 1224, (1940).

28. Pitzer, K. S., I & EC, 36, No. 9, 829, (1944).

29. Pitzer, K.S., "Quantum Chemistry," Prentice-Hall, Inc., (1953).

30. Prengle, H. W., Jr., Mauk, C.E., Technical Note. "Partition Function and Configurational Energy for Liquids," Chemical Engineering Department, University of Houston, May, 1963.

31. Prengle, H.W., Jr., private communication, (Nov. 1970).

32. Reid, R. C., Sherwood, T.K., "The Properties of Gases and Liquids," Second Edition, McGraw-Hill, New York, N.Y., (1966).

33. Ruehrivien, R. A., Huffman, H.M., J. Am. Chem. Soc., 65, 1620, (1943).

34. Sakiadis, B.C., Coates, J., AICHE Journ., 2, No. 1, 88, (1956).

35. Smith, L.B., Keyes, F.G., Proc. Am. Acad. Arts and Sci., 69, 285, (1934).

36. Todd, S.,S., Oliver, G.D., Huffman, H.M., J. Am. Chem. Soc., 69, 1519, (1947).

37. Tseng, T.T., Prengle, H.W., Jr., Computer Program: "Saturated Liquid Densities and Mole Volumes by Francis Equations."

38. Tseng, T. T., Prengle, H.W., Jr., Computer Program: "Evaluation of Gamson-Watson Constants from Experimental Vapor Pressure or Bubble Point Data."

APPENDIX A

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL METHODS INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

LIST OF EQUATIONS

Translation

1. $H^{o} - H_{o}^{o} = 2.5RT$
2. $Cp^{o} = 2.5R$
3. $F^{o} - H_{o}^{o} = T(-2.9841\ \ln M + 7.28295 - 4.9735\ \ln T)$
4. $S^{o} = 2.9841\ \ln M - 2.31498 + 4.9735\ \ln T$

External Rotation

For linear molecules (AI = BI, CI = 0)

5. $H^{o} - H_{o}^{o} = RT$
6. $Cp^{o} = R$
7. for $\sigma = 1$ $F^{o} - H_{o}^{o} = T\left[-1.9894(\ln AI \times 10^{39}) + 4.14506 - 1.9894\ \ln T\right]$
8. $S^{o} = 1.9894\ \ln(AI \times 10^{39}) - 2.15787 + 1.9894\ \ln T$
9. for $\sigma > 1$ $F^{o} - H_{o}^{o} = T\left[-1.9894\ \ln(AI \times 10^{39}) + 2.76764 - 1.9894\ \ln T\right]$
10. $S^{o} = 1.9894\ \ln(AI \times 10^{39}) - 0.78045 + 1.9894\ \ln T$

For non-linear molecules

11. $H^{o} - H_{o}^{o} = 1.5RT$
12. $Cp^{o} = 1.5R$
13. $F^{o} - H_{o}^{o} = T\left[-0.9947(\ln(AI \times 10^{39}) + \ln(BI \times 10^{39}) + \ln(CI \times 10^{39})) + 1.9894\ \ln\sigma + 3.01407 - 2.9841\ \ln T\right]$

14. $S^{o} = 0.9947(\ln(AI \times 10^{39}) + \ln(BI \times 10^{39}) + \ln(CI \times 10^{39}))$
$- 1.9894 \ln\sigma - 0.03329 + 2.9841 \ln T$

Internal Rotation

15. (free rotation) $F^{o} - H_{o}^{o} = -RT(0.5 \ln T) + 0.5 \ln(I_{red} \times 10^{40})$
$- \ln n - 1.275$

16. (free rotation) $S^{o} = R(0.5 \ln T + 0.5 \ln(I_{red} \times 10^{40})$
$- \ln n - 0.775$

17. $Q_f = 2.7935(10^{38} I_{red} T)^{\frac{1}{2}}/n$

Pitzers Corrections* to Internal Rotation:

The following tables are read in as data in a form to correspond to the appropriate values of V/RT and $1/Q_f$ ($Q_f \equiv$ partition function for free rotation calculated by equation 17).

Heat Capacity, C

Heat Content, H/T

Entropy , S

Entropy Decrease from Free Rotation, $S_f - S$

Free Energy, -F/T

Free Energy Increase from Free Rotation, $F - F_f/T$

Values for V/RT and $1/Q_f$ are read in as data from the tables also.

V_o/RT and $1/Q_f$ are calculated and compared to the table values until V_o/RT and $1/Q_f$ are less than the table values. The program then chooses the largest values for V/RT and $1/Q_f$

*See Pitzer, K. S., Quantum Chemistry, Prentice Hall, N. Y. (1953).

from the table that are smaller than the calculated values. The appropriate numbers for C and H/T are then picked by the program.

If $1/Q_f$ is less than 0.25 the free rotation values for S and -F/T are calculated. The correction factors are picked from the tables for $(A_f - S)$ and $(F - F_f/T)$.

If $1/Q_f$ is 0.25 or greater the program moves to the left five columns and picks the corresponding values for S and -F/T.

Vibrational

18. $Y = 1.4387\tilde{\nu}/T$

19. $S^o = \frac{RY}{e^Y - 1.0} - R\ln(1.0 - e^{-Y})$

20. $H^o - H_o^o = \frac{RTY}{e^Y - 1.0}$

21. $Cp^o = \frac{RY^2 e^Y}{(e^Y - 1.0)^2}$

22. $F^o - H_o^o = (H^o - H_o^o) - S^o T$

Input Variables Definition:

MW = Molecular Weight

K = No. of Temperatures read in

T = Temperatures

AI,BI,CI = External Moments of Inertia

SIG = No. of Equivalent Positions, σ

Z = No. of Rotating Groups

VO = Potential Barriers

REDI = Reduced Internal Moments of Inertia, I_{red}

NEQPO = No. of Min , n (Integer)

SIGNU = Also No. of Minima, n (Real)

J = No. of Different Vibrational Frequencies

FNU = Frequencies, ν

G = Degeneracy of the Frequencies

Note: Input Variables: C, H, S, F, SOF, FOF, VCOL, & QROW are from Pitzers tables for restricted internal rotation and are the same for all substances. Handle this data as if it were part of the body of the program.

APPENDIX B

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION -- LIST OF EQUATIONS

Francis Equation

1. $P = A - (B \times T) - (C / (E - T))$ $\quad T < Tmin$

2. $PS = G\ (TC - T)$

3. $LNPS = Ln\ (PS)/HF$

4. $P = EXP\ (LNPS) + P_c$ $\quad T > Tmin$

Antoine Equation

5. $Log\ P = A - B / C - 273.16 + T$

6. $DLNP = 2.30259\ B / (C - 273.16 + T)^2$

Gamson - Watson Equation

7. $Log\ P = (- GWA \times TC/T) + GWB - EXP\ -20(T/TC - b)^2$

8. $DLNP = 2.30259\ GWA \times TC/(T)^2 + (40\ (T/TC) - b) \times EXP\ -20\ (T/TC - b)^2$

Liquid and Gas Volumes

9. $V_L = MW / (\rho \times 1000)$

10. $VG = Z \times R \times T / P$

11. $V_L\ (c) = V_G\ (c)$

Vaporization

12. $\Delta E^V = P\,(VG - VL)\left[(T \times DLNP) - 1.0\right]$

13. $\Delta H^V = \Delta E^V + P\,(VG - VL)$

14. $\Delta S^V = \Delta H^V / T$

Configurational

15. $E_{ER} = 1.5\ R \times T$

16. $E_C = -\ \Delta E\Big|_o^{SV} - \Delta E^V$

17. $S_c^* = -\ \Delta S\Big|_o^{SV} - \Delta S^V + R \ln \frac{RT/P^o}{V_L}$

18. $E_L = E^o - \Delta E\Big|_o^{SV} - \Delta E^V$

19. $S_L = S^o - \Delta S\Big|_o^{SV} - \Delta S^V$

Input Variables Definitions

K = No. of temperatures read in

XMW = Molecular weight

OMEGA = Acentric factor,

T_C = Critical temperature

T = Temperatures

VDELE = $E^o - E^{SV}$

EPG = $E^o - E^o_o$

SPG = S^o

Z = Compressibility factors

VDELS = $S^o - S^{SV}$

A, B, C = Antoine Constants

GWA, GWB = Gamson - Watson Constants, A and B

GWBL = Gamson - Watson Constant, b

SER = Entropy of external rotation

AF, BF, CF, EF, GF, HF = Francis Constants

RHOC = ρ(critical)

TMIN = Tmin for Francis Equations

APPENDIX C-1

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: ARGON MOLECULAR WEIGHT: 39.9480 OMEGA: -0.0020

TRIPLE POINT: 83.96 K N-BOILING POINT: 87.46 K

CRITICAL POINT: 150.86 K 48.34 ATM 0.0740 L/GMOLE ZC 0.2900

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.61651 B= 304.22681 C= 267.31982 NC= 268.00635
GAMSON-WATSON: A= 2.3199 BL= 0.0 B= 6.8794

FRANCIS CONSTANTS: A= 1.9309 B= 0.4768E-02 C= 10.00 E= 167.83
G= 0.1144E-01 H= 2.39

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
83.96	3.00	250.30	30.72	0.9820	-0.73	30.72
87.46	6.00	260.70	30.93	0.9810	0.16	30.93
90.00	9.00	268.30	31.07	0.9800	0.70	31.07
100.00	24.00	298.10	31.59	0.9620	2.46	31.59
103.16	36.00	307.50	31.75	0.9510	3.08	31.75
113.16	54.00	337.30	32.21	0.9050	4.63	32.21
123.16	102.00	367.10	32.63	0.8340	6.08	32.63
133.16	167.00	396.90	33.02	0.7070	7.61	33.02
138.16	209.00	411.80	33.20	0.6500	8.37	33.20
143.16	275.00	426.70	33.38	0.5720	9.24	33.38
148.16	383.00	441.60	33.55	0.4600	10.43	33.55
150.86	603.00	449.70	33.64	0.2900	12.32	33.64

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
83.96	0.6940E 00	0.1148	0.02830	0.9749E 01	163.323	1411.	1574.	18.75
87.46	0.1019E 01	0.1052	0.02875	0.6907E 01	169.743	1391.	1561.	17.85
90.00	0.1321E 01	0.0989	0.02909	0.5480E 01	174.294	1377.	1551.	17.24
100.00	0.3152E 01	0.0806	0.03057	0.2504E 01	188.785	1334.	1523.	15.23
103.16	0.4035E 01	0.0758	0.03110	0.1995E 01	191.864	1308.	1500.	14.54
113.16	0.8049E 01	0.0629	0.03306	0.1044E 01	197.012	1206.	1403.	12.40
123.16	0.1435E 02	0.0541	0.03567	0.5573E 00	191.667	1062.	1254.	10.18
133.16	0.2346E 02	0.0454	0.03965	0.3293E 00	164.517	831.	996.	7.48
138.16	0.2920E 02	0.0422	0.04272	0.2524E 00	148.209	716.	864.	6.26
143.16	0.3580E 02	0.0393	0.04739	0.1877E 00	121.610	563.	685.	4.78
148.16	0.4329E 02	0.0367	0.05195	0.1292E 00	80.956	359.	440.	2.97
150.86	0.4772E 02	0.0354	0.07459	0.7459E-01	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
83.96	1.4113	-1163.39	-1413.69	12.70	19.80	-7.10	-8.47	-3.57
87.46	1.3895	-1136.63	-1397.33	12.92	19.96	-7.04	-8.04	-3.54
90.00	1.3733	-1117.82	-1386.12	13.13	20.07	-6.94	-7.75	-3.49
100.00	1.3067	-1059.62	-1357.72	13.91	20.48	-6.57	-6.83	-3.31
103.16	1.2844	-1036.15	-1343.65	14.13	20.61	-6.47	-6.55	-3.26
113.16	1.2084	-922.83	-1260.13	15.18	21.00	-5.83	-5.60	-2.93
123.16	1.1198	-797.37	-1164.47	16.37	21.41	-5.04	-4.76	-2.54
133.16	1.0076	-601.21	-998.11	17.93	21.85	-3.92	-3.77	-1.97
138.16	0.9351	-513.47	-926.27	18.57	22.11	-3.54	-3.37	-1.78
143.16	0.8430	-411.24	-837.94	19.36	22.42	-3.07	-2.95	-1.54
148.16	0.7690	-300.77	-742.37	20.15	22.71	-2.56	-2.52	-1.29
150.86	0.5356	-153.30	-603.00	21.32	23.48	-2.16	-2.01	-1.09

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: ARGON MW: 39,9480 TTP: 83.96K TNBP: 87.46K TTC: 150.86K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .0000+000 .0000+000 .0000+000 SYM NO: .00

INT ROT MOM: (1): .0000+000

INT ROT POT: (1): .00

VIB FREQ: (1): .00

FREQ DEGEN: 0

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
83.96	.15271+02	.4968+01	.41711+03	.30723+02	-.21624+04	166.84	.2503+03
87.46	.15373+02	.4968+01	.43450+03	.30927+02	-.22703+04	173.80	.2607+03
90.00	.15445+02	.4968+01	.44712+03	.31069+02	-.23491+04	178.85	.2683+03
100.00	.15706+02	.4968+01	.49690+03	.31593+02	-.26625+04	198.72	.2981+03
103.16	.15786+02	.4968+01	.51250+03	.31746+02	-.27626+04	205.00	.3075+03
113.16	.16017+02	.4968+01	.56218+03	.32206+02	-.30825+04	224.87	.3373+03
123.16	.16229+02	.4968+01	.61186+03	.32629+02	-.34067+04	244.74	.3671+03
133.16	.16424+02	.4968+01	.66154+03	.33017+02	-.37350+04	264.61	.3969+03
138.16	.16516+02	.4968+01	.68638+03	.33201+02	-.39006+04	274.55	.4118+03
143.16	.16605+02	.4968+01	.71122+03	.33377+02	-.40671+04	284.49	.4267+03
146.16	.16691+02	.4968+01	.73606+03	.33548+02	-.42344+04	294.42	.4416+03
150.86	.16736+02	.4968+01	.74947+03	.33638+02	-.43252+04	299.79	.4497+03
273.16	.18921+02	.4968+01	.13571+04	.36591+02	-.86381+04	542.82	.8142+03
298.16	.18439+02	.4968+01	.14813+04	.37026+02	-.95565+04	592.50	.8888+03

APPENDIX C-2

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: METHANE MOLECULAR WEIGHT: 16.0400 OMEGA: 0.0130

TRIPLE POINT: 90.68 K N-BOILING POINT: 111.70 K

CRITICAL POINT: 190.70 K 45.80 ATM 0.0995 L/GMOLE ZC 0.2900

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.61184 B= 389.92993 C= 266.00000 NC= 266.28369
GAMSON-WATSON: A= 2.3383 BL= 0.0477 B= 6.8787

FRANCIS CONSTANTS: A= 0.5925 B= 0.8749E-03 C= 9.00 E= 239.84
G= 0.2859E-03 H= 2.72

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
90.68	0.0	540.60	34.92	1.0000	-4.29	28.38
93.16	0.0	555.40	35.13	0.9990	-3.67	28.52
100.00	7.00	596.20	35.70	0.9900	-2.15	28.87
103.16	8.00	615.00	35.94	0.9850	-1.51	29.02
110.00	11.00	655.80	36.45	0.9680	-0.28	29.34
111.70	13.00	665.90	36.58	0.9640	0.22	29.42
113.16	15.00	674.60	36.68	0.9600	0.74	29.49
120.00	22.00	715.40	37.15	0.9450	1.63	29.78
123.16	26.00	734.20	37.35	0.9300	2.23	29.91
130.00	53.00	775.00	37.78	0.9050	3.10	30.18
133.16	57.00	793.90	37.99	0.8940	3.50	30.29
140.00	60.00	834.70	38.37	0.8690	4.25	30.54
143.16	72.00	853.60	38.55	0.8570	4.61	30.65
150.00	90.00	894.40	38.92	0.8240	5.39	30.89
153.16	109.00	913.30	39.09	0.8040	5.78	30.99
160.00	147.00	954.20	39.44	0.7580	6.52	31.21
163.16	174.00	973.10	39.59	0.7460	6.96	31.31
170.00	227.00	1014.00	39.92	0.6880	7.75	31.51
173.16	257.00	1033.00	40.07	0.6590	8.13	31.60
180.00	341.00	1074.00	40.38	0.5780	9.08	31.88
183.16	386.00	1093.00	40.52	0.5360	9.54	32.08
190.00	704.00	1134.00	40.81	0.3240	11.84	33.87
190.70	762.00	1139.00	40.84	0.2900	12.22	34.30

