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APPLICATIONS OF MULTIPROPERTY ANALYSIS IN THE PREDICTION OF COMPLEX-SYSTEM THERMOPHYSICAL BEHAVIOR

The University of Oklahoma PH.D. 1981

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THE UNIVERSITY OF OKLAHOMA

GRADUATE COLLEGE

APPLICATIONS OF MULTIPROPERTY ANALYSIS IN THE PREDICTION OF COMPLEX-SYSTEM THERMOPHYSICAL BEHAVIOR

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Michael Raoul Brule'

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APPLICATIONS OF MULTIPROPERTY ANALYSIS IN THE PREDICTION OF COMPLEX-SYSTEM THERMOPHYSICAL BEHAVIOR

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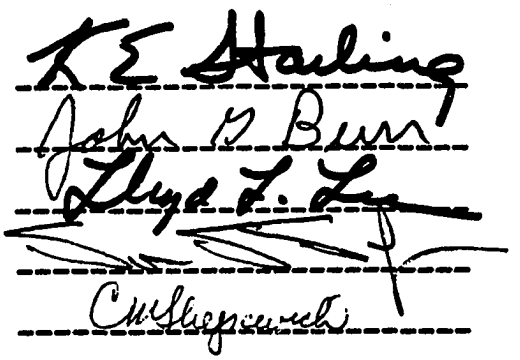

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ABSTRACT

A method has been developed for predicting compound characterization parameters used in multiparameter corresponding-states correlations. The technique employs multiproperty analysis of thermodynamic and transport data. Most of the property data utilized is similar to the inspection data obtained from industrial laboratory analyses for pseudocomponent fractions making up complex hydrocarbon mixtures. These property data include vapor pressure, density, and viscosity— the analogues for fraction inspection data such as average boiling temperature, API gravity, and Saybolt viscosity.

The objective of this work was to develop a method for obtaining correlation characterization parameters for high-molecular-weight compounds when these parameters have not been or cannot be measured. The new approach for determining correlation parameters altogether circumvents the need for critical-property data per se. The required correlation characterization parameters can be extracted using multiproperty regression analysis of the various types of inspection data. Multiproperty analysis is carried out, by simultaneous calculation of these properties, using several thermodynamic-property relations (e.g., density,

vapor pressure, enthalpy derived from an equation of state) and a viscosity correlation.

Accurate prediction of these properties has been successfully achieved by modifying the multiparameter corresponding-states correlations so that they utilize the same characterization parameters. Comprehensive applicability of the correlations has been achieved by determining universal correlation constants based on an extensive collection of low- and high-molecular-weight petroleum and coal organic compounds. These provisions have resulted in a unified framework of self-consistent correlations from which correlation characterization parameters can be determined in a self-consistent manner for predicting the thermophysical properties of complex, undefined fossil fluids.

Thermophysical-property data for over fifty organic compounds, including high-boiling-temperature hydrocarbons typical of coal-derived fluids, have been used to establish the feasibility of the technique. The overall average absolute relative deviations for the over 5000 data points analyzed are less than 2% for thermodynamic properties, and 5% for viscosity. The technique is successfully applied to complex undefined fluids from the Exxon Donor Solvent process. Volatility, density, and viscosity prediction deviations are 10% or less in most cases— sufficient for carrying out constructive process design.

APPLICATIONS OF MULTIPROPERTY ANALYSIS IN THE PREDICTION OF COMPLEX-SYSTEM THERMOPHYSICAL BEHAVIOR

Chapter I.

PROPERTIES PREDICTION FOR FOSSIL FLUIDS

Presently, most properties-correlation research is focusing on fossil fuels to rapidly develop practical properties-prediction capability for the coal demonstration-plant as well as future research programs. Fossil-fluid thermodynamic and transport properties are needed to design separation, heat-exchange, and other unit operations in coal-liquefaction plants. First-generation methodologies are being developed for predicting thermophysical properties of coal-derived fluids using current equation-of-state and transport-correlation technology (e.g., Chao et al 1980, Starling et al 1980, Hwang et al 1980, Wilson et al 1981). Previously, most equations of state and transport-property correlations could not be applied directly to coal fluids.

Recently, Starling and coworkers (1978 and 1980) developed an equation of state, cast in a multiparameter

corresponding-states (MPCS) framework, to predict the properties of organic compounds found in fossil fluids. Concurrently, transport correlations for viscosity and thermal conductivity were also developed (Chung 1980). The approach followed in these studies is unified in contrast to that pursued by other investigators in that the same correlation characterization parameters are used for both thermodynamic- and transport-property correlations (Starling et al 1978). That is, for all properties, three correlation characterization parameters, a molecular-size/separation parameter, a molecular-energy parameter, and a molecular-orientation parameter, are used to characterize nonpolar and slightly polar compounds. Using multiproperty analysis, a mutually consistent network of correlations can be developed with all correlations using the same chracterization parameters to make a respective property calculation. The use of common characterization parameters and multiproperty analysis in the development of these correlations afforded unique advantages and capabilities that made the research reported herein possible.

Capability for Predicting Coal-Fluid Properties

Completely new advances have been made in predicting the properties of high-molecular-weight fossil hydrocarbons. A three-parameter equation of state (Starling et al 1978),

based on perturbation theory (Pople 1954, Pitzer et al 1955) has been applied to predict the thermodynamic properties of pure coal chemicals (Brule' et al 1979). Less accurate estimates of properties are obtained for polar compounds (dipole moment > 2 debyes). A conformal-solution model (CSM) (Leland et al 1968, Smith 1972, Lee et al 1979) can be applied to describe the vapor/liquid-equilibrium (VLE) behavior of many defined binary and ternary coal-solvent systems (Watanasiri et al 1981).

This MPCS correlation is also able to reliably predict the density, enthalpy, and VLE of undefined distillable coal fluids. Equation-of-state characterization parameters have been estimated using empirical correlations which are functions of fraction average measurable properties such as normal boiling point and specific gravity. The degree of accuracy was found to be related to the amount of characterization data available (Brule' et al 1981, Watanasiri et al 1981).

Many problems exist in predicting complex-system thermophysical properties. The correlation framework must be capable of predicting properties of high-molecular-weight multifunctional organic compounds at extreme-temperature and -pressure operating conditions. A standard characterization procedure must be available for resolving a complex hydrocarbon mixture with hundreds of diverse organic compounds into a pseudocomponent mixture with twenty or so

fractions representing the overall properties of the parent full-range liquid (or gas). Once effective pseudocomponents are resolved, correlation characterization parameters must be determined for each of the fractions.

The technique presented herein focuses on the latter problem of determining fraction correlation characterization parameters for complex fractions. Of course, this problem is inextricably linked to the other two problems of properties correlation and pseudocomponent resolution. Correlations cannot be developed for complex-system thermophysical properties if the correlations are cast with parameters that cannot be determined for pseudocomponent fractions. Likewise, the resolution technique employed should not resolve fractions for which inspection-properties information cannot be obtained by using reasonably convenient methods.

Common correlation characterization parameters that are difficult to measure include compound critical properties used as characterization parameters in corresponding-states correlations. These parameters commonly include critical temperature, critical pressure or density, and a parameter related to molecular size and shape such as the acentric factor. Many high-molecular-weight organic compounds found in complex mixtures decompose far below their critical points (Johns et al 1962). Correlation characterization parameters have thus commonly been

estimated using empirical correlations that relate the characterization parameters to more easily measured inspection data such as normal boiling point and specific gravity (Wilson et al 1980, Brule' et al 1981). The problem with these correlations is that they are developed from critical vs inspection data; when critical properties are not available, correlations of this type are not possible.

Chapter II.

MULTIPARAMETER CORRESPONDING-STATES METHODOLOGY

The corresponding-states method used in this work is based on the concept of conformality. A reduced property is said to be conformal with the same reduced property of a second fluid if the reduced-property values for the two fluids are nearly equal at equivalent reduced temperature and density (Pitzer et al 1955, Rowlinson and Watson 1969). The classical example of conformality is provided by the thermodynamic behavior of monatomic fluids. For example, the compressibility factor of argon is almost the same as that of krypton at equal values of reduced temperature, T^*, and reduced density, ρ^* ,

$$Z(T^*,\rho^*)_{Ar} \simeq Z(T^*,\rho^*)_{Kr} \qquad (1)$$

These fluids are composed of relatively spherical molecules so intermolecular orientation has little effect on the fluid's properties. Such behavior is termed isotropic.

Polyatomic-fluid compressibility factors are generally not conformal. However, the compressibility factors (and other reduced properties) of many nonpolar,

polyatomic fluids can be correlated using the expression,

$$Z(T^*,\rho^*) = Z_o(T^*,\rho^*) + \omega Z_\omega(T^*,\rho^*) \qquad (2)$$

where ω is Pitzer's acentric factor (Pitzer et al 1955, Pitzer 1977). In eqn (2), Z_o and Z_ω are universal functions of T^* and ρ^*; i.e., Z_o and Z_ω are conformal for many nonpolar, polyatomic fluids. This expression is a perturbation expansion (Pople 1954) that has been simplified by truncating the higher-order terms (Pitzer et al 1955). The first term in eqn 2 represents the fluid behavior as if the fluid were comprised of quasispherical molecules with angle-independent interactions, and thus serves as the isotropic-reference-property contribution to the behavior of the real fluid. The remaining contributions to real-fluid behavior are lumped into the second term of eqn 2. The second term is the anisotropic contribution, a perturbation term which accounts for orientation effects due to molecular size and shape.

For polar, polyatomic fluids, compressibility factors can be correlated by extending the abbreviated form of the perturbation expansion with a fourth parameter:

$$Z(T^*,\rho^*) = Z_o(T^*,\rho^*) + \omega Z_\omega(T^*,\rho^*) + \mu^{*4} Z_\mu(T^*,\rho^*) \qquad (3)$$

where μ^* is the reduced dipole moment. Other polarity

parameters, such as Stiel's polarity factor (Halm and Stiel 1971), can also be used. In eqn (3), Z_o, Z_ω, and Z_μ are universal functions of (T^*, ρ^*) and therefore are conformal. Expansion of eqn (3) with the use of higher-order terms in ω and μ^*, as well as other corresponding-states characterization parameters, allows thermodynamic-properties correlation for fluids with many intermolecular effects (e.g., London dispersion forces, dipoles, quadrupoles, octupoles, etc...).

For routine process-design applications, a rigorous perturbation expansion, complete with the higher-order terms, would be too complicated and time consuming for calculation using the present generation of computing machines. This becomes especially evident when one considers, for example, that a distillation-column simulation may involve 1200 to 1600 flash calculations for 20 components or more (Boston and Mathias 1980). The tack that must be taken in developing correlations for engineering purposes must therefore involve a compromise between rigorous theory and practical calculation capability. For fluids with mild dipole moments (say less than ~2 debyes), and other effects in addition to those due to molecular shape and size, a convenient three-parameter approximation of the perturbation expansion is possible:

$$Z(T^*,\rho^*) = Z_o(T^*,\rho^*) + \gamma Z_\omega(T^*,\rho^*) \qquad (4)$$

where γ is an orientation parameter, similar to acentric factor but including other nonideal intermolecular effects such as weak steric and multipole anisotropies (Lee et al 1977, Starling et al 1978). Although relations of the type presented in eqns (2) and (3) can be derived from theoretical arguments (e.g., Gubbins et al 1977, Lee et al 1977, Brule' et al 1979), herein theory is used merely to provide a framework and starting point for the MPCS correlation of fluid thermodynamic behavior. In fact, an alternate, more empirical and usually simpler approach to MPCS correlation is to consider that reduced thermodynamic properties can be expressed by a generalized equation of state:

$$Z = Z(T^*, \rho^*, \{R\}, \{E\}) \tag{5}$$

where $\{E\}$ is a set of parameters, E_1, E_2,..., which are dependent on corresponding-states characterization parameters. The set $\{R\}$ comprises those characterization parameters used to reduce (and sometimes to further modify, e.g., Fisher and Leland 1970) T and ρ (or P),

$$\{R\} = (\varepsilon, \sigma, \ldots \quad or \quad T_c, P_c, \rho_c, \ldots) \tag{6}$$

The set of equation-of-state parameters $\{E\}$ are generalized with respect to different fluids:

$$\{E\} = E_i\ (\{K\}, \{C\}) \tag{7}$$

One method to accomplish the generalization is to use a set of universal constants, $\{C\}=(a_i,b_i,c_i,...)$, to calculate equation-of-state parameters $\{E\}$ as generalized functions of fluid characteristic properties $\{K\} =(\gamma,\mu^*,Q^*,...)$. For example, E_i could be of the form corresponding to eqn (3),

$$E_i = a_i + \omega b_i + \mu^{*4} c_i \tag{8}$$

The selection of characterization parameters is usually made with some basis in theory. The intermolecular potential energy is considered herein to involve a molecular-energy parameter, ε, a molecular-size parameter, σ, and an orientation parameter, γ. Fluid conditions, T and ρ, can be reduced by isotropic-reference-fluid force constants, ε and σ, in the following manner:

$$T^* = kT/\varepsilon \tag{9}$$

$$\rho^* = \rho\sigma^3 \tag{10}$$

The values of ε and σ can be estimated from critical properties when available,

$$\varepsilon = kT_c/1.2593 \qquad (11)$$

$$\sigma^3 = 0.3189/\rho_c \qquad (12)$$

These approximations are based on the values of ε and σ for monatomic fluids when the Lennard-Jones (12-6) intermolecular-potential function is assumed to represent the intermolecular potential. The parameters ε and σ are used to establish the isotropic contribution, Z_o, to the real-fluid compressibility factor, Z. The orientation parameter accounts for the anisotropic contribution, γZ_ω, to Z.

Casting the MPCS correlation in terms of molecular parameters, rather than the customary engineering parameters (e.g., T_c, ρ_c, P_c, etc...) has unique advantages. Both thermodynamic and transport properties can be simultaneously and self-consistently correlated using the same characterization parameters, since all properties are interrelated on the molecular level (Starling et al 1978). Molecular parameters also prove useful for characterizing complex, high-molecular-weight hydrocarbons when critical properties used in conventional equations of state have not been or cannot be measured (Brule' et al 1979). Molecular parameters also afford more correlation flexibility as they can be defined in other ways than just a function of critical properties. The absence of critical-properties information precludes the use of conventional equations of

state that are cast in the MPCS framework with critical properties used as the reducing parameters. This is the main problem addressed in the research reported herein.

Equation of State for Thermodynamic Properties

The equation of state used in this study is a modified Benedict-Webb-Rubin (MBWR) equation (Starling 1973) cast with a conformal-solution model for mixture-properties prediction (Starling et al 1978). Actually, any equation of state can be cast into the MPCS framework presented herein. Likewise, the CSM can be applied to predict the properties of mixtures using any equation of state that has been cast in the MPCS framework. The MBWR was selected because of its proven capability in accurately predicting both liquid- and vapor-phase thermodynamic properties at relative reduced temperatures as low as $T_r = 0.3$ and relative reduced densities as high as $\rho_r = 3$ (Starling 1973). The CSM was implemented to improve the accuracy and speed of VLE predictions over most previous BWR formulations (e.g., Han and Starling 1972). Thus, one correlation can be used to predict not only VLE for separation-equipment design, but also the enthalpies for heat-exchanger rating and densities for equipment sizing. Multiparameter corresponding states and conformal-solution model—MPCS and CSM—are generic methods used to build the framework. MBWR is a specific

equation of state to which these general methods have been applied. The combined methodology is thus indicated as CSM-MPCS-MBWR to illustrate the different levels on which the correlation is formulated. Further, the terms 3PCS, 4PCS, etc... (three-parameter, four-parameter) can be used to specifically indicate how many MPCS parameters have been used to formulate the equation of state.

The MBWR equation is:

$$Z = 1 + \rho^{*}(E_1 - E_2 T^{*-1} - E_3 T^{*-3} + E_9 T^{*-4} - E_{11} T^{*-5}) + \rho^{*2}(E_5 - E_6 T^{*-1} - E_{10} T^{*-2}) + \rho^{*5}(E_7 T^{*-1} + E_{12} T^{*-2}) + E_8 \rho^{*2} T^{*-3}(1 + E_4 \rho^{*2}) \exp(-E_4 \rho^{*2}) \qquad (13)$$

The use of the following relation for the coefficients E_i in eqn (13) corresponds to eqn (7) for nonpolar fluids and casts eqn (13) into the 3PCS form of eqn (4):

$$E_i = a_i + \gamma b_i \qquad (14)$$

The values of the universal constants, a_i and b_i, are listed in Table 1. The orientation parameter γ was forced to be equal to the acentric factor ω when determining the values of a_i and b_i from multiproperty regression analysis of experimental density, vapor pressure, and enthalpy data

Table 1.

Universal Constants a_i and b_i for Obtaining Parameters E_i for the CSM-3PCS-MBWR Equation of State

$$E = a_i + \gamma b_i$$

i	a_i	b_i
1	1.45907	0.32872
2	4.98813	-2.64399
3	2.20704	11.3293
4	4.86121	0.
5	4.59311	2.79979
6	5.06707	10.3901
7	11.4871	10.3730
8	9.22469	20.5388
9	0.094624	2.76010
10	1.48858	-3.11349
11	0.015273	0.18915
12	3.51486	0.94260

(Lin et al 1972) for the normal paraffins methane through decane (Starling et al 1978).

Use of eqn (13) allows the calculation of thermodynamic properties of a single-phase nonpolar or slightly polar fluid given the three characterization parameters, ε (or T_c), σ (or ρ_c), and γ for the fluid. This correlation has also been extended using a 4PCS formulation (eqn 3) to describe the thermodynamic behavior of a number of pure halocarbons, with dipole moments up to 2.3 debyes (Milani 1978).

Conformal-Solution Model

For mixtures, the conformal-solution formalism assumes that the mixture properties are the same as those of a hypothetical pure fluid characterized by parameters ε_x, σ_x, and γ_x. The following semiempirical mixing rules are used to obtain these three mixture characterization parameters as functions of composition (Lee et al 1979, Watanasiri et al 1981):

$$\sigma_x^{4.5} = \sum_i \sum_j x_i x_j \sigma_{ij}^{4.5} \tag{15}$$

$$\varepsilon_x \sigma_x^{4.5} = \sum_i \sum_j x_i x_j \varepsilon_{ij} \sigma_{ij}^{4.5} \tag{16}$$

$$\gamma_x \sigma_x^{3.5} = \sum_i \sum_j x_i x_j \gamma_{ij} \sigma_{ij}^{3.5} \tag{17}$$

The pair characterization parameters, σ_{ij}, ε_{ij}, and γ_{ij}, are functions of the pure-fluid characterization parameters σ, ε, and γ of components i and j, and are calculated using the following combining rules:

$$\sigma_{ij} = \xi_{ij} \, (\sigma_i \sigma_j)^{\frac{1}{2}} \tag{18}$$

$$\varepsilon_{ij} = \zeta_{ij} \, (\varepsilon_i \varepsilon_j)^{\frac{1}{2}} \tag{19}$$

$$\gamma_{ij} = \tfrac{1}{2}(\gamma_i + \gamma_j) \tag{20}$$

The binary-interaction parameters (BIPs), ξ_{ij} and ζ_{ij}, are indicative of deviations from ideal-solution behavior. BIPs are normally determined from regression analysis of binary-mixture thermodynamic data or can be correlated in terms of mixture-component characteristics.

The density is calculated implicitly by solving eqn (13). Other thermodynamic properties can be derived by the classical thermodynamic relations (see, e.g., Reid et al 1977). The following is the expression, derived from eqn (13), for the enthalpy departure, $H - H^{\circ}$:

$$\begin{aligned}\frac{(H-H^{\circ})}{R(\varepsilon_x/k)} &= \rho^*[E_1 T^* - 2E_2 - 4E_3 T^{*-2} + 5E_9 T^{*-3} - 6E_{11} T^{*-4}] \\ &+ \rho^{*2}[E_5 T^* - 1.5E_6 - 2E_{10} T^{*-1}] \\ &+ 0.2\rho^{*5}[6E_7 + 7E_{12} T^{*-1}] \\ &+ E_8[3 - (3 + 0.5E_4\rho^{*2} - E_4^2\rho^{*4})\exp(-E_4\rho^{*2})]E_4^{-1}T^{*-2}\end{aligned} \tag{21}$$

where H is the enthalpy of the fluid and H° is the ideal-gas-state enthalpy of the fluid at the system temperature. The ideal-gas enthalpy must be calculated to obtain the enthalpy. The expression for the entropy departure, $S - S^{\circ}$, is

$$\begin{aligned}\frac{(S-S^{\circ})}{R} = &-\ln[\rho^* R T^* \varepsilon_x / k\sigma_x^3] \\ &-\rho^*[E_1 + 2E_3 T^{*-3} - 3E_9 T^{*-4} + 4E_{11} T^{*-5}] \\ &-0.5\rho^{*2}[E_5 + E_{10} T^{*-2}] + 0.2E_{12}\rho^{*5} T^{*-2} \\ &+ 2E_8[1 - (1 + 0.5E_4\rho^{*2})\exp(-E_4\rho^{*2})]E_4^{-1} T^{*-3}\end{aligned} \tag{22}$$

where S is the entropy of the fluid and S° is the ideal-gas entropy of the fluid at system temperature and unit pressure (1 atm, 1 kPa, etc...).

The fugacity, $\hat{f}_i$, of the ith component in a mixture is

$$\begin{aligned}\ln\left(\frac{\hat{f}_i}{x_i f_i^{\circ}}\right) = &(1 + \bar{V}_i)\frac{H-H^{\circ}}{RT} - \frac{S-S^{\circ}}{R} + (\bar{R}_i - \bar{V}_i)(Z - 1) \\ &+ \rho^*[\bar{E}_{1,i} - \bar{E}_{2,i} T^{*-1} - \bar{E}_{3,i} T^{*-3} + \bar{E}_{9,i} T^{*-4} - \bar{E}_{11,i} T^{*-5}] \\ &+ \frac{\rho^{*2}}{2}[\bar{E}_{5,i} - \bar{E}_{6,i} T^{*-1} - \bar{E}_{10,i} T^{*-2}] + \frac{\rho^{*5}}{5}(\bar{E}_{7,i} T^{*-1} + \bar{E}_{12,i} T^{*-2}) \\ &+ \bar{E}_{8,i} T^{*-3}[1 - e^{-E_4\rho^{*2}} - \tfrac{1}{2}E_4\rho^{*2} e^{-E_4\rho^{*2}}]/E_4\end{aligned} \tag{23}$$

where f_i° is the standard-state reference fugacity, taken to

be unity. The derivatives in eqn (23) are

$$\bar{E}_{j,i} \equiv \left.\frac{\partial E_j}{\partial n_i}\right|_{T,V,n_{k\neq i}} = b_j \gamma_x \left[2\left(\frac{\sum_m x_m \gamma_{mi} \sigma_{mi}^{3.5}}{\gamma_x \sigma_x^{3.5}} - 1\right) - \frac{3.5}{3} \bar{R}_i \right] \tag{24}$$

$$\bar{R}_i \equiv \left.\frac{1}{\sigma^3} \frac{\partial \sigma^3}{\partial n_i}\right|_{T,V,n_{k\neq i}} = \frac{6}{4.5} \left[\frac{\sum_m x_m \sigma_{mi}^{4.5}}{\sigma_x^{4.5}} - 1 \right] \tag{25}$$

$$\bar{V}_i \equiv -\left.\frac{1}{T^*} \frac{\partial T^*}{\partial n_i}\right|_{T,V,n_{k\neq i}} = 2 \left[\frac{\sum_m x_m \varepsilon_{mi} \sigma_{mi}^{4.5}}{\varepsilon_x \sigma_x^{4.5}} - 1 \right] - \frac{4.5}{3} \bar{R}_i \tag{26}$$

Generalized Correlation of Thermodynamic Properties

The prediction of the thermodynamic properties of coal chemicals has been established for the CSM-3PCS-MBWR (Brule' et al 1979). Prediction results are given in Table 2 for a 'pilot' data set consisting of diverse high-molecular-weight compounds. A more extensive list of fossil compounds is given in Table 8 in Chapter 4.

The ability to predict the thermodynamic properties for compounds as complicated as those shown in Table 2 is impressive, considering that the CSM-MPCS-MBWR is based on data for the normal paraffins methane to n-decane. This attests to the comprehensive utility of the corresponding-states principle, as well as the superb capability of the Benedict-Webb-Rubin equation of state for predicting thermodynamic properties.