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
90.68	0.1154E 00	0.1287	0.03542	0.6446E 02	180.052	1921.	2102.	23.17
93.16	0.1574E 00	0.1214	0.03567	0.4852E 02	184.757	1905.	2089.	22.43
100.00	0.3396E 00	0.1042	0.03640	0.2392E 02	196.381	1849.	2046.	20.46
103.16	0.4669E 00	0.0974	0.03676	0.1786E 02	201.455	1823.	2025.	19.63
110.00	0.8698E 00	0.0849	0.03757	0.1005E 02	210.750	1757.	1968.	17.89.
111.70	0.1002E 01	0.0822	0.03778	0.8814E 01	213.005	1742.	1955.	17.50
113.16	0.1128E 01	0.0799	0.03797	0.7900E 01	214.782	1727.	1942.	17.16
120.00	0.1886E 01	0.0705	0.03889	0.4935E 01	223.513	1648.	1891.	15.76.
123.16	0.2379E 01	0.0679	0.03935	0.3950E 01	225.284	1659.	1884.	15.30
130.00	0.3603E 01	0.0609	0.04042	0.2614E 01	230.118	1590.	1820.	14.00
133.16	0.4456E 01	0.0580	0.04096	0.2102E 01	232.085	1560.	1792.	13.45
140.00	0.6496E 01	0.0524	0.04222	0.1537E 01	235.057	1490.	1725.	12.32
143.16	0.7638E 01	0.0501	0.04287	0.1318E 01	235.813	1456.	1692.	11.82
150.00	0.1059E 02	0.0456	0.04442	0.9574E 00	234.159	1369.	1603.	10.69
153.16	0.1220E 02	0.0438	0.04523	0.8282E 00	231.281	1319.	1551.	10.12
160.00	0.1625E 02	0.0401	0.04721	0.6205E 00	225.550	1222.	1447.	9.05
163.16	0.1840E 02	0.0386	0.04826	0.5428E 00	220.313	1166.	1386.	8.50
170.00	0.2370E 02	0.0355	0.05113	0.4049E 00	203.017	1023.	1226.	7.21
173.16	0.2647E 02	0.0342	0.05264	0.3538E 00	192.977	951.	1144.	6.61
180.00	0.3315E 02	0.0317	0.05708	0.2575E 00	160.877	757.	918.	5.10
183.16	0.3658E 02	0.0306	0.06016	0.2202E 00	141.760	653.	795.	4.34
190.00	0.4476E 02	0.0284	0.07799	0.1128E 00	37.780	166.	204.	1.07
190.70	0.4566E 02	0.0282	0.09901	0.9901E-01	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
90.68	0.4528	-1380.86	-1921.46	16.03	17.76	-8.26	-10.66	-4.16
93.16	0.4496	-1349.31	-1904.71	16.38	17.85	-8.09	-10.29	-4.07
100.00	0.4407	-1260.07	-1856.27	17.39	18.10	-7.54	-9.34	-3.80
103.16	0.4364	-1216.19	-1831.19	17.83	18.22	-7.30	-8.93	-3.68
110.00	0.4269	-1112.51	-1768.31	18.84	18.45	-6.72	-8.09	-3.38
111.70	0.4245	-1088.80	-1754.70	18.86	18.51	-6.81	-7.91	-3.43
113.16	0.4225	-1067.76	-1742.36	18.78	18.56	-6.97	-7.75	-3.51
120.00	0.4124	-974.39	-1689.79	19.76	18.78	-6.39	-7.09	-3.22
123.16	0.4076	-930.94	-1685.14	19.82	18.88	-6.50	-6.89	-3.27
130.00	0.4068	-868.36	-1643.36	20.68	19.10	-6.02	-6.36	-3.03
133.16	0.3916	-822.62	-1616.52	21.02	19.19	-5.85	-6.11	-2.95
140.00	0.3799	-715.05	-1549.75	21.80	19.40	-5.43	-5.57	-2.73
143.16	0.3742	-674.47	-1528.07	22.12	19.50	-5.27	-5.37	-2.65
150.00	0.3611	-564.52	-1458.92	22.85	19.71	-4.90	-4.89	-2.47
153.16	0.3547	-515.04	-1428.34	23.19	19.81	-4.72	-4.69	-2.38
160.00	0.3398	-414.72	-1368.92	23.87	20.02	-4.38	-4.31	-2.21
163.16	0.3324	-367.05	-1340.15	24.14	20.13	-4.28	-4.13	-2.15
170.00	0.3137	-236.18	-1250.18	24.96	20.36	-3.82	-3.70	-1.92
173.16	0.3047	-175.30	-1208.30	25.33	20.48	-3.61	-3.51	-1.82
180.00	0.2810	-23.81	-1097.81	26.20	20.84	-3.14	-3.07	-1.58
183.16	0.2666	54.08	-1038.92	26.64	21.11	-2.91	-2.85	-1.46
190.00	0.2057	263.62	-870.38	27.90	23.34	-2.39	-2.31	-1.20
190.70	0.1620	377.00	-762.00	28.62	24.24	-2.16	-2.01	-1.09

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. C. BUSH

SUBSTANCE: METHANE MW: 16.0420 TTP: [illegible]K TNBP: 111.70K TTC: 190.70K

[illegible]

EXTERNAL ROTATION MOMENTS: .5220-039 .5220-039 .5220-039 SYM NO:12.00

[illegible] (1): .0000+000

INT ROT [illegible] (1): .00

[illegible] (3): [illegible] 1440.00 1100.00

[illegible] 4 3 2

[illegible]

TEMP (DEG K)	LN Q	C(O)	H(O)-H(OO)	S(O)	F(O)-H(OO)	RT	E(O)-E(OO)
7[illegible]	.[illegible]72+0[illegible]	.7[illegible]+01	.[illegible]153+03	.33265+02	-.18480+04	145.38	.4361+03
[illegible]	[illegible]	.7543+01	.72073+03	.34317+02	-.24455+04	150.20	.5485+03
[illegible]	[illegible]	.7545+01	.74[illegible]52+03	[illegible]	[illegible]	185.13	.5554+03
200.00	[illegible]	.754[illegible]+01	.7[illegible]+03	.35[illegible]+02	-.27747+04	193.72	.5982+03
[illegible]	[illegible]	.7545+01	[illegible]	[illegible]44+02	-.[illegible]+04	[illegible]	.6150+03
[illegible]	[illegible]	.754[illegible]+01	.37437+03	.36454+02	-.31[illegible]+04	213.53	.[illegible]+03
111.70	.[illegible]+01	.754[illegible]+01	.[illegible]+03	[illegible]	-.3[illegible]77+04	221.57	.[illegible]+03
[illegible]	.1[illegible]47+[illegible]	.7540+01	[illegible]	[illegible]	-.32[illegible]+04	224.37	.6740+03
[illegible]	[illegible]	.75[illegible]+01	[illegible]	.37147+02	-.3[illegible]+04	[illegible].48	.7154+03
[illegible]	[illegible]	.7551+01	.373[illegible]+03	.37354+02	-.36215+04	244.74	.7342+03
[illegible]	[illegible]	.755[illegible]+01	.1[illegible]+04	.377[illegible]+02	-.3[illegible]+04	[illegible]	.775[illegible]+03
[illegible]	.1[illegible]+0[illegible]	.7555+01	.10[illegible]+04	.37975+02	-.39353+04	264.51	.7939+03
14[illegible]	[illegible]	.75[illegible]+01	.111[illegible]+0[illegible]	.3[illegible]74+02	-.41[illegible]+04	278.21	.8347+03
[illegible]	[illegible]	.7[illegible]+01	.11[illegible]+04	[illegible]	-.43810+04	[illegible].49	.[illegible]+03
[illegible]	[illegible]	.75[illegible]+01	[illegible]	[illegible]	-.46461+04	[illegible]	.8944+03
[illegible]	[illegible]	.7554+01	.12177+04	[illegible]	-.47694+04	304.36	.9133+03
[illegible]	[illegible]	.757[illegible]+01	.127[illegible]+04	[illegible]	-.50[illegible]+04	317.95	.9542+03
[illegible]	[illegible]	.757[illegible]+01	.12[illegible]73+04	[illegible]	-.51[illegible]+04	324.23	.9731+03
17[illegible]	[illegible]	.7[illegible]4+01	[illegible]	[illegible]	-.54347+04	337.82	.1014+04
[illegible]	[illegible]	[illegible]+01	.1377[illegible]+04	.40470+02	-.55513+04	344.10	.1033+04
[illegible]	[illegible]	[illegible]+01	.14572+04	.4[illegible]+02	-.5[illegible]44+04	36[illegible].97	.10[illegible]+04
[illegible]	[illegible]	[illegible]+01	.15176+04	.40[illegible]+02	-.62712+04	373.30	.1130+04
[illegible]	[illegible]	[illegible]+01	[illegible]+04	[illegible]	-.[illegible]+04	[illegible]	.1[illegible]54+04
[illegible]	.171[illegible]	.[illegible]7[illegible]+01	.[illegible]+04	.44[illegible]+02	-.10373+05	[illegible]	.1[illegible]21+04

APPENDIX C-3

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: NITROGEN MOLECULAR WEIGHT: 28.0160 OMEGA: 0.0400

TRIPLE POINT: 63.19 K N-BOILING POINT: 77.35 K

CRITICAL POINT: 126.20 K 33.50 ATM 0.0901 L/GMOLE ZC 0.2910

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 7.09816 B= 337.17676 C= 275.79977 NC= 274.93066
GAMSON-KATSON: A= 2.3903 BL= 0.1401 B= 6.7845

FRANCIS CONSTANTS: A= 1.1510 B= 0.3318E-02 C= 4.00 E= 146.62
G= 0.5030E-03 H= 3.36

INPUT DATA:

TEMP	H(0)-H(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
63.19	0.0	313.90	35.00	0.9994	-4.15	28.25
70.00	7.50	372.60	36.19	0.9500	-0.58	29.10
77.35	10.00	384.30	36.41	0.9285	0.22	29.26
100.00	65.00	496.80	36.20	0.8200	4.77	30.53
125.00	413.00	621.00	39.75	0.3800	10.57	31.64
126.20	504.00	627.00	39.82	0.2910	11.55	31.67

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
63.19	0.1237E 00	0.1794	0.03222	0.4190E 02	125.366	1296.	1421.	22.49
75.00	0.7452E 00	0.1289	0.03423	0.7846E 01	140.933	1222.	1363.	18.17
77.35	0.1000E 01	0.1215	0.03468	0.5894E 01	141.842	1191.	1333.	17.23
100.00	0.7709E 01	0.0696	0.04057	0.8729E 00	155.335	925.	1080.	10.60
125.00	0.3094E 02	0.0445	0.06653	0.1266E 00	44.537	203.	247.	1.98
126.20	0.3262E 02	0.0436	0.07008	0.900PE-01	0.0	0.	0.	0.0

TEMP	RHO	EI	LC	SL	STR*	SC*	EC/RT	SC*/R
63.19	0.8694	-981.70	-1295.60	16.67	18.15	-8.24	-10.32	-4.15
75.00	0.8184	-856.75	-1229.35	18.61	18.79	-7.27	-8.25	-3.66
77.35	0.8077	-816.47	-1200.77	18.96	18.90	-7.10	-7.81	-3.57
100.00	0.6905	-493.27	-990.07	22.62	19.98	-5.02	-4.98	-2.53
125.00	0.4211	5.06	-615.94	27.20	21.63	-2.54	-2.48	-1.28
126.20	0.3110	123.00	-504.00	28.27	22.26	-2.12	-2.01	-1.07

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

C SUBSTANCE: NITROGEN MW: 28.0130 TTP: 63.19K TNBP: 77.35K TTC: 126.20K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .1394-038 .1394-038 .0000+000 SYM NO: 2.00

INT ROT MOM: (1): .0000+000

INT ROT POT: (1): .00

VIB FREQ: (1): 2345.00

FREQ DEGEN: 1

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
63.19	.10946+03	.6955+01	.43950+03	.35002+02	-.17723+04	125.57	.3139+03
75.00	.11015+03	.6955+01	.52164+03	.36195+02	-.21930+04	149.04	.3726+03
77.35	.11027+03	.6955+01	.53798+03	.36410+02	-.22783+04	153.71	.3843+03
100.00	.11130+03	.6955+01	.69552+03	.38191+02	-.31243+04	198.72	.4968+03
125.00	.11219+03	.6955+01	.86940+03	.39752+02	-.40996+04	248.40	.6210+03
126.20	.11223+03	.6955+01	.87774+03	.39819+02	-.41474+04	250.78	.6270+03
150.00	.11292+03	.6955+01	.10433+04	.41022+02	-.51100+04	298.08	.7452+03
200.00	.11407+03	.6955+01	.13910+04	.43025+02	-.72139+04	397.44	.9936+03
250.00	.11496+03	.6956+01	.17386+04	.44578+02	-.94058+04	496.80	.1242+04
298.16	.11567+03	.6958+01	.20738+04	.45805+02	-.11563+05	592.50	.1481+04

APPENDIX C-4

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: CYCLOHEXANE MOLECULAR WEIGHT: 84.1560 OMEGA: 0.1860

TRIPLE POINT: 279.83 K N-BOILING POINT: 353.90 K

CRITICAL POINT: 553.67 K 40.00 ATM 0.3080 L/GMOLE ZC 0.2710

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.84498 B= 1203.52588 C= 222.86299 NC= 224.51636
GAMSON-WATSON: A= 2.8127 BL= 0.1805 B= 7.2905

FRANCIS CONSTANTS: A= 1.0584 B= 0.8395E-03 C= 10.00 E= 592.03
G= 0.5701E-03 H= 2.58

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
279.83	0.0	3232.00	69.68	0.9980	-5.85	38.93
290.00	0.0	3457.00	70.54	0.9940	-4.84	39.11
298.16	0.0	3645.00	71.23	0.9916	-4.08	39.25
300.00	0.0	3688.00	71.39	0.9900	-3.92	39.28
310.00	0.0	3930.00	72.25	0.9860	-3.07	39.44
323.16	0.0	4263.00	73.38	0.9800	-2.04	39.65
330.00	22.00	4443.00	73.98	0.9770	-1.55	39.75
348.16	33.00	4946.00	75.56	0.9690	-0.35	40.02
353.90	44.00	5112.00	76.07	0.9651	0.16	40.10
373.16	77.00	5694.00	77.78	0.9500	1.38	40.37
383.16	88.00	6012.00	78.67	0.9380	1.85	40.50
393.16	110.00	6340.00	79.57	0.9240	2.37	40.63
400.00	121.00	6570.00	80.18	0.9160	2.75	40.71
403.16	132.00	6678.00	80.47	0.9100	2.90	40.75
423.16	209.00	7384.00	82.27	0.8760	3.91	40.99
433.16	253.00	7752.00	83.18	0.8570	4.37	41.11
448.16	319.00	8322.00	84.54	0.8260	5.07	41.28
458.16	374.00	8714.00	85.45	0.8050	5.50	41.39
473.16	473.00	9319.00	86.81	0.7700	6.20	41.55
498.16	715.00	10370.00	89.08	0.7020	7.41	41.80
500.00	748.00	10450.00	89.25	0.6960	7.51	41.82
523.16	1045.00	11480.00	91.35	0.5960	8.74	42.05
548.16	1815.00	12640.00	93.60	0.3980	10.93	42.28
553.67	2399.00	12900.00	94.10	0.2710	12.28	42.33

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
279.83	0.5258E-01	0.0526	0.10633	0.4359E 03	554.682	7610.	8164.	29.18
290.00	0.8775E-01	0.0482	0.10764	0.2696E 03	572.448	7434.	8007.	27.61
298.16	0.1284E 00	0.0451	0.10872	0.1890E 03	587.031	7308.	7895.	26.48
300.00	0.1394E 00	0.0444	0.10897	0.1748E 03	589.673	7273.	7862.	26.21
310.00	0.2138E 00	0.0411	0.11034	0.1173E 03	606.674	7121.	7727.	24.93
323.16	0.3576E 00	0.0372	0.11222	0.7267E 02	628.200	6928.	7556.	23.38
330.00	0.4585E 00	0.0354	0.11323	0.5771E 02	639.265	6833.	7473.	22.64
348.16	0.8388E 00	0.0312	0.11606	0.3301E 02	667.860	6595.	7263.	20.86
353.90	0.1000E 01	0.0301	0.11700	0.2803E 02	675.711	6514.	7190.	20.32
373.16	0.1724E 01	0.0266	0.12032	0.1688E 02	699.256	6238.	6937.	18.59
383.16	0.2188E 01	0.0249	0.12217	0.1348E 02	707.547	6037.	6745.	17.60
393.16	0.2786E 01	0.0235	0.12411	0.1070E 02	713.344	5883.	6597.	16.78
400.00	0.3263E 01	0.0227	0.12551	0.9214E 01	718.000	5791.	6509.	16.27
403.16	0.3503E 01	0.0223	0.12617	0.8594E 01	718.159	5735.	6453.	16.01
423.16	0.5351E 01	0.0201	0.13069	0.5685E 01	719.505	5410.	6129.	14.48
433.16	0.6513E 01	0.0192	0.13320	0.4677E 01	716.486	5237.	5953.	13.74
448.16	0.8599E 01	0.0179	0.13736	0.3533E 01	706.829	4961.	5668.	12.65
458.16	0.1024E 02	0.0171	0.14048	0.2955E 01	697.885	4772.	5470.	11.94
473.16	0.1313E 02	0.0160	0.14584	0.2277E 01	677.448	4461.	5138.	10.86
498.16	0.1921E 02	0.0145	0.15722	0.1494E 01	621.628	3854.	4476.	8.98
500.00	0.1973E 02	0.0143	0.15823	0.1448E 01	615.791	3802.	4417.	8.83
523.16	0.2710E 02	0.0131	0.17497	0.9442E 00	504.652	2955.	3459.	6.61
548.16	0.3705E 02	0.0119	0.22139	0.4833E 00	234.870	1302.	1536.	2.80
553.67	0.3954E 02	0.0117	0.30826	0.3083E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
279.83	0.7915	-4377.63	-7609.63	46.35	28.25	-12.64	-13.68	-6.36
290.00	0.7818	-3977.34	-7434.34	47.76	28.38	-12.05	-12.90	-6.06
298.16	0.7741	-3663.09	-7308.09	48.83	28.49	-11.64	-12.33	-5.86
300.00	0.7723	-3584.75	-7272.75	49.10	28.51	-11.52	-12.20	-5.80
310.00	0.7627	-3190.76	-7120.76	50.38	28.63	-11.05	-11.56	-5.56
323.16	0.7499	-2664.91	-6927.91	52.04	28.79	-10.48	-10.79	-5.27
330.00	0.7432	-2412.36	-6855.36	52.88	28.87	-10.21	-10.45	-5.14
348.16	0.7251	-1682.13	-6628.13	55.05	29.08	-9.57	-9.58	-4.82
353.90	0.7193	-1445.84	-6557.84	55.60	29.14	-9.52	-9.32	-4.79
373.16	0.6994	-620.66	-6314.66	57.81	29.36	-8.96	-8.52	-4.51
383.16	0.6889	-113.11	-6125.11	59.22	29.47	-8.42	-8.04	-4.24
393.16	0.6781	346.80	-5993.20	60.42	29.58	-8.10	-7.67	-4.08
400.00	0.6705	657.69	-5912.31	61.16	29.65	-7.96	-7.44	-4.01
403.16	0.6670	811.19	-5866.81	61.56	29.68	-7.84	-7.32	-3.94
423.16	0.6439	1765.09	-5618.91	63.88	29.90	-7.30	-6.68	-3.67
433.16	0.6318	2262.03	-5489.97	65.06	30.01	-7.01	-6.38	-3.53
448.16	0.6127	3042.19	-5279.81	66.82	30.17	-6.61	-5.93	-3.33
458.16	0.5991	3567.88	-5146.12	68.01	30.28	-6.33	-5.65	-3.19
473.16	0.5771	4385.38	-4933.62	69.75	30.45	-5.96	-5.25	-3.00
498.16	0.5353	5800.87	-4569.13	72.69	30.75	-5.34	-4.62	-2.69
500.00	0.5319	5900.48	-4549.52	72.91	30.78	-5.30	-4.58	-2.67
523.16	0.4810	7480.40	-3999.60	76.00	31.11	-4.42	-3.85	-2.22
548.16	0.3801	9523.42	-3116.58	79.87	31.72	-3.17	-2.86	-1.60
553.67	0.2730	10501.00	-2399.00	81.82	32.41	-2.36	-2.18	-1.19

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: CYCLOHEXANE MW: 84.1560 TTP: 279.83K TNBP: 353.90K TTC: 553.67K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .2326-037 .2326-037 .2326-037 SYM NO: 6.00