In any case, many equations of state may be modified to predict thermodynamic properties for coal chemicals. An adequate density dependence is important for calculating the many thermodynamic properties that are calculated from density. The MPCS viscosity correlation utilized herein is also constructed with extensive density dependence. Accurate density prediction is also thus required for calculating accurate transport properties, since MPCS transport correlations are not capable of yielding densities from an implicit iterative-search procedure (e.g., see

Table 2.

Prediction Deviations of Pilot Data Set Usins the CSM-3PCS-MBWR Equation of State

	CSM-3PCS-MBWR Equation of State %AARD*		
Fluid Name	Vapor Pressure	Liquid Density	Heat of Vaporization
Benzene	0.73	1.15	0.79
Toluene	1.64	1.17	1.44
m-Cresol	1.83	1.28	2.56
Indene	0.82	1.69	0.87
Naphthalene	1.33	1.01	1.21
Tetralin	1.26	1.30	1.76
1-Methylnaphthalene	0.92	0.60	—
Acenaphthene	0.74	0.64	—
Biphenyl	1.25	0.44	1.96
n-Dodecane	0.43	0.42	0.74
Fluorene	2.08	—	—
Anthracene	5.72	7.26	4.18
Phenanthrene	2.60	2.24	3.55
Dimethylphenanthrene	0.28	0.27	—
Octanthrene	0.38	1.00	—
Pyrene	3.23	—	—
Fluoranthene	3.59	—	—
Hexahydropyrene	0.37	1.91	—
n-Hexadecane	1.01	0.86	0.32
Triphenylene	2.12	0.76	—
n-Eicosane	0.19	0.88	0.23

**Average Absolute Relative Deviation = $|(exp - calc)/ exp|$ x 100*

Starling 1973) in the same way that an equation of state is. Equations of state that do not accurately predict densities are thus unsuitable for simultaneous correlation of thermodynamic and transport properties.

Generalized MPCS Viscosity Correlation

The Chung-Lee-Starling (CLS) viscosity correlation (Chung 1980) is also a multiparameter corresponding-states expression. The construction of the CLS viscosity correlation closely parallels that of the CSM-MPCS-MBWR insofar as the CLS correlation is also cast as a perturbation expansion using isotropic viscosity (based on monatomic fluids in the dilute-gas state) as reference (Chung 1980). The CLS correlation also employs the conformal-solution model to represent the composition dependence of viscosity. The viscosity-correlation analogue of the CSM-MPCS-MBWR equation of state might thus be called the CSM-MPCS-CLS viscosity correlation.

Compatibility of Thermodynamic and Transport Correlations

Starling (1973b) purposely prescribed the use of the same characterization parameters for the viscosity (as well as for other transport-property correlations) as for the equation of state. However, early developments of the CSM-MPCS-CLS viscosity correlation also involved the use of the acentric factor, ω, to estimate the orientation parameter, γ (Starling et al 1978). Apparently, the impetus in the early development of the MPCS viscosity correlation was to develop an extremely accurate expression in terms of the 3PCS

characterization parameters, $\varepsilon(T_c)$, $\sigma(\rho_c)$, and ω. This correlation was not compatible (except for the normal paraffins methane through n-decane) for use with the CSM-3PCS-MBWR. Further, the harmonic function that was used to correlate γ as a function of ω, yields anomalous estimates for γ outside the range over which the ω-to-γ converting equation was developed.

Chung (1980) formulated new transport-property correlations and extended the number of characterization parameters to 5 ($\varepsilon, \sigma, \gamma, \mu^*, \kappa$) where μ^* and κ are the reduced dipole moment and association factor, respectively. The harmonic function was dropped and ω was used directly as the parameter accounting for molecular-shape effects. Using this approach, very accurate results were obtained for many fluids, both polar and hydrogen-bonding. In addition, extensive density dependence was incorporated to enable the CSM-5PCS-CLS to predict viscosities over the whole fluid range from dilute gases to dense liquids. The main limitation reported by Chung (1980) is failure to accurately predict viscosity at low reduced temperature, where the temperature dependency of viscosity becomes very significant.

The CSM-MPCS-CLS thus appeared to be the best vehicle for a viscosity correlation as needed in this study. However, the CSM-5PCS-CLS could not be used conjunctively with the CSM-3PCS-MBWR to simultaneously predict both

thermodynamic and transport properties. In the CSM-5PCS-CLS correlation, the acentric factor was used in lieu of the orientation parameter in order to effectively separate different molecular effects to be described by the use of the 5 characterization parameters. The basic problem in using the orientation parameter lies in the way in which it is determined using multiproperty analysis. The orientation parameter can change, depending on what and how many characterization parameters are being used in the MPCS correlation. In contrast, the value of the acentric factor depends on a relatively static operational definition involving the difference in vapor-pressure-curve characteristics between the real fluid and an isotropic reference fluid. In other words, γ is correlation specific, while ω is not. This implies that the CSM-5PCS-CLS correlation is incompatible with the CSM-3PCS-MBWR correlation, even when μ^* and κ are zero, since ω and γ are not necessarily the same quantity.

Applicability of the Viscosity Correlation to Different Fluid Types

Another problem develops when attempting to apply the CSM-MPCS-CLS correlation to predict the viscosities of coal chemicals. The nonequilibrium-property CSM-MPCS-CLS correlation has some distinctly different characteristics compared to its equilibrium-property counterpart, the CSM-

MPCS-MBWR. Viscosity predictions for fluid types not originally in the viscosity-correlation data base cannot be well predicted. Viscosity predictions were quite poor (ca 50 to 100%) even for simple aromatics such as naphthalene and tetralin. Interestingly, the original CSM-MPCS-CLS correlation appears to predict viscosities over much wider ranges of temperature and pressure than over what the CSM-MPCS-MBWR can predict. This is not absolutely the case for all thermodynamic properties, but, e.g., if enthalpy predictions are compared with viscosity predictions, at high temperatures and pressures, the CSM-MPCS-CLS correlation will generally surpass the CSM-MPCS-MBWR in prediction accuracy. This is perhaps because the CSM-MPCS-CLS correlation only has to predict one transport property, while the CSM-MPCS-MBWR has to be able to predict several thermodynamic properties.

Modification of the Viscosity Correlation

The CSM-MPCS-CLS correlation was thus modified to solve both the problems of incompatible characterization parameters and nongeneral prediction capability. First the CSM-MPCS-CLS was recast with the same characterization parameters used by the CSM-3PCS-MBWR correlation. Then the CSM-3PCS-CLS coefficients were redetermined using an extensive data base with both paraffins and aromatics for

which T_c, ρ_c, and γ are well known. One of the novel features of the CSM-MPCS-CLS, as compared to other viscosity correlations, is that the CSM-MPCS-CLS can make excellent predictions for fluids over a wide molecular-weight-range, as well as for conditions over wide temperature and pressure ranges (Chung 1980, Lin and Lu 1981). Thus, a special effort was made to take advantage of this feature by incorporating data for hydrocarbon, sour, and acid gases, and both high-molecular-weight petroleum paraffins and coal-fluid polycyclic aromatic hydrocarbons (PCAHs). No other correlation in the open literature can predict viscosity, as a function of temperature and density, for so many fluid types.

There are many more data for light gases than for heavy hydrocarbons, so some of the light-gas data were deleted to 'groom' a more balanced data set of linear and cyclic organic compounds. So that viscosities could be calculated in terms of the more frequently specified conditions of temperature and pressure, the CSM-3PCS-MBWR was used to calculate the densities, as a function of T and P, needed for viscosity prediction. This provision yielded an unexpected bonus as viscosities for the normal paraffins n-undecane through n-eicosane were better predicted by using densities generated by the CSM-3PCS-MBWR correlation than by using densities generated by the Hankinson-Thomson correlation (1979) as were used in the original viscosity-

correlation work by Chung (1980). This may be due to the increased accuracy of densities generated by the CSM-3PCS-MBWR over the accuracy that can be achieved using the Hankinson-Thomson correlation. In addition, a viscosity correlation that uses temperature and pressure, rather than temperature and density as the independent variables, is of much greater practical use since density is not an easily and routinely measured quantity. The coupling of the CSM-3PCS-MBWR and the CSM-3PCS-CLS in this manner is also a necessary step in establishing the consistency needed to simultaneously correlate both thermodynamic and transport properties using the same correlation characterization parameters.

The Chung-Lee-Starling viscosity correlation as modified (hence, the CSM-3PCS-CLS) for use in the work herein is:

$$\eta^* = \eta_o^* \left[1/GN(Y) + E_6 \cdot Y\right] + E_7 \cdot Y^2 \cdot GN(Y) \cdot e^{E(T^*)} \qquad (27)$$

where $Y = (\pi/6)\rho\sigma^3$ is the reduced density

$$G = (1-0.5Y)/(1-Y)^3$$

$$GN(Y) = \left[E_1(1-e^{-E_4 Y})/Y + E_2 \cdot G \cdot e^{E_5 Y} + E_3 \cdot G\right] E_1 \cdot E_4 + E_2 + E_3$$

$$E(T^*) = E_8 + A_9/T^* + A_{10}/T^{*2} \qquad (28)$$

In eqn (27), all properties are in SI units (σ is in $\mathring{A}$). Equation parameters E_i are calculated using the same relation given by eqn (14). Univeral constants, a_i and b_i, are given in Table 3. The isotropic-reference-fluid viscosity, η_o^*, is expressed as

$$\eta_o^* = E_{11}\eta_{CE}^* \tag{29}$$

The Chapman-Enskog relation for the dilute-gas viscosity, η_{CE}^*, is

$$\eta_{CE}^* = 5/16\ \sqrt{\pi MRT}/[(\pi\sigma^2)\cdot\Omega(2,2)^*] \tag{30}$$

where η_{CE}^* = viscosity in Pa·s

T = temperature in K

T^* = reduced temperature defined by eqn (9)

M = molecular weight

σ = collision diameter in $\mathring{A}$

The collision integral, $\Omega(2,2)^*$, is evaluated using the Lennard-Jones (12-6) intermolecular-potential model (Neufeld et al 1972) as given in Table 4.

The capability of the the CSM-3PCS-CLS to predict the viscosities of both heavy paraffins typical of petroleum and polycyclic aromatic hydrocarbons preponderant in coal fluids

Table 3.

Universal Constants a_i and b_i for Obtaining Parameters E_i for the CSM-3PCS-CLS Viscosity Correlation

$$E_i = a_i + \gamma b_i$$

i	a_i	b_i
1	17.9765	39.1118
2	-0.506421E-3	0.701739E-2
3	43.1637	158.397
4	4.23084	-43.5696
5	3.95645	60.9599
6	0.618000E-2	66.4271
7	20.7488	-1.48606
8	1.05785	3.15007
9	-0.420218E-1	-3.57541
10	0.268786	1.17365
11	1.	-0.163563

Table 4.

Coefficients for Calculating the Transport Collision Integrals for the Lennard-Jones 12-6 Potential

$$\Omega(2,2)^* = (A/T^{*B})+[C/\exp(DT^*)]+[E/\exp(FT^*)]+RT^{*B}\sin(ST^{*W}-P)$$

Coefficients	Values
A	1.16145
B	0.14874
C	0.52487
D	0.77320
E	2.16178
F	2.43787
R x 10	-6.435
S	18.0323
W	-0.76830
P	7.27371

is remarkable. The viscosity of light gases, and petroleum and coal hydrocarbons, in both the liquid and vapor phases, can be well predicted over wide ranges of temperature and pressure. Most of the heavy hydrocarbons shown in Table 5 can be predicted to within 10% of experiment. Many are predicted under 5%, well within the range of error for experimental viscosity measurements of these complicated compounds. Note that although thermodynamic properties are generally predicted in the 1 to 2% range, transport-property-prediction deviations can be somewhat higher and still will be suitable for engineering purposes. For instance, the viscosities appearing in the Sieder-Tate equation yield a composite power of only about 1/2, which affects only slightly estimates for heat-transfer coefficients. The accuracy of the viscosities used is not nearly as critical as that of the enthalpy, which dictates the overall duty, in sizing and designing the heat exchanger. The accuracy criterion for transport vs thermodynamic properties can thus be relaxed; larger errors in transport-property predictions, say an order of magnitude from that of thermodynamic properties, can be tolerated in most process-design applications.

Viscosity for some polar and hydrogen-bonding (e.g., quinoline and m-cresol) are predicted with acceptable error only at high temperatures and moderate pressures. This is due to the limitations of a three-parameter formulation as

Table 5.

Prediction Deviations of Pilot Data Set Using Different Formulations of the CSM-3PCS-CLS Viscosity Correlation

	CSM-MPCS-CLS Viscosity Correlation %AARD				
				Modified $E(T^*)$ Dependence	
Fluid Name	Original w/ New Constants	Abbrev Data Set (PCAHs only)	Modified and eqns 31,32	eqn 33	eqn 34
Benzene	4.91	5.44	3.95	4.83	4.89
Toluene	6.66	11.5	10.3	8.68	8.54
m-Cresol	5.11	6.62	4.86	4.88	4.40
Indene	4.44	1.69	2.71	3.00	3.28
Naphthalene	2.78	4.65	4.43	4.01	3.53
Tetralin	5.87	8.33	2.73	2.41	2.87
1-Methylnaphthalene	6.84	14.4	14.9	15.4	16.6
Acenaphthene	2.07	3.61	2.11	2.75	2.13
Biphenyl	6.93	4.39	10.3	10.0	9.70
n-Dodecane	1.28	--	1.61	1.83	1.91
Fluorene	1.11	5.03	2.56	3.05	2.53
Anthracene	4.34	3.17	4.51	4.60	4.57
Octanthrene	9.68	15.2	13.9	13.2	11.5
Pyrene	6.03	4.80	2.68	2.88	2.55
n-Hexadecane	1.51	--	2.20	1.77	1.58
Triphenylene	4.16	0.93	1.62	1.30	0.69
n-Eicosane	0.94	--	1.04	1.61	1.30

Table 5. (continued)

'Trouble' PCAHs Fluid Name	CSM-MPCS-CLS Viscosity Correlation %AARD				
	Original w/ New Constants	Abbrev Data Set (PCAHs only)	Modified and eqns 31,32	Modified E(T*) Dependence	
				eqn 33	eqn 34
Cyclohexane	33.5	27.3	33.7	34.0	33.8
Phenanthrene	14.9	16.2	--	20.0	19.9
Dimethyl-phenanthrene	37.8	43.8	41.2	43.3	43.7
Dimethyldihydro-phenanthrene	45.4	46.9	47.0	47.1	44.7
Fluoranthene	23.7	26.4	23.9	23.9	23.3
Hexahydropyrene	18.8	1.40	--	8.96	5.74

dicussed in Chapter 1. Viscosity for some heavy polycyclic aromatic hydrocarbons (PCAHs) are not well predicted by the CSM-3PCS-CLS, even after regression using the new petroleum- and coal-data base (see Table 5). The reason for this is not entirely clear since many PCAHs in the data base, which are similar in structure and molecular weight to the poorly predicted PCAHs, are very well predicted. Curiously, there was no trouble in predicting the viscosities of high-molecular-weight paraffins, such as n-eicosane (C20). Also, vapor pressure and density for the troublesome PCAHs are very well predicted by the companion CSM-3PCS-MBWR equation of state.

Two issues can be considered in attempting to solve the problem of viscosity prediction for these 'trouble' PCAHs. Since many high-molecular-weight PCAHs with just as complicated structures as those of the trouble PCAHs are well predicted, the obvious impulse would be to suspect the data. Indeed, data-compilation experts have cited the abundance of erroneous viscosity data in the open literature (Viswanath 1981). Another piece of evidence makes the data suspect not because of the way the data were measured, but because of the fluids on which the measurements were made. A few of the compounds for which viscosity is poorly predicted come from the API-42 Project (API 1966). These compounds have not been certified to be more than 90 to 95% pure (Eisenbraun 1981); thus, errors could creep in from the

fluid not actually being what it was supposed to be. Also, these fluids are quite unstable and could have pyrolyzed during the viscosity measurements. A change in the molecular weight alone would produce drastic effects on density and viscosity predictions to the extent that density and viscosity calculations would be difficult to make in a mutually consistent manner using the CSM-3PCS-MBWR and CSM-MPCS-CLS simultaneously.

The other possible explanation for the poor predictions is the *inadequacy* of the CSM-3PCS-CLS to predict the viscosity of these compounds. The deterioration of prediction capability at low reduced temperatures, an inherent weakness of the correlation, might be the problem. Some, but not all, of the trouble PCAHs are represented by data at relatively low reduced temperatures (ca T_r=0.4). For instance, dodecahydrochrysene has a viscosity of 512 cp at 37.8 C, which may be in the non-Newtonian region where the CSM-3PCS-CLS hardly applies.

Four approaches were tried to solve the prediction problem for the trouble PCAHs. As shown in Table 5, none of these significantly improved prediction capability. The first attempted solution involved determining coefficients using a data base for only the PCAHs. This was done to 'take some of the strain off' the correlation from having to predict viscosity for too many fluid types. There was some marked improvement, but only for those compounds whose

predictions were already satisfactory using the original data base for fluids of all types.

The second attempt involved redefining ε and σ as a function of γ:

$$\varepsilon = (1 + a\gamma)kT_c/1.2593 \qquad (31)$$

$$\sigma = (1 + b\gamma)0.3189/\rho_c \qquad (32)$$

This was done to give the correlation characterization parameters more flexibility in the way they are defined, allowing them to move in the regression calculations. Prediction was improved for fluids that were already well predicted using the original CSM-3PCS-MBWR, but not for any of the trouble PCAHs in Table 5.

Since the problem of low-temperature dependence of viscosity is a basic weakness of the CSM-3PCS-CLS viscosity correlation, two studies were carried out to modify the temperature dependence of the CSM-3PCS-CLS viscosity correlation. Both these studies involved modifying E(T*) in eqn (27):

$$E(T^*) = E_8 + E_9/T^* + E_{10}/T^{*2} + E_{11}/T^{*3} \qquad (33)$$

$$E(T^*) = E_8 + E_9/T^* + E_{10}/T^{*2} + E_{11}/T^{*3} + E_{12}/T^{*5} \qquad (34)$$

where E_i is defined by eqn (14).

The E(T*) term was chosen for modification since it is the

dominant term in eqn (27). Again, predictions for some of the already well predicted compounds were slightly improved, but the trouble was that PCAHs such as dimethyldihydrophenanthrene and fluoranthene would not budge from 20% to 40% prediction deviations.

The conclusion is, therefore, that the viscosity data for these PCAHs are bogus. This conclusion is qualified by observations that (1) viscosity for similarly complicated organic compounds are well predicted, (2) the reliability of both synthesis and viscosity-measurement of these complicated hydrocarbons is uncertain, and (3) all attempted modifications of the CSM-3PCS-CLS correlation did not improve its capability to predict the viscosities of these fluids. Data for the troublesome PCAHs were subsequently removed from the data base (17 points out of a total of 384). The final correlation coefficients, determined for the original version of eqn (27), are given in Table 3.

Although, the CSM-3PCS-CLS has unfortunately not been ascertained to have prediction capability commensurate with the CSM-3PCS-MBWR, general prediction capability using MPCS thermodynamic and transport correlations has nonetheless been established, for the first time, for many model high-molecular-weight petroleum and coal organic compounds. As a result, the correlation vehicles, necessary for the simultaneous prediction of the thermodynamic and transport properties of complex, undefined fluids, have been put in a very useful working order.

Chapter III.

MULTIPROPERTY ANALYSIS OF THERMODYNAMIC AND TRANSPORT PROPERTIES

The method described herein depends on the capability to calculate many different properties using the same correlation characterization parameters. This idea indirectly stems from the earlier concepts of multiproperty analysis and its application. The method also has roots in findings concerning the determinancy of potential parameters using different types of data.

The thermodynamic and transport correlations used herein are cast with the same characterization parameters. This approach has theoretical grounds in molecular theory (e.g., Mo and Starling 1976, Lee et al 1977) and suggests the feasibility of simultaneously correlating thermodynamic and transport properties in a self-consistent manner (Starling et al 1978).

Much work on the use of multiproperty analysis in equation-of-state development preceded the extension of multiproperty analysis to correlation development for thermodynamic and transport properties. To understand the

implications of multiproperty analysis in the research at hand, it is valuable to recount the development of multiproperty-analysis techniques for improving equations of state.

The first ideas leading to multiproperty anlaysis first came about in work dealing with complex mixtures some fifteen years ago (Starling 1966). The systems under study involved reservoir-condensate fluids comprised of high-molecular-weight paraffins for which equation-of-state characterization parameters could not be measured and were otherwise unavailable. The equation of state and expressions for the correlation characterization parameters were developed by regression analysis of P-V-T data for low-molecular-weight components and phase-equilibria data for high-molecular-weight pseudocomponents. This approach is unique in that K-value data were used in lieu of density data for the high-molecular-weight pseudocomponents. This was done because not enough material for P-V-T measurements can be obtained from analysis of the high-boiling fractions, using, e.g., gas chromatography. The method was successful and sparked more ideas on the simultaneous use of many different data types in equation-of-state development.

Density and enthalpy data of pure fluids (Cox et al 1971), and then pure-fluid density and enthalpy, and mixture VLE (Lin et al 1972) were next incorporated via multiproperty analysis to develop a modified BWR equation of

state. The result was a generalized correlation that predicted all thermodynamic properties with exceptional accuracy. Ancillary investigations were carried out to determine which types of data were more important in insuring overall prediction capability, and which parts of the correlation were most affected by the different types of data. For example, enthalpy data are useful in determining the temperature dependency of an equation of state (Cox et al 1971); heat-capacity data enhances the accuracy of the temperature derivatives (Wang et al 1976). Phase-equilibrium data are valuable in determining the composition dependency of an equation of state (Lin et al 1972). Inclusion of all these properties in correlation development enhances the capability of the correlation to predict all these property types.

Eventually the development of the multiproperty-analysis concept expanded to include both thermodynamic and transport properties (Starling 1973b). Using multiproperty analysis, a network of thermodynamic- and transport-property correlations, either theoretical or semiempirical, can be developed using the same characterization parameters. Molecular parameters can be used since all properties can be interrelated by the molecular-distribution functions of statistical mechanics. For example, nonequilibrium properties have been related by the use of time-correlation functions (Kubo et al 1957, Kubo 1958, Mo and Starling 1976,

Lee 1981); equilibrium-property relationships have been developed with the use of perturbation and other theories (Twu and Gubbins 1978, Lee et al 1977, Starling et al 1978). Of course, thermodynamic properties can be related on the macroscopic level by the well known thermodynamic relationships (e.g., see Reid et al 1977), whereas transport properties cannot. This presents a great difficulty in simultaneously predicting thermodynamic and transport properties using semiempirical methods. For quite some time, the only seemingly viable method of correlating thermodynamic and transport properties within the same framework was to resort to fundamental statistical-mechanical expressions for both types of thermophysical properties. However, not all of these theoretical functions can be evaluated analytically, even at the present time, and engineers have had to resort to desultory, mostly empirical approaches involving unrelated correlations specific to each transport property. This provisional approach to transport-property correlation is at great disadvantage to that of thermodynamic-property correlation since the self-consistency that can be achieved between thermodynamic-property relationships cannot be achieved with transport-property relationships.

Starling (1973b) proposed the development of a unified, semiempirical approach to thermodynamic- and transport-property correlation. First, the typical

engineering-correlation characterization parameters (such as T_c, ρ_c, and γ) for the thermodynamic-property correlation were translated to molecular parameters used in transport correlations derived from fundamental kinetic theory for dilute gases. Next, perturbation theory was used to develop three-parameter corresponding-states viscosity and thermal-conductivity correlations, using the same characterization parameters as the equation of state. The tack was thus taken to develop semiempirical correlations for both thermodynamic properties (e.g., the CSM-MPCS-MBWR) and transport properties (e.g., the CSM-MPCS-CLS viscosity correlation) (Starling et al 1978). Although these properties are not inextricably linked within the network of correlations to the degree implied by statistical mechanics (i.e., one property cannot be analytically derived in terms of the other), the different property correlations can still be closely related in their development. That is, the thermodynamic correlations can serve as 'companions' to the transport correlations, and vice versa, to enhance overall prediction capability. This is shown schematically in the companion-correlation network of Figure 1. For instance, both the CSM-MPCS-CLS viscosity and thermal-conductivity correlations utilize density, which can be predicted by the CSM-MPCS-MBWR. Density must also be predicted to calculate all the thermodynamic properties such as enthalpy and fugacity. Thus, the accurate prediction of

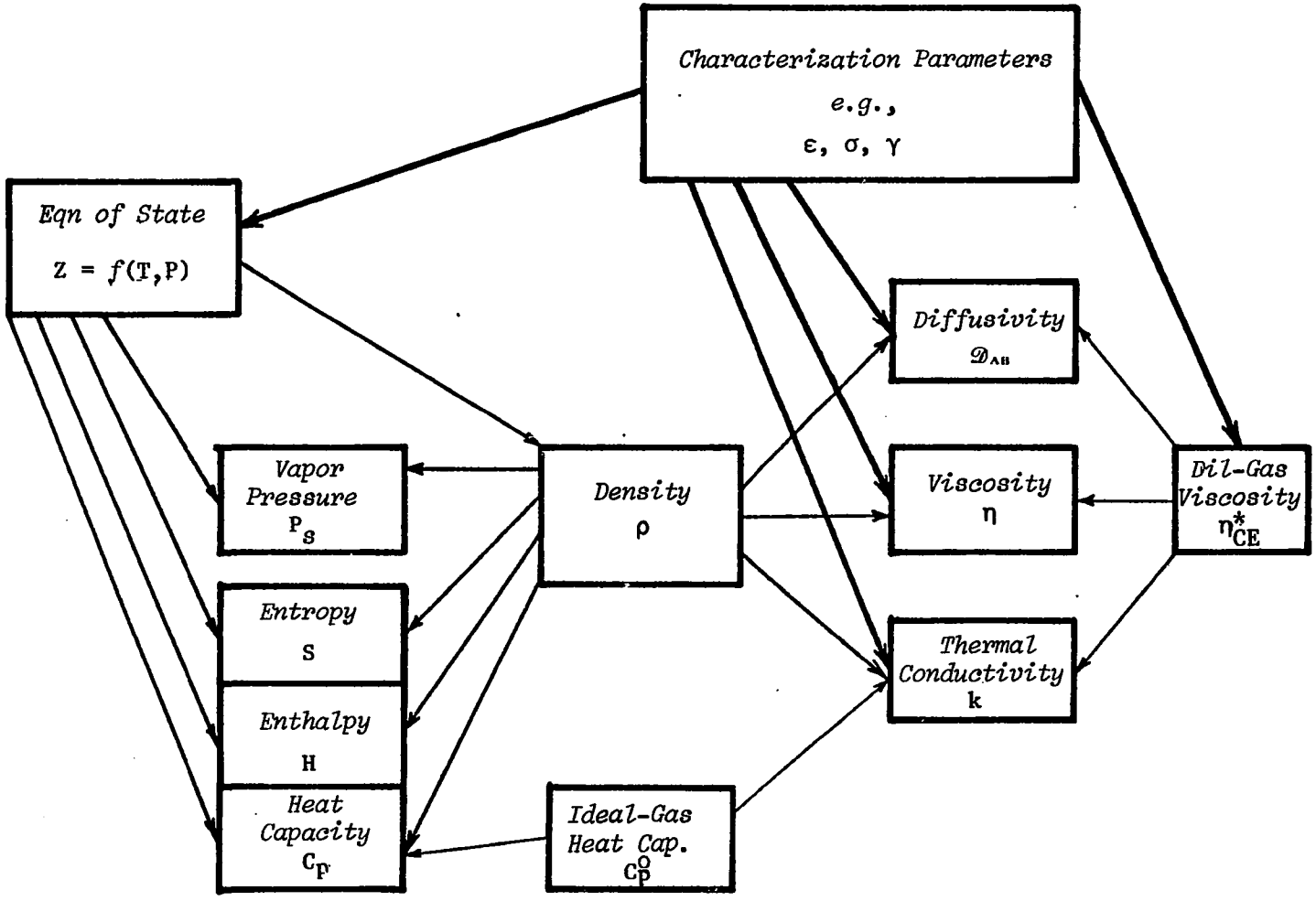

Figure 1. Companion-Correlation Network—
Interrelationships amongst Thermophysical-Property Correlations
Using the Multiparameter Corresponding-States Principle

density by the CSM-MPCS-MBWR is necessary for accurate prediction of all thermodynamic and transport properties.

Clearly, density is the central linking property in the correlation network of Figure 1. All the correlations are co-anchored, within the multiparameter corresponding-states framework, by using the same correlation characterization parameters. Other links between the various property correlations are also evident. Since the thermodynamic-property correlation and the transport-property correlations all use the same correlation characterization parameters, it follows that the values of the respective parameters must be such that all the correlations in the network will be able to predict their respective properties. Insofar as many of the correlations have their own unique mathematical behavior, it would seem plausible that unique correlation parameters could be extracted via regression, of different types of data, in constraint with the behavior of the respective correlations in the network. This hypothesis has been found to be true for determining at least one of the correlation parameters used in the CSM-MPCS-MBWR. The orientation parameter, γ, can be reliably obtained for prediction of thermodynamic and transport properties by regressing only vapor-pressure data. In fact, one vapor-pressure datum, which may conveniently be the normal boiling point, can be used to determine γ (Brule' et al 1981). Sensitivity analysis, rather than regression

analysis, has to be used when dealing with only the one point (see Figure 2). This technique is effective as shown in Table 6.

There arises the need to be able to determine all the correlation characterization parameters when making a property calculation for defined compounds, as well as complex, undefined fluids, for which critical data are not available. A logical extension of the work in determining the orientation parameter would be to incorporate several diversified types of data in multiproperty analysis to determine the other characterization parameters as well. However, the basis for such an approach is open to question. For instance, it is not unreasonable to imagine that γ can be obtained by regressing vapor-pressure data since the acentric factor (to which the orientation parameter was purposely made similar) is a mathematical definition based on vapor pressure. However, potential parameters σ, representative of molecular size, and ε, representive of the strength of intermolecular attraction, are calculated herein using critical parameters and not any of the thermodynamic and/or transport properties per se. One might surmise that multiproperty analsis within the network of correlations may be able to deliver unique parameters since the parameters must satisfy the many different correlations simultaneously. The regression problem for even three variables is highly dimensional, i.e., many solutions might

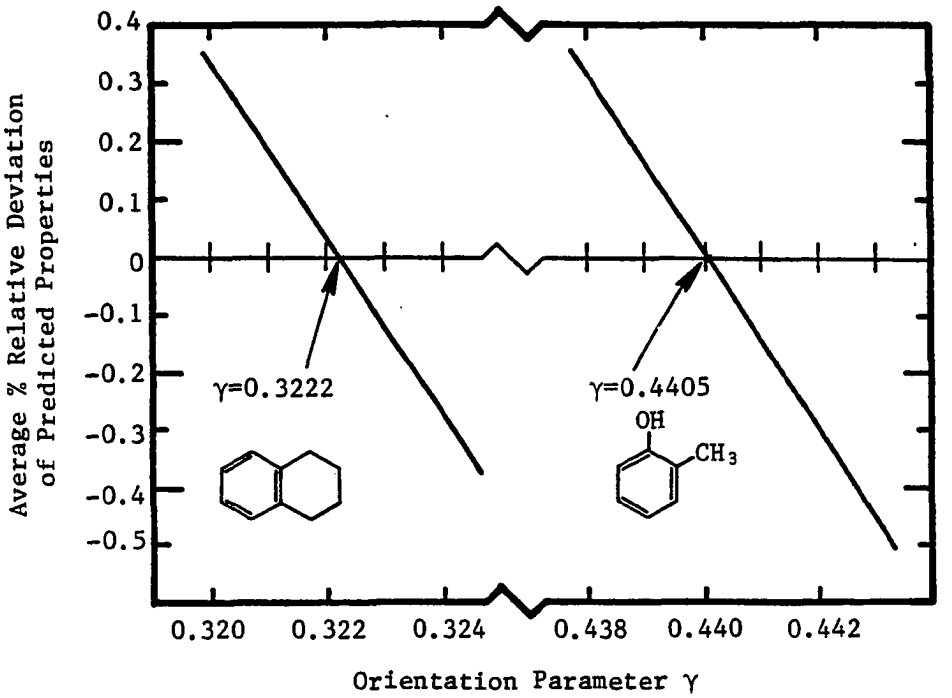

Figure 2. Sensitivity Analysis of the Normal Boiling Point to the Orientation Parameter

Table 6. Comparison of Thermodynamic-Property-Prediction Results Using Orientation Parameters from Vapor-Pressure Data Sets of Varying Sizes

Orientation Parameter γ from:		P_s = Normal Boiling Point		P_s to 2 atm		P_s to critical		*All* Properties to Critical	
PCAHs	Properties	γ	% AARD	γ	% AARD	γ	% AARD	γ	% AARD
Toluene	P_s	0.2694	1.80	0.2664	1.44	0.2660	1.46	0.2665	1.45
	ρ		0.86		0.91		0.92		0.91
	$H-H^0$		3.42		3.02		3.00		2.99
Tetralin	P_s	0.3222	1.18	0.3236	1.08	0.3230	1.11	0.3232	1.89
	ρ		1.94		1.99		2.02		1.10
o-Cresol	P_s	0.4401	2.08	0.4394	2.12	0.4417	2.04	0.4478	2.23

possibly exist even within the network of correlations. There is only partial justification for the proposed approach from the mathematical viewpoint just stated. If this approach can indeed deliver unique parameters, or at least a reasonably well valued trio suitable for calculating thermophysical properties using the three-parameter corresponding-states correlations studied herein, additional substantive reasoning for why this occurs must come from theory.

Determinancy of Potential Parameters

During the same period of time that the first concepts and applications were being developed for multiproperty analysis, some observations were being made concerning the problem of determining potential parameters for intermolecular-potential models using second-virial-coefficient (B_2) vs viscosity (η) data for dilute gases (Reid 1968). It was found that if B_2 data were used to regress potential parameters ε and σ in the Lennard-Jones 12-6 intermolecular-potential model (LJ) (see Figure 3), an infinite number of sets of ε and σ would yield identically satisfactory predictions of B_2 calculated from the integrated LJ expression. The same was found if ε and σ were determined using the integrated form of the LJ function for η. However, if both B_2 and η data for dilute gases are used simultaneously in the regression analysis, a 'unique' set of ε and σ are determined satisfying both sets of data (Tee et al 1966, Reid 1968, Reichenberg 1973, Reid et al 1977). This is shown graphically in Figure 4. Potential parameters ε and σ are not uniquely determined from B_2 and η separately since these properties are each given by integrals of the pair potential, and the areas of the integrals, which yield B_2 and η, are weak conditions on ε and σ (see Figure 3). The only apparent use that was made of this discovery was in ancillary investigations to provide

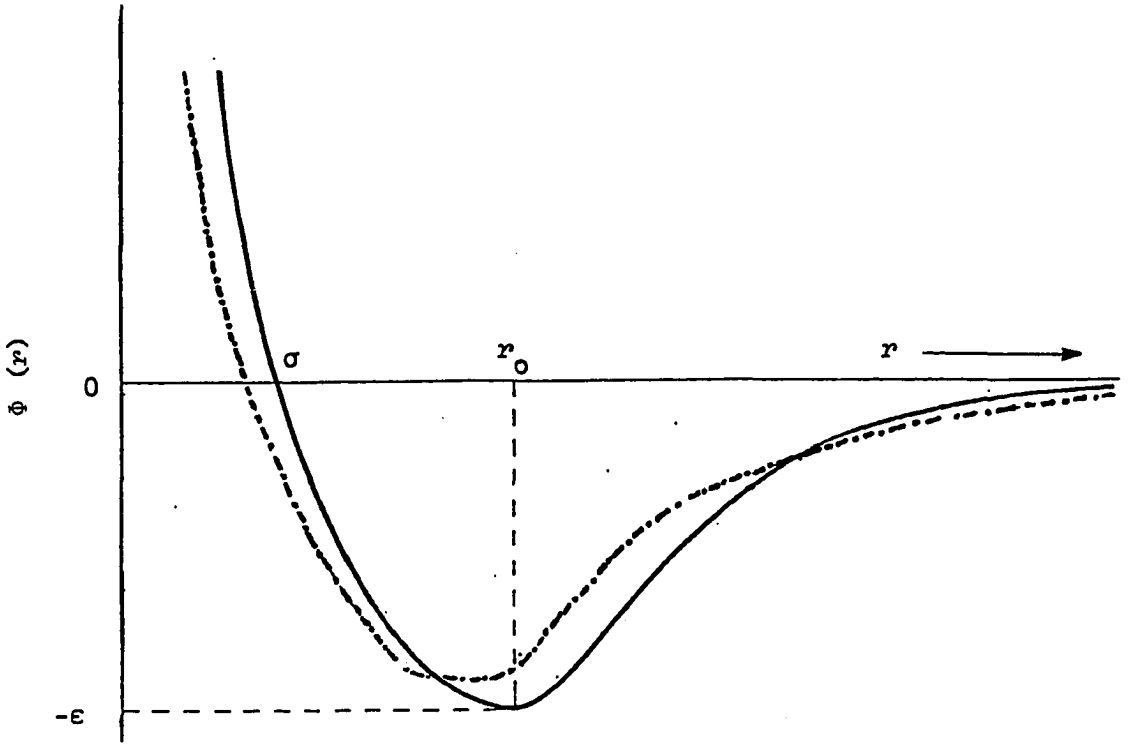

Figure 3. Topology of the L-J Intermolecular-Potential Function

Second Virial Coefficient B_2 and viscosity η are calculated from the area under the curves representing the integrand of the potential function. The areas under each of the curves can be equal, although ε and σ, used to generate each curve, can be different. In fact, an infinite number of sets of (ε,σ) are possible that will yield equal areas encompassed by the $\phi(r)$ curve. This is mathematically termed as the independent variables (ε,σ) being a 'weak condition' on the function $\phi(r)$.

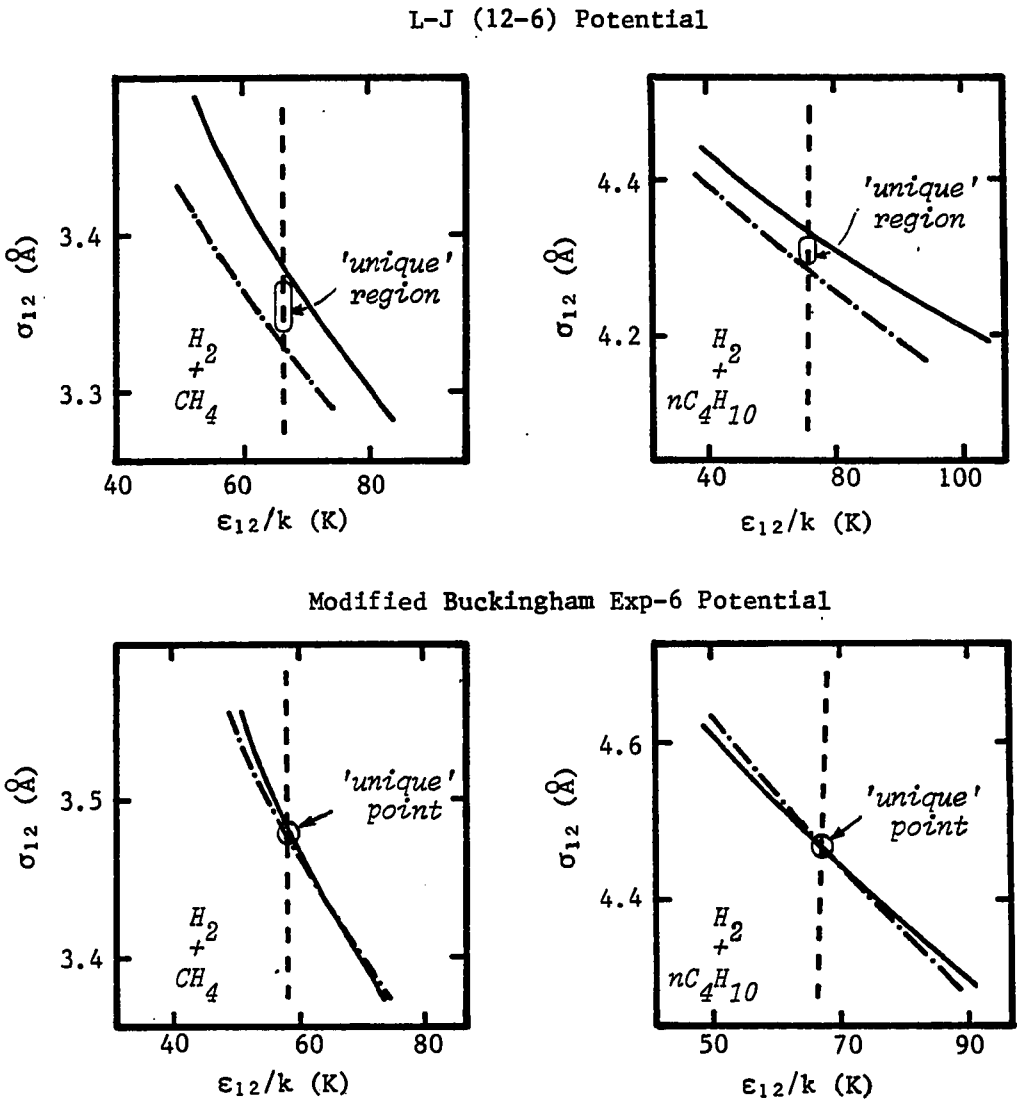

Figure 4. Determination of Force Constants σ and ε for 2 Potential Functions Using Mixture B_{12} and η Data (Chu *et al* 1975)

Key: - - - - - - Second Virial Coefficient
- • - • - • Diffusivity
———— Viscosity

insight into mixing rules for ε and σ (Hu et al 1970, Chu et al 1975).

In addition to the point of potential-parameter indeterminancy, certain thermodynamic and transport data affect different parts of the intermolecular-potential curve as shown in Figure 3 (Dymond and Alder 1969). This has been found by inversion of the derived B_2 and η equations, after regression analysis of B_2 and η data, back to the parent intermolecular-potential expression. For example, η affects the slope of the outer wall of the attractive bowl of the potential function. The depth and shape of the attractive bowl is emphasized by both B_2 and η data in certain temperature ranges. Although the LJ or any other two-parameter potential function is hardly rigorous for real molecules, equations derived from any potential function are rigorous with respect to their relationship with the parent potential-function expression. That is, regardless of what potential-function expression is used, certain types of data dictate the shape of the $\phi(r)$ curve. The extrapolation of these findings to polyatomic fluids such as those studied herein is uncertain, because the correct form of the intermolecular-potential function would necessarily involve additional terms to account for angle dependency, polar effects, etc.... Some connection still exists, however, since the perturbation-theory method used to develop the correlations studied herein is also based on isotropic

reference fluids described by a two-parameter intermolecular-potential function.

Another point must necessarily be made in passing. The determination of characterization parameters ε and σ, by using multiproperty analysis of thermodynamic and transport data and semiempirical corresponding-states correlations, cannot be construed to be a viable methodology for determimining the true values of ε and σ, and subsequently, the correct shape of the pair-potential curve. The methodology presented herein delivers parameters ε and σ that must be labeled as 'effective'— effective from the narrow but functional standpoint that when these parameters are used with the correlations presented herein, thermophysical properties can be accurately predicted. More fundamental insight into the true nature of the pair potential can be garnered from past and ongoing works of Smith, Aziz, and other investigators who have devoted a great many years to intermolecular-potential studies.

Development of the Therm-Trans Concept

Concepts from both multiproperty analysis and the determinancy of potential parameters led to the proposed idea of extracting correlation characterization parameters from multiproperty analysis of thermodynamic and viscosity data for real fluids. The proposed new use of multiproperty

analysis would be of a sort different than that practiced before in equation-of-state development. In general correlation development, multiproperty analysis insures that the universal constants delivered from regression would enable the correlation to predict all properties accurately. In the application at hand, multiproperty analysis would be used to deliver correlation characterization parameters that would enable the companion thermodynamic and transport correlations to simultaneously predict accurate thermophysical properties. Findings on the determinancy of potential parameters using both second-virial-coefficient and viscosity data suggest the simultaneous use of both thermodynamic and transport data to deliver unique correlation characterization parameters. Having an equation of state and a companion transport-property correlation that use the same correlation parameters provides the necessary vehicles for performing simultaneous and self-consistent multiproperty analysis of thermodynamic and transport data. For ease of reference, this concept is referred to herein as "Therm-Trans". Proof of the feasibility of the Therm-Trans technique could eventually lead to a new characterization technique with which correlation characterization parameters for high-molecular-weight organic compounds as well as undefined, complex fractions could be determined via multiproperty analysis of vapor pressure (average normal boiling point), density (specific gravity), and viscosity (SSU viscosity) data from typical fraction inspection analyses.

Chapter IV.

DETERMINATION OF CHARACTERIZATION PARAMETERS

Application of any property correlation to pure coal chemicals and defined hydrocarbon mixtures is of limited practical use in coal-liquefaction-process design per se. However, properties calculations for known-component systems are necessary to develop and test methods before applying them to undefined fluids. This also holds true for the development of correlations for estimating MPCS characterization parameters for both pure and complex fossil fluids. Information for defined pure coal chemicals that coincides with the information commonly obtained for complex systems is the most useful in developing the overall correlation strategy. The availability of the types of information for complex fractions must be the main criterion for developing the parameter-estimation techniques. Parameter-estimation correlations that require rarely determined information is of little use in the prediction of complex-system thermophysical properties. For example, Lydersen's method is commonly used to estimate the critical

temperature, critical density, and critical pressure for pure organic compounds (Reid et al 1977). However, Lydersen's method relies on knowledge of the structure of the compound, information that is usually unavailable for a complex fraction. Thus, for present needs, parameter-estimation methods should not rely on structural information for complex fluids. Of course, with new advances in ^{13}C-NMR and mass-spectroscopy analytical techniques, structural information will become more and more available, and group-contribution methods will subsequently be useful.

For applying MPCS correlations to undefined coal fluids, average properties of pseudocomponent fractions making up the coal fluid are often used to estimate correlation characterization parameters. The usual strategy for developing characterization correlations is to first develop a data set consisting of MPCS parameters (e.g., critical temperature and pressure, and acentric factor) vs measurable properties (e.g., TBP-distillation inspection data such as average boiling point, specific gravity, SSU viscosity, etc...) for selected pure compounds representative of those in fossil-fuels processing. Using this known-component-data base, generalized correlations can be developed for estimating MPCS characterization parameters from complex-fraction inspection data. This is the most widely taken approach to estimate the characterzation parameters for complex fluids.

As complex fluids get higher in molecular weight, the determination of characterization parameters at the normal boiling point is not feasible. This presents quite a problem, especially for many of the pure coal chemicals investigated herein, since only low-temperature, subatmospheric vapor-pressure data are available. If the usual approach of developing parameter-estimation equations were extended to higher-boiling-temperature fluids, many correlations would have to be developed, each covering a specific range identified by some reference-boiling-temperature (i.e., there would have to be a correlation for T_b at e.g., 100, 40, 10, and 0.1 mm Hg of pressure). However, even this unwieldy approach is doomed; direct correlations of critical properties vs subatmospheric data is not possible since critical-property data for high-molecular-weight compounds is virtually nonexistent. The lack of critical data for high-molecular-weight organic compounds is a major stumbling block for correlating the properties of complex fluids using MPCS formulations. This is perhaps an insurmountable problem as many polycyclic organic compounds in coal fluids decompose far below their critical point as shown in Table 7.

The present state of the art for handling these heavy systems is to simply extrapolate subatmospheric boiling-point information to atmospheric conditions and use the resulting normal boiling point to calculate MPCS

TABLE 7. STABILITY OF PCAHs IN THE CONDENSED AND VAPOR PHASES AND SOME PRODUCTS OF DECOMPOSITION (Johns, McElhill, and Smith 1962, Madison and Roberts 1958)

PCAH	Vapor-Phase Decomp Temp °C (Rate: 1 mol%/hr)	Liquid-Phase Decomp Temp °C (Rate: 1 mol%/hr)	Critical Temperature °C	Decomposition Products
Benzene	600	–	290	Biphenyl
Toluene	565-590	–	319	methane, hydrogen
Thiophene	590-620	–	306	–
Pyridine	620-650	–	347	–
Naphthalene	620-650	570	475	2,2'-Binaphthalene
Biphenyl	510-540	543	516	p-Terphenyl
Diphenylmethane	–	454	497	Fluorene
Quinoline	650	510-535	521	2,2'-Biquinoline, Pyridine
Isoquinoline	–	438-63	530	–
Dibenzofuran	–	518	*536***	–
Pyrene	500*	–	*665*	–
Chrysene	500*	–	*720*	–
Fluoranthene	500*	–	*638*	–
Triphenylene	500*	–	*740*	–
Coronene	–	453	*516*	p-Terphenyl

* *Pyrolysis reactions were studied at constant temperatures*
** *Italicized critical constants estimated by Lydersen's method*

characterization parameters (API 1980). Extrapolation of vapor pressures for well-behaved homologous series such as the paraffins is not too risky as evidenced by the widespread use of these procedures by the petroleum industry. However, coal fluids with a diversity of multifunctional organic compounds are not amenable to this treatment.