INT ROT MOM: (1): .0000+000

INT ROT POT: (1): .00

VIB FREQ: (5): 2950.00 1450.00 1100.00 1000.00 335.00

FREQ DEGEN: 12 6 18 6 6

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
279.83	.92517+03	.2360+02	.37883+04	.69677+02	-.15709+05	556.08	.3232+04
290.00	.10110+04	.2460+02	.40334+04	.70538+02	-.16423+05	576.29	.3457+04
298.16	.10841+04	.2543+02	.42375+04	.71232+02	-.17001+05	592.50	.3645+04
300.00	.11012+04	.2561+02	.42844+04	.71389+02	-.17132+05	596.16	.3688+04
310.00	.11972+04	.2664+02	.45457+04	.72246+02	-.17851+05	616.03	.3930+04
323.16	.13328+04	.2800+02	.49052+04	.73382+02	-.18809+05	642.18	.4263+04
330.00	.14075+04	.2872+02	.50991+04	.73976+02	-.19313+05	655.77	.4443+04
348.16	.16203+04	.3062+02	.56379+04	.75565+02	-.20671+05	691.86	.4946+04
353.90	.16919+04	.3122+02	.58154+04	.76071+02	-.21106+05	703.27	.5112+04
373.16	.19484+04	.3323+02	.64360+04	.77779+02	-.22588+05	741.54	.5694+04
383.16	.20913+04	.3426+02	.67735+04	.78671+02	-.23370+05	761.41	.6012+04
393.16	.22412+04	.3529+02	.71212+04	.79567+02	-.24161+05	781.28	.6340+04
400.00	.23477+04	.3598+02	.73650+04	.80182+02	-.24708+05	794.88	.6570+04
403.16	.23980+04	.3630+02	.74792+04	.80466+02	-.24962+05	801.16	.6678+04
423.16	.27328+04	.3829+02	.82251+04	.82272+02	-.26589+05	840.90	.7384+04
433.16	.29109+04	.3926+02	.86129+04	.83178+02	-.27417+05	860.77	.7752+04
448.16	.31916+04	.4069+02	.92126+04	.84539+02	-.28675+05	890.58	.8322+04
458.16	.33879+04	.4163+02	.96242+04	.85448+02	-.29525+05	910.45	.8714+04
473.16	.36961+04	.4300+02	.10259+05	.86811+02	-.30817+05	940.26	.9319+04
498.16	.42460+04	.4521+02	.11362+05	.89083+02	-.33016+05	989.94	.1037+05
500.00	.42892+04	.4537+02	.11445+05	.89250+02	-.33180+05	993.59	.1045+05
523.16	.48443+04	.4732+02	.12519+05	.91349+02	-.35271+05	1039.62	.1148+05
548.16	.54888+04	.4933+02	.13727+05	.93605+02	-.37583+05	1089.30	.1264+05
553.67	.56372+04	.4976+02	.14000+05	.94100+02	-.38101+05	1100.25	.1290+05

APPENDIX C-5

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: CARBON TETRACHLORIDE MOLECULAR WEIGHT:153.8400 OMEGA: 0.2020

TRIPLE POINT: 250.30 K N-BOILING POINT: 349.70 K

CRITICAL POINT: 556.40 K 45.00 ATM 0.2760 L/GMOLE ZC 0.2710

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.88750 B= 1214.33984 C= 226.53999 NC= 223.83844
GAMSON-WATSON: A= 2.7796 BL= 0.1237 B= 7.3062

FRANCIS CONSTANTS: A= 2.1832 B= 0.1880E-02 C= 10.00 E= 571.32
G= 0.1780E-02 H= 3.27

INPUT DATA:

TEMP	E(O)-E(SV)	E(O)-E(OO)	S(O)	Z(VAP)	S(O)-S(SV)	STR
250.30	0.0	2689.00	70.68	0.9900	-9.31	40.18
298.16	0.0	3517.00	74.05	0.9884	-3.76	41.05
300.00	0.0	3550.00	74.18	0.9879	-3.60	41.08
349.70	22.00	4473.00	77.33	0.9710	0.14	41.84
350.00	25.00	4478.00	77.34	0.9700	0.14	41.85
373.16	64.00	4926.00	78.71	0.9660	1.51	42.17
398.16	110.00	5418.00	80.12	0.9220	2.86	42.49
400.00	121.00	5455.00	80.22	0.9180	2.98	42.51
423.16	210.00	5921.00	81.46	0.8780	4.09	42.77
448.16	309.00	6431.00	82.75	0.8290	5.23	43.03
473.16	464.00	6949.00	83.98	0.7740	6.36	43.35
498.16	697.00	7473.00	85.16	0.7090	7.53	43.60
500.00	719.00	7512.00	85.25	0.7030	7.61	43.62
523.16	995.00	8003.00	86.30	0.6090	8.80	43.85
548.16	1614.00	8548.00	87.39	0.4460	10.63	44.08
556.40	2410.00	8716.00	87.74	0.2710	12.50	44.15

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
250.30	0.9216E-02	0.0692	0.09149	0.2206E 04	492.270	8037.	8529.	34.08
298.16	0.1510E 00	0.0442	0.09700	0.1601E 03	585.119	7125.	7710.	25.86
300.00	0.1637E 00	0.0436	0.09722	0.1485E 03	588.165	7097.	7685.	25.62
349.70	0.1000E 01	0.0304	0.10390	0.2786E 02	672.075	6482.	7154.	20.46
350.00	0.1009E 01	0.0304	0.10394	0.2760E 02	671.934	6473.	7145.	20.41
373.16	0.1940E 01	0.0262	0.10749	0.1524E 02	711.090	6247.	6958.	18.65
398.16	0.3469E 01	0.0226	0.11173	0.8084E 01	719.930	5744.	6464.	15.24
400.00	0.3615E 01	0.0223	0.11206	0.8335E 01	719.697	5711.	6431.	16.08
423.16	0.5892E 01	0.0199	0.11653	0.5174E 01	721.492	5360.	6081.	14.37
448.16	0.9427E 01	0.0177	0.12215	0.3230E 01	709.328	4930.	5664.	12.58
473.16	0.1435E 02	0.0159	0.12908	0.2095E 01	682.732	4457.	5139.	10.86
498.16	0.2093E 02	0.0144	0.13860	0.1385E 01	631.444	3863.	4514.	9.06
500.00	0.2149E 02	0.0142	0.13948	0.1342E 01	629.746	3831.	4457.	8.91
523.16	0.2946E 02	0.0130	0.15508	0.8876E 00	522.368	3033.	3556.	6.80
548.16	0.4018E 02	0.0119	0.18492	0.5015E 00	307.999	1693.	2001.	3.65
556.40	0.4424E 02	0.0115	0.27619	0.2762E 00	0.0	0.	0.	0.0

TEMP	RHO	FL	FC	SL	STR*	SC*	EC/RT	SC*/R
250.30	1.6815	-5348.16	-8037.16	45.92	29.42	-14.00	-16.16	-7.09
298.16	1.5861	-3607.55	-7124.55	51.95	30.06	-11.11	-12.02	-5.59
300.00	1.5823	-3546.62	-7096.62	52.16	30.08	-11.02	-11.90	-5.56
349.70	1.4806	-2031.04	-6504.04	56.73	30.67	-9.43	-9.36	-4.74
350.00	1.4800	-2019.66	-6497.66	56.79	30.68	-9.38	-9.34	-4.72
373.16	1.4312	-1387.22	-6313.22	58.55	30.93	-8.93	-8.51	-4.49
398.16	1.3769	-836.50	-5964.50	61.02	31.20	-7.81	-7.60	-3.93
400.00	1.3728	-797.35	-5842.35	61.16	31.22	-7.77	-7.54	-3.91
423.16	1.3202	351.10	-5560.90	63.00	31.47	-7.14	-6.62	-3.59
448.16	1.2595	1191.66	-5239.34	64.93	31.74	-6.47	-5.86	-3.26
473.16	1.1913	2028.33	-4920.67	66.76	32.01	-5.88	-5.23	-2.96
498.16	1.1100	2893.28	-4579.72	68.57	32.30	-5.29	-4.63	-2.66
500.00	1.1030	2961.80	-4550.20	68.73	32.33	-5.23	-4.58	-2.63
523.16	0.9920	3974.59	-4026.41	70.70	32.67	-4.42	-3.97	-2.23
548.16	0.8319	5231.08	-3306.92	73.11	33.16	-3.36	-3.09	-1.69
556.40	0.5570	6306.00	-2410.00	75.24	34.00	-2.35	-2.18	-1.18

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. HUSH

SUBSTANCE: CARBON TETRACHLORIDE MW:153,8400 TTP: 250,30K TNBP: 349,70K TTC: 556,40K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: ,4990-037 ,4990-037 ,4990-037 SYM NO:12,00

INT ROT NON: (1): ,0000+000

INT ROT POT: (1): ,00

VIB FREQ: (4): 775,00 450,00 311,00 230,00

FREQ DEGEN: 3 1 3 2

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
250,30	,81200+03	,1857+02	,31867+04	,70683+02	-,14505+05	497,39	,2689+04
298,16	,12114+04	,1994+02	,41095+04	,74055+02	-,17971+05	592,50	,3517+04
300,00	,12286+04	,1998+02	,41462+04	,74178+02	-,18107+05	596,16	,3550+04
349,70	,17442+04	,2107+02	,51677+04	,77327+02	-,21874+05	694,92	,4473+04
350,00	,17476+04	,2108+02	,51740+04	,77346+02	-,21897+05	695,52	,4478+04
373,16	,20201+04	,2150+02	,56672+04	,78710+02	-,23704+05	741,54	,4926+04
398,16	,23361+04	,2190+02	,62097+04	,80116+02	-,25690+05	791,22	,5418+04
400,00	,23603+04	,2192+02	,62500+04	,80219+02	-,25838+05	794,88	,5455+04
423,16	,26746+04	,2225+02	,67616+04	,81463+02	-,27710+05	840,90	,5921+04
448,16	,30330+04	,2256+02	,73218+04	,82749+02	-,29763+05	890,58	,6431+04
473,16	,34124+04	,2283+02	,78893+04	,83982+02	-,31846+05	940,26	,6949+04
498,16	,38114+04	,2308+02	,84632+04	,85164+02	-,33962+05	989,94	,7473+04
500,00	,38415+04	,2309+02	,85057+04	,85250+02	-,34119+05	993,59	,7512+04
523,16	,42294+04	,2329+02	,90429+04	,86300+02	-,36106+05	1039,62	,8003+04
548,16	,46657+04	,2349+02	,96277+04	,87393+02	-,38277+05	1089,30	,8536+04
556,40	,48134+04	,2355+02	,98215+04	,87744+02	-,38999+05	1105,67	,8716+04

APPENDIX C-6

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: BENZENE MOLECULAR WEIGHT: 78.1100 OMEGA: 0.2150

TRIPLE POINT: 278.69 K N-BOILING POINT: 353.30 K

CRITICAL POINT: 562.10 K 48.60 ATM 0.2600 L/GMOLE ZC 0.2740

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.90565 B= 1211.03296 C= 220.78999 NC= 223.46680
GAMSON-WATSON: A= 2.8152 BL= 0.1924 B= 7.3835

FRANCIS CONSTANTS: A= 1.1928 B= 0.9575E-03 C= 10.00 E= 599.49
G= 0.6250E-03 H= 2.70

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
278.69	0.0	2492.00	63.01	1.0000	-6.07	38.69
293.16	0.0	2733.00	63.95	0.9960	-4.60	38.94
298.16	0.0	2820.00	64.28	0.9928	-4.13	39.03
300.00	0.0	2852.00	64.40	0.9910	-3.96	39.06
323.16	11.00	3283.00	65.93	0.9810	-2.05	39.43
348.16	33.00	3796.00	67.60	0.9680	-0.32	39.80
353.30	44.00	3907.00	67.95	0.9670	0.12	39.87
373.16	67.00	4356.00	69.30	0.9490	1.35	40.14
398.16	111.00	4963.00	71.00	0.9200	2.72	40.47
400.00	122.00	5010.00	71.13	0.9190	2.84	40.49
423.16	178.00	5615.00	72.71	0.8860	3.99	40.77
448.16	290.00	6310.00	74.42	0.8380	5.15	41.05
473.16	413.00	7044.00	76.12	0.7860	6.24	41.32
500.00	659.00	7875.00	77.94	0.7170	7.53	41.60
523.16	915.00	8626.00	79.50	0.6320	8.64	41.82
548.16	1485.00	9468.00	81.16	0.5380	10.29	42.06
562.10	2401.00	9954.00	82.09	0.2740	12.69	42.18

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
278.69	0.4719E-01	0.0544	0.08729	0.4846E 03	553.565	7845.	8399.	30.14
293.16	0.9695E-01	0.0481	0.08882	0.2421E 03	579.869	7596.	8176.	27.89
298.16	0.1252E 00	0.0462	0.08936	0.1940E 03	587.809	7502.	8090.	27.13
300.00	0.1363E 00	0.0455	0.08956	0.1791E 03	590.342	7463.	8054.	26.85
323.16	0.3570E 00	0.0380	0.09220	0.7288E 02	629.016	7101.	7730.	23.92
348.16	0.8523E 00	0.0319	0.09530	0.3245E 02	667.579	6740.	7408.	21.28
353.30	0.1001E 01	0.0308	0.09597	0.2800E 02	676.401	6682.	7359.	20.83
373.16	0.1777E 01	0.0271	0.09871	0.1635E 02	699.290	6372.	7071.	18.95
398.16	0.3339E 01	0.0234	0.10252	0.9005E 01	719.446	5983.	6702.	16.83
400.00	0.3484E 01	0.0232	0.10282	0.8658E 01	721.627	5964.	6685.	16.71
423.16	0.5772E 01	0.0205	0.10687	0.5331E 01	729.909	5608.	6338.	14.98
448.16	0.9396E 01	0.0182	0.11197	0.3294E 01	720.747	5160.	5881.	13.12
473.16	0.1430E 02	0.0163	0.11824	0.2121E 01	697.651	4682.	5380.	11.37
500.00	0.2177E 02	0.0146	0.12731	0.1352E 01	645.129	4058.	4704.	9.41
523.16	0.3006E 02	0.0133	0.13927	0.9027E 00	555.523	3314.	3870.	7.40
548.16	0.4130E 02	0.0121	0.16527	0.5860E 00	420.651	2376.	2796.	5.10
562.10	0.4870E 02	0.0115	0.26037	0.2604E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
278.69	0.8948	-5353.21	-7845.21	38.94	27.63	-13.00	-14.17	-6.54
293.16	0.8795	-4862.93	-7595.93	40.66	27.81	-12.16	-13.04	-6.12
298.16	0.8741	-4681.84	-7501.84	41.27	27.87	-11.85	-12.66	-5.96
300.00	0.8722	-4611.26	-7463.26	41.51	27.90	-11.72	-12.52	-5.90
323.16	0.8472	-3829.12	-7112.12	44.06	28.18	-10.62	-11.07	-5.35
348.16	0.8196	-2977.19	-6773.19	46.65	28.47	-9.63	-9.79	-4.84
353.30	0.8139	-2819.11	-6726.11	47.00	28.52	-9.60	-9.58	-4.83
373.16	0.7913	-2082.75	-6438.75	49.00	28.74	-8.90	-8.68	-4.48
398.16	0.7619	-1130.57	-6093.57	51.45	29.01	-8.10	-7.70	-4.08
400.00	0.7597	-1075.79	-6085.79	51.57	29.03	-8.10	-7.66	-4.07
423.16	0.7309	-171.23	-5786.23	53.74	29.28	-7.48	-6.88	-3.76
448.16	0.6976	859.55	-5450.45	56.15	29.54	-6.76	-6.12	-3.40
473.16	0.6605	1948.54	-5095.46	58.51	29.81	-6.10	-5.42	-3.07
500.00	0.6135	3157.59	-4717.41	61.00	30.12	-5.46	-4.75	-2.75
523.16	0.5609	4396.76	-4229.23	63.46	30.44	-4.65	-4.07	-2.34
548.16	0.4725	5607.37	-3860.63	65.77	30.91	-4.25	-3.54	-2.14
562.10	0.3000	7553.00	-2401.00	69.40	31.89	-2.40	-2.15	-1.21

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: BENZENE MW: 78.1100 TTP: 278.69K TNBP: 353.30K TTC: 562.10K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .7750-038 .7750-038 .2000-037 SYM NO: 6.00

INT ROT MOM: (1): .0000+000

INT ROT POT: (1): .00

VIB FREQ: (6):	3000.00	1025.00	1050.00	1500.00	390.00	850.00
FREQ DEGEN:	6	12	3	3	3	3

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
278.69	.49322+03	.1804+02	.30461+04	.63008+02	-.14514+05	553.81	.2492+04
293.16	.55603+03	.1916+02	.33152+04	.63949+02	-.15432+05	582.56	.2733+04
298.16	.57957+03	.1955+02	.34120+04	.64277+02	-.15753+05	592.50	.2820+04
300.00	.58848+03	.1970+02	.34481+04	.64398+02	-.15871+05	596.16	.2852+04
323.16	.71218+03	.2151+02	.39253+04	.65930+02	-.17381+05	642.18	.3283+04
348.16	.87096+03	.2345+02	.44874+04	.67605+02	-.19050+05	691.86	.3796+04
353.30	.90700+03	.2385+02	.46090+04	.67952+02	-.19398+05	702.07	.3907+04
373.16	.10575+04	.2535+02	.50976+04	.69297+02	-.20761+05	741.54	.4356+04
398.16	.12732+04	.2718+02	.57545+04	.71001+02	-.22515+05	791.22	.4963+04
400.00	.12903+04	.2731+02	.58046+04	.71127+02	-.22646+05	794.88	.5010+04
423.16	.15190+04	.2893+02	.64560+04	.72710+02	-.24312+05	840.90	.5615+04
448.16	.17958+04	.3059+02	.72001+04	.74418+02	-.26151+05	890.56	.6310+04
473.16	.21042+04	.3215+02	.79846+04	.76122+02	-.28033+05	940.26	.7044+04
500.00	.24708+04	.3374+02	.88691+04	.77940+02	-.30101+05	993.59	.7875+04
523.16	.28169+04	.3502+02	.96655+04	.79497+02	-.31924+05	1039.62	.8626+04
548.16	.32217+04	.3634+02	.10558+05	.81163+02	-.33933+05	1089.30	.9468+04
562.16	.34626+04	.3704+02	.11071+05	.82089+02	-.35076+05	1117.12	.9954+04

APPENDIX C-7

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: 2,3 DIMETHYLBUTANE MOLECULAR WEIGHT: 86.1700 OMEGA: 0.2570

TRIPLE POINT: 145.19 K N-BOILING POINT: 331.20 K

CRITICAL POINT: 499.90 K 30.90 ATM 0.3580 L/GMOLE ZC 0.2700

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.80983 B= 1127.18677 C= 228.89999 NC= 241.89180
GAMSON-WATSON: A= 2.8915 BL= 0.1866 B= 7.2554