The proposed Therm-Trans analysis can aid in the problem of determining correlation characterization parameters when the widely used parameter-estimation techniques fail. Characterization parameters would be extracted by multiproperty analysis of vapor pressure, density, and viscosity data for the fluid. The temperature and pressure ranges over which the thermophysical-property data are available, would not have to depend on some reference conditions like those to which characterization-parameter equations are anchored. As pointed out in Chapter 3, the Therm-Trans concept is predicated on the capability to determine reliable correlation parameters by simultaneously analyzing both thermodynamic- and transport-property data using multiproperty analysis. The purpose of the following studies for pure coal chemicals is to examine the ability of Therm-Trans to extract unique (or as a practical compromise, reliable) correlation characterization parameters. At the same time the general prediction capability of the 3PCS correlations presented herein can be

assessed.

Brief mention will be made of the Therm-Trans computer program developed to carry out these studies, to focus not so much on how the program relates to this work, but on how the program can serve many general purposes. The program determines any number or combination of characterization parameters by multiproperty analysis of any type of data whether thermodynamic, transport, or thermochemical. A description of the program as well as the master data bank is given in Appendix A.

Properties Prediction for Pure Coal Chemicals

The development of the concept of characterizing via Therm-Trans begins with examining correlation behavior when predicting the properties of defined organic compounds. The examination is conducted with knowledge of critical properties, so that correlation-behavior patterns can be identified.

To calculate the thermophysical properties of pure coal chemicals using the CSM-3PCS-MBWR and CSM-MPCS-CLS correlations, critical temperature, critical molar density (or inversely, volume), and the orientation parameter are required. When critical properties are available, only the orientation parameter has to be determined, either from multiproperty analysis of all the available different types of property data or regression analysis of only vapor-pressure data. In most cases, the orientation parameter can be determined emphasizing only vapor pressure (Brule' et al 1979). This is usually sufficient for determining an orientation parameter with which vapor pressure, density, enthalpy, and viscosity can be accurately predicted for most fossil chemicals as shown in Table 8. Detailed listings for PCAHs known to be present in concentrations greater than about two percent in coal fluids are given in Appendix A. The overall average absolute deviations for the over 5000 data points analyzed are 1.13% for density, 1.78% for vapor

Table 8

Prediction of Thermophysical Properties of Defined Coal Chemicals Using the Generalized 3PCS-MBWR Equation of State and 3PCS-CLS Viscosity Correlation

Coal Chemicals		Characterization parameters					No. of	Range		For P and ρ, %AARD;	
Emp form.	Fluid name	Mol wt	Crit temp K	Crit vol cm3/mol	Orient. param	Prop.	Data pts	Temp C	Pres kPa	for H-H, AAD	Data References
N2	Nitrogen	28.016	126.17	90.10	0.0263	P_s	19	-184~-147	200~3392	0.90	Canjar & Manning 1967
						ρ	41	-196~116	101~61614	0.27	
						$H-H^o$	79	-184~10	1379~17237	2.02	
						η	13	25~500	167~17633	2.49	Vargaftik 1975
CH4	Methane	16.042	190.69	99.50	0.01289	P_s	30	-199~-82	1~4613	0.68	Douslin et al 1964
						ρ	41	-148~350	889~16030	0.65	Vennix 1966
						$H-H^o$	35	-157~10	1724~13789	1.34	Yesavage 1968
						η	26	38~238	690~20685	1.93	Vargaftik 1975
CO	Carbon monoxide	28.011	132.89	93.04	0.04385	P_s	25	-203~-143	20~3039	1.52	Vargaftik 1975
						ρ	40	-205~-143	20~3039	1.06	
H2S	Hydrogen sulfide	34.076	373.56	95.00	0.1092	P_s	24	-60~101	101~9004	0.72	Reamer et al 1950
						ρ	41	4~171	689~13789	1.85	
						η	8	100~527	101~174	1.32	
CO2	Carbon dioxide	44.01	304.17	94.00	0.2093	P_s	33	-56~29	517~7115	0.76	Canjar & Manning 1967
						ρ	41	-30~140	1517~31923	0.65	
						$H-H^o$	39	-30~140	3041~50678	3.16	
						η	6	25~600	101~15500	1.26	
COS	Carbonyl sulfide	60.070	378.78	135.13	0.1070	P_s	23	-103~106	2~6349	1.22	Robinson & Senturk 1979
C6H6	Benzene	78.115	562.16	259.	0.2143	P_s	68	6.9~289	8~4895	0.74	API-44/TRC Project
						ρ	19	10~260	6~3403	1.15	Chao 1978
						ΔH_v	19	10~260	6~3403	0.79	
						η	24	69~277	32~4218	4.83	
C7H8	Toluene	92.142	591.7	316.	0.2647	P_s	33	0~310	0.9~3774	1.64	Vargaftik 1975
						ρ	1.17	0~110	1~99	1.17	API-44/TRC
						$H-H^o$	84	10~371	346~17237	3.03	Eakin et al 1972
						η	17	0~600	0.9~516	6.64	
C7H8O	m-Cresol	108.140	705.83	312.14	0.4667	P_s	20	140~300	14.3~770	1.82	Kudchadker et al 1978a
						ρ	23	40~400	0.06~3110	1.29	
						ΔH_v	12	100~300	2.5~770	2.55	
						η	3	160~190	29~90	5.06	
C7H16	n-Heptane	100.21	540.29	426.13	0.3499	P_s	43	-68~258	0.004~2413	0.75	API-44/TRC
						ρ	41	-68~238	101~21243	0.65	
						$H-H^o$	16	267~374	545~16292	2.13	
						η	14	25~275	507~20271	1.81	
C8H10	o-Xylene	106.169	630.20	369.	0.3081	P_s	82	0~358	0.2~3808	0.76	API-44/TRC
						ρ	59	20~275	100~40000	1.47	
						ΔH_v					
						η	12	30~140	1.2~90	8.17	Vargaftik 1975

Table 8 (continued)

Coal Chemicals		Characterization parameters					No. of	Range		For P and ρ, %AARD; for H-H, AAD	Data References
Emp form.	Fluid name	Mol wt	Crit temp K	Crit vol cm3/mol	Orient. param	Prop.	Data pts	Temp C	Pres kPa		
C8H10O	2,5-Xylenol	122.166	707.05	333.93	0.4970	P_s	16	180~434	43~4900	5.99	Kudchadker et al 1978b
						ρ	7	80~200	0.7~200	14.1	
						ΔH_v	17	100~400	2~3200	5.19	
						η	10	90~180	101	7.87	
C8H18	n-Octane	114.224	568.59	486.20	0.4004	P_s	63	-57~293	0.002~2413	1.16	API-44/TRC
						ρ	54	-57~266	101~1655	1.18	
						$H-H^o$	66	24~316	1379~9653	3.17	
						η	13	50~296	101~20271	3.38	
C8H6S	Thianaphthene	134.20	752.0	405.72	0.3092	P_s	29	158~357	19~1060	0.55	Kobayashi 1979
C9H7N	Quinoline	129.163	782.15	357.07	0.3455	P_s	28	30~480	0.01~3531	2.36	Wilson et al 1979
						ρ	16	30~240	0.01~107	5.83	Viswanath 1979
						ΔH_v	18	70~360	0.2~876	2.34	
C9H8	Indene	116.162	702.49	368.34	0.2765	P_s	12	100~422	7.8~3800	0.70	Kudchadker et al 1980
						ρ	13	100~422	7.8~3800	2.30	
						ΔH_v	14	100~320	7.8~1440	0.70	
						η	6	70~120	101	5.00	
C9H10	Indan	118.178	685.61	381.66	0.3013	P_s	19	100~412	9.2~3950	0.29	Kudchadker et al 1980
						ρ	22	0~412	9.2 3950	1.03	
						ΔH_v	19	10~240	0.07~379	1.24	
						η	10	30~120	101	3.60	
C10H8	Naphthalene	128.175	748.35	401.29	0.3010	P_s	50	100~475	2.5~4050	1.61	Kudchadker et al 1978d
						ρ	25	100~440	2.5~2730	1.78	
						ΔH_v	20	100~460	2.5~3340	1.72	
						η	16	90~280	101~345	2.98	
C10H12	Tetralin	132.207	720.0	430.54	0.3455	P_s	34	100~447	3.4~3300	1.26	Wilson et al 1980
						ρ	17	100~400	3.4~2169	1.30	Kudchadker et al 1978c
						ΔH_v	14	100~340	3.4~1057	1.76	
						η	9	40~140	101	5.65	
C10H22	n-Decane	142.276	617.56	602.01	0.4880	P_s	24	-29~204	0.001~207	0.77	API-44/TRC
						ρ	32	38~238	1379~41368	1.09	
C11H10	1-Methylnaphthalene	142.201	772.00	453.03	0.3519	P_s	34	174~482	16~3027	1.19	Wilson et al 1980
						ρ	21	0~99	101~962	1.36	Camin & Rossini 1955
						η	3	38~99	101	6.04	API-42 (1966)
C11H24	n-Undecane	156.313	638.80	660.	0.5291	P_s	22	30~367	0.08~1940	0.66	Vargaftik 1975
						ρ	3	220~30	101	0.10	
						ΔH_v	2	25~196	0.05~101	0.23	
						η	16	-10~180	101	2.35	

Table 8 (continued)

Coal Chemicals		Characterization parameters						Range		For P and , %AARD; for H-H, AAD	Data References
Emp form.	Fluid name	Mol wt	Crit temp K	Crit vol cm3/mol	Orient. param	Prop.	No. of Data pts	Temp C	Pres kPa		
C12H10	Acenaphthene	154.214	824.13	460.05	0.3564	P_s	15	182~288	8.5~126	0.74	Mortimer & Murphy 1922
						ρ	1	99	101	0.64	Anderson & Wu 1963
						η	6	99~140	101	1.89	Coal Tar Data Book 1965
C12H9N	Carbazole	167.210	900.	616.48	0.4569	P_s	50	245~358	7.4~108	0.54	Senseman & Nelson 1923
C12H10	Biphenyl	154.214	789.	480.54	0.3222	P_s	12	123~328	2~400	1.25	Kobayashi 1979
						ρ	13	100~380	0.6~380	0.44	Vargaftik 1975
						ΔH_v	8	240~380	71~880	1.96	Chipman & Peltier 1929
						η	10	75~210	101	6.55	
C12H22	Bicyclohexyl	166.31	731.4	626.14	0.3830	P_s	23	151~304	10~347	0.45	Kobayashi 1979
C12H26	n-Dodecane	170.340	658.30	522.75	0.5690	P_s	51	40~386	0.05~1810	0.39	Vargaftik 1975
						ρ	23	0~210	101	0.45	
						ΔH_v	2	25~216	0.02~101	0.74	
						η	8	10~100	101	1.63	Stephan & Lucas 1979
C13H9N	Acridine	179.211	905.56	542.85	0.4044	P_s	9	166~346	1~101	4.82	Coal Tar Data Book 1965
C13H10	Fluorene	166.225	843.54	542.23	0.3604	P_s	10	161~300	2~108	2.08	Mortimer & Murphy 1923
						η	11	114~202	101	1.28	Coal Tar Data Book 1965
C13H12	Diphenylmethane	168.241	775.34	543.25	0.4258	P_s	32	151~454	4~1827	0.78	Kobayashi 1979
						ρ	3	38~99	101	0.21	
C13H28	n-Tridecane	184.367	675.80	786.31	0.6070	P_s	19	70~403	0.2~1723	0.68	Vargaftik 1975
						ρ	25	0~230	101	0.62	
						ΔH_v	2	25~235	0.004~101	1.53	
						η	16	0~200	101	1.07	
C14H10	Anthracene	178.233				P_s	13	216~400	4.9~261	5.89	Kudchadker 1979a
						ρ	7	216~320	4.9~67	4.23	
						ΔH_v	13	216~400	4.9~261	4.84	
						η	10	220~310	101	4.56	
C14H10	Phenanthrene	178.233	890.	540.23	0.4123	P_s	12	180~454	200~320	2.73	Wilson et al 1980
						ρ	7	200~320	3~69	3.26	
						ΔH_v	11	200~360	3~143	3.22	
						η	10	100~316	101	19.4	
C14H12	9,10-Dihydro-phenanthrene	180.25	846.1	606.1	0.4181	P_s					API-42 1966
						ρ	3				
						η	2				
C14H30	n-Tetradecane	198.394	694.	846.16	0.6365	P_s	16	120~421	1.2~1621	0.26	Vargaftik 1975
						ρ	26	10~250	101	0.66	
						ΔH_v	1	254	101	0.43	
						η	10	10~100	101	0.93	
C15H32	n-Pentadecane	212.421	707.	911.22	0.6869	P_s	16	140~434	1.6~1520	0.76	
						ρ	27	10~260	101	0.74	
						ΔH_v	1	271	101	0.14	
						η	9	20~100	101	0.48	

Table 8 (continued)

Coal Chemicals		Characterization parameters					No. of	Range		For P and ρ, %AARD; for H-H, AAD	Data References
Emp form.	Fluid name	Mol wt	Crit temp K	Crit vol cm3/mol	Orient. param	Prop.	Data pts	Temp C	Pres kPa		
C16H10	Pyrene	202.258	985.00	590.14	0.3804	P_s	9	260~400	5~110	3.32	Kudchadker et al 1979b
						η	7	158~213	101	3.31	
C16H10	Fluoranthene	202.258	956.74	652.97	0.3700	P_s	9	229~384	3~101	5.11	Boublik et al 1973
						η	5	120~179	101	28.1	Coal Tar Data Book 1965
C16H14	1,2,3,4-Tetrahydrofluoranthene	206.3	954.4	625.5	0.3211	P_s	5	127~196	0.1~1.4	0.34	API-42 1942-1966
C16H16	1,2,2a,3,4,5-Hexahydropyrene	208.3	987.67	608.17	0.3000	P_s	5	138~201	0.07~1.3	7.25	API-42
						ρ	2	115~135	101	4.68	
						η	2	115~135	101	18.8	
C16H34	n-Hexadecane	226.448	717.00	973.42	0.7548	P_s	11	190~444	7~1419	0.97	Varsaftik 1975
						ρ	28	20~280	101	0.79	
						ΔH_v	1	287	101	0.29	
						η	16	20~240	101	0.93	
C17H36	n-Heptadecane	240.475	733.	1038.75	0.7687	P_s	16	160~460	1.2~1317	0.84	Varsaftik 1975
						ρ	28	30~300	101	0.99	
						ΔH_v	1	302	101	0.34	
						η	18	30~300	101	1.22	
C18H12	Triphenylene	228.296	1083.18	749.14	0.2804	P_s	15	260~500	1.9~500	2.25	API-42
						η	6	200~250	101	2.36	
C18H24	1,2,3,4,5,6,7,8,13,14,14,16-Dodecahydrochrysene	240.4	923.3	781.3	0.4795	P_s	5	149~217	0.1~1.4	0.61	API-42
C18H38	n-Octadecane	254.502	591.6	1101.1	0.8094	P_s	15	190~472	2.6~1206	0.75	Varsaftik 1975
						ρ	28	30~300	101	0.93	
						ΔH_v	1	316	101	0.18	
						η	8	30~100	101	0.33	
C20H26	1,2,3,3a,4,5,6,7,8,9,9a,10,11,12-Tetradecahydroperylene	266.4	929.4	889.3	0.6591	P_s	5	184~252	0.1~1.4	1.66	API-42
C20H42	n-Eicosane	282.556	767.	1228.2	0.8851	P_s	16	200~502	1.5~502	1.08	Varsaftik 1975
						ρ	27	40~300	101	0.93	
						ΔH_v	1	343	101	0.25	
						η	12	40~220	101	0.68	

pressure, 1.89% for heat of vaporization, 2.09% for enthalpy, and 4.24% for viscosity.

When critical properties are not available, characterization parameters for pure fluids are usually determined by using Lydersen's critical-property-estimation method (see Reid et al 1977). However, Lydersen's method is not supposed to be applied to compounds with molecular weight beyond 100, especially those compounds that are multifunctional. For these cases, Therm-Trans can be used to extract the characterization parameters. In the work herein, Lydersen's method has been used to generate guesses for the characerization parameters to effect a stable regression in the Therm-Trans analysis. A guess for the orientation parameter can be generated by using eqn (37) given in the next chapter.

Extracting Characterization Parameters

If only vapor-pressure data are available for regressing all three characterization parameters, the regression can become unstable. This has been circumvented in most cases by first fixing γ and regressing T_c and ρ_c, and then fixing the resulting regressed values of T_c and ρ_c and regressing only γ. This was done in the case of phenylcyclohexane (see Appendix A), but a good intitial guess of γ was required. The 'flip-flop' technique does not

always work using just vapor pressure if the regression guess for Y is inadequate. However, this approach works if density data are also available for analysis, even if the choice of the value for Y is poor. This lends support to the hypothesis that the more types of data that are incorporated in the regression analysis, the more likely that effective characterization parameters can be determined.

The interesting part about the techniques just outlined is the effect of viscosity. Simultaneous regression of both vapor-pressure and viscosity data can in many cases deliver parameters which facilitate the reliable prediction of the other properties. This is evidenced in the cases of acenaphthene, fluorene, triphenylene, pyrene, indene, as well as other coal-fluid compounds. When only one type of property is available for regression analysis, the values of the three characterization parameters can wander to completely unrealistic values in obvious disaccord with physical principles. If viscosity data are included in the Therm-Trans analysis, the analysis will deliver reasonably well-behaved parameters. This holds only for those cases in which the viscosity data have been ascertained to be reliable. The inclusion of density data yields a slightly different set of parameters. Viscosity data indirectly forces the parameters to deliver realistic densities since density is required to calculate viscosity

(recall the correlation network of Figure 1). Apparently, γ is somewhat dependent on P_s when only the equation of state is considered. However, when viscosity is included, γ then becomes dependent on the behavior of the viscosity correlation as well. Although relatively small, there can still be a compensatory effect in the viscosity correlation that allows some error in density calculations. Thus, density should be provided in the Therm-Trans analysis to delete that degree of freedom.

As a result of these studies, the recommendation is to use vapor pressure, density, and viscosity to yield the best possible set of parameters. These data appear to be the most reliable for determining parameters that enable the 3PCS correlations presented herein to predict properties over an extended range of temperature and pressure.

Chapter V.

PREDICTION OF COMPLEX-SYSTEM THERMOPHYSICAL PROPERTIES

For applying MPCS correlations to undefined coal fluids, average properties (inspection data) of pseudocomponent fractions making up the coal fluid have often been used to estimate correlation characterization parameters. To use the inspection data, ancillary correlations traditionally have been developed to relate fraction average inspection properties to MPCS characterization parameters. Although in widespread use, characterization-parameter correlations have several shortcomings, which can be circumvented by the use of Therm-Trans.

Correlation of Corresponding-States Characterization Parameters with Fraction Average Measurable Properties

To obtain estimates of MPCS characterization parameters for undefined, distillable coal-fluid fractions, correlations have been developed in the manner commonly practiced in dealing with petroleum fractions. Most

established correlations for distillable fluids are based on petroleum hydrocarbons (e.g., Riazi and Daubert 1980, Sim and Daubert 1980). In order to be at all applicable to coal fluids, these correlations must be re-evaluated and modified using a data base which includes organic compounds typical of coal fluids.

For most distillable-coal-fluid systems for which data have been reported in the open literature, the average normal boiling point T_b and specific gravity S are the typically reported inspection data. Average molecular weight M is also important for characterizing high-molecular-weight fluids, as heavy-hydrocarbon S changes only slightly as M increases, whereas molar density continues to decrease uniformly as M increases. Unfortunately, M is only sometimes available. As M is that important piece of information that allows conversion of weight to moles, M should always be included as part of the inspection data. A great deal of uncertainty is introduced into any properties calculation when M is not available.

Viscosity as a Key Characterizing Parameter

Additional inspection data such as viscosity could potentially improve correlation accuracy; e.g., petroleum fluids and coal fluids with the same Watson characterization factor can have very different viscosities at ambient

temperature and pressure. The viscosity of a fluid is very much affected by the shape of its molecules. Compounds with the same empirical formula, or even of similar structure, can exhibit quite disparate viscosity behavior. Several investigators have recognized that viscosity offers additional information that can aid in the characterization of high-molecular-weight fluids. Suggestions to include viscosity as an additional parameter in parameter-estimation equations have followed (e.g., Kesler and Lee 1977). As illustrated in Chapter 4, viscosity also proves useful when determining characterization parameters using the Therm-Trans approach. Unfortunately, additional inspection data such as viscosity and M are not always available, and thus, most of the extant empirical characterization formulas express corresponding-states parameters as functions of only T_b and S (e.g., Wilson et al 1980).

Empirical Correlations for Estimating Characterization Parameters

Empirical equations for estimating characterization parameters have been developed using a coal-chemical data base (Starling et al 1980, Brule' et al 1981). These characterization correlations are based on data for more than 130 pure cyclic aromatic hydrocarbons as well as multifunctional NOS (nitrogen, oxygen, sulfur) organic compounds (Lin et al 1980a,b,&c). Using these correlations,

estimates can be obtained for critical temperature T_c, critical molar volume V_c, and orientation parameter γ — the characterization parameters used for the three-parameter corresponding-states correlations presented herein. Note that these parameter-estimation equations are not applicable for those cases in which only subatmospheric data are available, but nonetheless can produce 'ballpark' regression guesses for use in a Therm-Trans analysis of the subatmospheric data. Furthermore, empirical correlations of this type are not able to distinguish between the many chemical types of organic cyclic compounds, whether aromatic vs paraffinic or hydrocarbon vs multifunctional, which may be present in a coal fluid. This can be partly illustrated by the behavior of empirical characterization correlations.

The equation used for many years in the petroleum industry (Cavett 1962) has been modified for predicting T_c of distillable coal fluids:

$$T_c = 429.138 + 0.886861\,T_b - 4.596433 \times 10^{-4} T_b^2 - 2.410089 \times 10^{-3} API \times T_b + 1.630489 \times 10^{-7} T_b^3 - 9.323778 \times 10^{-7} API \times T_b^2 - 1.430628 \times 10^{-8} API^2 \times T_b^2 \qquad (35)$$

where T_c is in kelvins, $T_b = 1.8\,T_b(^{\circ}C) + 32$ or $T_b = T_b(^{\circ}F)$, and API = 141.5/S - 131.5. This correlation is based on S @ 20/20 °C (68/68 °F) since most PCAH specific-gravity data reported in the literature are usually for fluids at 20 °C,

rather than the U.S. customary reference temperature of 60 °F (15.6 °C). The difference between S for most aromatic hydrocarbons at the two reference temperatures is small, ca 0.3 %, and therefore can be neglected for most engineering calculations. Hall and Yarbrough's correlation for V_c (1973) has been modified using a data base including coal cyclic organic compounds:

$$V_c = 3.01514\ M^{1.02247} S^{-0.054476} \tag{36}$$

where V_c is in $cm^3/gmol$. If M is not available (and this is frequently the case), M can be estimated using eqn (37). Estimates for γ can be obtained from

$$\gamma = 333.333 + 151.244(T_c/T_b) - 519.841(T_b/T_c) + 38.9063(T_b/T_c)^4 + 1255.01 \log_{10}(T_b/T_c) \tag{37}$$

where both T_b and T_c are in the same absolute units, i.e., in kelvins or degrees Rankine. The expression given by Kesler and Lee (1976) for calculating M for petroleum fractions has been modified for coal fluids:

$$M = -12421.7 + 9316.25\ S + (7.753212 - 5.362614\ S)\ T_b + (1.0 - 0.753344\ S - 0.0173543\ S^2)(1.42072 - 405.3994/T_b)(5.5556 \times 10^6/T_b) + (1.0 - 0.888972\ S + 0.118591\ S^2)(1.66192 - 46.7525/T_b) \times (1.714678 \times 10^{11}/T_b^3) \tag{38}$$

where T_b is in kelvins.

Equations (35), (36), (37), and (38) have been successfully used to estimate the characterization parameters for distillable coal-fluid fractions in calculations of thermodynamic properties using the CSM-PCS-MBWR (Brule' et al 1981, Watanasiri et al 1981). Caution should be exercised when extrapolating beyond a boiling temperature of about 350 °C; little data were available for correlation development beyond this temperature.

The behavior of each of these correlations is shown graphically in Figure 5. The curves shown in these figures represent smoothly monotonic functions of correlation parameter vs normal boiling point at different specific gravities. This is not always the case, especially for coal liquids. Even though the correlations are based on more coal-chemical data than any chracterization correlations presented to date, the correlations are still not able to distinguish the difference in behavior between the different types of cyclic organic compounds found in coal fluids. This disparate behavior has been illustrated many times in simulated-distillation (simdis) analyses (e.g., ASTM D-2889). When a boiling-point-vs-retention-time curve is plotted from a simdis analysis of a whole coal liquid, several independent curves result as compared to one main curve that would result from simdis of a petroleum liquid. Each of the curves represent a separate chemical family,

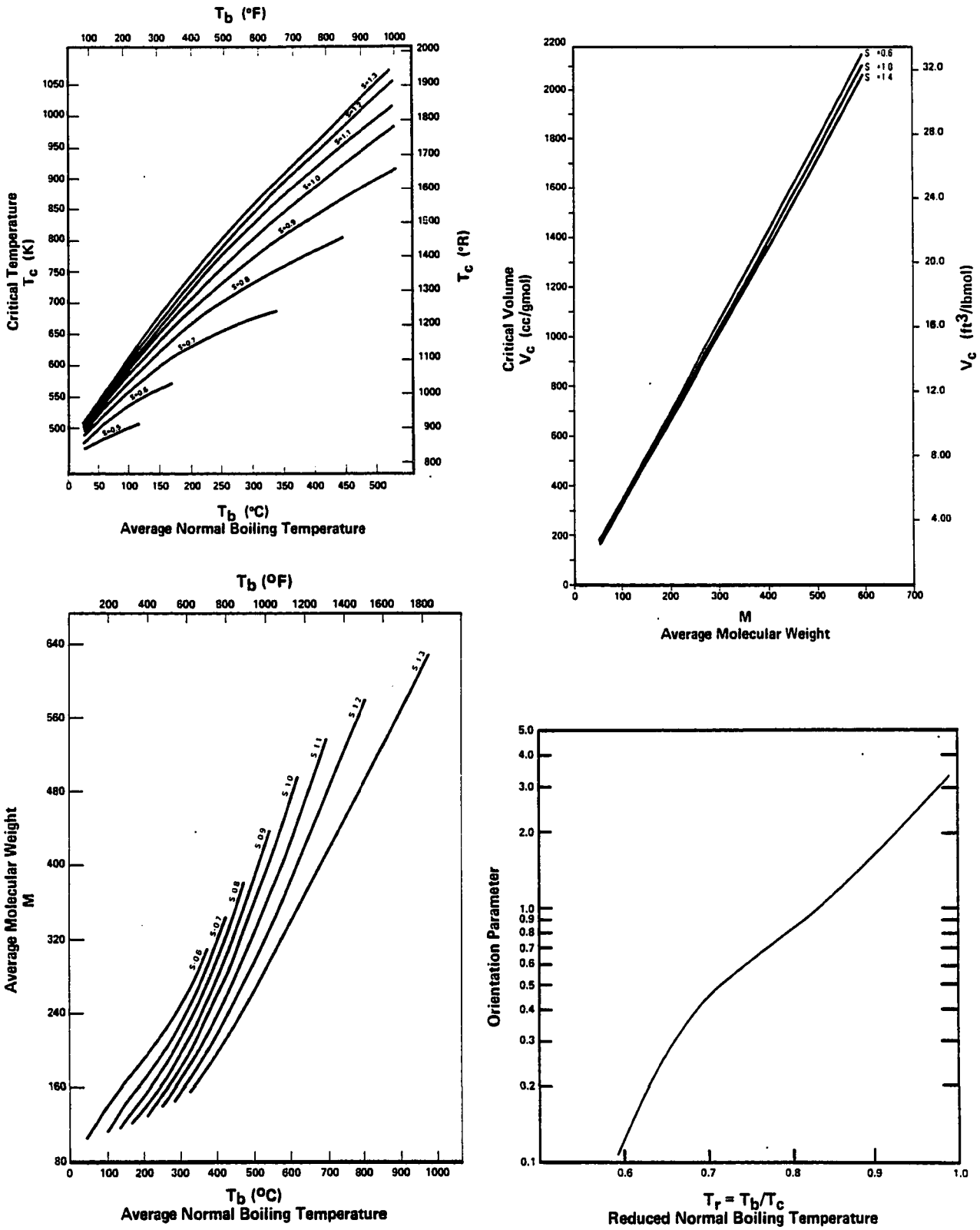

Figure 5. Characterization Parameter vs Normal Boiling Point at Constant Specific Gravity (Brulé *et al* 1981).

none of which can be deconvoluted using any single reference standard. This problem is usually circumvented by first separating the coal liquid into several chemical classes such as saturates, aromatics, acids, and bases, as shown in Figure 6. Then a simdis analysis of each of the separated fractions is done, using separate standards appropriate to the each particular chemical class making up the the parent coal fluid.

Characterization via Therm-Trans

More options are open for characterizing coal fluids if Therm-Trans is used. These include multiproperty analysis of many types of data to extract characterization parameters as illustrated in Chapter 4 for pure components. Procedures are now prescribed for carrying out the Therm-Trans analysis.

Application of the MPCS thermophysical correlations presented herein, to complex coal fluids, requires the use of the characterization parameters for the undefined fluid. Reasonable guesses for the parameters should be supplied to insure the success of the Therm-Trans analysis. The characterization parameters, T_c, ρ_c, and γ, as well as M, can be first estimated using eqns (35) through (38).

For a given coal-fluid fraction, all the information required to estimate the parameters, i.e., T_b, S, and M, may

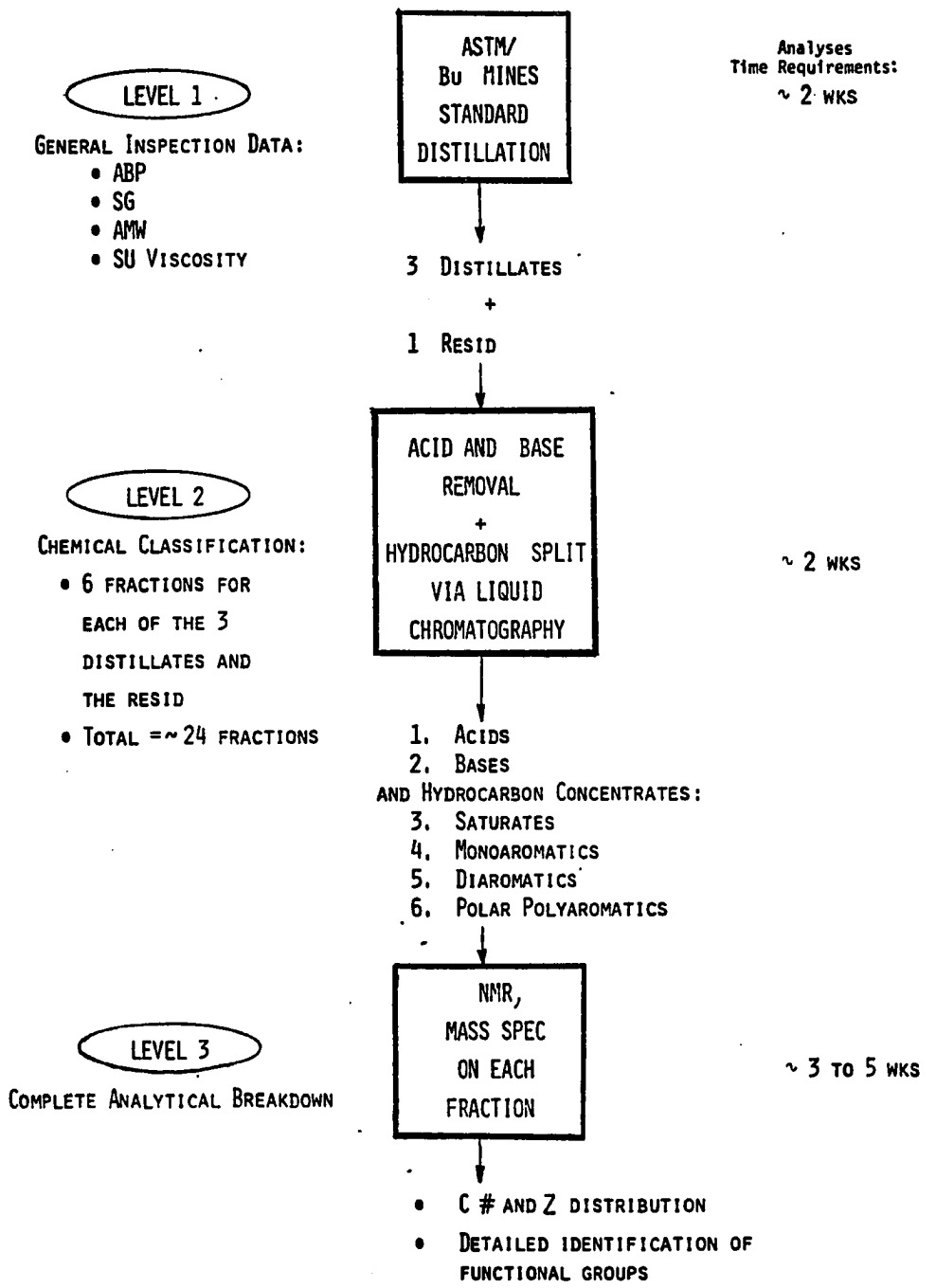

Figure 6. Various Levels of Complex-Fluid Analyses

not always be available. The following procedures can be used to estimate this information. When T_b, S, and M are available, use eqns (35), (36), and (37) to estimate T_c, ρ_c, and γ. When only T_b and S are available, use eqn (38) to estimate M. Then use the estimated M in eqns (35), (36), and (37) to calculate T_c, ρ_c, and γ.

Depending on what inspection data are available, the coal fluid may be treated either as a single pseudocomponent or as a mixture. Generally more pseudocomponents need to be specified when calculating properties for multiphase systems rather than for bulk (single-phase) systems (Brule' et al 1981, Watanasiri et al 1981). When the T_b, S, and M for just the whole fluid are given, the fluid can be treated as a single pseudocomponent having characterization parameters estimated by using the procedures prescribed above. If the whole coal fluid is characterized by separating it into different TBP fractions, with inspection data for each fraction, the fluid can be treated as a mixture with each fraction represented as a pseudocomponent.

If S of each fraction is not available, but S of the whole fluid is given, use the whole-fluid S to calculate the M of each fraction using eqn (38); then estimate T_c, ρ_c, and γ from M and eqns (34), (35), and (36). The mole fraction of each pseudocomponent in the coal-fluid mixture can be estimated by various procedures depending on the available information. If the weight percent (wt%) and M of each

fraction are given, then

$$x_i = \frac{wt\%_i / M_i}{\sum_j (wt\%_j / M_j)} \qquad (39)$$

If only the wt% of each fraction is available, but not M, use T_b and S to estimate M using eqn (38). Then calculate x_i per eqn (39). If percent volume distilled, v%, S, and T_b of each fraction distilled are given, which is the usual inspection data included in a ASTM-distillation analysis, use T_b and S to estimate M using eqn (38). Then the mole fraction, x_i, is calculated by

$$x_i = \frac{v\%_i S_i / M_i}{\sum_j (v\%_j S_j / M_j)} \qquad (40)$$

If v% and T_b of each fraction and S of the whole fluid before analysis are given, use the whole-fluid S for all the fractions. The x_i can then be estimated by using eqn (40).

Coal-Liquid Volatility Predictions

The CSM-MPCS-MBWR has been used to predict the volatility (vapor pressure) of several coal liquids. The experimental data reported were measured at conditions ranging from 21 to 454°C and 6.8 to 218 atm (70 to 850 °F and 100 to 3200 psia) (Wilson et al 1979). Only M for each liquid is given. Each coal fluid can be treated as a single

pseudocomponent (not as a mixture). Characterization parameters can first be estimated using eqns (35), (36), and (37), assuming as S=1 as a rough estimate, and extrapolating the vapor-pressure data to yield an estimate of the normal boiling point. Then, the parameters can be regressed using the flip-flop treatment (regress T_c and ρ_c holding γ constant; then regress γ holding T_c and ρ_c constant) given in the previous chapter. The volatility predictions for 6 coal liquids are summarized in Table 9. These predictions are quite good in light of the poor predictions (ca 20%) obtained when parameter regression is not used. Parameters might be adequately estimated, without regression, by using characterization equations (35) through (38), but neither the normal boiling point or the specific gravity was available for making the necessary calculations. Although viscosity data was also unavailable to aid in the analysis, the regression that was performed on the vapor-pressure data enabled reliable predictions of vapor pressure to be made. This does not guarantee that density or viscosity predictions made using these parameters will be accurate.

Coal-Liquid Density and Viscosity Predictions

The densities and viscosities of several coal liquids from the Exxon Donor Solvent process have been reported (Hwang et al 1980). The experimental data were measured at conditions

Table 9.

Comparison of Coal-Fluid Volatility Measurements with Prediction via the CSM-3PCS-MBWR Equation of State

Exxon Coal-liquid Designation	No. of Points	Avg Mol Wt	%AARD
N-1	16	164	3.74
N-2	14	205	4.85
S-1	15	134	1.16
S-2	17	176	4.19
U-1	17	158	1.29
U-2	17	225	5.41

ranging from 21 to 454 °C and 6.8 to 218 atm (70 to 850 °F and 100 to 3200 psia). The T_b and M, but not S, is given for each liquid. Characterization parameters were first roughly estimated using eqns (35) through (37). A Therm-Trans analysis was performed on the single boiling point, and all of the density and viscosity data. Therm-Trans proved remarkably effective in yielding effective characterization parameters for predicting the densities and viscosities of these liquids. The regression was very stable, and reasonably valued parameters were delivered as indicated in Table 10 and Appendix B.

The use of Therm-Trans as a direct characterization method was next studied. One vapor pressure (normal boiling point), three densities, and three viscosities were selected for each of the Exxon coal fluids. The data were selected in accordance with what could be easily measured for a fraction in routine laboratory analyses, i.e., only moderate temperature and low pressure. A Therm-Trans analysis was then carried out to determine the three characterization parameters from the seven data points for each coal liquid. Both the density and viscosity predictions are quite good as shown in Table 10.

The pressure effect on liquid density was exceptionally well predicted by the CSM-3PCS-MBWR equation of state. This is especially encouraging since all the other properties require density for their calculation. The

CSM-3PCS-CLS is a powerful companion correlation in that it not only predicts the viscosity of coal liquids reliably, but is also able to predict light-gas viscosity. This bodes well for predicting the viscosity of coal fluids in admixture with lighter components.

Table 10.

Comparison of Coal-Fluid Density and Viscosity Data with Prediction via the CSM-3PCS-MBWR Equation of State and the CSM-MPCS-CLS Viscosity Correlation

Exxon Coal-liquid Designation	Prop.	No. of Points	Tb at 50 wt% Dist	Avg MW	All Data %AARD	Insp Data %AARD
IHS	Tb	1	271 C	179	0.83	0.22
	ρ	33	(520 F)		1.11	1.08
	η	25			7.57	8.28
IA-10	Tb	1	244	164	0.39	0.25
	ρ	32	(471)		1.03	1.09
	η	30			4.46	4.58
IA-6	Tb	1	260	172	2.12	0.57
	ρ	36	(500)		0.71	1.26
	η	20			7.47	7.09
IA-3	Tb	1	246	167	0.80	0.29
	ρ	30	(475)		0.53	1.12
	η	8			8.53	7.55
WV-1	Tb	1	276	192	0.29	1.05
	ρ	26	(528)		0.49	1.75
	η	5			10.6	10.3

I = Illinois No. 6 coal
W = Wyoming Wyodak Coal

Chapter VI.

CONCLUSIONS AND RECOMMENDATIONS

Simultaneous prediction of coal-fluid thermophysical properties using multiparameter corresponding-states correlations has been demonstrated. A corresponding-states viscosity correlation has been successfully modified to predict the viscosities of dense fossil fluids, while preserving the ability of the correlation to predict light-gas viscosity as well.

A new approach to coal-fluid characterization has been successfully implemented. This characterization procedure is based on multiproperty analysis of vapor pressure, density, and viscosity inspection data for a coal-fluid fraction. Viscosity appears to be a very important piece of information necessary for characterizing a multiplicity of chemical families found in coal liquids. Properly used, the new characterization procedure is able to deliver effective characterization parameters that can be used to predict many thermophysical properties reliably.

Both the correlations and characterization procedure

have been applied to typical coal liquids from the Exxon Donor Solvent process. The potential of the Therm-Trans technique is evident as the properties of these coal liquids were very well predicted with very little conventional characterization information. This approach offers an advantage that parameter-estimation equations cannot offer: a more reliable method of insuring that ultimately thermophysical properties are accurately predicted.

As more experimental data become available, the Therm-Trans characterization method should undergo further testing. In addition, new work should begin to explore the redefinition of the orientation parameter (or acentric factor) based on viscosity in addition to vapor pressure. A priori calculation of the orientation parameter would enhance the reliability of the Therm-Trans technique.

NOMENCLATURE

Roman

API	$^{\circ}API = 141.5/S - 131.5$
C_p^o	Heat capacity in ideal-gas state
E_i	Generalized ith equation-of-state parameter
a_i, b_i	Universal constants in expression for E_i
f_i, f_i^o	Fugacity of component i, standard-state reference fugacity of component i
$H - H^o$	Specific enthalpy departure of fluid
H^o	Specific enthalpy of fluid in ideal-gas state
ij	Subscript denoting binary pair
k	Boltzmann constant (1.38054×10^{-23} J/K)
K	Watson characterization factor
k_i	Equilibrium vaporization ratio y_i/x_i
M	Fraction average molecular weight
P	Absolute pressure
P_c	Critical pressure
P_s	Vapor pressure
Q^*	Reduced quadrupole moment
S	Specific gravity
$S - S^o$	Specific entropy departure of fluid
S^o	Specific entropy of fluid in ideal-gas state
T	Absolute temperature

T^*	Reduced temperature = kT/ε
T_b	Normal boiling temperature
T_{b_r}	Relative reduced normal boiling temperature = T_b/T_c
T_c	Critical temperature
T_r	Relative reduced temperature = T/T_c
V_c	Critical volume
x	Subscript denoting mixture
x_i	Liquid-phase mole fraction
y_i	Vapor-phase mole fraction
Z	Fluid compressibility factor
Z_o	Isotropic-reference-fluid compressibility factor
$Z_{\omega,\gamma}$	First-order perturbation contribution to compressibility factor

Greek

ε	Characteristic molecular-energy parameter
γ	Molecular orientation parameter
μ^*	Reduced dipole moment
ρ	Density
ρ_c	Critical density
ρ^*	Reduced number density
ρ_r	Relative reduced density
ω	Acentric factor
σ	Characteristic molecular-size parameter
ξ_{ij}	Molecular-size binary-interaction parameter
ζ_{ij}	Molecular-energy binary-interaction parameter

LITERATURE CITED

Ambrose, D., B.E. Broderick, and R. Townsend, "The Critical Temperatures and Pressures of Thirty Organic Compounds," J Appl Chem Biotechnol 24: 359-372 (1974).

American Petroleum Institute (API), "Properties of Hydrocarbons of High Molecular Weight," Research Project 42, New York (1940-1966).

API-44/TRC Data Project, "Selected Values of Properties of Hydrocarbons and Related Compounds," Thermodynamics Research Center, Texas A&M Univ, College Station TX (looseleaf data sheets extant 1978).

API Division of Refining, Technical Data Book— Petroleum Refining, 2nd ed., New York (1970) and extant supplements (1980).

Anderson, H.C and W.R.K. Wu, "Properties of Compounds in Coal-Carbonization Products," BuMines Bulletin 606, U.S. Gov Printing Office, Washington, DC (1963).

Andon, R.J. L., D.P. Biddiscombe, J.D. Cox, R. Handley, D. Harrop, E.F.G. Herington, and J.F. Martin, "Thermodynamic Properties of Organic Oxygen Compounds. Part I. Preparation and Physical Properties of Pure Phenol, Cresols, and Xylenols," J Chem Soc (London) Part IV-1009: 5246-5254 (1960).

Boston, J.F. and P.M. Mathias, "Phase Equilibria in a Third-Generation Simulator," paper delivered to 2nd Int Conf on Phase Equilibria and Fluid Properties in the Process Industries, West Berlin (Mar. 1980).

Boublik, T., V. Fried, and E. Hala, The Vapor Pressures of Pure Substances, Elsevier Pub. Co, New York (1973).

Brule', M.R., L.L. Lee, and K.E. Starling, "Predicting thermodynamic properties for fossil-fuel chemicals," Chem Eng: 155-164 (19 Nov 1979).

Brule', M.R., D.E. Rhodes, and K.E. Starling, "Development of a Standardized Method to Characterize Fossil Fluids for Process Design," in press, Fuel (1980).

Brule', M.R., C.T. Lin, L.L. Lee, and K.E. Starling, "Multiparameter Corresponding-States Correlation of Coal-Fluid Thermodynamic Properties," in press, AIChE J (1981).

Camin, D.L. and F.D. Rossini, "Physical Properties of 14 American Petroleum Institute Hydrocarbons, C9 to C15," J Phys Chem 59: 1173-1179 (1955).

Canjar, L.N. and F.S. Manning, Thermodynamic Properties and Reduced Correlations for Gases, Gulf Pub. Co, Houston TX (1967).

Cavett, R.H., "Physical Data for Distillation Calculations--Vapor-Liquid Equilibria," API Div Ref 42-III: 351-366 (1962).

Chaback, J.J., cis- and trans-Decalin, API Monograph 706, (Oct 1978).

Chao, J., "Benzene," TRC Key Chemicals Data Books, Texas A&M Univ, College Station TX (Jan. 1978).

Chao, K.C., H.M. Lin, H.M. Sebastian, J.J. Simnick, et al, "Phase Equilibrium in Coal Liquefaction Processes," EPRI Research Project AF-466 Final Report for period 1977-1979 (1980).

Chipman, J. and S.B. Peltier, "Vapor Pressure and Heat of Vaporization of Diphenyl," I&EC 21-11: 1106-1108 (1929).

Chu, T.C., P.S. Chappelear, and R. Kobayashi, "Unlike Pair Potential Interaction Force Constants for Hydrogen—Light Hydrocarbon Systems," AIChE J 21-1: 173-175 (1975).

Coal Tar Research Assn, Coal Tar Data Book, 2nd Ed., Oxford Road, Gomersal, Leeds, England (1965).

Chung, T.H., "Applications of Multiparameter Corresponding States Theory for Prediction of Polar, Polyatomic Fluid Transport Properties," PhD dissertation, Univ of Oklahoma (1980).

Cox, K.W., J.L. Bono, Y.C. Kwok, and K.E. Starling, "Multiproperty Analysis. Modified BWR Equation for Methane PVT and Enthalpy Data," I&EC Fundam 10: 245-250 (May 1971).

Douslin, D.R., R.H. Harrison, R.T. Moore, and J.P. McCullough,

"P-V-T Relations for Methane," J Chem Eng Data 9-3: 358 (1964).

Dymond, J.H., and B.J. Alder, "Pair Potential for Argon," J Chem Physics 51-1: 309-320 (Jul 1969).

Eakin, B.E., G.M. Wilson, and W.E. Devaney, NGPA Research Report RR-6, Project 661, Natural Gas Processors Association, Tulsa OK (1966).

Edwards, D., C.G. Van de Rostyne, J. Winnick, and J.M. Prausnitz, "Estimation of Vapor Pressures of High-Boiling Fractions in Liquefied Fossil Fuels Containing Heteroatoms of Nitrogen or Sulfur," I&EC Proc Des & Dev 20-1: 138-143 (1981).

Eisenbraun, E.J., personal communication at the Workshop on Design Properties of Coal Liquids, Checotah, OK (4 Mar. 1981).

Fisher, G.D. and T.W. Leland, "Corresponding States Principle Using Shape Factors," I&EC Fundam 9-4:537-544 (1970).

Frith, J.F.S., S. Viswanathan, and A. Gupta, "Solvent-Refined Coal Process: Data Correlation and Analysis," Final Report for EPRI Research Project 915, Lummus Co, Bloomfield NJ (Aug 1979).

Green, M.S., J Chem Phys 20: 1281 (1952).

Green, M.S., J Chem Phys 22: 398 (1954).