FRANCIS CONSTANTS: A= 0.9283 B= 0.7774E-03 C= 10.00 E= 549.70
G= 0.2600E-03 H= 2.93

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
145.19	0.0	1587.00	68.87	1.0000	-27.30	35.74
160.00	0.0	1849.00	70.81	1.0000	-22.87	36.22
180.00	0.0	2231.00	73.32	1.0000	-18.05	36.81
200.00	0.0	2670.00	75.86	1.0000	-14.19	37.33
220.00	0.0	3100.00	77.98	1.0000	-11.03	37.81
240.00	0.0	3570.00	80.02	1.0000	-8.37	38.24
260.00	0.0	4233.00	83.43	1.0000	-5.93	38.64
273.16	0.0	4567.00	84.79	1.0000	-4.55	38.88
280.00	4.00	4740.00	85.32	0.9950	-3.90	39.01
298.16	7.90	5319.00	87.48	0.9795	-2.34	39.32
300.00	16.90	5370.00	87.63	0.9780	-2.19	39.35
323.16	24.00	6039.00	89.65	0.9610	-0.51	39.72
331.20	39.00	6282.00	90.29	0.9550	0.18	39.84
348.16	79.00	6951.00	92.58	0.9300	1.31	40.09
373.16	139.00	8044.00	94.89	0.8970	2.80	40.44
393.16	218.00	8777.00	96.74	0.8580	3.86	40.70
400.00	248.00	9037.00	97.38	0.8420	4.21	40.78
423.16	387.00	9999.00	100.26	0.7860	5.37	41.06
448.16	615.00	11040.00	102.58	0.7130	6.76	41.35
458.16	725.00	11470.00	103.51	0.6740	7.29	41.46
473.16	933.00	12140.00	104.90	0.5970	8.21	41.62
498.16	1907.00	13300.00	107.21	0.3360	11.11	41.87
499.90	2175.00	13380.00	107.37	0.2700	11.78	41.89

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
145.19	0.1083E-05	0.2000	0.10898	0.1100E 08	288.445	8087.	8375.	57.68
160.00	0.1004E-04	0.1628	0.11072	0.1308E 07	317.867	7962.	8280.	51.75
180.00	0.1136E-03	0.1266	0.11319	0.1300E 06	357.600	7794.	8152.	45.29
200.00	0.7921E-03	0.1010	0.11579	0.2072E 05	397.331	7626.	8023.	40.12
220.00	0.3884E-02	0.0821	0.11854	0.4648E 04	437.056	7457.	7894.	35.88
240.00	0.1481E-01	0.0677	0.12146	0.1330E 04	476.757	7274.	7751.	32.30
260.00	0.5061E-01	0.0558	0.12458	0.4215E 03	516.381	6970.	7487.	28.80
273.16	0.1011E 00	0.0495	0.12676	0.2218E 03	542.368	6797.	7339.	26.87
280.00	0.1405E 00	0.0467	0.12793	0.1628E 03	553.051	6679.	7232.	25.83
298.16	0.3087E 00	0.0403	0.13121	0.7763E 02	579.221	6374.	6953.	23.32
300.00	0.3323E 00	0.0397	0.13155	0.7246E 02	581.830	6345.	6927.	23.09
323.16	0.7717E 00	0.0334	0.13614	0.3302E 02	614.429	6011.	6625.	20.50
331.20	0.1002E 01	0.0315	0.13786	0.2591E 02	625.032	5901.	6526.	19.70
348.16	0.1659E 01	0.0281	0.14172	0.1601E 02	637.568	5601.	6238.	17.92
373.16	0.3155E 01	0.0241	0.14817	0.8705E 01	653.668	5224.	5878.	15.75
393.16	0.4780E 01	0.0216	0.15421	0.5558E 01	651.573	4886.	5537.	14.08
400.00	0.5759E 01	0.0209	0.15652	0.4799E 01	647.289	4754.	5402.	13.50
423.16	0.9088E 01	0.0186	0.16561	0.3003E 01	624.335	4292.	4916.	11.62
448.16	0.1410E 02	0.0166	0.17899	0.1860E 01	573.724	3689.	4262.	9.51
458.16	0.1658E 02	0.0159	0.18957	0.1528E 01	537.393	3367.	3905.	8.52
473.16	0.2087E 02	0.0149	0.20301	0.1110E 01	458.593	2768.	3226.	6.82
498.16	0.2971E 02	0.0134	0.27513	0.4623E 00	134.630	765.	900.	1.81
499.90	0.3041E 02	0.0133	0.35755	0.3576E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
145.19	0.7907	-6499.78	-8086.78	38.48	26.41	-21.06	-28.03	-10.60
160.00	0.7783	-6113.20	-7962.20	41.93	26.73	-19.39	-25.04	-9.76
180.00	0.7613	-5562.98	-7793.98	46.08	27.13	-17.56	-21.79	-8.84
200.00	0.7442	-4955.71	-7625.71	49.93	27.49	-16.08	-19.19	-8.09
220.00	0.7269	-4357.34	-7457.34	53.13	27.82	-14.87	-17.06	-7.48
240.00	0.7094	-3704.29	-7274.29	56.10	28.13	-13.81	-15.25	-6.95
260.00	0.6917	-2737.38	-6970.38	60.57	28.42	-12.65	-13.49	-6.36
273.16	0.6798	-2229.55	-6796.55	62.47	28.60	-12.03	-12.52	-6.05
280.00	0.6735	-1943.12	-6683.12	63.39	28.69	-11.61	-12.01	-5.84
298.16	0.6568	-1062.81	-6381.81	66.50	28.93	-10.59	-10.77	-5.33
300.00	0.6550	-991.86	-6361.86	66.73	28.95	-10.50	-10.67	-5.29
323.16	0.6329	4.14	-6034.86	69.66	29.24	-9.51	-9.40	-4.79
331.20	0.6251	342.40	-5939.60	70.41	29.34	-9.38	-9.02	-4.72
348.16	0.6080	1271.41	-5679.59	73.35	29.55	-8.68	-8.21	-4.37
373.16	0.5815	2680.66	-5363.34	76.34	29.84	-7.96	-7.23	-4.00
393.16	0.5588	3673.36	-5103.64	78.80	30.08	-7.33	-6.53	-3.69
400.00	0.5509	4034.53	-5002.47	79.67	30.16	-7.09	-6.29	-3.57
423.16	0.5203	5320.33	-4678.67	83.27	30.44	-6.36	-5.56	-3.20
448.16	0.4814	6736.42	-4303.57	86.31	30.76	-5.69	-4.83	-2.86
458.16	0.4546	7377.65	-4092.35	87.70	30.94	-5.30	-4.49	-2.67
473.16	0.4245	8439.41	-3700.59	89.87	31.18	-4.59	-3.94	-2.31
498.16	0.3132	10628.11	-2671.89	94.29	31.93	-2.98	-2.70	-1.50
499.90	0.2410	11205.00	-2175.00	95.59	32.47	-2.36	-2.19	-1.19

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: 2,3 DIMETHYLBUTANE MW: 86.1700 TTP: 145.19K TNBP: 331.20K TTC: 499.90K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: 0.3315E-37 0.3316E-37 0.1932E-37 SYM NO: 1.00

INT ROT MOM: (5): 0.52E-39 0.52E-39 0.52E-39 0.52E-39 0.55E-38

INT ROT POT: (5): 4100.00 4100.00 4100.00 4100.00 2100.00

VIB FREQ: (6): 2950.00 1405.00 1074.00 989.00 465.00 330.00

FREQ DEGEN: 14 16 8 5 4 2

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
145.19	0.25278E+03	0.1937E+02	0.18759E+04	0.68571E+02	-0.81236E+04	288.52	0.1587E+04
160.00	0.27291E+03	0.2067E+02	0.21666E+04	0.70611E+02	-0.91631E+04	317.95	0.1849E+04
180.00	0.30969E+03	0.2241E+02	0.25889E+04	0.73320E+02	-0.10609E+05	357.69	0.2231E+04
200.00	0.35884E+03	0.2413E+02	0.30674E+04	0.75858E+02	-0.12103E+05	397.44	0.2670E+04
220.00	0.42164E+03	0.2574E+02	0.35371E+04	0.77979E+02	-0.13617E+05	437.18	0.3100E+04
240.00	0.49936E+03	0.2745E+02	0.40471E+04	0.80024E+02	-0.15159E+05	476.93	0.3570E+04
260.00	0.59320E+03	0.2979E+02	0.47496E+04	0.83436E+02	-0.16944E+05	516.67	0.4233E+04
273.16	0.66432E+03	0.3078E+02	0.51097E+04	0.84786E+02	-0.18051E+05	542.82	0.4567E+04
280.00	0.70437E+03	0.3136E+02	0.52967E+04	0.85321E+02	-0.18593E+05	556.41	0.4740E+04
298.16	0.82130E+03	0.3327E+02	0.59118E+04	0.87481E+02	-0.20172E+05	592.50	0.5319E+04
300.00	0.83404E+03	0.3344E+02	0.59663E+04	0.87626E+02	-0.20322E+05	596.16	0.5370E+04
323.16	0.10088E+04	0.3545E+02	0.66814E+04	0.89645E+02	-0.22289E+05	642.18	0.6039E+04
331.20	0.10759E+04	0.3620E+02	0.69406E+04	0.90292E+02	-0.22964E+05	658.16	0.6282E+04
348.16	0.12289E+04	0.3803E+02	0.76426E+04	0.92579E+02	-0.24591E+05	691.86	0.6951E+04
373.16	0.14836E+04	0.4047E+02	0.87860E+04	0.94891E+02	-0.26623E+05	741.54	0.8044E+04
393.16	0.17131E+04	0.4238E+02	0.95587E+04	0.96745E+02	-0.28477E+05	781.28	0.8777E+04
400.00	0.17971E+04	0.4303E+02	0.98316E+04	0.97380E+02	-0.29119E+05	794.88	0.9037E+04
423.16	0.21027E+04	0.4498E+02	0.10839E+05	0.10026E+03	-0.31584E+05	840.90	0.9999E+04
448.16	0.24701E+04	0.4728E+02	0.11932E+05	0.10258E+03	-0.34038E+05	890.55	0.1104E+05
458.16	0.26281E+04	0.4819E+02	0.12386E+05	0.10351E+03	-0.35036E+05	910.45	0.1147E+05
473.16	0.28774E+04	0.4953E+02	0.13031E+05	0.10490E+03	-0.36551E+05	940.26	0.1214E+05
498.16	0.33255E+04	0.5170E+02	0.14285E+05	0.10721E+03	-0.39121E+05	989.94	0.1330E+05
499.90	0.33583E+04	0.5185E+02	0.14371E+05	0.10737E+03	-0.39302E+05	993.40	0.1338E+05
500.00	0.33602E+04	0.5186E+02	0.14376E+05	0.10738E+03	-0.39313E+05	993.59	0.1338E+05

APPENDIX C-8

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: CIS-PENTENE-2 MOLECULAR WEIGHT: 70.1300 OMEGA: 0.2800

TRIPLE POINT: 121.80 K N-BOILING POINT: 310.10 K

CRITICAL POINT: 475.56 K 40.40 ATM 0.2950 L/GMOLE ZC 0.2660

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.87274 B= 1067.95093 C= 230.58499 NC= 246.55499
GANSON-WATSON: A= 2.9633 BL= 0.2272 B= 7.4491

FRANCIS CONSTANTS: A= 0.9184 B= 0.8060E-03 C= 6.00 E= 468.57
G= 0.3299E-03 H= 2.95

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
121.80	0.0	1217.00	65.40	1.0000	-33.07	34.25
125.00	0.0	1255.00	65.69	1.0000	-31.70	34.38
150.00	0.0	1604.00	68.67	1.0000	-23.02	35.29
200.00	0.0	2347.00	73.36	1.0000	-12.15	36.72
250.00	0.0	3230.00	77.94	0.9980	-5.29	37.83
273.16	0.0	3616.00	79.96	0.9940	-2.93	38.27
298.16	19.00	4226.00	82.57	0.9840	-0.85	38.71
300.00	28.00	4266.00	82.70	0.9830	-0.72	38.74
310.10	38.00	4496.00	83.40	0.9750	0.16	38.90
323.16	57.00	4804.00	84.33	0.9610	1.05	39.11
348.16	113.00	5464.00	86.33	0.9140	2.60	39.48
350.00	122.00	5512.00	86.46	0.9090	2.74	39.50
373.16	236.00	6141.00	88.11	0.8490	4.35	39.82
398.16	434.00	6866.00	89.90	0.7700	6.08	40.14
400.00	444.00	6921.00	90.03	0.7640	6.20	40.17
423.16	708.00	7669.00	91.95	0.6760	7.75	40.45
448.16	1058.00	8485.00	93.85	0.5460	9.38	40.73
450.00	1096.00	8547.00	93.99	0.5350	9.48	40.75
473.16	1984.00	9345.00	95.75	0.3030	12.06	41.00
475.56	2136.00	9466.00	95.93	0.2660	12.48	41.03

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
121.80	0.5934E-07	0.2714	0.08734	0.1684E 09	241.977	7756.	7998.	65.66
125.00	0.1182E-06	0.2571	0.08764	0.8682E 08	248.334	7732.	7980.	63.84
150.00	0.9334E-05	0.1755	0.09006	0.1319E 07	298.000	7547.	7845.	52.30
200.00	0.2206E-02	0.0953	0.09543	0.7440E 04	397.328	7176.	7573.	37.87
250.00	0.6971E-01	0.0572	0.10172	0.2937E 03	495.502	6584.	7080.	28.32
273.16	0.2293E 00	0.0462	0.10506	0.9716E 02	538.839	6269.	6807.	24.92
298.16	0.6508E 00	0.0376	0.10909	0.3699E 02	581.149	5942.	6523.	21.88
300.00	0.6972E 00	0.0371	0.10941	0.3471E 02	584.022	5918.	6502.	21.67
310.10	0.9999E 00	0.0344	0.11121	0.2481E 02	597.971	5773.	6371.	20.55
323.16	0.1534E 01	0.0312	0.11372	0.1661E 02	612.751	5572.	6185.	19.14
348.16	0.3269E 01	0.0274	0.11928	0.7987E 01	622.753	5311.	5934.	17.04
350.00	0.3437E 01	0.0270	0.11974	0.7595E 01	622.095	5267.	5889.	16.82
373.16	0.6162E 01	0.0235	0.12656	0.4219E 01	610.521	4748.	5358.	14.36
398.16	0.1067E 02	0.0205	0.13347	0.2357E 01	574.591	4124.	4699.	11.80
400.00	0.1108E 02	0.0203	0.13407	0.2263E 01	571.155	4077.	4648.	11.62
423.16	0.1729E 02	0.0181	0.14321	0.1358E 01	508.348	3394.	3902.	9.22
448.16	0.2653E 02	0.0162	0.15944	0.7569E 00	383.723	2396.	2779.	6.20
450.00	0.2733E 02	0.0160	0.16117	0.7230E 00	371.662	2309.	2681.	5.96
473.16	0.3890E 02	0.0145	0.21522	0.3025E 00	82.161	481.	564.	1.19
475.56	0.4027E 02	0.0143	0.29591	0.2959E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
121.80	0.8029	-6538.59	-7755.59	32.81	24.83	-23.18	-32.04	-11.66
125.00	0.8002	-6476.89	-7731.89	33.55	24.92	-22.68	-31.13	-11.41
150.00	0.7787	-5942.52	-7546.52	39.39	25.52	-19.51	-25.32	-9.82
200.00	0.7349	-4828.74	-7175.74	47.65	26.49	-15.48	-18.05	-7.79
250.00	0.6894	-3354.45	-6584.45	54.92	27.28	-12.48	-13.25	-6.28
273.16	0.6675	-2652.56	-6268.56	57.96	27.61	-11.34	-11.55	-5.71
298.16	0.6429	-1734.64	-5960.64	61.54	27.95	-10.27	-10.06	-5.17
300.00	0.6410	-1679.52	-5945.52	61.74	27.97	-10.19	-9.97	-5.13
310.10	0.6306	-1315.23	-5811.23	62.70	28.10	-9.91	-9.43	-4.99
323.16	0.6167	-825.26	-5629.26	64.14	28.27	-9.36	-8.77	-4.71
348.16	0.5880	40.10	-5423.90	66.69	28.59	-8.76	-7.84	-4.41
350.00	0.5857	123.40	-5388.60	66.90	28.61	-8.67	-7.75	-4.37
373.16	0.5541	1157.40	-4983.60	69.40	28.91	-7.80	-6.72	-3.93
398.16	0.5254	2307.96	-4558.04	72.02	29.21	-6.95	-5.76	-3.50
400.00	0.5231	2400.30	-4520.70	72.21	29.24	-6.89	-5.69	-3.47
423.16	0.4897	3566.93	-4102.07	74.97	29.54	-6.06	-4.88	-3.05
448.16	0.4398	5031.50	-3453.50	78.27	29.92	-4.77	-3.88	-2.40
450.00	0.4351	5141.88	-3405.12	78.56	29.95	-4.64	-3.81	-2.33
473.16	0.3259	6879.66	-2465.34	82.50	30.68	-2.93	-2.62	-1.47
475.56	0.2370	7330.00	-2136.00	83.45	31.33	-2.78	-2.26	-1.40

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: CIS-PENTENE-2 MW: 70.1300 TTP: 121.80 K TNBP: 310.10K TTC: 475.36K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: 0.2320E-37 0.2320E-37 0.1615E-37 SYM NO: 1.00

INT ROT MOM: (3): 0.45E-39 0.43E-38 0.45E-39

INT ROT POT: (3): 800.00 800.00 4100.00

VIB FREQ: (6): 3000.00 1440.00 950.00 1000.00 1600.00 320.00

FREQ DEGEN: 10 7 12 3 1 3

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
121.80	0.21866E+03	0.1493E+02	0.14594E+04	0.65401E+02	-0.65063E+04	242.04	0.1217E+04
125.00	0.22103E+03	0.1505E+02	0.15029E+04	0.65689E+02	-0.67081E+04	248.40	0.1255E+04
150.00	0.24599E+03	0.1608E+02	0.19017E+04	0.68671E+02	-0.83991E+04	298.08	0.1604E+04
200.00	0.33641E+03	0.1803E+02	0.27447E+04	0.73358E+02	-0.11927E+05	397.44	0.2347E+04
250.00	0.49401E+03	0.2111E+02	0.37266E+04	0.77943E+02	-0.15759E+05	496.80	0.3230E+04
273.16	0.59451E+03	0.2242E+02	0.41591E+04	0.79959E+02	-0.17682E+05	542.82	0.3616E+04
298.16	0.72524E+03	0.2446E+02	0.48180E+04	0.82566E+02	-0.19801E+05	592.50	0.4226E+04
300.00	0.73533E+03	0.2460E+02	0.48626E+04	0.82696E+02	-0.19947E+05	596.16	0.4266E+04
310.10	0.79639E+03	0.2537E+02	0.51120E+04	0.83405E+02	-0.20753E+05	616.23	0.4496E+04
323.16	0.88099E+03	0.2638E+02	0.54461E+04	0.84327E+02	-0.21806E+05	642.18	0.4804E+04
348.16	0.10635E+04	0.2837E+02	0.61561E+04	0.86329E+02	-0.23901E+05	691.86	0.5464E+04
350.00	0.10781E+04	0.2851E+02	0.62079E+04	0.86460E+02	-0.24054E+05	695.52	0.5512E+04
373.16	0.12744E+04	0.3023E+02	0.68828E+04	0.88112E+02	-0.25998E+05	741.54	0.6141E+04
398.16	0.15149E+04	0.3215E+02	0.76568E+04	0.89902E+02	-0.28140E+05	791.22	0.6866E+04
400.00	0.15339E+04	0.3228E+02	0.77156E+04	0.90034E+02	-0.28299E+05	794.88	0.6921E+04
423.16	0.17862E+04	0.3387E+02	0.85034E+04	0.91947E+02	-0.30398E+05	840.90	0.7669E+04
448.16	0.20890E+04	0.3561E+02	0.93758E+04	0.93853E+02	-0.32684E+05	890.58	0.8485E+04
450.00	0.21126E+04	0.3573E+02	0.94412E+04	0.93993E+02	-0.32854E+05	894.24	0.8547E+04
473.16	0.24241E+04	0.3728E+02	0.10285E+05	0.95749E+02	-0.35018E+05	940.26	0.9345E+04
475.56	0.24580E+04	0.3744E+02	0.10411E+05	0.95930E+02	-0.35209E+05	945.03	0.9466E+04

APPENDIX C-9

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: N-HEXANE MOLECULAR WEIGHT: 86.1720 OMEGA: 0.2900

TRIPLE POINT: 177.84 K N-BOILING POINT: 341.90 K

CRITICAL POINT: 507.90 K 29.92 ATM 0.3680 L/GMOLE ZC 0.2640

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.87776 B= 1171.52979 C= 224.36600 NC= 235.09067
GAMSON-WATSON: A= 2.9978 BL= 0.2110 B= 7.3480

FRANCIS CONSTANTS: A= 0.9183 B= 0.7492E-03 C= 10.00 E= 545.67
G= 0.4726E-03 H= 2.57

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
177.84	0.0	2781.00	77.46	1.0000	-20.06	36.75
180.00	0.0	2841.00	78.13	1.0000	-19.58	36.81
190.00	0.0	3043.00	79.06	1.0000	-17.48	37.08
200.00	0.0	3252.00	79.97	1.0000	-15.58	37.33
210.00	0.0	3555.00	82.19	1.0000	-13.87	37.58
220.00	0.0	3784.00	83.10	1.0000	-12.31	37.81
230.00	0.0	4046.00	84.29	1.0000	-10.89	38.03
240.00	0.0	4302.00	85.73	1.0000	-9.59	38.24
250.00	0.0	4558.00	86.63	0.9970	-8.35	38.44
260.00	0.0	4836.00	87.85	0.9960	-7.09	38.64
273.16	0.0	5192.00	89.50	0.9910	-5.60	38.88
298.16	0.0	6045.00	92.70	0.9852	-3.21	39.32
300.00	0.0	6103.00	93.07	0.9840	-3.05	39.35
323.16	2.02	6891.00	95.76	0.9650	-1.25	39.72
341.90	18.16	7561.00	97.86	0.9505	0.18	40.00
348.16	26.24	7790.00	98.45	0.9460	0.52	40.07
373.16	70.65	8747.00	100.32	0.9130	1.95	40.44
398.16	151.40	9769.00	103.21	0.8770	3.64	40.76
400.00	160.00	9847.00	103.39	0.8760	3.80	40.78
423.16	260.40	10780.00	106.51	0.8170	4.89	41.06
473.16	773.10	13180.00	111.53	0.6380	7.61	41.62
498.16	1130.00	14440.00	114.02	0.4800	9.68	41.87
500.00	1170.00	14530.00	114.20	0.4760	8.78	41.89
507.90	2300.00	14860.00	115.31	0.2640	11.86	41.97

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
177.84	0.4122E-04	0.1361	0.11370	0.3540E 06	353.309	8323.	8676.	48.79
180.00	0.5243E-04	0.1346	0.11397	0.2807E 06	357.601	8307.	8665.	48.14
190.00	0.1516E-03	0.1201	0.11523	0.1028E 06	377.467	8234.	9612.	45.32
200.00	0.3930E-03	0.1077	0.11652	0.4176E 05	397.333	8161.	8559.	42.79
210.00	0.9305E-03	0.0971	0.11785	0.1852E 05	417.198	8089.	8506.	40.50
220.00	0.2037E-02	0.0879	0.11922	0.8361E 04	437.061	8016.	8453.	38.42
230.00	0.4168E-02	0.0799	0.12064	0.4528E 04	456.922	7943.	9400.	36.52
240.00	0.8033E-02	0.0729	0.12210	0.2452E 04	476.777	7870.	8347.	34.78
250.00	0.1494E-01	0.0666	0.12360	0.1372E 04	496.625	7798.	8295.	33.06
260.00	0.2819E-01	0.0605	0.12516	0.7538E 03	514.362	7573.	8098.	31.11
273.16	0.5963E-01	0.0536	0.12729	0.3725E 03	537.610	7332.	7859.	28.91
298.16	0.1930E 00	0.0434	0.13166	0.1211E 03	582.944	6957.	7540.	25.29
300.00	0.2154E 00	0.0427	0.13200	0.1124E 03	585.776	6926.	7512.	25.04
323.16	0.5333E 00	0.0358	0.13651	0.4798E 02	617.778	6536.	7154.	22.14
341.90	0.1000E 01	0.0314	0.14056	0.2667E 02	642.216	6252.	6894.	20.17
348.16	0.1212E 01	0.0301	0.14200	0.2230E 02	650.160	6163.	6813.	19.57
373.16	0.2414E 01	0.0256	0.14838	0.1158E 02	668.175	5708.	6396.	17.09
398.16	0.4383E 01	0.0223	0.15605	0.6538E 01	677.160	5325.	6002.	15.07
400.00	0.4565E 01	0.0220	0.15668	0.6209E 01	678.813	5308.	5986.	14.97
423.16	0.7300E 01	0.0196	0.16583	0.3839E 01	657.166	4801.	5458.	12.90
473.16	0.1775E 02	0.0157	0.20233	0.1395E 01	512.768	3288.	3960.	8.03
498.16	0.2575E 02	0.0141	0.24123	0.7620E 00	324.663	1960.	2286.	4.59
500.00	0.2643E 02	0.0140	0.24792	0.7391E 00	314.217	1889.	2203.	4.41
507.90	0.2947E 02	0.0136	0.36826	0.4683E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
177.84	0.7579	-5541.72	-8322.72	48.74	27.10	-19.07	-23.55	-9.60
180.00	0.7561	-5466.00	-8307.00	49.57	27.14	-18.89	-23.22	-9.51
190.00	0.7478	-5191.21	-8234.21	51.21	27.33	-18.10	-21.81	-9.11
200.00	0.7395	-4909.42	-8161.42	52.76	27.50	-17.38	-20.54	-8.75
210.00	0.7312	-4533.59	-8088.59	55.56	27.67	-16.73	-19.38	-8.42
220.00	0.7228	-4231.77	-8015.77	56.99	27.83	-16.13	-18.34	-8.12
230.00	0.7143	-3896.90	-7942.90	58.66	27.99	-15.59	-17.39	-7.85
240.00	0.7058	-3567.93	-7869.93	60.34	28.14	-15.09	-16.50	-7.59
250.00	0.6972	-3210.41	-7768.41	61.92	28.29	-14.55	-15.54	-7.32
260.00	0.6885	-2737.16	-7573.16	63.83	28.43	-13.80	-14.66	-6.95
273.16	0.6770	-2139.76	-7331.76	66.39	28.61	-12.93	-13.61	-6.51
298.16	0.6545	-912.05	-6957.05	70.62	28.94	-11.70	-11.74	-5.89
300.00	0.6528	-823.34	-6926.34	71.08	28.96	-11.60	-11.62	-5.84
323.16	0.6312	352.58	-6538.42	74.87	29.25	-10.42	-10.18	-5.24
341.90	0.6131	1290.59	-6270.41	77.51	29.48	-9.62	-9.23	-4.94
348.16	0.6068	1600.52	-6189.48	78.35	29.55	-9.35	-8.95	-4.81
373.16	0.5808	2868.75	-5778.24	81.78	29.85	-8.44	-7.79	-4.29
398.16	0.5522	4292.76	-5476.23	84.50	30.14	-8.09	-6.92	-4.07
400.00	0.5500	4379.43	-5467.57	84.62	30.16	-8.15	-6.88	-4.10
423.16	0.5196	5718.52	-5061.48	88.72	30.44	-7.17	-6.02	-3.61
473.16	0.4257	9119.33	-4060.67	95.39	31.17	-5.20	-4.32	-2.61
498.16	0.3572	11349.64	-3090.36	100.75	31.67	-3.07	-3.12	-1.54
500.00	0.3476	11470.86	-3059.14	101.01	31.74	-3.03	-3.08	-1.53
507.90	0.2340	12560.00	-2300.00	103.43	32.57	-2.48	-2.28	-1.25

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: N-HEXANE MW: 86.1720 TTP: 177.84K TNBP: 341.90K TTC: 507.90K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .1733-037 .1733-037 .4000-038 SYM NO: 1.00

INT ROT [illegible] ([illegible]): .4510-038 .4510-038 .1650-038 .1650-038 .4430-038

INT ROT POT: ([illegible]): 2000.00 2000.00 1600.00 1600.00 1600.00

VIB FREQ: ([illegible]): [illegible] 1400.00 950.00 330.00 300.00

[illegible]: 14 10 16 [illegible] 4

TOTAL QUANTITIES

TEMPERATURE	LN(Q)	C(P)	H(O)-H(OO)	S(O)	F(O)-H(OO)	RT	E(O)-E(OO)
177.84	.33727+[illegible]	.2431+02	.31345+04	.77450+02	-.10041+05	353.40	.2781+04
[illegible]	.3[illegible]42+02	.2438+02	.31330+04	.75127+02	-.10855+05	357.69	.2941+04
[illegible]	.[illegible]+[illegible]	.2[illegible]+02	.34267+04	.70857+02	-.11501+05	377.57	.3043+04
[illegible]	.[illegible]+02	.2[illegible]+02	.36404+04	.72074+02	-.12347+05	397.44	.3252+04
[illegible]	.40[illegible]1+02	.2[illegible]+02	.39720+04	.[illegible]+02	-.13208+05	417.31	.3555+04
[illegible]	.47[illegible]+02	.2774+02	.4220[illegible]+04	.83027+02	-.14050+05	437.18	.3784+04
[illegible]	.[illegible]+[illegible]	.2[illegible]+02	.45[illegible]+04	.[illegible]+02	-.14[illegible]+05	457.05	.4040+04
[illegible]	.[illegible]7[illegible]+02	.[illegible]+02	.47735+04	.87727+02	-.15795+05	476.93	.4302+04
[illegible]	.[illegible]+[illegible]	.[illegible]+02	.[illegible]+04	.[illegible]+02	-.15551+05	496.30	.4555+04
[illegible]	.[illegible]+02	.30[illegible]+02	.[illegible]+04	.87387+02	-.17471+05	516.67	.4838+04
[illegible]	.7457[illegible]+[illegible]	.317[illegible]+02	.57[illegible]+04	.[illegible]+02	-.1[illegible]721+05	542.62	.5192+04
[illegible]	.[illegible]41+02	.34[illegible]+02	.[illegible]74+04	.92330+02	-.21051+05	592.50	.5945+04
[illegible]	.[illegible]70[illegible]+[illegible]	.344[illegible]+02	.[illegible]+04	.[illegible]+02	-.21[illegible]+05	596.16	.6[illegible]3+04
[illegible]	.1[illegible]+04	.[illegible]+02	.7[illegible]+04	.[illegible]+02	-.23411+05	642.13	.6891+04
[illegible]	.[illegible]+04	.[illegible]+02	.[illegible]+04	.[illegible]+02	-.25217+05	679.42	.7561+04
[illegible]	.1[illegible]+04	.[illegible]7+02	.[illegible]+04	.[illegible]+02	-.25734+05	691.35	.7730+04
[illegible]	.16740+[illegible]	.4[illegible]+02	.[illegible]+04	.[illegible]+03	-.28134+05	741.54	.8747+04
[illegible]	.[illegible]+04	.4[illegible]+02	.10[illegible]+05	.10[illegible]+03	-.30534+05	791.22	.9703+04
[illegible]	.[illegible]+04	.441[illegible]+02	.[illegible]+05	.10[illegible]+03	-.[illegible]+05	794.82	.9847+04
[illegible]	.[illegible]+04	.[illegible]+02	.[illegible]+05	.[illegible]+03	-.33445+05	840.90	.1073+05
473.[illegible]	.[illegible]+04	.4[illegible]+02	.[illegible]+05	.11150+03	-.31[illegible]4+05	940.20	.1318+05
[illegible]	.[illegible]7[illegible]+04	.[illegible]+02	.[illegible]+05	.114[illegible]+03	-.41374+05	939.94	.1444+05
[illegible]	.[illegible]+04	.[illegible]+02	.15514+05	.1142[illegible]+03	-.41577+05	993.59	.1450+05
507.[illegible]	.[illegible]767+04	.[illegible]+02	.15374+05	.11[illegible]+03	-.41[illegible]+05	1009.29	.1460+05

APPENDIX C-10

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: 2,2,4 TRIMETHYLPENTANE MOLECULAR WEIGHT:114.2200 OMEGA: 0.3100

TRIPLE POINT: 165.78 K N-BOILING POINT: 372.40 K

CRITICAL POINT: 543.60 K 25.40 ATM 0.4820 L/GMOLE ZC 0.2740

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.81189 B= 1257.83984 C= 220.73499 NC= 235.53909
GAMSON-WATSON: A= 3.0760 BL= 0.0 B= 7.3614

FRANCIS CONSTANTS: A= 0.9371 B= 0.7162E-03 C= 10.00 E= 585.25
G= 0.4167E-03 H= 2.68

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
165.78	0.0	2429.00	80.44	1.0000	-26.92	37.24
180.00	0.0	2838.00	83.22	1.0000	-23.15	37.65
200.00	0.0	3380.00	86.23	1.0000	-18.75	38.18
220.00	0.0	3991.00	89.37	1.0000	-15.15	38.65
240.00	0.0	4584.00	91.72	1.0000	-12.15	39.08
273.16	0.0	5916.00	97.79	0.9980	-8.09	39.73
298.16	0.0	6883.00	101.27	0.9916	-5.43	40.16
300.00	0.0	6952.00	101.46	0.9910	-5.26	40.19
323.16	0.0	7983.00	104.85	0.9860	-3.27	40.56
348.16	22.00	9148.00	108.38	0.9740	-1.47	40.93
358.16	43.00	9851.00	109.42	0.9680	-0.84	41.07
372.40	65.00	10520.00	111.17	0.9568	0.26	41.27
390.91	86.00	11470.00	113.72	0.9480	1.30	41.51
393.16	97.00	11590.00	114.01	0.9310	1.43	41.54
400.00	108.00	11940.00	114.85	0.9250	1.75	41.62
423.16	194.00	13280.00	118.43	0.8820	2.98	41.90
448.16	302.00	14730.00	122.17	0.8240	4.21	42.19
458.16	367.00	15320.00	123.40	0.8010	4.67	42.30
473.16	475.00	16220.00	125.25	0.7620	5.43	42.46
498.16	756.00	18020.00	129.73	0.6820	6.76	42.71
500.00	766.00	18140.00	129.95	0.6740	6.88	42.73
523.16	1145.00	19740.00	132.79	0.5490	8.31	42.96
533.16	1463.00	20420.00	134.01	0.4690	9.24	43.05
543.60	2323.00	21140.00	135.28	0.2740	11.34	43.15

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
165.78	0.1307E-05	0.1763	0.14376	0.1041E 08	329.350	9299.	9628.	58.08
180.00	0.8717E-05	0.1480	0.14578	0.1694E 07	357.600	9167.	9525.	52.91
200.00	0.7969E-04	0.1180	0.14874	0.2059E 06	397.333	8982.	9379.	46.90
220.00	0.4877E-03	0.0960	0.15186	0.3702E 05	437.066	8797.	9234.	41.97
240.00	0.2209E-02	0.0794	0.15514	0.8916E 04	476.792	8612.	9089.	37.87
273.16	0.1709E-01	0.0594	0.16100	0.1309E 04	541.526	8251.	8793.	32.19
298.16	0.6492E-01	0.0480	0.16584	0.3737E 03	587.108	7809.	8396.	28.16
300.00	0.7087E-01	0.0473	0.16621	0.3443E 03	590.352	7778.	8369.	27.90
323.16	0.1928E 00	0.0395	0.17112	0.1356E 03	632.225	7441.	8073.	24.98
348.16	0.4762E 00	0.0331	0.17693	0.5843E 02	671.655	7072.	7744.	22.24
358.16	0.6560E 00	0.0310	0.17944	0.4337E 02	685.926	6926.	7612.	21.25
372.40	0.1000E 01	0.0283	0.18322	0.2924E 02	703.438	6707.	7410.	19.90
390.81	0.1636E 01	0.0253	0.18855	0.1858E 02	728.566	6473.	7202.	18.43
393.16	0.1736E 01	0.0249	0.18928	0.1730E 02	719.229	6335.	7054.	17.94
400.00	0.1996E 01	0.0241	0.19144	0.1521E 02	725.815	6261.	6987.	17.47
423.16	0.3381E 01	0.0215	0.19957	0.9058E 01	725.143	5873.	6598.	15.59
448.16	0.5617E 01	0.0192	0.21028	0.5395E 01	705.051	5352.	6057.	13.52
458.16	0.6775E 01	0.0183	0.21539	0.4445E 01	693.749	5136.	5830.	12.72
473.16	0.8844E 01	0.0172	0.22440	0.3346E 01	668.245	4769.	5438.	11.49
498.16	0.1330E 02	0.0155	0.24584	0.2096E 01	595.779	4009.	4605.	9.24
500.00	0.1369E 02	0.0154	0.24770	0.2020E 01	587.425	3936.	4523.	9.05
523.16	0.1925E 02	0.0141	0.29137	0.1225E 01	439.486	2795.	3234.	6.18
533.16	0.2210E 02	0.0135	0.30998	0.9286E 00	330.946	2059.	2390.	4.48
543.60	0.2538E 02	0.0130	0.48194	0.4819E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
165.78	0.7945	-6869.55	-9298.55	49.28	28.20	-22.11	-28.23	-11.13
180.00	0.7835	-6329.01	-9167.01	53.45	28.47	-20.59	-25.63	-10.36
200.00	0.7679	-5601.96	-8981.96	58.09	28.83	-18.80	-22.60	-9.46
220.00	0.7522	-4805.93	-8796.93	62.55	29.15	-17.32	-20.12	-8.72
240.00	0.7362	-4027.78	-8611.78	66.00	29.46	-16.09	-18.06	-8.10
273.16	0.7094	-2335.45	-8251.45	73.69	29.92	-14.29	-15.20	-7.19
298.16	0.6887	-925.95	-7808.95	78.54	30.24	-12.80	-13.18	-6.44
300.00	0.6872	-826.38	-7778.38	78.83	30.26	-12.70	-13.05	-6.39
323.16	0.6675	542.08	-7440.92	83.14	30.54	-11.69	-11.59	-5.88
348.16	0.6456	2053.72	-7094.28	87.61	30.83	-10.66	-10.25	-5.37
358.16	0.6366	2881.80	-6969.20	89.00	30.94	-10.28	-9.79	-5.18
372.40	0.6234	3747.97	-6772.03	91.02	31.10	-9.99	-9.15	-5.03
390.81	0.6058	4910.54	-6559.46	93.99	31.30	-9.52	-8.45	-4.79
393.16	0.6035	5158.07	-6431.93	94.64	31.33	-9.16	-8.23	-4.61
400.00	0.5966	5570.79	-6369.21	95.64	31.40	-8.99	-8.01	-4.53
423.16	0.5723	7213.10	-6066.90	99.35	31.65	-8.32	-7.21	-4.19
448.16	0.5432	9075.84	-5654.16	104.44	31.93	-7.46	-6.35	-3.76
458.16	0.5303	9816.74	-5503.26	106.01	32.04	-7.14	-6.04	-3.59
473.16	0.5090	10975.60	-5244.40	108.33	32.22	-6.68	-5.58	-3.36
498.16	0.4646	13255.11	-4764.89	113.73	32.55	-5.84	-4.81	-2.94
500.00	0.4611	13438.03	-4701.97	114.03	32.58	-5.77	-4.73	-2.90
523.16	0.4059	15800.09	-3939.90	118.30	32.97	-4.50	-3.79	-2.27
533.16	0.3685	16893.03	-3526.97	120.29	33.22	-3.89	-3.33	-1.96
543.60	0.2370	18817.00	-2323.00	123.94	34.15	-2.34	-2.15	-1.18