Gubbins, K.E. and C.H. Twu, "Polar and Quadrupolar Fluid Mixtures," ACS Adv Chem Ser 60: 344-366 (1977).

Hales, J.L. and R. Townsend, "Liquid densities from 293 to 490 K of nine aromatic hydrocarbons," J Chem Thermodynamics 4: 763-772 (1972).

Hall, K.R. and L. Yarborough, "New, Simple Correlation for Predicting Critical Volume," Chem Eng: 76-77 (1 Nov 1971).

Halm, R.L. and L.I. Stiel, "Second Virial Coefficients of Polar Fluids and Mixtures," AICHE J 17-2: 259-265 (1971).

Han, M.S. and K.E. Starling, "Thermo Data Refined for LPG. Part 14: Mixtures," Hyd Proc 51-6: 107 (1972).

Hu, A.T., P.S. Chappelear, and R. Kobayashi, "Determination of Unlike Pair Potential Interaction Force Constants from Dilute Gas Thermodynamic and Transport Property Data," AIChE J 16-3: 490-492 (1970).

Hwang, S.C., C. Tsonopoulos, J.R. Cunningham, and G.M. Wilson, "Density, Viscosity, and Surface Tension of Coal Liquids at High Temperatures and Pressures," AIChE 88th National Meeting, Philadelphia PA (Jun 1980).

Johns, I.B., E.A. McElhill, and J.O. Smith, "Thermal Stability of Some Organic Compounds," J Chem Eng Data 7-2: 277-281 (1962).

Institute of Gas Technology (IGT), "Preparation of A Coal Conversion Systems Technical Data Book," Annual Reports prepared for DOE, by IGT, Chicago IL (extant 1980).

Kesler, M.G. and B.I. Lee, "Improve Prediction of Enthalpy of Fractions," Hyd Proc: 153 (Mar. 1976).

Kesler, M.G. and B.I. Lee, "On the Development of an Equation of State for Vapor-Liquid Equilibrium Calculations," ACS Sym Ser 60: 236-240 (1977).

Kobayashi, R., et al, "Physical Properties of Coal Liquids," EPRI Research Project 633-1, Report AF-1209 (Nov 1979).

Kubo, R., M. Yohota, and S. Nakajima, J Phys Soc Japan 11: 1029 (1957).

Kubo, R., in Lectures in Theoretical Physics 1: 120, Wiley, New York (1958).

Kudchadker, A.P., S.A. Kudchadker, and R.C. Wilhoit, "Phenol," Key Coal Chemicals Data Books, Thermodynamics Research Center, Texas A&M Univ (Dec 1977).

Kudchadker, A.P., S.A. Kudchadker, and R.C. Wilhoit, "Cresols," Key Coal Chemicals Data Books, Thermodynamics Research Center, Texas A&M Univ (Jan. 1978a).

Kudchadker, A.P., S.A. Kudchadker,"Xylenols," Key Chemicals Data Books, Thermodynamics Research Center, Texas A&M Univ (Mar. 1978b).

Kudchadker, A.P., S.A. Kudchadker, and R.C. Wilhoit, "Furan, Dihydrofuran,and Tetrahydrofuran," Key Coal Chemicals Data Books,Thermodynamics Research Center, Texas A&M Univ(May 1978c).

Kudchadker, A.P., S.A. Kudchadker, and R.C Wilhoit, "Tetralin," API Monograph 705 (Oct 1978d).

Kudchadker, A.P., S.A. Kudchadker, and R.C Wilhoit, "cis- and and trans-Decalin," API Monograph 706 (Oct 1978e).

Kudchadker, A.P., S.A. Kudchadker, and R.C Wilhoit, "Naphthalene,"

API Monograph 707 (Oct 1978f).

Kudchadker, A.P., S.A. Kudchadker, and R.C Wilhoit, "Anthracene and Phenanthrene," API Monograph 708 (Jan. 1979a).

Kudchadker, A.P., S.A. Kudchadker, and R.C Wilhoit, "Four-Ring Condensed Aromatic Compounds," API Monograph 709 (Mar. 1979b).

Kudchadker, A.P., S.A. Kudchadker, and R.C. Wilhoit, "Pyridine and Phenylpyridines," API Monograph 710 (Jul 1979c).

Kudchadker, A.P. and S.A. Kudchadker, "Indan and Indene," API Monograph Series 709 (Apr 1980).

Lee, L.L., K.C. Mo, and K.E. Starling, "Multiparameter Conformal Solution Theory— Application to Hydrocarbon Pure Fluid and Mixture Thermodynamic Properties," Bunsen-Gesellschaft fur Physikalische Chemie 81: 1043 (1977).

Lee, T.J., L.L. Lee, and K.E. Starling, "Conformal Solution Theory Parameter Mixing Rules," ACS Adv Chem Ser 182: 125-141 (1979).

Lee, L.L., The Statistical Mechanics of Fluids— An Introduction for Engineers, in press, Pittman Press (1980).

Leland, T.W., J.S. Rowlinson, and G.A. Sather, "Statistical Thermodynamics of Mixtures of Molecules of Different Sizes," Trans Faraday Soc 64: 1447 (1968).

Lenoir, J.M., G.K. Kuravila, and H.G. Hipkin, paper presented at 34th Midyear Meeting of API Division of Refining, Philadelphia PA (May 1969).

Lin, C.J., Y.C. Kwok, and K.E. Starling, "Multiproperty Analysis of PVT, Enthalpy, and Phase Equilibrium Data," Can. J Chem Eng 50: 644-650 (1972).

Lin, C.T., M.R. Brule', F.K. Young, L.L. Lee, K.E. Starling, and J. Chao, "Data bank for synthetic fuels, Part 1— Basic data needed for predicting the properties of coal-derived fluids," Hyd Proc 59-5: 229-233 (May 1980a).

Lin, C.T., F.K. Young, M.R. Brule', L.L. Lee, K.E. Starling, and J. Chao, "Data bank for synthetic fuels, Part 2— Properties constants for 161 one- and two-ring coal chemicals," Hyd Proc 59-8: 117-123 (Aug 1980b).

Lin, C.T., F.K. Young, M.R. Brule', L.L. Lee, K.E. Starling, and J. Chao, "Data bank for synthetic fuels, Part 3— Properties constants for 137 more coal chemicals,"

Hyd Proc 59-11: 225-232 (Nov 1980c).

Lin, C.T. and K.C. Lu, "Corresponding States Prediction of Transport Properties for Hydrocarbon Mixtures," submitted for publication (1981).

Madison, J.J. and R.M. Roberts, "Pyrolysis of Aromatics and Related Heterocyclics," I&EC 50-2: 237-250 (1958).

Milani, J.S., "Determination of MBWR Equation of State Parameters for Halogenated Hydrocarbons Using Multiproperty Regression Analysis," Masters Thesis, Univ Oklahoma (1979).

Mortimer, F.S. and R.V. Murphy, "The Vapor Pressures of Some Substances Found in Coal Tar," I&EC 15-11: 1140-1142 (1923).

Nasir, P., S.C. Hwang, and R. Kobayashi, "Development of an Apparatus to Measure Vapor Pressures at High Temperatures and Its Application to Three Higher-Boiling Compounds," J Chem Eng Data 25-4: 208-301 (1980).

Nelson, O.A. and C.E. Senseman, "Vapor Pressure Determinations on Naphthalene, Anthracene, Phenanthrene, and Anthraquinone between Their Melting and Boiling Points," I&EC 14-1: 58-62 (1922).

Neufeld, P.D., A.R. Janzene, and R.A. Aziz, "Empirical Equations to Calculate 16 of the Transport Collision Integrals (l,s) for the Lennard-Jones (12-6) Potential," J Chem Phys 57: 1100 (1972).

Passut, C.A., and R.P. Danner, "Correlation of Ideal Gas Enthalpy, Heat Capacity, and Entropy, I&EC Proc Des & Dev 11: 543-546 (1972).

Pitzer, K.S., D.Z. Lippmann, R.F. Curl, C.M. Huggins, and D.E. Petersen, "The Volumetric and Thermodynamic Properties of Fluids, J Am Chem Soc 77: 3433 (1955).

Pitzer, K.S., "Origin of the Acentric Factor", ACS Sym Ser 60: 1-10 (1977).

Pople, J.A., "The Statistical Mechanics of Assemblies of Axially Symmetric Molecules, I. General Theory," Proc R Soc London, Ser A 221: 498 (1954).

Reamer, H.H., B.H. Sage, and W.N. Lacey, "Volumetric Behavior of Hydrogen Sulfide," I&EC 42-1: 140 (1950).

Reichenberg, D., "The Indeterminancy of the Values of Potential Parameters as Derived from Transport and Virial Coefficients,"

AIChE J 19-4: 854-856 (Jul 1973).

Reid, R.C., "Present, past, and future property estimation techniques," Chem Eng Prog Monograph Series 64-5, AIChE, New York (1968).

Reid, R.C., J.M. Prausnitz, and T.K. Sherwood, The Properties of Gases and Liquids, McGraw-Hill (1977).

Riazi, M.R. and T.E. Daubert, "Simplify property predictions," Hyd Proc 115-116 (Mar. 1980).

Robinson, D.B. and N.H. Senturk, "The vapor pressure and critical properties of carbonyl sulfide," J Chem Therm 11: 461-467 (1979).

Rowlinson, J.S., and I.D. Watson, "The Principle of Corresponding States and Its Extensions," Chem Eng Sci 24: 1565 (1969).

Sage, B.H., and W.N. Lacey, "Some Properties of the Lighter Hydrocarbons, Hydrogen Sulfide and Carbon Dioxide," American Petroleum Institute (1955).

Sim, W.J., and T.E. Daubert, Prediction of Vapor—Liquid Equilibria of Undefined Mixtures," I&EC Proc Des & Dev 19-3: 386-393 (1980).

Smith, W.R., "Perturbation Theory and One-Fluid Corresponding States Theories for Fluid Mixtures," Can. J Chem Eng 50: 271 (1972).

Starling, K.E., "A New Approach for Determination of Equation-of-State Parameters Using Phase Equilibria Data," Soc Pet. Eng J 6-4: 363-371 (1966).

Starling, K.E., Fluid Thermodynamic Properties for Light Petroleum Systems," Gulf Pub. Co (1973a).

Starling, K.E., "Multiproperty Analysis of Thermodynamic and and Transport Properties," lectures at the University of Leuven, Belgium (1973b).

Starling, K.E., L.L. Lee, K.C. Mo, C.H. Twu, et al, "Self-Consistent Correlation of Thermodynamic and Transport Properties," Final Report GRI/AGA/BR-111-1/77-36, Gas Research Institute and American Gas Association, Arlington VA (1978).

Starling, K.E., M.R. Brule', C.T. Lin, and S. Watanasiri, "Calculation of Distillable-Coal-Fluid Thermophysical Properties

Using Multiparameter Corresponding-States Correlations," Report OU/IGT/S-14366/1 to the Institute of Gas Technology, Chicago IL (1980).

Stephan, K. and K. Lucas, Viscosity of Dense Fluids, Plenum Press, New York and London (1979).

Vargaftik, N.B., Tables on the Thermophysical Properties of Gases and Liquids, 2nd Ed., Hemisphere Pub. Co, Washington, D.C. (1975).

Viswanath, D.S., "Quinoline," API Monograph Series 711 (Dec 1979a).

Viswanath, D.S., and R.C. Wilhoit, "Isoquinoline," API Monograph Series 712 (Dec 1979b).

Viswanath, D.S., and R.C. Wilhoit, "Indanols," API Monograph Series 713 (Mar. 1980).

Viswanath, D.S., personal communication from Univ Missouri at Columbia (18 Feb 1981).

Wang, J.S., and W. Van Dael, and K.E. Starling, "Use of Velocity of Sound and Heat Capacity Data in Ethane Equation of State Correlation," Can. J Chem Eng 54: 241-244 (Jun 1976).

Watanasiri, S., M.R. Brule', and K.E. Starling, "Correlation of Phase-Separation Data for Coal-Conversion Systems," presented at the AIChE 90th National Meeting, Houston TX. Submitted for publication (1981).

Wieczorek, S.A. and R. Kobayashi, "Vapor Pressure Measurements of Diphenylmethane, Thianaphthene, and Bicyclohexyl at Elevated Temperatures," J Chem Eng Data 25-4: 302-305 (1980).

Wilson, G.M., R.H. Johnston, S.C. Hwang, and C. Tsonopoulos, "Volatility of Coal Liquids at High Temperatures and Pressures," I&EC Proc Des & Dev 20-1: 94-104 (1981).

Yaws, C.L., Physical Properties, McGraw-Hill, New York (1978).

Yesavage, V.F., PhD Thesis, Univ Michigan (1968).

Appendix A.

DETAILED LISTINGS OF CALCULATIONS FOR PURE FOSSIL CHEMICALS

The Therm-Trans Computer Program

Brief mention will be made of the computer program developed to carry out these studies, not so much as it relates to these studies, but how this program can serve many general purposes. The program determines any number or combination of characterization parameters by multiproperty analysis of any type of data whether thermodynamic, transport, or thermochemical. The many types of data that the program can handle include density or volume, vapor pressure, either departure or base enthalpy, heat capacity, heat of vaporization, compressibility factor, second and third virial coefficients, surface tension, absolute or kinematic viscosity, self-diffusion coefficient, thermal conductivity, and ideal-gas heat capacity, enthalpy, Gibb's free energy, and equilibrium constant. As the program can easily be set up to automatically handle any additional property-calculation routines, multiproperty analysis can be practiced on a grand scale. The program is also amenable to

making mixture calculations for all these properties; this feature will be incorporated in the near future. A special provision has been made to generate vapor pressure, in the cases where the condition is specified as only the temperature of the saturated liquid. This allows automatic calculation of the extensive property in either of the cases where the intensive variables are specified as either T or T and P.

The program is also capable of reading data directly from master files for each compound. Each data point in the file has a 5-digit code which tells the program what the property is as well as what units the property is in. The program automatically decodes the property identifier and converts the property units to SI for internal calculation in the program. The master data bank is among the most extensive in existence. The bank is set up on a central directory and is under access to members in the Coal-Calc Project. Contributions are easily made to the data file, without the bother of having to convert units, by any member in the central directory.

Interpreting the Output Given in the Tables

The single-alphabet, four-digit character first read on the calculations listing is the numerical code as established in the Physics and Chemistry Handbook (Chemical Rubber Publishing Company). Next, common and formal

nomenclature are given for the compound. CONST stands for references or methods from which the characterization parameters were obtained; these values are listed next as INPUT. FITTED indicates those parameter values which were fitted via mulitproperty analysis. A detailed listing of experimental vs calculated data points, at temperature and pressure, follows. The property CODE can be identified in the SUMMARY of deviations, which follows the detailed listing.

The average relative deviation (AAD) is defined as the calculated property value minus the experimental value. Percent average absolute relative deviation (%AARD) is defined as the absolute quotient (times 100) of the calculated value minus the experimental value divided by the experimental value.

B2214 C6H6 BENZENE

CONST: REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 342, 2. CHAO 1978

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	78.115	562.16	446.41	259.00	5.157	0.21250
FITTED:						0.21425

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
6.85		4	5.300	5.301	0.001	0.025	1
16.85		4	8.770	8.801	0.031	0.359	1
26.85		4	13.900	14.037	0.137	0.983	1
36.85		4	21.500	21.644	0.144	0.672	1
46.85		4	32.200	32.320	0.120	0.371	1
56.85		4	46.700	46.872	0.172	0.368	1
66.85		4	66.200	66.268	0.068	0.103	1
76.85		4	91.700	91.542	-0.158	-0.173	1
86.85		4	124.300	123.827	-0.473	-0.380	1
96.85		4	165.400	164.372	-1.028	-0.621	1
106.85		4	216.400	214.501	-1.899	-0.878	1
116.85		4	278.600	275.611	-2.989	-1.073	1
126.85		4	353.600	349.190	-4.410	-1.247	1
131.85		4	396.300	391.135	-5.165	-1.303	1
136.85		4	442.800	436.788	-6.012	-1.358	1
141.85		4	493.200	486.351	-6.849	-1.389	1
146.85		4	547.900	540.041	-7.859	-1.434	1
151.85		4	606.900	598.065	-8.835	-1.456	1
156.85		4	670.400	660.644	-9.756	-1.455	1
161.85		4	738.800	728.008	-10.792	-1.461	1
166.85		4	812.100	800.380	-11.720	-1.443	1
171.85		4	890.600	877.998	-12.602	-1.415	1
176.85		4	974.600	961.104	-13.496	-1.385	1
181.85		4	1064.000	1049.936	-14.064	-1.322	1
186.85		4	1160.000	1144.773	-15.227	-1.313	1
191.85		4	1261.000	1245.825	-15.175	-1.203	1
196.85		4	1369.000	1353.406	-15.594	-1.139	1
201.85		4	1484.000	1467.785	-16.215	-1.093	1
206.85		4	1606.000	1589.238	-16.762	-1.044	1
211.85		4	1734.000	1718.031	-15.969	-0.921	1
216.85		4	1870.000	1854.510	-15.490	-0.828	1
221.85		4	2014.000	1998.982	-15.018	-0.746	1
226.85		4	2166.000	2151.773	-14.227	-0.657	1
231.85		4	2327.000	2313.240	-13.760	-0.591	1
236.85		4	2496.000	2483.717	-12.283	-0.492	1
241.85		4	2674.000	2663.593	-10.407	-0.389	1
246.85		4	2862.000	2853.268	-8.732	-0.305	1

B2214 C6H6 BENZENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
251.85		4	3060.000	3053.135	-6.865	-0.224	1
256.85		4	3269.000	3263.599	-5.401	-0.165	1
261.85		4	3488.000	3484.996	-3.004	-0.086	1
266.85		4	3719.000	3717.588	-1.412	-0.038	1
271.85		4	3962.000	3961.250	-0.750	-0.019	1
276.85		4	4218.000	4214.869	-3.131	-0.074	1
281.85		4	4487.000	4475.082	-11.918	-0.266	1
286.85		4	4771.000	4780.377	9.377	0.197	1
287.85		4	4830.000	4838.430	8.430	0.175	1
288.85		4	4889.000	4868.415	-20.585	-0.421	1
289.45		4	4924.000	4910.765	-13.235	-0.269	1
66.85	66.200	21	0.355	0.311	-0.044	-12.522	1
86.85	124.300	21	0.299	0.265	-0.034	-11.471	1
106.85	216.400	21	0.246	0.228	-0.018	-7.151	1
126.85	353.600	21	0.205	0.199	-0.006	-3.063	1
146.85	547.900	21	0.173	0.174	0.001	0.408	1
166.85	812.100	21	0.148	0.152	0.004	2.726	1
186.85	1160.000	21	0.128	0.133	0.005	3.702	1
206.85	1606.000	21	0.112	0.115	0.003	2.723	1
226.85	2166.000	21	0.098	0.098	0.000	0.341	1
246.85	2862.000	21	0.084	0.081	-0.003	-3.415	1
266.85	3719.000	21	0.069	0.062	-0.007	-10.480	1
46.85	32.200	-21	0.008	0.008	-0.000	-3.504	1
66.85	66.200	-21	0.009	0.009	-0.000	-3.447	1
86.85	124.300	-21	0.009	0.009	-0.000	-3.463	1
106.85	216.400	-21	0.010	0.010	-0.000	-3.423	1
126.85	353.600	-21	0.011	0.010	-0.000	-4.625	1
146.85	547.900	-21	0.011	0.011	-0.001	-4.619	1
166.85	812.100	-21	0.012	0.011	-0.001	-5.803	1
186.85	1160.000	-21	0.013	0.012	-0.001	-6.205	1
206.85	1606.000	-21	0.014	0.013	-0.001	-6.212	1
226.85	2166.000	-21	0.015	0.014	-0.001	-6.428	1
246.85	2862.000	-21	0.016	0.016	-0.001	-4.803	1
266.85	3719.000	-21	0.018	0.018	0.000	0.065	1
276.85	4218.000	-21	0.020	0.021	0.001	5.257	1
10.00		4	6.070	6.210	0.140	2.314	2
20.00		4	10.027	10.207	0.180	1.800	2
30.00		4	15.915	16.132	0.217	1.366	2
40.00		4	24.379	24.622	0.243	0.996	2
50.00		4	36.186	36.426	0.240	0.664	2
60.00		4	52.218	52.408	0.190	0.364	2
70.00		4	73.470	73.537	0.067	0.092	2
79.68		4	100.000	99.902	-0.098	-0.098	2
80.00		4	101.040	100.889	-0.151	-0.149	2

B2214 C6H6 BENZENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
90.00		4	136.130	135.636	-0.494	-0.363	2
100.00		4	180.030	179.044	-0.986	-0.548	2
120.00		4	299.760	297.317	-2.443	-0.815	2
140.00		4	472.030	467.457	-4.573	-0.969	2
160.00		4	709.710	702.400	-7.310	-1.030	2
180.00		4	1026.600	1016.277	-10.323	-1.006	2
200.00		4	1437.600	1424.579	-13.021	-0.906	2
220.00		4	1958.400	1944.543	-13.857	-0.708	2
240.00		4	2606.500	2595.905	-10.595	-0.406	2
260.00		4	3403.400	3401.741	-1.659	-0.049	2
280.00		4	4382.600	4378.292	-4.308	-0.098	2
10.00	6.070	1	889.500	874.553	-14.947	-1.680	2
20.00	10.027	1	878.900	863.921	-14.979	-1.704	2
30.00	15.915	1	868.300	853.414	-14.886	-1.714	2
40.00	24.379	1	857.600	843.001	-14.599	-1.702	2
50.00	36.186	1	846.800	832.648	-14.152	-1.671	2
60.00	52.218	1	835.900	822.323	-13.577	-1.624	2
70.00	73.470	1	824.800	811.993	-12.807	-1.553	2
79.68	100.000	1	814.000	801.958	-12.042	-1.479	2
80.00	101.040	1	813.600	801.625	-11.975	-1.472	2
90.00	136.130	1	802.300	791.186	-11.114	-1.385	2
100.00	180.030	1	790.700	780.637	-10.063	-1.273	2
120.00	299.760	1	767.100	759.058	-8.042	-1.048	2
140.00	472.030	1	742.400	736.532	-5.868	-0.790	2
160.00	709.710	1	716.200	712.604	-3.596	-0.502	2
180.00	1026.600	1	688.200	686.640	-1.560	-0.227	2
200.00	1437.600	1	657.300	657.670	0.370	0.056	2
220.00	1958.400	1	622.600	624.002	1.402	0.225	2
240.00	2606.500	1	582.000	582.108	0.108	0.019	2
260.00	3403.400	1	530.700	521.970	-8.730	-1.645	2
10.00	6.070	5	444.089	437.824	-6.264	-1.411	2
20.00	10.027	5	436.805	431.333	-5.472	-1.253	2
30.00	15.915	5	429.610	424.698	-4.912	-1.143	2
40.00	24.379	5	422.454	417.960	-4.494	-1.064	2
50.00	36.186	5	415.285	411.139	-4.146	-0.998	2
60.00	52.218	5	408.091	404.242	-3.849	-0.943	2
70.00	73.470	5	400.807	397.262	-3.544	-0.884	2
79.68	100.000	5	393.638	390.417	-3.221	-0.818	2
80.00	101.040	5	393.394	390.187	-3.208	-0.815	2
90.00	136.130	5	385.829	382.995	-2.834	-0.734	2
100.00	180.030	5	378.045	375.660	-2.385	-0.631	2
120.00	299.760	5	362.350	360.438	-1.913	-0.528	2
140.00	472.030	5	345.068	344.216	-0.852	-0.247	2
160.00	709.710	5	326.365	326.602	0.237	0.073	2

B2214 C6H6 BENZENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
180.00	1026.600	5	305.793	307.070	1.277	0.418	2
200.00	1437.600	5	282.673	284.855	2.182	0.772	2
220.00	1958.400	5	255.969	258.731	2.763	1.079	2
240.00	2606.500	5	223.709	226.339	2.631	1.176	2
260.00	3403.400	5	181.514	181.710	0.195	0.108	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.15 %AARD FOR 19 POINTS
4	VAPOR PRESSURE	KPA	0.74 %AARD FOR 68 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.79 %AARD FOR 19 POINTS
-21	VAPOR VISCOSITY	CP	4.45 %AARD FOR 13 POINTS
21	LIQUID VISCOSITY	CP	5.27 %AARD FOR 11 POINTS

B2214 C6H12 CYCLOHEXANE
NOTES: LIQUID VISCOSITY PROBLEM
CONST: REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 301, 2. EAKIN ET AL 1972
3. STEPHAN AND LUCAS