PERFECT-GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: 2,2,4 TRIMETHYLPENTANE MW: 114.22 TTP: 165.78 K TNBP: 372.40 K TC: 543.60 K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: 0.6700E-37 0.1200E-36 0.1330E-36 SYM NO: 1.00

INT ROT MOM: (7): 0.52E-39 0.53E-39 0.53E-39 0.41E-38 0.41E-38 0.53E-39 0.52E-39

INT ROT POT: (7): 4800.00 4800.00 4800.00 3400.00 3400.00 3800.00 3800.00

VIB FREQ: (5): 3000.00 1440.00 1100.00 1000.00 400.00

FREQ DEGEN: 18 16 15 7 9

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
165.78	0.33565E+03	0.2720E+02	0.2758E+04	0.8043E+02	-0.10577E+05	329.44	0.2409E+04
180.00	0.37799E+03	0.2924E+02	0.3196E+04	0.8321E+02	-0.11782E+05	357.69	0.2838E+04
200.00	0.45437E+03	0.3157E+02	0.3778E+04	0.8622E+02	-0.13468E+05	397.44	0.3380E+04
220.00	0.55265E+03	0.3410E+02	0.4428E+04	0.8937E+02	-0.15233E+05	437.18	0.3991E+04
240.00	0.67268E+03	0.3681E+02	0.5060E+04	0.9172E+02	-0.16952E+05	476.93	0.4664E+04
273.16	0.92754E+03	0.4113E+02	0.6459E+04	0.9779E+02	-0.20254E+05	542.52	0.5916E+04
298.16	0.11685E+04	0.4438E+02	0.7475E+04	0.1012E+03	-0.22719E+05	592.50	0.6883E+04
300.00	0.11880E+04	0.4460E+02	0.7548E+04	0.1014E+03	-0.22891E+05	596.16	0.6952E+04
323.16	0.14546E+04	0.4786E+02	0.8625E+04	0.1048E+03	-0.25259E+05	642.18	0.7933E+04
348.16	0.17884E+04	0.5127E+02	0.9839E+04	0.1083E+03	-0.27895E+05	691.86	0.9148E+04
358.16	0.19368E+04	0.5285E+02	0.1056E+05	0.1094E+03	-0.28626E+05	711.73	0.9851E+04
372.40	0.21598E+04	0.5465E+02	0.1126E+05	0.1111E+03	-0.30138E+05	740.03	0.1052E+05
390.81	0.24745E+04	0.5703E+02	0.1224E+05	0.1137E+03	-0.32197E+05	776.61	0.1147E+05
393.16	0.25167E+04	0.5733E+02	0.1236E+05	0.1140E+03	-0.32455E+05	781.28	0.1159E+05
400.00	0.26423E+04	0.5819E+02	0.1273E+05	0.1148E+03	-0.33208E+05	794.88	0.1194E+05
423.16	0.30978E+04	0.6123E+02	0.1412E+05	0.1184E+03	-0.35989E+05	840.90	0.1326E+05
448.16	0.36427E+04	0.6405E+02	0.1562E+05	0.1221E+03	-0.39126E+05	890.56	0.1473E+05
458.16	0.38743E+04	0.6525E+02	0.1623E+05	0.1234E+03	-0.40308E+05	910.45	0.1532E+05
473.16	0.42439E+04	0.6700E+02	0.1716E+05	0.1252E+03	-0.42103E+05	940.26	0.1622E+05
498.16	0.49025E+04	0.6941E+02	0.1901E+05	0.1297E+03	-0.45610E+05	989.94	0.1802E+05
500.00	0.49533E+04	0.6962E+02	0.1913E+05	0.1299E+03	-0.45839E+05	993.50	0.1814E+05
523.16	0.56191E+04	0.7214E+02	0.2078E+05	0.1337E+03	-0.48685E+05	1039.62	0.1974E+05
533.16	0.59271E+04	0.7322E+02	0.2148E+05	0.1340E+03	-0.49966E+05	1059.49	0.2042E+05
543.60	0.62485E+04	0.7432E+02	0.2221E+05	0.1352E+03	-0.51317E+05	1080.24	0.2114E+05

APPENDIX C-11

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: WATER MOLECULAR WEIGHT: 18.0200 OMEGA: 0.3480

TRIPLE POINT: 273.16 K N-BOILING POINT: 373.16 K

CRITICAL POINT: 647.00 K 218.30 ATM 0.0560 L/GMOLE ZC 0.2300

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 7.84819 B= 1614.00000 C= 224.92000 NC= 227.56396
GAMSON-WATSON: A= 3.1287 BL= 0.1700 B= 8.3468

FRANCIS CONSTANTS: A= 1.2637 B= 0.8835E-03 C= 9.00 E= 91.44
G= 0.1226E-02 H= 2.51

SMITH-KEYLS CONSTANTS: A= -0.31515479 B=-0.12033738E-02 C=0.74890799E-12 D= 0.13424885
E=-0.39462596E-02 F= 3.1975 G= 647.27

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
273.16	0.0	1629.00	44.42	1.0000	-9.72	34.21
298.16	0.0	1779.00	45.12	1.0000	-6.82	34.65
300.00	0.0	1790.00	45.17	1.0000	-6.60	34.68
350.00	13.00	2092.00	46.41	1.0000	-1.74	35.45
373.16	13.00	2233.00	46.92	0.9990	0.04	35.77
375.00	26.00	2244.00	46.96	0.9980	0.17	35.79
398.16	39.00	2386.00	47.45	0.9850	1.76	36.09
400.00	51.00	2397.00	47.49	0.9840	1.91	36.11
423.16	64.00	2540.00	47.95	0.9667	3.24	36.39
448.16	154.00	2695.00	48.42	0.9400	4.65	36.68
473.16	270.00	2852.00	48.87	0.9100	5.98	36.95
498.16	411.00	3010.00	49.30	0.8750	7.23	37.20
500.00	424.00	3022.00	49.33	0.8730	7.31	37.22
523.16	591.00	3170.00	49.71	0.8330	8.43	37.45
548.16	797.00	3331.00	50.10	0.7770	9.62	37.68
573.16	1067.00	3494.00	50.48	0.7040	10.77	37.90
598.16	1491.00	3658.00	50.85	0.6250	12.26	38.11
623.16	2057.00	3824.00	51.20	0.5130	13.67	38.32
635.00	2167.45	3903.00	51.36	0.4370	14.37	38.41
647.00	3844.00	3984.00	51.53	0.2320	17.29	38.50

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
273.16	0.7497E-02	0.0718	0.01802	0.2990E 04	542.675	10096.	10638.	38.95
298.16	0.3231E-01	0.0595	0.01808	0.7573E 03	592.331	9916.	10508.	35.24
300.00	0.3602E-01	0.0586	0.01809	0.6835E 03	595.985	9887.	10483.	34.94
350.00	0.4157E 00	0.0408	0.01850	0.6909E 02	695.148	9235.	9930.	28.37
373.16	0.1000E 01	0.0352	0.01880	0.3059E 02	740.149	8982.	9723.	26.05
375.00	0.1067E 01	0.0348	0.01883	0.2879E 02	743.024	8955.	9698.	25.86
398.16	0.2307E 01	0.0306	0.01919	0.1395E 02	778.075	8702.	9480.	23.81
400.00	0.2440E 01	0.0303	0.01922	0.1324E 02	780.818	8676.	9457.	23.64
423.16	0.4711E 01	0.0267	0.01965	0.7126E 01	810.443	8334.	9145.	21.61
448.16	0.8809E 01	0.0235	0.02020	0.3924E 01	832.617	7945.	8777.	19.59
473.16	0.1535E 02	0.0210	0.02084	0.2303E 01	847.668	7561.	8409.	17.77
498.16	0.2522E 02	0.0188	0.02161	0.1418E 01	852.773	7153.	8006.	16.07
500.00	0.2611E 02	0.0187	0.02167	0.1372E 01	853.483	7128.	7982.	15.96
523.16	0.3948E 02	0.0171	0.02255	0.9058E 00	844.223	6689.	7533.	14.40
548.16	0.5930E 02	0.0155	0.02373	0.5894E 00	812.098	6098.	6910.	12.61
573.16	0.8594E 02	0.0142	0.02529	0.3853E 00	749.008	5344.	6093.	10.63
598.16	0.1207E 03	0.0130	0.02755	0.2541E 00	662.185	4498.	5160.	8.63
623.16	0.1650E 03	0.0120	0.03179	0.1589E 00	508.061	3292.	3800.	6.10
635.00	0.1897E 03	0.0116	0.03546	0.1200E 00	388.406	2463.	2851.	4.49
647.00	0.2174E 03	0.0111	0.05596	0.5596E-01	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
273.16	0.9998	-8466.55	-10095.55	15.20	20.05	-15.06	-18.60	-7.58
298.16	0.9968	-8136.95	-9915.95	16.70	20.32	-14.09	-16.74	-7.09
300.00	0.9964	-8097.41	-9887.41	16.83	20.34	-14.00	-16.59	-7.05
350.00	0.9738	-7155.68	-9247.68	19.78	20.85	-12.03	-13.30	-6.05
373.16	0.9584	-6762.43	-8995.43	20.83	21.07	-11.40	-12.13	-5.74
375.00	0.9571	-6737.30	-8981.30	20.93	21.09	-11.33	-12.05	-5.70
398.16	0.9390	-6355.09	-8741.09	21.80	21.30	-10.79	-11.05	-5.43
400.00	0.9375	-6330.15	-8727.15	21.94	21.32	-10.76	-10.98	-5.42
423.16	0.9169	-5958.50	-8398.50	23.10	21.53	-9.99	-9.99	-5.03
448.16	0.8922	-5403.61	-8098.61	24.18	21.76	-9.32	-9.09	-4.69
473.16	0.8647	-4979.40	-7831.40	25.12	21.98	-8.79	-8.33	-4.42
498.16	0.8339	-4554.35	-7564.35	26.00	22.21	-8.31	-7.64	-4.18
500.00	0.8315	-4530.34	-7552.34	26.05	22.23	-8.28	-7.60	-4.17
523.16	0.7992	-4109.84	-7279.84	26.88	22.44	-7.82	-7.00	-3.94
548.16	0.7594	-3563.70	-6894.70	27.88	22.68	-7.23	-6.33	-3.64
573.16	0.7125	-2916.63	-6410.63	29.08	22.94	-6.44	-5.63	-3.24
598.16	0.6540	-2331.26	-5989.26	29.96	23.24	-6.01	-5.04	-3.03
623.16	0.5668	-1525.21	-5349.21	31.43	23.64	-5.10	-4.32	-2.56
635.00	0.5082	-727.09	-4630.09	32.50	23.92	-4.37	-3.67	-2.20
647.00	0.3220	140.00	-3844.00	34.24	24.88	-3.67	-2.99	-1.85

[illegible] GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY [illegible]

SUBSTANCE: [illegible] MW: 18.0150 TTP: 273.16K TNBP: 373.16K TTC: 647.00K

[illegible]

INTERNAL ROTATION MOMENTS: .1023-[illegible] .1921-039 .2944-039 SYM NO: 2.00

[illegible] (1 [illegible]): .0000+000

[illegible] (1 [illegible]): .00

VIB FREQ: (1 [illegible]): [illegible]5.00 1594.00 3930.00

[illegible] 1 1 1

TOTAL QUANTITIES

TEMP DEG K	[illegible]	C(O)	H(O)-H(OO)	S(O)	F(O)-H(OO)	RT	E(O)-E(OO)
[illegible]	.15731+01	.7151+01	.15990+04	[illegible]	-.67077+04	397.44	.1182+04
273.[illegible]	[illegible]	.7574+01	.21721+04	.44421+02	-.09620+04	542.32	.1623+04
[illegible]	[illegible]	[illegible]	[illegible]	.45121+02	-.11007+05	592.50	.1779+04
[illegible]	[illegible]	[illegible]	.23363+04	.45179+02	-.11165+05	596.13	.1790+04
350.[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.13455+05	695.52	.2092+04
373.[illegible]	[illegible]	.8037+01	[illegible]	.46325+02	-.14535+05	741.54	.2233+04
375.[illegible]	[illegible]	[illegible]	.29891+04	[illegible]	-.14027+05	745.20	.2244+04
[illegible]	[illegible]	[illegible]	[illegible]	.47452+02	-.15719+05	791.22	.2385+04
400.[illegible]	[illegible]	.8134+01	[illegible]	.47402+02	-.15004+05	794.88	.2397+04
423.[illegible]	[illegible]	.8173+01	[illegible]	.47349+02	-.16393+05	840.90	.2540+04
[illegible]	[illegible]	.8271+01	[illegible]	[illegible]	-.18124+05	890.58	.2655+04
473.[illegible]	[illegible]	[illegible]	.37024+04	[illegible]	-.19330+05	940.25	.2852+04
[illegible]	[illegible]	.8344+01	[illegible]	[illegible]	-.21552+05	989.94	.3010+04
[illegible]	[illegible]	[illegible]	[illegible]	.49028+02	-.20949+05	993.59	.3022+04
[illegible]	[illegible]	.8404+01	[illegible]	[illegible]	[illegible]	1039.62	.3179+04
[illegible]	[illegible]	[illegible]	.44264+04	.50102+02	-.23044+05	1089.30	.3331+04
573.[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.24201+05	1128.98	.3424+04
[illegible]	[illegible]	[illegible]	[illegible]	.50347+02	-.23553+05	1138.66	.3553+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.26044+05	1238.34	.3824+04
[illegible]	[illegible]	[illegible]	[illegible]	.51504+02	-.27451+05	1251.37	.3903+04
647.[illegible]	[illegible]	.8917+01	[illegible]	[illegible]	[illegible]	1285.71	.3964+04

APPENDIX C-12

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: N-OCTANE MOLECULAR WEIGHT:114.2200 OMEGA: 0.4030

TRIPLE POINT: 216.38 K N-BOILING POINT: 398.83 K

CRITICAL POINT: 569.40 K 24.60 ATM 0.4860 L/GMOLE ZC 0.2560

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.92377 B= 1355.12598 C= 209.51700 NC= 219.05653
GAMSON-WATSON: A= 3.2266 BL= 0.2364 B= 7.4928

FRANCIS CONSTANTS: A= 0.0446 B= 0.7158E-03 C= 10.00 E= 608.12
G= 0.4288E-03 H= 2.61

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
216.38	0.0	4843.00	98.75	1.0000	-19.71	38.57
250.00	0.0	5987.00	103.94	0.9980	-13.97	39.29
298.16	0.0	7926.00	111.62	0.9896	-7.94	40.16
300.00	0.0	8003.00	111.84	0.9890	-7.73	40.19
323.16	0.0	9002.00	115.60	0.9870	-5.39	40.56
348.16	31.70	10180.00	118.72	0.9800	-3.29	40.93
373.16	61.10	11580.60	122.69	0.9710	-1.53	41.28
393.16	92.80	12940.00	125.85	0.9590	-0.04	41.60
398.83	95.00	12970.00	125.93	0.9563	0.02	41.61
400.00	107.00	13040.00	126.08	0.9550	0.11	41.62
423.16	158.00	14340.00	130.13	0.9310	1.71	41.90
448.16	248.00	15860.00	133.42	0.8910	2.96	42.19
473.16	362.00	17600.00	137.00	0.8220	4.17	42.46
498.16	565.00	19280.00	140.26	0.7470	5.43	42.71
500.00	588.00	19400.00	140.50	0.7360	5.54	42.73
523.16	859.00	21030.00	143.50	0.6700	6.78	42.96
548.16	1323.00	22320.00	147.71	0.5480	8.43	43.19
569.40	2750.00	23890.00	150.41	0.2560	11.80	43.38