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	84.162	553.40	439.45	308.00	5.464	0.21300
FITTED:						0.21596

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
10.00		4	6.331	6.398	0.067	1.056	1
20.00		4	10.335	10.407	0.072	0.693	1
25.00		4	13.010	13.080	0.070	0.538	1
30.00		4	16.229	16.292	0.062	0.385	1
40.00		4	24.623	24.651	0.027	0.112	1
50.00		4	36.237	36.182	-0.055	-0.152	1
60.00		4	51.889	51.680	-0.209	-0.402	1
70.00		4	72.505	72.036	-0.468	-0.646	1
80.00		4	99.096	98.229	-0.866	-0.874	1
90.00		4	132.720	131.318	-1.402	-1.056	1
100.00		4	174.620	172.450	-2.170	-1.243	1
110.00		4	226.000	222.835	-3.165	-1.400	1
120.00		4	288.100	283.755	-4.345	-1.508	1
130.00		4	362.200	356.556	-5.644	-1.558	1
140.00		4	449.800	442.656	-7.144	-1.588	1
150.00		4	552.000	543.521	-8.479	-1.536	1
160.00		4	670.300	660.699	-9.601	-1.432	1
170.00		4	805.900	795.798	-10.102	-1.254	1
180.00		4	960.100	950.509	-9.591	-0.999	1
190.00		4	1134.000	1126.610	-7.390	-0.652	1
200.00		4	1330.000	1326.016	-3.984	-0.300	1
210.00		4	1552.000	1550.799	-1.201	-0.077	1
220.00		4	1801.000	1803.111	2.111	0.117	1
230.00		4	2082.000	2085.375	3.375	0.162	1
240.00		4	2396.000	2400.138	4.138	0.173	1
250.00		4	2745.000	2750.125	5.125	0.187	1
260.00		4	3132.000	3137.729	5.729	0.183	1
270.00		4	3561.000	3561.243	0.243	0.007	1
10.00	101.325	1	787.950	788.319	0.369	0.047	1
20.00	101.325	1	778.570	778.589	0.019	0.002	1
25.00	101.325	1	773.870	773.765	-0.105	-0.014	1
30.00	101.325	1	769.150	768.962	-0.188	-0.024	1
40.00	101.325	1	759.600	759.404	-0.196	-0.026	1
50.00	101.325	1	749.930	749.884	-0.046	-0.006	1
60.00	101.325	1	740.100	740.369	0.269	0.036	1
70.00	101.325	1	730.100	730.825	0.725	0.099	1
80.00	101.325	1	719.900	721.217	1.317	0.183	1

B2214 C6H12 CYCLOHEXANE
NOTES: LIQUID VISCOSITY PROBLEM
(CONTINUED)

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
148.89	9652.660	2	-313.545	-315.582	-2.037	0.650	2
160.00	9652.660	2	-307.265	-310.134	-2.870	0.934	2
171.11	1378.951	2	-303.776	-307.611	-3.835	1.262	2
171.11	9652.660	2	-300.984	-304.690	-3.705	1.231	2
182.22	1378.951	2	-297.263	-301.129	-3.866	1.301	2
182.22	9652.660	2	-293.774	-299.219	-5.445	1.853	2
193.33	1378.951	2	-290.517	-294.279	-3.762	1.295	2
193.33	9652.660	2	-288.657	-293.688	-5.032	1.743	2
204.44	1378.951	-2	-39.542	-38.250	1.292	-3.269	2
204.44	2068.427	2	-282.842	-287.317	-4.475	1.582	2
204.44	9652.660	2	-281.679	-288.061	-6.382	2.266	2
215.55	1378.951	-2	-36.751	-35.384	1.367	-3.720	2
215.55	2068.427	2	-276.096	-279.452	-3.356	1.215	2
215.55	9652.660	2	-275.864	-282.293	-6.429	2.331	2
226.66	1378.951	-2	-34.657	-32.977	1.681	-4.849	2
226.66	2068.427	2	-267.025	-270.403	-3.378	1.265	2
226.66	9652.660	2	-267.723	-276.332	-8.610	3.216	2
237.78	1378.951	-2	-33.262	-30.935	2.327	-6.996	2
237.78	2068.427	-2	-54.894	-52.749	2.145	-3.907	2
237.78	2757.903	2	-258.884	-261.651	-2.767	1.069	2
237.78	9652.660	2	-262.140	-270.118	-7.978	3.044	2
248.89	2068.427	-2	-53.033	-48.891	4.142	-7.810	2
248.89	2757.903	2	-247.719	-248.201	-0.482	0.195	2
248.89	9652.660	2	-256.790	-263.576	-6.786	2.642	2
260.00	2757.903	-2	-67.687	-67.937	-0.250	0.369	2
260.00	3447.378	2	-240.043	-235.603	4.440	-1.850	2
260.00	4054.117	2	-240.508	-241.296	-0.787	0.327	2
260.00	6894.757	2	-246.556	-252.419	-5.863	2.378	2
260.00	9652.660	2	-251.208	-256.614	-5.406	2.152	2
271.11	1378.951	-2	-27.912	-25.778	2.134	-7.646	2
271.11	2068.427	-2	-44.659	-41.922	2.737	-6.129	2
271.11	2757.903	-2	-60.941	-61.429	-0.488	0.800	2
271.11	3447.378	-2	-96.529	-96.013	0.516	-0.535	2
271.11	4054.117	2	-227.250	-219.645	7.606	-3.347	2
271.11	4826.330	2	-233.530	-230.895	2.636	-1.129	2
271.11	5515.806	2	-234.693	-236.267	-1.573	0.670	2
271.11	6894.757	2	-236.554	-242.685	-6.131	2.592	2
271.11	9652.660	2	-244.695	-249.119	-4.424	1.808	2
282.22	2068.427	-2	-42.101	-39.290	2.810	-6.676	2
282.22	2757.903	-2	-57.685	-56.872	0.813	-1.410	2
282.22	3447.378	-2	-85.829	-83.092	2.738	-3.190	2
282.22	4054.117	-2	-127.465	-128.325	-0.860	0.675	2
282.22	5515.806	2	-224.692	-219.821	4.870	-2.168	2
282.22	6894.757	2	-230.507	-231.196	-0.689	0.299	2

B2214 C6H12 CYCLOHEXANE
NOTES: LIQUID VISCOSITY PROBLEM
(CONTINUED)

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
282.22	9652.660	2	-237.717	-240.962	-3.245	1.365	2
293.33	2068.427	-2	-37.914	-36.674	1.239	-3.269	2
293.33	2757.903	-2	-53.033	-52.615	0.417	-0.787	2
293.33	3447.378	-2	-76.991	-74.182	2.809	-3.648	2
293.33	4054.117	-2	-105.600	-102.538	3.062	-2.900	2
293.33	5515.806	-2	-203.990	-197.003	6.987	-3.425	2
293.33	6894.757	-2	-217.946	-217.257	0.689	-0.316	2
293.33	9652.660	-2	-229.576	-232.001	-2.425	1.056	2
304.44	1378.951	-2	-23.958	-21.986	1.972	-8.231	2
304.44	2068.427	-2	-36.286	-34.685	1.601	-4.411	2
304.44	2757.903	-2	-50.242	-49.259	0.983	-1.957	2
304.44	3447.378	-2	-69.780	-67.515	2.265	-3.246	2
304.44	4054.117	-2	-91.179	-88.443	2.736	-3.000	2
304.44	4826.330	-2	-130.489	-129.092	1.397	-1.071	2
304.44	5515.806	-2	-167.937	-167.823	0.114	-0.068	2
304.44	6894.757	-2	-205.153	-200.726	4.427	-2.158	2
304.44	9652.660	-2	-221.900	-222.137	-0.237	0.107	2
315.55	1378.951	-2	-22.562	-20.898	1.664	-7.377	2
315.55	2068.427	-2	-34.657	-32.866	1.791	-5.168	2
315.55	2757.903	-2	-46.985	-46.176	0.809	-1.721	2
315.55	3447.378	-2	-63.035	-62.029	1.005	-1.595	2
315.55	4054.117	-2	-80.247	-79.031	1.216	-1.516	2
315.55	4826.330	-2	-106.298	-106.735	-0.436	0.410	2
315.55	5515.806	-2	-142.351	-140.786	1.565	-1.100	2
315.55	6894.757	-2	-189.802	-182.730	7.071	-3.726	2
315.55	9652.660	-2	-213.062	-211.379	1.683	-0.790	2
326.66	1378.951	-2	-20.469	-19.791	0.678	-3.311	2
326.66	2068.427	-2	-32.331	-31.096	1.235	-3.820	2
326.66	2757.903	-2	-44.194	-43.483	0.711	-1.610	2
326.66	3447.378	-2	-57.220	-57.456	-0.236	0.413	2
326.66	4054.117	-2	-71.641	-71.963	-0.322	0.450	2
326.66	4826.330	-2	-96.064	-95.144	0.919	-0.957	2
326.66	5515.806	-2	-125.139	-121.493	3.646	-2.914	2
326.66	6894.757	-2	-174.450	-165.026	9.424	-5.402	2
326.66	9652.660	-2	-209.340	-200.053	9.287	-4.436	2
337.78	1378.951	-2	-18.375	-18.721	-0.346	1.881	2
337.78	2068.427	-2	-29.773	-29.415	0.358	-1.201	2
337.78	2757.903	-2	-40.938	-40.947	-0.009	0.022	2
337.78	3447.378	-2	-53.265	-53.782	-0.516	0.969	2
337.78	4054.117	-2	-64.663	-66.303	-1.640	2.536	2
337.78	4826.330	-2	-87.458	-86.369	1.089	-1.245	2
337.78	5515.806	-2	-110.485	-107.333	3.152	-2.853	2
337.78	6894.757	-2	-156.307	-148.311	7.996	-5.115	2
337.78	9652.660	-2	-195.849	-188.314	7.535	-3.848	2

B2214 C6H12 CYCLOHEXANE
NOTES: LIQUID VISCOSITY PROBLEM
(CONTINUED)

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
348.89	1378.951	-2	-16.049	-17.610	-1.561	9.727	2
348.89	2068.427	-2	-27.912	-27.949	-0.037	0.134	2
348.89	2757.903	-2	-38.146	-38.694	-0.548	1.436	2
348.89	3447.378	-2	-49.544	-50.520	-0.977	1.971	2
348.89	4054.117	-2	-60.709	-62.035	-1.327	2.185	2
348.89	4826.330	-2	-80.712	-79.522	1.191	-1.475	2
348.89	5515.806	-2	-98.390	-96.695	1.694	-1.722	2
348.89	6894.757	-2	-138.862	-133.404	5.458	-3.930	2
348.89	9652.660	-2	-186.313	-176.807	9.506	-5.102	2
360.00	1378.951	-2	-15.119	-16.810	-1.691	11.184	2
360.00	2068.427	-2	-25.353	-26.445	-1.092	4.307	2
360.00	2757.903	-2	-35.123	-36.555	-1.433	4.079	2
360.00	3447.378	-2	-46.753	-47.741	-0.988	2.113	2
360.00	4054.117	-2	-58.383	-58.573	-0.190	0.326	2
360.00	4826.330	-2	-73.734	-73.600	0.134	-0.182	2
360.00	5515.806	-2	-87.225	-88.060	-0.835	0.957	2
360.00	6894.757	-2	-119.324	-119.876	-0.552	0.463	2
360.00	9652.660	-2	-175.846	-165.712	10.133	-5.763	2
10.00	6.331	5	399.000	398.250	-0.750	-0.188	1
20.00	10.335	5	394.000	392.143	-1.857	-0.471	1
30.00	16.229	5	388.500	385.917	-2.583	-0.665	1
40.00	24.623	5	383.100	379.602	-3.498	-0.913	1
50.00	36.237	5	377.600	373.212	-4.388	-1.162	1
60.00	51.889	5	372.100	366.746	-5.354	-1.439	1
70.00	72.505	5	366.200	360.194	-6.006	-1.640	1
80.00	99.096	5	360.200	353.541	-6.659	-1.849	1
90.00	132.720	5	353.700	346.764	-6.936	-1.961	1
100.00	174.620	5	346.800	339.833	-6.967	-2.009	1
110.00	226.000	5	339.300	332.717	-6.583	-1.940	1
120.00	288.100	5	331.300	325.382	-5.918	-1.786	1
130.00	362.200	5	322.900	317.788	-5.112	-1.583	1
140.00	449.800	5	313.900	309.885	-4.015	-1.279	1
150.00	552.000	5	304.000	301.631	-2.369	-0.779	1
160.00	670.300	5	293.500	292.961	-0.539	-0.184	1
170.00	805.900	5	282.600	283.811	1.211	0.429	1
180.00	960.100	5	271.100	274.100	3.000	1.107	1
190.00	1134.000	5	259.200	263.733	4.533	1.749	1
200.00	1330.000	5	246.800	252.535	5.735	2.324	1
210.00	1552.000	5	233.800	240.230	6.430	2.750	1
220.00	1801.000	5	220.400	226.571	6.171	2.800	1
230.00	2082.000	5	206.500	211.028	4.528	2.193	1
240.00	2396.000	5	189.000	192.849	3.849	2.037	1
250.00	2745.000	5	171.100	170.983	-0.117	-0.069	1
46.85	100.000	21	0.628	0.326	-0.302	-48.154	3

B2214 C6H12 CYCLOHEXANE
NOTES: LIQUID VISCOSITY PROBLEM
(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
56.85	100.000	21	0.560	0.298	-0.262	-46.860	3
66.85	100.000	21	0.502	0.273	-0.229	-45.563	3
76.85	100.000	21	0.452	0.252	-0.200	-44.258	3
-0.00	100.000	-21	0.007	0.006	-0.000	-1.861	1
25.00	100.000	-21	0.007	0.007	-0.000	-1.650	1
50.00	100.000	-21	0.008	0.008	-0.000	-1.206	1
75.00	100.000	-21	0.008	0.008	0.000	0.557	1
100.00	100.000	-21	0.009	0.009	0.000	0.478	1
150.00	100.000	-21	0.010	0.010	0.000	1.710	1
200.00	100.000	-21	0.011	0.011	0.000	3.027	1
250.00	100.000	-21	0.012	0.012	0.001	4.230	1
300.00	100.000	-21	0.013	0.014	0.001	5.084	1
400.00	100.000	-21	0.015	0.016	0.001	6.399	1
500.00	100.000	-21	0.017	0.018	0.001	6.916	1
600.00	100.000	-21	0.019	0.020	0.001	6.682	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.05 %AARD FOR 9 POINTS
-2	VAPOR ENTHALPY DEPARTURE	KJ/KG	2.18 AAD FOR 76 POINTS
2	LIQUID ENTHALPY DEPARTURE	KJ/KG	1.64 %AARD FOR 30 POINTS
4	VAPOR PRESSURE	KPA	0.72 %AARD FOR 28 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.41 %AARD FOR 25 POINTS
-21	VAPOR VISCOSITY	CP	3.32 %AARD FOR 12 POINTS
21	LIQUID VISCOSITY	CP	46.21 %AARD FOR 4 POINTS

B2214 C7H8 TOLUENE. METHYLBENZENE. PHENYLMETHANE.

CONST: REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 347, 2. EAKIN ET AL 1972

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	92.141	591.70	469.86	316.00	5.510	0.25700
FITTED:						0.26472

TEMP C	PRES KPA	CODE	PROPERTY EXPM	CALC	AAD	%AARD	REF
-0.00		4	0.896	0.897	0.001	0.100	1
10.00		4	1.657	1.655	-0.002	-0.128	1
20.00		4	2.912	2.908	-0.003	-0.119	1
25.00		4	3.792	3.791	-0.001	-0.021	1
30.00		4	4.889	4.891	0.002	0.046	1
40.00		4	7.887	7.909	0.022	0.276	1
50.00		4	12.282	12.345	0.064	0.518	1
60.00		4	18.518	18.664	0.146	0.786	1
70.00		4	27.158	27.420	0.262	0.964	1
80.00		4	38.823	39.248	0.425	1.094	1
90.00		4	54.222	54.871	0.649	1.197	1
100.00		4	74.167	75.093	0.926	1.249	1
110.00		4	99.538	100.797	1.258	1.264	1
120.00		4	131.200	132.932	1.732	1.320	1
130.00		4	170.400	172.541	2.141	1.256	1
140.00		4	218.000	220.701	2.701	1.239	1
150.00		4	275.200	278.573	3.373	1.226	1
160.00		4	343.300	347.378	4.078	1.188	1
170.00		4	423.300	428.381	5.081	1.200	1
180.00		4	516.500	522.923	6.423	1.244	1
190.00		4	624.100	632.399	8.299	1.330	1
200.00		4	747.400	758.275	10.875	1.455	1
210.00		4	909.400	902.708	-6.692	-0.736	1
220.00		4	1093.000	1066.655	-26.345	-2.410	1
230.00		4	1298.000	1251.817	-46.183	-3.558	1
240.00		4	1526.000	1460.055	-65.945	-4.321	1
250.00		4	1777.000	1693.333	-83.667	-4.708	1
260.00		4	2050.000	1953.774	-96.226	-4.694	1
270.00		4	2348.000	2243.771	-104.229	-4.439	1
280.00		4	2669.000	2565.838	-103.162	-3.865	1
290.00		4	3015.000	2922.576	-92.424	-3.065	1
300.00		4	3382.000	3315.089	-66.911	-1.978	1
310.00		4	3774.000	3732.514	-41.486	-1.099	1
-0.00	101.325	1	885.500	878.012	-7.488	-0.846	1
10.00	101.325	1	876.200	867.764	-8.436	-0.963	1
20.00	101.325	1	866.900	857.695	-9.205	-1.062	1
25.00	101.325	1	862.300	852.719	-9.581	-1.111	1

B2214 C7H8 TOLUENE. METHYLBENZENE. PHENYLMETHANE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
30.00	101.325	1	857.600	847.776	-9.824	-1.145	1
40.00	101.325	1	848.300	837.981	-10.319	-1.216	1
50.00	101.325	1	838.800	828.280	-10.520	-1.254	1
60.00	101.325	1	829.300	818.649	-10.651	-1.284	1
70.00	101.325	1	819.700	809.060	-10.640	-1.298	1
80.00	101.325	1	809.900	799.485	-10.415	-1.286	1
90.00	101.325	1	800.000	789.896	-10.104	-1.263	1
100.00	101.325	1	790.000	780.265	-9.735	-1.232	1
110.00	101.325	1	779.800	770.559	-9.241	-1.185	1
-0.00	0.896	5	423.000	428.779	5.779	1.366	1
10.00	1.657	5	419.000	423.952	4.952	1.182	1
20.00	2.912	5	414.400	418.616	4.216	1.017	1
30.00	4.889	5	409.400	412.918	3.518	0.859	1
40.00	7.887	5	404.000	406.964	2.964	0.734	1
50.00	12.282	5	399.000	400.829	1.829	0.458	1
60.00	18.518	5	393.500	394.563	1.063	0.270	1
70.00	27.158	5	388.100	388.198	0.098	0.025	1
80.00	38.823	5	382.200	381.748	-0.452	-0.118	1
90.00	54.222	5	376.700	375.221	-1.479	-0.393	1
100.00	74.167	5	370.800	368.612	-2.188	-0.590	1
110.00	99.538	5	364.400	361.909	-2.491	-0.684	1
120.00	131.200	5	358.500	355.101	-3.399	-0.948	1
130.00	170.400	5	352.200	348.155	-4.045	-1.149	1
140.00	218.000	5	345.300	341.056	-4.244	-1.229	1
150.00	275.200	5	338.500	333.771	-4.729	-1.397	1
160.00	343.300	5	331.700	326.262	-5.438	-1.639	1
170.00	423.300	5	324.000	318.499	-5.501	-1.698	1
180.00	516.500	5	315.800	310.436	-5.364	-1.698	1
190.00	624.100	5	307.200	302.027	-5.173	-1.684	1
200.00	747.400	5	298.100	293.211	-4.889	-1.640	1
210.00	909.400	5	288.500	283.155	-5.345	-1.853	1
220.00	1093.000	5	278.500	272.418	-6.082	-2.184	1
230.00	1298.000	5	267.200	260.921	-6.279	-2.350	1
240.00	1526.000	5	255.400	248.492	-6.908	-2.705	1
250.00	1777.000	5	242.200	234.946	-7.254	-2.995	1
260.00	2050.000	5	227.600	220.055	-7.545	-3.315	1
270.00	2348.000	5	211.800	203.291	-8.509	-4.018	1
-0.00	0.896	21	0.768	0.842	0.074	9.621	1
10.00	1.657	21	0.667	0.727	0.060	9.000	1
20.00	2.912	21	0.586	0.636	0.050	8.461	1
30.00	4.889	21	0.522	0.562	0.040	7.578	1
40.00	7.887	21	0.466	0.501	0.035	7.451	1
50.00	12.282	21	0.420	0.450	0.030	7.155	1
60.00	18.518	21	0.381	0.407	0.026	6.905	1

B2214 C7H8 TOLUENE. METHYLBENZENE. PHENYLMETHANE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
70.00	27.158	21	0.348	0.371	0.023	6.565	1
80.00	38.823	21	0.319	0.339	0.020	6.397	1
100.00	74.167	21	0.271	0.288	0.017	6.264	1
120.00	131.200	21	0.231	0.248	0.017	7.192	1
140.00	218.000	21	0.199	0.215	0.016	7.998	1
160.00	343.300	21	0.172	0.188	0.016	9.106	1
180.00	516.500	21	0.150	0.164	0.014	9.556	1
200.00	100.000	-21	0.011	0.011	-0.000	-1.226	1
400.00	100.000	-21	0.015	0.016	0.000	1.162	1
600.00	100.000	-21	0.019	0.020	0.000	1.283	1
10.00	344.738	2	-421.704	-423.837	-2.133	0.506	2
10.00	689.476	2	-421.239	-423.571	-2.332	0.554	2
10.00	1378.951	2	-420.773	-423.039	-2.265	0.538	2
10.00	2757.903	2	-419.378	-421.972	-2.594	0.619	2
10.00	4136.854	2	-417.982	-420.903	-2.921	0.699	2
10.00	5515.806	2	-416.819	-419.831	-3.012	0.723	2
10.00	6894.757	2	-415.424	-418.757	-3.333	0.802	2
10.00	10342.135	2	-412.167	-416.060	-3.893	0.944	2
10.00	17236.892	2	-405.654	-410.622	-4.968	1.225	2
37.78	344.738	2	-404.724	-408.556	-3.832	0.947	2
37.78	689.476	2	-404.491	-408.294	-3.803	0.940	2
37.78	1378.951	2	-404.491	-407.768	-3.277	0.810	2
37.78	2757.903	2	-402.631	-406.714	-4.084	1.014	2
37.78	4136.854	2	-401.468	-405.656	-4.189	1.043	2
37.78	5515.806	2	-400.537	-404.595	-4.057	1.013	2
37.78	6894.757	2	-398.909	-403.529	-4.620	1.158	2
37.78	10342.135	2	-395.653	-400.849	-5.197	1.313	2
37.78	17236.892	2	-389.372	-395.429	-6.056	1.555	2
65.55	344.738	2	-387.977	-392.141	-4.164	1.073	2
65.55	689.476	2	-387.744	-391.886	-4.142	1.068	2
65.55	1378.951	2	-387.046	-391.374	-4.328	1.118	2
65.55	2757.903	2	-385.883	-390.347	-4.464	1.157	2
65.55	4136.854	2	-384.720	-389.314	-4.593	1.194	2
65.55	5515.806	2	-383.557	-388.274	-4.717	1.230	2
65.55	6894.757	2	-382.394	-387.230	-4.835	1.265	2
65.55	10342.135	2	-379.371	-384.595	-5.225	1.377	2
65.55	17236.892	2	-373.090	-379.239	-6.148	1.648	2
93.33	344.738	2	-370.997	-375.771	-4.774	1.287	2
93.33	689.476	2	-370.997	-375.528	-4.531	1.221	2
93.33	1378.951	2	-370.532	-375.041	-4.509	1.217	2
93.33	2757.903	2	-369.369	-374.060	-4.691	1.270	2
93.33	4136.854	2	-368.206	-373.070	-4.864	1.321	2
93.33	5515.806	2	-367.275	-372.071	-4.796	1.306	2
93.33	6894.757	2	-366.345	-371.064	-4.719	1.288	2