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
216.38	0.4923E-04	0.1185	0.14947	0.3607E 05	429.875	10592.	11022.	50.94
250.00	0.3831E-03	0.0856	0.15483	0.2318E 05	495.670	10109.	10605.	42.42
298.16	0.1839E-01	0.0567	0.16342	0.1317E 04	586.111	9329.	9915.	33.25
300.00	0.2040E-01	0.0559	0.16378	0.1194E 04	589.363	9286.	9876.	32.92
323.16	0.6626E-01	0.0463	0.16842	0.3350E 03	633.396	8850.	9483.	29.35
348.16	0.1906E 00	0.0385	0.17387	0.1469E 03	677.043	8409.	9086.	26.10
373.16	0.4621E 00	0.0326	0.17989	0.6434E 02	717.833	8007.	8725.	23.38
398.16	0.9817E 00	0.0279	0.18664	0.3192E 02	754.144	7619.	8373.	21.03
398.43	0.1000E 01	0.0278	0.18684	0.3136E 02	754.779	7606.	8360.	20.96
400.00	0.1033E 01	0.0276	0.18718	0.3034E 02	754.224	7566.	8321.	20.80
423.16	0.1878E 01	0.0241	0.19437	0.1722E 02	773.834	7131.	7905.	18.68
448.16	0.3237E 01	0.0213	0.20349	0.1012E 02	777.350	6633.	7410.	16.53
473.16	0.5348E 01	0.0190	0.21477	0.5968E 01	744.880	5944.	6689.	14.14
498.16	0.8388E 01	0.0171	0.22978	0.3738E 01	712.422	5348.	6060.	12.17
500.00	0.8654E 01	0.0169	0.23112	0.3584E 01	702.537	5251.	5954.	11.91
523.16	0.1259E 02	0.0155	0.24958	0.2315E 01	629.634	4465.	5095.	9.74
548.16	0.1821E 02	0.0141	0.28537	0.1354E 01	470.973	3165.	3635.	6.63
569.40	0.2429E 02	0.0130	0.48604	0.4860E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
216.38	0.7642	-5748.68	-10591.68	67.52	29.07	-21.73	-24.63	-10.94
250.00	0.7377	-4122.40	-10109.40	75.49	29.57	-18.74	-20.35	-9.43
298.16	0.6989	-1402.52	-9328.52	86.31	30.21	-15.36	-15.74	-7.73
300.00	0.6974	-1283.22	-9286.22	86.66	30.23	-15.22	-15.58	-7.66
323.16	0.6782	152.14	-8849.86	91.65	30.51	-13.90	-13.78	-6.99
348.16	0.6569	1739.29	-8440.70	95.92	30.79	-12.66	-12.20	-6.37
373.16	0.6349	3512.72	-8067.88	100.84	31.07	-11.64	-10.83	-5.86
398.16	0.6120	5225.52	-7711.48	104.86	31.34	-10.73	-9.75	-5.40
398.43	0.6113	5269.33	-7700.67	104.95	31.34	-10.72	-9.72	-5.39
400.00	0.6102	5366.58	-7673.42	105.17	31.36	-10.64	-9.69	-5.36
423.16	0.5876	7050.68	-7289.32	109.74	31.60	-10.09	-8.67	-5.08
448.16	0.5613	8979.50	-6880.50	113.93	31.86	-9.17	-7.73	-4.61
473.16	0.5318	11294.31	-6305.69	118.69	32.13	-7.98	-6.71	-4.01
498.16	0.4971	13366.97	-5913.03	122.66	32.42	-7.30	-5.97	-3.67
500.00	0.4942	13560.87	-5839.13	123.05	32.44	-7.16	-5.88	-3.60
523.16	0.4576	15706.00	-5324.00	126.98	32.73	-6.29	-5.12	-3.16
548.16	0.4003	17832.48	-4487.52	132.65	33.13	-5.01	-4.12	-2.52
569.40	0.2350	21140.00	-2750.00	136.61	34.31	-2.73	-2.43	-1.37

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: N-OCTANE MW:114.2240 TTP: 216.38K TNBP: 398.83K TTC: 569.40

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .5650-037 .5650-037 .1000-037 SYM NO: 1.00

INT ROT MOM: (7): .4510-039 .1600-038 .4400-038 .5000-038 .4400-038 .1600-038 .4510-039

INT ROT POT: (7): 4200.00 1600.00 1600.00 1600.00 1600.00 1600.00 4200.00

VIB FREQ: (5): 3000.00 1440.00 950.00 1000.00 280.00

FREQ DEGEN: 18 12 22 7 6

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
216.38	.70201+03	.3574+02	.52727+04	.98758+02	-.16097+05	429.99	.4843+04
250.00	.96850+03	.3923+02	.64833+04	.10394+03	-.19501+05	496.80	.5987+04
298.16	.14866+04	.4521+02	.85164+04	.11162+03	-.24763+05	592.50	.7926+04
300.00	.15101+04	.4547+02	.85991+04	.11184+03	-.24955+05	596.16	.8003+04
323.16	.18266+04	.4767+02	.96443+04	.11560+03	-.27712+05	642.18	.9002+04
348.16	.22168+04	.5121+02	.10870+05	.11872+03	-.30461+05	691.86	.1010+05
373.16	.26660+04	.5497+02	.12319+05	.12269+03	-.33462+05	741.54	.1158+05
398.16	.31705+04	.5836+02	.13728+05	.12585+03	-.36380+05	791.22	.1294+05
398.83	.31846+04	.5842+02	.13767+05	.12593+03	-.36459+05	792.55	.1297+05
400.00	.32097+04	.5861+02	.13835+05	.12608+03	-.36598+05	794.88	.1304+05
423.16	.37536+04	.6051+02	.15178+05	.13013+03	-.39889+05	840.90	.1434+05
448.16	.43971+04	.6365+02	.16749+05	.13342+03	-.43046+05	890.58	.1566+05
473.16	.50419+04	.6661+02	.18540+05	.13700+03	-.46284+05	940.26	.1760+05
493.16	.57867+04	.6946+02	.20268+05	.14026+03	-.49605+05	989.94	.1928+05
500.00	.59462+04	.6967+02	.20398+05	.14050+03	-.49653+05	993.59	.1940+05
523.16	.65983+04	.7215+02	.22066+05	.14350+03	-.53008+05	1039.62	.2103+05
548.16	.74702+04	.7349+02	.24410+05	.14771+03	-.57557+05	1089.30	.2232+05
569.40	.82605+04	.7659+02	.25024+05	.15041+03	-.60629+05	1131.51	.2389+05

APPENDIX C-13

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: METHYL ALCOHOL MOLECULAR WEIGHT: 32.0400 OMEGA: 0.5560

TRIPLE POINT: 175.48 K N-BOILING POINT: 337.80 K

CRITICAL POINT: 512.28 K 78.70 ATM 0.1180 L/GMOLE ZC 0.2240

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 7.89750 B= 1474.07983 C= 229.12999 NC= 243.70482
WAMSON-WATSON: A= 3.6072 BL= 0.2222 B= 8.3802

FRANCIS CONSTANTS: A= 1.0493 B= 0.7827E-03 C= 6.00 E= 507.77
G= 0.1010E-02 H= 2.47

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
175.48	0.0	1223.00	53.27	1.0000	-23.24	33.73
273.16	0.0	1900.00	56.26	0.9760	-6.48	35.93
298.16	0.0	2126.00	57.29	0.9640	-3.59	36.37
300.00	0.0	2140.00	57.35	0.9620	-3.40	36.40
323.16	20.00	2345.00	58.18	0.9530	-1.21	36.77
337.86	41.00	2471.00	58.60	0.9474	0.12	36.99
348.16	71.00	2587.00	59.06	0.9400	0.97	37.14
373.16	143.00	2816.00	59.76	0.9210	2.86	37.48
398.16	264.00	3064.00	60.58	0.8920	4.53	37.81
400.00	274.00	3082.00	60.63	0.8900	4.69	37.83
423.16	437.00	3348.00	61.45	0.8380	6.18	38.11
448.16	682.00	3616.00	62.11	0.7590	7.83	38.40
473.16	1058.00	3896.00	62.76	0.6510	9.64	38.66
498.16	1689.00	4176.00	63.54	0.4960	11.80	38.92
500.00	1761.00	4198.00	63.59	0.4800	12.02	38.94
512.28	3207.00	4347.00	63.90	0.2240	15.60	39.06

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
175.48	0.8396E-05	0.1592	0.03584	0.1723E 07	348.621	9389.	9738.	55.49
273.16	0.3831E-01	0.0647	0.03956	0.5711E 03	529.617	8823.	9353.	34.24
298.16	0.1645E 00	0.0526	0.04070	0.1434E 03	570.859	8375.	8945.	30.00
300.00	0.1811E 00	0.0518	0.04078	0.1308E 03	573.173	8335.	8908.	29.69
323.16	0.5441E 00	0.0436	0.04194	0.4644E 02	611.284	7994.	8606.	26.63
337.86	0.9990E 00	0.0393	0.04275	0.2627E 02	634.875	7798.	8433.	24.96
348.16	0.1478E 01	0.0367	0.04334	0.1816E 02	648.626	7638.	8287.	-23.80
373.16	0.3478E 01	0.0311	0.04496	0.8108E 01	678.993	7200.	7879.	21.12
398.16	0.7180E 01	0.0271	0.04692	0.4059E 01	697.427	6814.	7512.	18.87
400.00	0.7545E 01	0.0268	0.04708	0.3872E 01	698.655	6788.	7487.	18.72
423.16	0.1354E 02	0.0238	0.04951	0.2148E 01	688.255	6254.	6942.	16.41
448.16	0.2376E 02	0.0212	0.05321	0.1175E 01	645.167	5487.	6132.	13.68
473.16	0.3925E 02	0.0190	0.05908	0.6440E 00	555.807	4444.	5000.	10.57
498.16	0.6164E 02	0.0171	0.07105	0.3289E 00	384.845	2903.	3287.	6.60
500.00	0.6361E 02	0.0170	0.07264	0.3096E 00	364.939	2741.	3106.	6.21
512.28	0.7801E 02	0.0162	0.11779	0.1178E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
175.48	0.8939	-8166.24	-9389.24	21.02	21.82	-20.34	-26.93	-10.24
273.16	0.8099	-6923.41	-8823.41	28.50	23.33	-15.16	-16.25	-7.63
298.16	0.7873	-6248.62	-8374.62	30.88	23.65	-13.70	-14.13	-6.89
300.00	0.7856	-6194.54	-8334.54	31.05	23.67	-13.57	-13.98	-6.83
323.16	0.7639	-5669.41	-8014.41	32.76	23.95	-12.60	-12.48	-6.34
337.86	0.7495	-5367.90	-7838.90	33.52	24.12	-12.21	-11.68	-6.15
348.16	0.7392	-5122.28	-7709.28	34.29	24.24	-11.87	-11.14	-5.97
373.16	0.7127	-4527.31	-7343.31	35.78	24.52	-11.01	-9.90	-5.54
398.16	0.6829	-4014.14	-7078.14	37.19	24.80	-10.39	-8.95	-5.23
400.00	0.6805	-3979.89	-7061.89	37.23	24.82	-10.40	-8.88	-5.23
423.16	0.6472	-3342.82	-6690.82	38.86	25.09	-9.56	-7.96	-4.81
448.16	0.6022	-2553.01	-6169.01	40.60	25.40	-8.52	-6.93	-4.29
473.16	0.5423	-1606.14	-5502.14	42.56	25.77	-7.31	-5.85	-3.68
498.16	0.4509	-415.59	-4591.59	45.14	26.29	-5.77	-4.64	-2.90
500.00	0.4411	-303.95	-4501.95	45.36	26.35	-5.64	-4.53	-2.84
512.28	0.2720	1140.00	-3207.00	48.30	27.38	-3.92	-3.15	-1.97

IDEAL GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

COMPOUND: METHYL ALCOHOL   MW: 32.043[illegible]   TTP: 175.43K   TNBP: 337.80K   TTC: 512.28K

[illegible]

INTERNAL ROTATION MOMENTS: .[illegible]-0[illegible] .3[illegible]-0[illegible]3 .0[illegible]5-0[illegible] SYM NO: 1.00

[illegible] ( ): .[illegible]-0[illegible]

[illegible] ( ): [illegible].00

[illegible] ( ): [illegible].00 [illegible].00 1033.00 3420.00 1[illegible].00

[illegible]: 3 3 1 1 3

[illegible]

TEMP	[illegible]	C(P)	H(T)-H(0)	S(T)	F(T)-H(00)	RT	E(T)-E(00)
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.7777[illegible]+04	348.71	.1227+04
[illegible]	.177[illegible]	[illegible]	.2[illegible]	[illegible]	-.12925+05	542.32	.1909+04
[illegible]	[illegible]	[illegible]	.27[illegible]	[illegible]	-.14305+05	592.50	.2126+04
[illegible]	[illegible]	.1072+02	.27[illegible]+04	.57[illegible]1+02	-.1445[illegible]+05	595.10	.2140+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	642.17	.2345+04
[illegible]	[illegible]	.11[illegible]+02	[illegible]	[illegible]	-.1[illegible]57+05	671.30	.2471+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	691.50	.2527+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.1874[illegible]+05	741.34	.2810+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	791.22	.3004+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.2037[illegible]+05	794.33	.3032+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	845.95	.3240+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.2333[illegible]+05	890.53	.3510+04
[illegible]	[illegible]	.1277+[illegible]	[illegible]	[illegible]	-.24[illegible]1+05	940.26	.3890+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]44+02	-.2546[illegible]+05	933.34	.4175+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.2[illegible]+05	991.59	.4128+04
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	-.27371+05	1018.00	.4347+04

APPENDIX C-14

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: N-DECANE MOLECULAR WEIGHT:142.2800 OMEGA: 0.5860

TRIPLE POINT: 243.51 K N-BOILING POINT: 447.30 K

CRITICAL POINT: 617.60 K 20.80 ATM 0.6020 L/GMOLE ZC 0.2470

VAPOR PRESSURE CONSTANTS:
ANTOINE: A= 6.95367 B= 1501.26782 C= 194.48000 NC= 206.01999
GAMSON-WATSON: A= 3.4177 BL= 0.0 B= 7.6037

FRANCIS CONSTANTS: A= 0.9491 B= 0.6899E-03 C= 6.00 E= 615.33
G= 0.5379E-03 H= 2.39

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
243.51	0.0	7216.00	120.10	0.9700	-20.31	39.81
250.00	0.0	7500.00	121.07	0.9700	-19.16	39.94
273.16	0.0	8580.00	126.11	0.9690	-15.51	40.38
298.16	0.0	9919.00	130.53	0.9686	-12.19	40.82
300.00	0.0	10020.00	130.81	0.9680	-11.97	40.85
323.16	0.0	11240.00	135.64	0.9660	-9.38	41.22
348.16	6.00	12730.00	139.52	0.9640	-6.85	41.59
373.16	11.00	14500.00	144.27	0.9600	-4.69	41.93
398.16	33.00	16220.00	148.23	0.9560	-2.87	42.26
400.00	38.00	16350.00	148.52	0.9550	-2.74	42.28
423.16	62.00	17940.00	152.58	0.9470	-1.31	42.56
447.28	123.00	19780.00	157.52	0.9351	0.36	42.83
448.16	135.00	19850.00	157.66	0.9310	0.44	42.84
473.16	271.00	22000.00	162.03	0.9130	1.90	43.11
498.16	371.00	24110.00	166.09	0.8743	3.12	43.37
500.00	392.00	24270.00	166.37	0.8637	3.26	43.39
523.16	515.00	26310.00	170.10	0.7900	4.49	43.61
548.16	695.00	27830.00	175.35	0.7160	5.92	43.85
573.16	1202.00	30150.00	179.30	0.6160	7.33	44.07
598.16	1816.00	32550.00	183.20	0.4820	9.00	44.28
600.00	1902.00	32730.00	183.49	0.4660	9.18	44.29
617.60	3199.00	34500.00	186.55	0.2470	11.84	44.44

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
243.51	0.3638E-04	0.1111	0.18600	0.5328E 06	469.260	12229.	12699.	52.15
250.00	0.6482E-04	0.1047	0.18716	0.3070E 06	481.766	12125.	12607.	50.43
273.16	0.4081E-03	0.0854	0.19147	0.5323E 05	525.854	11742.	12268.	44.91
298.16	0.2164E-02	0.0696	0.19639	0.1095E 05	573.735	11337.	11911.	39.95
300.00	0.2420E-02	0.0686	0.19676	0.9946E 04	576.917	11300.	11877.	39.59
323.16	0.3892E-02	0.0575	0.20164	0.2881E 04	620.140	10907.	11527.	35.67
348.16	0.3176E-01	0.0476	0.20727	0.8672E 03	666.619	10381.	11048.	31.73
373.16	0.9437E-01	0.0399	0.21335	0.3115E 03	711.204	9868.	10579.	28.35
398.16	0.2365E 00	0.0339	0.21998	0.1321E 03	754.948	9425.	10180.	25.57
400.00	0.2516E 00	0.0335	0.22049	0.1246E 03	757.565	9388.	10146.	25.36
423.16	0.5186E 00	0.0291	0.22731	0.6342E 02	793.269	8985.	9778.	23.11
447.28	0.9999E 00	0.0254	0.23562	0.3432E 02	825.223	8566.	9391.	21.00
448.16	0.1023E 01	0.0253	0.23593	0.3348E 02	823.071	8517.	9346.	20.84
473.16	0.1850E 01	0.0222	0.24559	0.1916E 02	847.231	8058.	8906.	19.82
498.16	0.3060E 01	0.0196	0.25724	0.1168E 02	846.219	7410.	8256.	16.57
500.00	0.3172E 01	0.0194	0.25820	0.1117E 02	838.116	7309.	8147.	16.29
523.16	0.4877E 01	0.0178	0.27183	0.6953E 01	788.984	6541.	7330.	14.01
548.16	0.7451E 01	0.0162	0.29113	0.4323E 01	727.219	5721.	6442.	11.76
573.16	0.1097E 02	0.0148	0.31925	0.2641E 01	616.648	4612.	5229.	9.12
598.16	0.1563E 02	0.0136	0.37018	0.1513E 01	432.666	3083.	3516.	5.68
600.00	0.1603E 02	0.0135	0.37610	0.1431E 01	407.525	2908.	3317.	5.53
617.60	0.2019E 02	0.0127	0.60238	0.6029E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
243.51	0.7650	-5013.29	-12229.29	88.26	30.52	-22.54	-25.27	-11.34
250.00	0.7602	-4625.27	-12125.27	89.81	30.61	-21.93	-24.41	-11.04
273.16	0.7431	-3161.91	-11741.91	96.71	30.92	-19.94	-21.63	-10.03
298.16	0.7245	-1617.78	-11336.78	102.78	31.23	-18.17	-19.13	-9.14
300.00	0.7231	-1280.30	-11300.30	103.19	31.25	-19.02	-18.96	-9.07
323.16	0.7056	333.27	-10906.73	109.36	31.52	-16.59	-16.98	-8.35
348.16	0.6864	2342.77	-10387.23	114.64	31.80	-15.09	-15.01	-7.59
373.16	0.6669	4621.02	-9878.98	120.61	32.06	-13.79	-13.32	-6.94
398.16	0.6468	6761.62	-9438.38	125.53	32.32	-12.77	-11.95	-6.42
400.00	0.6451	6923.95	-9426.05	125.90	32.34	-12.68	-11.85	-6.38
423.16	0.6259	8892.79	-9047.21	131.78	32.56	-11.81	-10.76	-5.94
447.28	0.6039	11091.16	-8688.84	136.16	32.80	-11.32	-9.78	-5.70
448.16	0.6041	11197.73	-8652.27	136.39	32.81	-11.25	-9.72	-5.66
473.16	0.5793	13671.22	-8328.78	141.31	33.05	-10.66	-8.86	-5.36
498.16	0.5531	16369.08	-7740.92	146.39	33.30	-9.62	-7.62	-4.84
500.00	0.5510	16569.14	-7700.86	146.92	33.32	-9.48	-7.75	-4.77
523.16	0.5234	19254.17	-7055.83	151.60	33.55	-8.44	-6.79	-4.25
548.16	0.4887	21214.36	-6515.64	157.67	33.83	-7.67	-6.07	-3.86
573.16	0.4457	24335.65	-5814.35	162.89	34.15	-6.53	-5.10	-3.29
598.16	0.3844	27651.12	-4898.88	168.32	34.57	-5.17	-4.12	-2.60
600.00	0.3783	27920.21	-4809.79	168.78	34.61	-5.02	-4.04	-2.53
617.60	0.2360	31301.00	-3199.00	174.71	35.63	-3.03	-2.61	-1.53

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: N-DECANE MW:142.2760 TTP: 243.51K TNBP: 447.28K TTC: 617.60K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: .2680-036 .2680-036 .3780-038 SYM NO: 1.00

INT ROT MOM: (9): .4400-039 .1600-038 .4400-038 .5000-038 .5500-038 .5000-038 .4400-038 .1600-038 .4400-039

INT ROT POT: (9): 4200.00 1600.00 1600.00 1600.00 1600.00 1600.00 1600.00 1600.00 4200.00

VIB FREQ: (5): 3000.00 1440.00 950.00 1000.00 280.00

FREQ DEGEN: 22 14 28 9 8

HECK

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(0)	H(0)-H(00)	S(0)	F(0)-H(00)	RT	E(0)-E(00)
243.51	.11531+04	.4760+02	.76998+04	.12010+03	-.21545+05	483.90	.7216+04
250.00	.12287+04	.4864+02	.79965+04	.12107+03	-.22269+05	496.80	.7500+04
273.16	.15297+04	.5148+02	.91227+04	.12611+03	-.25327+05	542.82	.8580+04
298.16	.19123+04	.5602+02	.10511+05	.13053+03	-.28410+05	592.50	.9919+04
300.00	.19429+04	.5635+02	.10612+05	.13081+03	-.28634+05	596.16	.1002+05
323.16	.23588+04	.5897+02	.11886+05	.13564+03	-.31945+05	642.18	.1124+05
348.16	.28731+04	.6343+02	.13420+05	.13952+03	-.35155+05	691.86	.1273+05
373.16	.34582+04	.6809+02	.15245+05	.14427+03	-.38592+05	741.54	.1450+05
398.16	.41167+04	.7235+02	.17010+05	.14823+03	-.42007+05	791.22	.1622+05
400.00	.41681+04	.7266+02	.17144+05	.14852+03	-.42262+05	794.88	.1635+05
423.16	.48508+04	.7483+02	.18776+05	.15358+03	-.46213+05	840.90	.1794+05
447.28	.56321+04	.7862+02	.20669+05	.15752+03	-.49786+05	888.83	.1978+05
448.16	.56620+04	.7876+02	.20740+05	.15766+03	-.49918+05	890.58	.1985+05
473.16	.65514+04	.8245+02	.22944+05	.16203+03	-.53723+05	940.26	.2200+05
498.16	.75200+04	.8601+02	.25102+05	.16608+03	-.57632+05	989.94	.2411+05
500.00	.75944+04	.8626+02	.25265+05	.16637+03	-.57923+05	993.59	.2427+05
523.16	.85682+04	.8939+02	.27347+05	.17010+03	-.61641+05	1039.62	.2631+05
548.16	.96962+04	.9086+02	.28920+05	.17535+03	-.67199+05	1089.30	.2783+05
573.16	.10904+05	.9392+02	.31291+05	.17930+03	-.71474+05	1138.98	.3015+05
598.16	.12192+05	.9683+02	.33738+05	.18320+03	-.75846+05	1188.66	.3255+05
600.00	.12290+05	.9704+02	.33921+05	.18349+03	-.76172+05	1192.31	.3273+05
617.60	.13248+05	.9878+02	.35726+05	.18655+03	-.79489+05	1227.29	.3450+05

APPENDIX C-15

CONFIGURATIONAL ENERGY, ENTHALPY, AND ENTROPY AT SATURATION

PROGRAM DEVELOPED BY K. E. BUSH AND H. W. PRENGLE, JR.

SUBSTANCE: ISOPROPYL ALCOHOL MOLECULAR WEIGHT: 60.0900 OMEGA: 0.7730

TRIPLE POINT: 185.20 K N-BOILING POINT: 355.39 K

CRITICAL POINT: 508.32 K 53.00 ATM 0.2200 L/GMOLE ZC 0.2480

VAPOR PRESSURE CONSTANTS:

ANTOINE: A= 8.14504 B= 1581.00977 C= 218.09999 NC= 235.41866

GAMSON-WATSON: A= 3.8997 BL= 0.3128 B= 8.5015

FRANCIS CONSTANTS: A= 1.0171 B= 0.6472E-03 C= 9.00 E= 507.39
G= 0.6650E-03 H= 2.89

INPUT DATA:

TEMP	E(0)-E(SV)	E(0)-E(00)	S(0)	Z(VAP)	S(0)-S(SV)	STR
185.20	0.0	1678.00	65.40	1.0000	-24.97	35.88
273.16	0.0	3062.00	72.11	1.0000	-8.99	37.81
298.16	0.0	3530.00	73.97	0.9990	-5.67	38.24
300.00	0.0	3561.00	74.07	0.9890	-5.45	38.28
324.56	10.00	4002.00	75.36	0.9700	-2.76	38.67
339.23	20.00	4346.00	76.59	0.9500	-1.37	38.89
355.39	40.00	4684.00	77.64	0.9438	0.61	39.12
373.16	70.00	5159.00	78.56	0.9200	1.55	39.36
398.16	151.00	5718.00	80.01	0.8870	3.34	39.68
400.00	161.00	5760.00	80.11	0.8710	3.48	39.71
423.16	262.00	6354.00	81.98	0.8350	4.95	39.99
448.16	454.00	6981.00	83.41	0.7820	6.54	40.27
473.16	777.00	7640.00	84.83	0.6760	8.29	40.54
498.16	1474.00	8329.00	86.24	0.4840	10.77	40.80
500.00	1565.00	8380.00	86.34	0.4620	11.03	40.82
508.32	2546.00	8689.00	87.47	0.2480	13.61	40.90

TEMP	P ATM	D(LN P)/DT	VL, L/GMOLE	VG, L/GMOLE	P(VG-VL)	DEL E(V)	DEL H(V)	DEL S(V)
185.20	0.3488E-05	0.1674	0.06912	0.4358E 07	367.931	11040.	11408.	61.60
273.16	0.1083E-01	0.0761	0.07494	0.2069E 04	542.658	10741.	11283.	41.31
298.16	0.5764E-01	0.0616	0.07693	0.4241E 03	591.645	10275.	10867.	36.45
300.00	0.6450E-01	0.0607	0.07708	0.3775E 03	589.324	10138.	10728.	35.76
324.56	0.2499E 00	0.0501	0.07929	0.1034E 03	624.969	9542.	10167.	31.33
339.23	0.5019E 00	0.0451	0.08076	0.5269E 02	639.260	9137.	9776.	28.82
355.39	0.1000E 01	0.0404	0.08255	0.2753E 02	664.364	8865.	9529.	26.81
373.16	0.1968E 01	0.0360	0.08481	0.1431E 02	677.996	8424.	9102.	24.39
398.16	0.4267E 01	0.0298	0.08866	0.6792E 01	692.469	7527.	8219.	20.64
400.00	0.4506E 01	0.0295	0.08897	0.6345E 01	682.450	7367.	8049.	20.12
423.16	0.8544E 01	0.0259	0.09341	0.3393E 01	682.644	6803.	7486.	17.69
448.16	0.1570E 02	0.0229	0.09993	0.1832E 01	658.262	6093.	6751.	15.06
473.16	0.2696E 02	0.0204	0.11013	0.9735E 00	563.566	4887.	5451.	11.52
498.16	0.4379E 02	0.0184	0.13340	0.4519E 00	337.591	2758.	3096.	6.21
500.00	0.4529E 02	0.0183	0.13701	0.4186E 00	308.700	2512.	2820.	5.64
508.32	0.5259E 02	0.0177	0.22011	0.2201E 00	0.0	0.	0.	0.0

TEMP	RHO	EL	EC	SL	STR*	SC*	EC/RT	SC*/R
185.20	0.8693	-9362.26	-11040.26	28.77	25.16	-25.91	-30.00	-13.04
273.16	0.8019	-7678.75	-10740.75	39.80	26.48	-20.99	-19.79	-10.56
298.16	0.7811	-6744.91	-10274.91	43.20	26.79	-19.32	-17.34	-9.72
300.00	0.7795	-6577.37	-10138.37	43.76	26.82	-18.85	-17.01	-9.49
324.56	0.7578	-5549.91	-9551.91	46.79	27.11	-17.01	-14.81	-8.56
339.23	0.7440	-4810.86	-9156.86	49.14	27.28	-15.84	-13.58	-7.97
355.39	0.7279	-4221.02	-8905.02	50.22	27.46	-15.76	-12.61	-7.93
373.16	0.7085	-3335.20	-8494.20	52.62	27.66	-14.24	-11.45	-7.17
398.16	0.6778	-1959.67	-7677.67	56.02	27.94	-12.24	-9.70	-6.16
400.00	0.6754	-1767.67	-7527.67	56.51	27.96	-11.85	-9.47	-5.97
423.16	0.6433	-711.39	-7065.39	59.34	28.23	-10.88	-8.40	-5.48
448.16	0.6013	433.99	-6547.01	61.81	28.53	-9.86	-7.35	-4.96
473.16	0.5456	1975.67	-5664.33	65.02	28.89	-8.15	-6.02	-4.10
498.16	0.4504	4096.64	-4232.36	69.25	29.42	-5.61	-4.28	-2.82
500.00	0.4380	4303.32	-4076.68	69.67	29.49	-5.34	-4.10	-2.69
508.32	0.2730	6143.00	-2546.00	73.86	30.48	-3.19	-2.52	-1.60

PERFECT GAS STATE THERMODYNAMIC PROPERTIES BY STATISTICAL THERMODYNAMIC METHODS

INCLUDING HINDERED INTERNAL ROTATION CORRECTIONS BY PITZER

DEVELOPED BY K. E. BUSH

SUBSTANCE: ISOPROPYL ALCOHOL MW: 60.0970 TTP: 185.20K TNBP: 355.39K TTC: 508.3?K

ASSIGNMENTS

EXTERNAL ROTATION MOMENTS: 0.2700E-37 0.2700E-37 0.1170E-37 SYM NO: 1.00

INT ROT MOM: (3): 0.50E-39 0.50E-39 0.13E-39

INT ROT POT: (3): 4000.00 4000.00 800.00

VIB FREQ: (6): 3020.00 1423.00 1173.00 917.00 500.00 400.00

FREQ DEGEN: 8 7 5 4 2 1

TOTAL QUANTITIES

TEMP DEG K	LN Q	C(O)	H(O)-H(OO)	S(O)	F(O)-H(OO)	RT	E(O)-E(OO)
185.20	0.22645E+03	0.1488E+02	0.20465E+04	0.65400E+02	-0.10066E+05	368.03	0.1678E+04
273.16	0.37151E+03	0.1961E+02	0.36052E+04	0.72112E+02	-0.16093E+05	542.82	0.3062E+04
298.16	0.44284E+03	0.2103E+02	0.41221E+04	0.73975E+02	-0.17934E+05	592.50	0.3530E+04
300.00	0.44871E+03	0.2113E+02	0.41575E+04	0.74071E+02	-0.18064E+05	596.16	0.3561E+04
324.56	0.53562E+03	0.2242E+02	0.46469E+04	0.75360E+02	-0.19812E+05	644.96	0.4002E+04
339.23	0.59548E+03	0.2331E+02	0.50203E+04	0.76590E+02	-0.20962E+05	674.11	0.4346E+04
355.39	0.66866E+03	0.2420E+02	0.53902E+04	0.77644E+02	-0.22205E+05	706.23	0.4684E+04
373.16	0.75821E+03	0.2526E+02	0.59001E+04	0.78563E+02	-0.23416E+05	741.54	0.5159E+04
398.16	0.90097E+03	0.2659E+02	0.65091E+04	0.80007E+02	-0.25346E+05	791.22	0.5718E+04
400.00	0.91228E+03	0.2669E+02	0.65552E+04	0.80113E+02	-0.25490E+05	794.88	0.5760E+04
423.16	0.10641E+04	0.2784E+02	0.71951E+04	0.81982E+02	-0.27496E+05	840.90	0.6354E+04
448.16	0.12484E+04	0.2912E+02	0.78719E+04	0.83410E+02	-0.29509E+05	890.58	0.6931E+04
473.16	0.14543E+04	0.3035E+02	0.85800E+04	0.84823E+02	-0.31557E+05	940.26	0.7640E+04
498.16	0.16825E+04	0.3154E+02	0.93185E+04	0.86236E+02	-0.33641E+05	989.94	0.8329E+04
500.00	0.17002E+04	0.3163E+02	0.93740E+04	0.86341E+02	-0.33796E+05	993.59	0.8380E+04
508.32	0.17816E+04	0.3178E+02	0.96992E+04	0.87467E+02	-0.34761E+05	1010.13	0.8689E+04

APPENDIX D--CONFIGURATIONAL ENTROPY

In a manner similar to the energy the entropy can be represented by,

$$S_L = S_{TR} + S_{ER} + S_I + S_C$$

$$= S_{TR}(liq) + S^\circ_{ER} + S_I{}^\circ + S_C \qquad (D\text{-}1)$$

or,

$$S_C = S_L - S_{TR}(liq) - S^\circ_{ER} - S_I{}^\circ \qquad (D\text{-}2)$$

The important difference is that $S_{TR}(liq) \neq S^\circ_{TR}$! How can it be calculated?

By analogy with the translational partition function for a perfect gas, a liquid phase partition function might be defined as,

$$q_{TR}(liq) = \left(\frac{2\pi mkT}{h^2}\right)^{\frac{3N}{2}} \frac{(V^f)^N}{N!} = \left(\frac{2\pi mkT}{h^2}\right)^{\frac{3N}{2}} \frac{(V_L)^N}{N!} \left(\frac{V^f}{V_L}\right)^N \qquad (D\text{-}3)$$

where conceptually V^f is a free volume in which the liquid translates. Then,

$$\ln q_{TR} = \frac{3N}{2} \ln T + \ln \left(\frac{2\pi mk}{h^2}\right)^{\frac{3N}{2}} \frac{(V^L)^N}{N!} \left(\frac{V^f}{V_L}\right)^N \qquad (D\text{-}4)$$

$$\left(\frac{\partial \ln q_{TR}}{\partial T}\right)_V = \frac{3N}{2T} \qquad (D\text{-}5)$$

Now, $S_{TR}(liq) = k\left[\ln q_{TR} + T \left(\frac{\partial \ln q_{TR}}{\partial T}\right)_V\right]$ (D-6)

Substituting (4) and (5) into (6) gives,

$$S_{TR}(liq) = \frac{5R}{2} + R \ln \frac{kT}{P^\circ} \left(\frac{2\pi mkT}{h^2}\right)^{3/2} + R \ln \frac{V^f}{RT/P^\circ} \qquad (D\text{-}7)$$

The first two terms on the right are recognized as S°_{TR}; then,

$$S_{TR}(liq) = S^\circ_{TR} - R \ln \frac{RT/P^\circ}{V_L} + R \ln \frac{V^f}{V_L} \qquad (D\text{-}8)$$

Substituting into (2) gives,

$$S_C = S_L - (S^\circ_{TR} - R \ln \frac{RT/P^\circ}{V_L}) - R \ln \frac{V^f}{V_L} - S^\circ_{ER} - S^\circ_I$$

and

$$(S_C + R \ln \frac{V^f}{V_L}) = S_L - (S^\circ_{TR} - R \ln \frac{RT/P^\circ}{V_L}) - S^\circ_{ER} - S^\circ_I \qquad \text{(D-9)}$$

Now since V^f is unknown, let (left hand side),

$$S_C^* \equiv S_C + R \ln \frac{V^f}{V_L} \qquad \text{(D-10)}$$

Finally, the calculatable configurational entropy can be represented as,

$$S_C^* = S_L - (S^\circ_{TR} - R \ln \frac{RT/P^\circ}{V_L}) - S^\circ_{ER} - S^\circ_I \qquad \text{(D-11)}$$

APPENDIX E

NOMENCLATURE

A, B, C = Antione Constants

AF, BF, CF, EF, GF, HF, = Francis Constants

AG, BG, b = Gamson - Watson Constants

C_p^o = Heat capacity of the perfect gas

E_o^o = Energy of the perfect gas at 0^oK

E^o = Energy of the perfect gas

E_{TR}^o = Translation energy of the perfect gas

E_{ER}^o = External rotational energy of the perfect gas

E_{IR}^o = Internal rotational energy of the perfect gas

E_{VIB}^o = Vibrational energy of the perfect gas

E_{EL}^o = Electronic energy of the perfect gas

E_L = Total energy of the liquid

E_C = Configurational energy of the liquid

E_{CTP} = Configurational energy at the triple point

E_I = Internal energy of the liquid

E_{TR} = Translational energy of the liquid

E^{sv} = Energy of the saturated vapor

$\Delta E \Big|_o^{sv}$ = Energy difference between the perfect gas and the saturated vapor

ΔE^{V} = Energy of vaporization

$\Delta E_{\Delta V}$ = Energy difference between the saturated liquid and the liquid at a point above saturation pressure

f = Fugacity

F^{O} = Free energy of the perfect gas

Ff = Free energy of free rotation

H_{o}^{o} = Enthalpy of the perfect gas at 0^{o} K

H^{O} = Enthalpy of the perfect gas

H^{SV} = Enthalpy of the saturated vapor

ΔH^{V} = Enthalpy of vaporization

I = Moment of inertia of the molecule

I_X = Moment of inertia of the molecule about the X axis

I_Y = Moment of inertia of the molecule about the Y axis

I_Z = Moment of inertia of the molecule about the Z axis

I_R = Reduced moment of internal rotation

M = Molecular weight

n = Number of maximi of the potential barrier to internal rotation per rotation

N = Number of atoms in the molecule

NC = Modified Antoine Equation constant

N_{TR} = Number of degrees of freedom of translational motion

N_{ER} = Number of degrees of freedom of external rotation

N_{IR} = Number of degrees of freedom of internal rotation

P = Vapor pressure

P^{O} = Pressure at which a substance exists as a perfect gas

P^{SV} = Vapor pressure of saturated vapor

Q = Partition function

q = Mode partition function

R = Gas constant

S^o = Entropy of the perfect gas

S_f = Entropy of free internal rotation

S_c = Configurational entropy of the liquid

$S_c^* = S_c + R \ln \frac{V^f}{V_L}$

S_{cTP} = Configurational entropy at the triple point

S_L = Total entropy of the liquid

S_{ER} = External rotational entropy of the liquid

S^{sv} = Entropy of the saturated vapor

ΔS^v = Entropy of vaporization

$\Delta S \Big|_o^{sv}$ = Entropy difference between the perfect gas and the saturated vapor

T = Temperature

T_C = Critical temperature

T_R = Reduced temperature

T_{TP} = Triple point temperature

V = Potential of restricted internal rotation as defined by Pitzer

V^f = Free volume of the system

V_G = Gas volume

V_L = Liquid volume

X = NC -273.16 + T

Y = Dummy variable, 1.4387 ν/T

Z = Compressibility factor

ρ = Liquid density

ρ_c = Critical Density

ρ_{TP} = Density at the triple point

σ = Number of equivalent positions of the molecule

ν = Frequency of the molecular vibration

ω = Acentric factor