B2214 C7H8 TOLUENE. METHYLBENZENE. PHENYLMETHANE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
93.33	10342.135	2	-363.554	-368.512	-4.958	1.364	2
93.33	17236.892	2	-357.739	-363.281	-5.542	1.549	2
121.11	344.738	2	-354.017	-359.836	-5.819	1.644	2
121.11	689.476	2	-354.017	-359.614	-5.597	1.581	2
121.11	1378.951	2	-353.552	-359.167	-5.615	1.588	2
121.11	2757.903	2	-352.622	-358.262	-5.640	1.599	2
121.11	4136.854	2	-351.691	-357.342	-5.651	1.607	2
121.11	5515.806	2	-350.761	-356.408	-5.648	1.610	2
121.11	6894.757	2	-350.063	-355.462	-5.399	1.542	2
121.11	10342.135	2	-347.504	-353.045	-5.540	1.594	2
121.11	17236.892	2	-342.155	-348.021	-5.867	1.715	2
148.89	344.738	2	-337.037	-344.309	-7.271	2.157	2
148.89	689.476	2	-336.805	-344.120	-7.316	2.172	2
148.89	1378.951	2	-336.572	-343.739	-7.166	2.129	2
148.89	2757.903	2	-336.107	-342.955	-6.848	2.037	2
148.89	4136.854	2	-335.177	-342.147	-6.971	2.080	2
148.89	5515.806	2	-334.711	-341.317	-6.606	1.974	2
148.89	6894.757	2	-334.014	-340.466	-6.452	1.932	2
148.89	10342.135	2	-331.920	-338.257	-6.337	1.909	2
148.89	17236.892	2	-327.268	-333.552	-6.284	1.920	2
176.66	689.476	2	-319.360	-328.754	-9.395	2.942	2
176.66	1378.951	2	-319.127	-328.481	-9.354	2.931	2
176.66	2757.903	2	-319.127	-327.899	-8.772	2.749	2
176.66	4136.854	2	-318.662	-327.272	-8.610	2.702	2
176.66	5515.806	2	-318.429	-326.606	-8.177	2.568	2
176.66	6894.757	2	-317.964	-325.904	-7.940	2.497	2
176.66	10342.135	2	-316.336	-324.016	-7.680	2.428	2
176.66	17236.892	2	-312.847	-319.785	-6.938	2.218	2
204.44	1378.951	2	-300.984	-312.858	-11.873	3.945	2
204.44	2757.903	2	-301.682	-312.629	-10.947	3.629	2
204.44	4136.854	2	-301.915	-312.311	-10.396	3.443	2
204.44	5515.806	2	-301.915	-311.917	-10.002	3.313	2
204.44	6894.757	2	-301.915	-311.456	-9.541	3.160	2
204.44	10342.135	2	-301.217	-310.066	-8.849	2.938	2
204.44	17236.892	2	-298.891	-306.538	-7.647	2.558	2
232.22	4136.854	2	-283.539	-296.586	-13.047	4.601	2
232.22	5515.806	2	-284.702	-296.680	-11.977	4.207	2
232.22	6894.757	2	-285.400	-296.634	-11.234	3.936	2
232.22	10342.135	2	-287.261	-296.054	-8.793	3.061	2
232.22	17236.892	2	-285.400	-293.576	-8.176	2.865	2
260.00	2757.903	2	-259.814	-277.115	-17.301	6.659	2
260.00	4136.854	2	-263.303	-278.778	-15.474	5.877	2
315.55	2757.903	-2	-54.196	-56.317	-2.121	3.914	2
343.33	1378.951	-2	-22.330	-21.429	0.901	-4.035	2

B2214 C7H8 TOLUENE. METHYLBENZENE. PHENYLMETHANE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
343.33	2757.903	-2	-50.009	-48.380	1.629	-3.258	2
343.33	4136.854	-2	-90.016	-88.591	1.425	-1.583	2
343.33	6894.757	-2	-187.243	-197.950	-10.707	5.718	2
343.33	10342.135	-2	-215.388	-225.345	-9.957	4.623	2
343.33	17236.892	-2	-233.065	-238.684	-5.619	2.411	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.17 %AARD FOR 13 POINTS
-2	VAPOR ENTHALPY DEPARTURE	KJ/KG	4.62 AAD FOR 7 POINTS
2	LIQUID ENTHALPY DEPARTURE	KJ/KG	1.94 %AARD FOR 76 POINTS
4	VAPOR PRESSURE	KPA	1.64 %AARD FOR 33 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.44 %AARD FOR 28 POINTS
-21	VAPOR VISCOSITY	CP	1.22 %AARD FOR 3 POINTS
21	LIQUID VISCOSITY	CP	7.80 %AARD FOR 14 POINTS

T4990 C7H8O M-CRESOL

CONST: KUDCHADKER ET AL 1978A
PROP.: 1. KUDCHADKER ET AL 1978A, 2. NASIR ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	108.140	705.85	560.51	312.00	5.487	0.45000
FITTED:				328.96	5.585	0.44822

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
40.00	0.055	1	1008.400	1028.282	19.882	1.972	1
50.00	0.120	1	1002.500	1018.178	15.678	1.564	1
60.00	0.246	1	996.400	1008.230	11.830	1.187	1
70.00	0.472	1	990.000	998.421	8.421	0.851	1
80.00	0.863	1	983.000	988.736	5.736	0.583	1
90.00	1.505	1	977.000	979.159	2.159	0.221	1
100.00	2.521	1	969.000	969.676	0.676	0.070	1
120.00	6.362	1	954.000	950.928	-3.072	-0.322	1
140.00	14.261	1	938.000	932.369	-5.631	-0.600	1
160.00	29.011	1	921.000	913.872	-7.128	-0.774	1
180.00	54.451	1	903.000	895.305	-7.695	-0.852	1
200.00	95.521	1	883.000	876.522	-6.478	-0.734	1
201.77	100.000	1	881.000	874.839	-6.161	-0.699	1
220.00	158.240	1	862.000	857.361	-4.639	-0.538	1
240.00	249.630	1	839.000	837.632	-1.368	-0.163	1
260.00	376.000	1	815.000	817.098	2.098	0.257	1
280.00	540.000	1	789.000	795.444	6.444	0.817	1
300.00	770.000	1	760.000	772.295	12.295	1.618	1
320.00	1060.000	1	730.000	747.007	17.007	2.330	1
340.00	1430.000	1	696.000	718.620	22.620	3.250	1
360.00	1910.000	1	658.000	685.460	27.460	4.173	1
380.00	2470.000	1	616.000	643.132	27.132	4.405	1
400.00	3110.000	1	565.000	574.695	9.695	1.716	1
140.00		4	14.261	14.704	0.443	3.109	1
160.00		4	29.011	29.487	0.476	1.641	1
180.00		4	54.451	54.687	0.236	0.433	1
200.00		4	95.521	94.946	-0.575	-0.602	1
201.77		4	100.000	99.421	-0.579	-0.579	1
220.00		4	158.240	155.878	-2.362	-1.493	1
240.00		4	249.630	244.026	-5.604	-2.245	1
260.00		4	376.000	366.778	-9.222	-2.453	1
280.00		4	540.000	532.314	-7.686	-1.423	1
300.00		4	770.000	750.453	-19.547	-2.539	1
100.00	2.521	5	530.424	507.499	-22.924	-4.322	1
120.00	6.362	5	509.802	493.611	-16.191	-3.176	1
140.00	14.261	5	491.308	478.944	-12.363	-2.516	1
160.00	29.011	5	474.200	463.847	-10.353	-2.183	1

T4990 C7H8O M-CRESOL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
180.00	54.451	5	458.017	448.468	-9.549	-2.085	1
200.00	95.521	5	442.205	432.825	-9.380	-2.121	1
201.77	100.000	5	440.817	431.427	-9.391	-2.130	1
220.00	158.240	5	420.751	416.840	-3.911	-0.929	1
240.00	249.630	5	399.482	400.369	0.887	0.222	1
260.00	376.000	5	376.364	383.265	6.901	1.834	1
280.00	540.000	5	352.321	365.471	13.150	3.732	1
300.00	770.000	5	328.278	345.925	17.647	5.376	1
156.29		4	25.337	26.052	0.716	2.825	2
167.90		4	37.430	37.951	0.521	1.391	2
187.33		4	67.950	67.457	-0.493	-0.726	2
203.40		4	106.384	103.788	-2.596	-2.441	2
216.72		4	149.431	144.364	-5.067	-3.391	2
160.00	101.325	21	0.512	0.460	-0.052	-10.219	1
180.00	101.325	21	0.411	0.395	-0.016	-3.811	1
190.00	101.325	21	0.372	0.368	-0.004	-1.051	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.29 %AARD FOR 23 POINTS
4	VAPOR PRESSURE	KPA	1.82 %AARD FOR 15 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	2.55 %AARD FOR 12 POINTS
21	LIQUID VISCOSITY	CP	5.03 %AARD FOR 3 POINTS

B0660 C8H10 O-XYLENE

CONST: REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 356

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	106.168	630.20	500.44	369.00	5.803	0.31400
FITTED:						0.30814

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
-0.00		4	0.167	0.167	0.001	0.414	1
10.00		4	0.340	0.337	-0.003	-0.803	1
20.00		4	0.651	0.642	-0.008	-1.269	1
30.00		4	1.181	1.165	-0.017	-1.399	1
40.00		4	2.045	2.020	-0.025	-1.241	1
50.00		4	3.398	3.365	-0.033	-0.976	1
60.00		4	5.440	5.406	-0.033	-0.610	1
70.00		4	8.425	8.404	-0.020	-0.243	1
80.00		4	12.663	12.678	0.015	0.120	1
90.00		4	18.530	18.611	0.081	0.435	1
100.00		4	26.466	26.650	0.185	0.697	1
110.00		4	36.976	37.308	0.332	0.899	1
120.00		4	50.636	51.160	0.525	1.036	1
130.00		4	68.084	68.846	0.763	1.120	1
140.00		4	90.023	91.064	1.041	1.157	1
150.00		4	117.200	118.569	1.369	1.168	1
160.00		4	150.500	152.175	1.675	1.113	1
170.00		4	190.700	192.739	2.039	1.069	1
180.00		4	238.800	241.179	2.379	0.996	1
190.00		4	295.600	298.448	2.848	0.963	1
200.00		4	362.200	365.562	3.362	0.928	1
210.00		4	439.000	443.557	4.557	1.038	1
220.00		4	528.000	533.578	5.578	1.056	1
230.00		4	630.500	636.790	6.290	0.998	1
240.00		4	750.000	754.477	4.477	0.597	1
250.00		4	882.000	887.764	5.764	0.654	1
260.00		4	1032.000	1038.135	6.135	0.594	1
270.00		4	1200.000	1207.008	7.008	0.584	1
280.00		4	1390.000	1396.004	6.004	0.432	1
290.00		4	1602.000	1606.783	4.783	0.299	1
300.00		4	1835.000	1841.155	6.155	0.335	1
310.00		4	2095.000	2101.246	6.246	0.298	1
320.00		4	2379.000	2389.176	10.176	0.428	1
330.00		4	2687.000	2706.895	19.895	0.740	1
340.00		4	3032.000	3052.913	20.913	0.690	1
350.00		4	3436.000	3407.086	-28.914	-0.842	1
355.00		4	3650.000	3616.376	-33.624	-0.921	1

B0660 C8H10 O-XYLENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
356.00		4	3696.000	3683.496	-12.504	-0.338	1
357.00		4	3742.000	3764.862	22.862	0.611	1
358.00		4	3788.000	3779.165	-8.835	-0.233	1
358.44		4	3808.000	3772.632	-35.368	-0.929	1
25.00	100.000	1	876.000	865.338	-10.662	-1.217	1
25.00	5000.000	1	879.500	867.987	-11.513	-1.309	1
25.00	10000.000	1	882.500	870.611	-11.889	-1.347	1
25.00	15000.000	1	886.000	873.159	-12.841	-1.449	1
25.00	20000.000	1	889.000	875.638	-13.362	-1.503	1
25.00	25000.000	1	892.000	878.051	-13.949	-1.564	1
25.00	30000.000	1	895.000	880.404	-14.596	-1.631	1
25.00	35000.000	1	898.000	882.699	-15.301	-1.704	1
25.00	40000.000	1	901.000	884.941	-16.059	-1.782	1
50.00	100.000	1	855.500	841.985	-13.515	-1.580	1
50.00	5000.000	1	859.000	845.183	-13.817	-1.608	1
50.00	10000.000	1	863.000	848.327	-14.673	-1.700	1
50.00	15000.000	1	867.000	851.360	-15.640	-1.804	1
50.00	20000.000	1	870.500	854.293	-16.207	-1.862	1
50.00	25000.000	1	873.500	857.132	-16.368	-1.874	1
50.00	30000.000	1	877.000	859.885	-17.115	-1.952	1
50.00	35000.000	1	880.000	862.558	-17.442	-1.982	1
50.00	40000.000	1	883.000	865.157	-17.843	-2.021	1
100.00	100.000	1	811.000	796.925	-14.075	-1.735	1
100.00	5000.000	1	816.000	801.558	-14.442	-1.770	1
100.00	10000.000	1	821.000	806.023	-14.977	-1.824	1
100.00	15000.000	1	826.000	810.256	-15.744	-1.906	1
100.00	20000.000	1	830.500	814.285	-16.215	-1.952	1
100.00	25000.000	1	835.000	818.132	-16.868	-2.020	1
100.00	30000.000	1	839.000	821.817	-17.183	-2.048	1
100.00	35000.000	1	843.000	825.355	-17.645	-2.093	1
100.00	40000.000	1	847.000	828.760	-18.240	-2.153	1
150.00	5000.000	1	772.000	758.585	-13.415	-1.738	1
150.00	10000.000	1	779.000	764.948	-14.052	-1.804	1
150.00	15000.000	1	785.500	770.827	-14.673	-1.868	1
150.00	20000.000	1	792.000	776.303	-15.697	-1.982	1
150.00	25000.000	1	797.000	781.435	-15.565	-1.953	1
150.00	30000.000	1	802.500	786.274	-16.226	-2.022	1
150.00	35000.000	1	807.500	790.857	-16.643	-2.061	1
150.00	40000.000	1	812.500	795.214	-17.286	-2.128	1
200.00	5000.000	1	723.500	713.635	-9.865	-1.364	1
200.00	10000.000	1	733.000	722.982	-10.018	-1.367	1
200.00	15000.000	1	742.000	731.266	-10.734	-1.447	1
200.00	20000.000	1	750.000	738.739	-11.261	-1.501	1
200.00	25000.000	1	757.000	745.569	-11.431	-1.510	1

B0660 C8H10 O-XYLENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
200.00	30000.000	1	764.000	751.876	-12.124	-1.587	1
200.00	35000.000	1	770.000	757.744	-12.256	-1.592	1
200.00	40000.000	1	776.000	763.242	-12.758	-1.644	1
250.00	5000.000	1	667.000	662.836	-4.164	-0.624	1
250.00	10000.000	1	682.500	677.574	-4.926	-0.722	1
250.00	15000.000	1	695.500	689.703	-5.797	-0.833	1
250.00	20000.000	1	706.500	700.109	-6.391	-0.905	1
250.00	25000.000	1	716.000	709.277	-6.723	-0.939	1
250.00	30000.000	1	724.500	717.507	-6.993	-0.965	1
250.00	35000.000	1	732.000	724.999	-7.001	-0.956	1
250.00	40000.000	1	740.000	731.893	-8.107	-1.095	1
275.00	5000.000	1	635.000	632.994	-2.006	-0.316	1
275.00	10000.000	1	656.000	652.449	-3.551	-0.541	1
275.00	15000.000	1	671.500	667.485	-4.015	-0.598	1
275.00	20000.000	1	684.000	679.918	-4.082	-0.597	1
275.00	25000.000	1	695.000	690.607	-4.393	-0.632	1
275.00	30000.000	1	705.000	700.038	-4.962	-0.704	1
275.00	35000.000	1	714.000	708.508	-5.492	-0.769	1
275.00	40000.000	1	722.000	716.219	-5.781	-0.801	1
250.00	882.000	5	259.900	266.110	6.210	2.389	1
-0.00		4	0.167	0.167	0.001	0.414	1
10.00		4	0.340	0.337	-0.003	-0.803	1
20.00		4	0.651	0.642	-0.008	-1.269	1
30.00		4	1.181	1.165	-0.017	-1.399	1
40.00		4	2.045	2.020	-0.025	-1.241	1
50.00		4	3.398	3.365	-0.033	-0.976	1
60.00		4	5.440	5.406	-0.033	-0.610	1
70.00		4	8.425	8.404	-0.020	-0.243	1
80.00		4	12.663	12.678	0.015	0.120	1
90.00		4	18.530	18.611	0.081	0.435	1
100.00		4	26.466	26.650	0.185	0.697	1
110.00		4	36.976	37.308	0.332	0.899	1
120.00		4	50.636	51.160	0.525	1.036	1
130.00		4	68.084	68.846	0.763	1.120	1
140.00		4	90.023	91.064	1.041	1.157	1
150.00		4	117.200	118.569	1.369	1.168	1
160.00		4	150.500	152.175	1.675	1.113	1
170.00		4	190.700	192.739	2.039	1.069	1
180.00		4	238.800	241.179	2.379	0.996	1
190.00		4	295.600	298.448	2.848	0.963	1
200.00		4	362.200	365.562	3.362	0.928	1
210.00		4	439.000	443.557	4.557	1.038	1
220.00		4	528.000	533.578	5.578	1.056	1
230.00		4	630.500	636.790	6.290	0.998	1

B0660 C8H10 O-XYLENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
240.00		4	750.000	754.477	4.477	0.597	1
250.00		4	882.000	887.764	5.764	0.654	1
260.00		4	1032.000	1038.135	6.135	0.594	1
270.00		4	1200.000	1207.008	7.008	0.584	1
280.00		4	1390.000	1396.004	6.004	0.432	1
290.00		4	1602.000	1606.783	4.783	0.299	1
300.00		4	1835.000	1841.155	6.155	0.335	1
310.00		4	2095.000	2101.246	6.246	0.298	1
320.00		4	2379.000	2389.176	10.176	0.428	1
330.00		4	2687.000	2706.895	19.895	0.740	1
340.00		4	3032.000	3052.913	20.913	0.690	1
350.00		4	3436.000	3407.086	-28.914	-0.842	1
355.00		4	3650.000	3616.376	-33.624	-0.921	1
356.00		4	3696.000	3683.496	-12.504	-0.338	1
357.00		4	3742.000	3764.862	22.862	0.611	1
358.00		4	3788.000	3779.165	-8.835	-0.233	1
358.44		4	3808.000	3772.632	-35.368	-0.929	1
30.00	1.181	21	0.708	0.784	0.076	10.693	1
40.00	2.045	21	0.625	0.688	0.063	10.030	1
50.00	3.398	21	0.557	0.609	0.052	9.391	1
60.00	5.440	21	0.501	0.544	0.043	8.674	1
70.00	8.425	21	0.453	0.490	0.037	8.197	1
80.00	12.663	21	0.412	0.444	0.032	7.793	1
90.00	18.530	21	0.376	0.405	0.029	7.635	1
100.00	26.466	21	0.345	0.371	0.026	7.434	1
110.00	36.976	21	0.318	0.341	0.023	7.215	1
120.00	50.636	21	0.294	0.315	0.021	7.080	1
130.00	68.084	21	0.272	0.292	0.020	7.224	1
140.00	90.023	21	0.254	0.271	0.017	6.677	1

B0660 C8H10 O-XYLENE

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.47 %AARD FOR 59 POINTS
4	VAPOR PRESSURE	KPA	0.76 %AARD FOR 82 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	2.39 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	8.17 %AARD FOR 12 POINTS

B0680 C8H10O 2,5-XYLENOL. 2,5-DIMETHYLPHENOL.
1,4-DIMETHYL-2-HYDROXY-BENZENE.
CONST: KUDCHADKER AND KUDCHADKER 1978B
PROP.: 1. KUDCHADKER AND KUDCHADKER 1978B

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	122.166	707.05	561.46	390.00	5.911	0.56800
FITTED:				333.93	5.613	0.49696

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
180.00		4	43.202	44.148	0.946	2.190	1
200.00		4	75.944	78.511	2.567	3.380	1
210.61		4	100.000	103.979	3.979	3.979	1
220.00		4	125.990	131.650	5.660	4.492	1
240.00		4	198.900	209.961	11.061	5.561	1
260.00		4	301.000	320.816	19.816	6.583	1
280.00		4	500.000	474.666	-25.334	-5.067	1
300.00		4	700.000	676.993	-23.007	-3.287	1
320.00		4	1000.000	941.024	-58.976	-5.898	1
340.00		4	1400.000	1278.128	-121.872	-8.705	1
360.00		4	1800.000	1700.677	-99.323	-5.518	1
380.00		4	2500.000	2229.697	-270.303	-10.812	1
400.00		4	3200.000	2882.334	-317.666	-9.927	1
420.00		4	4100.000	3613.714	-486.286	-11.861	1
430.00		4	4600.000	4318.271	-281.729	-6.125	1
433.90		4	4900.000	4776.588	-123.412	-2.519	1
100.00	1.958	5	474.191	473.027	-1.164	-0.245	1
120.00	4.982	5	455.118	459.900	4.782	1.051	1
140.00	11.234	5	438.011	445.973	7.963	1.818	1
160.00	22.949	5	422.212	431.638	9.425	2.232	1
180.00	43.202	5	407.151	417.088	9.938	2.441	1
200.00	75.944	5	392.417	402.388	9.971	2.541	1
210.61	100.000	5	384.641	394.521	9.880	2.569	1
220.00	125.990	5	377.355	387.508	10.152	2.690	1
240.00	198.900	5	360.166	372.358	12.193	3.385	1
260.00	301.000	5	335.609	356.794	21.185	6.312	1
280.00	500.000	5	319.238	338.563	19.325	6.054	1
300.00	700.000	5	294.681	320.985	26.304	8.926	1
320.00	1000.000	5	270.124	300.536	30.412	11.258	1
340.00	1400.000	5	245.568	276.744	31.177	12.696	1
360.00	1800.000	5	221.011	252.406	31.396	14.206	1
380.00	2500.000	5	196.454	211.496	15.042	7.657	1
400.00	3200.000	5	155.526	152.095	-3.432	-2.206	1
80.00	0.663	1	966.000	1108.171	142.171	14.717	1
100.00	1.958	1	949.000	1086.864	137.864	14.527	1
120.00	4.982	1	931.000	1065.910	134.910	14.491	1
140.00	11.234	1	915.000	1045.177	130.177	14.227	1

B0680 C8H10O 2,5-XYLENOL. 2,5-DIMETHYLPHENOL.
1,4-DIMETHYL-2-HYDROXY-BENZENE.
(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
160.00	22.949	1	899.000	1024.527	125.527	13.963	1
180.00	43.202	1	884.000	1003.816	119.816	13.554	1
200.00	75.944	1	869.000	982.884	113.884	13.105	1
90.00	101.325	21	1.200	1.016	-0.184	-15.364	1
100.00	101.325	21	1.020	0.907	-0.113	-11.127	1
110.00	101.325	21	0.880	0.815	-0.065	-7.418	1
120.00	101.325	21	0.770	0.737	-0.033	-4.317	1
130.00	101.325	21	0.680	0.670	-0.010	-1.479	1
140.00	101.325	21	0.600	0.612	0.012	2.028	1
150.00	101.325	21	0.540	0.562	0.022	4.042	1
160.00	101.325	21	0.480	0.518	0.038	7.838	1
170.00	101.325	21	0.430	0.479	0.049	11.288	1
180.00	101.325	21	0.390	0.444	0.054	13.782	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	14.08 %AARD FOR 7 POINTS
4	VAPOR PRESSURE	KPA	5.99 %AARD FOR 16 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	5.19 %AARD FOR 17 POINTS
21	LIQUID VISCOSITY	CP	7.87 %AARD FOR 10 POINTS

Q0034 C9H7N QUINOLINE. 1-BENZAZINE. BENZO(B)PYRIDINE.

CONST: VISWANATH 1979
PROP.: 1. VISWANATH 1979, 2. KOBAYASHI 1979,
3. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	129.161	782.15	621.10	403.00	5.976	0.33000
FITTED:				357.07	5.740	0.34553

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
30.00	0.012	1	1086.100	1162.248	76.148	7.011	1
40.00	0.027	1	1078.300	1151.475	73.175	6.786	1
50.00	0.057	1	1070.400	1140.918	70.518	6.588	1
60.00	0.113	1	1062.500	1130.560	68.060	6.406	1
70.00	0.213	1	1054.600	1120.386	65.786	6.238	1
80.00	0.383	1	1046.700	1110.379	63.679	6.084	1
90.00	0.660	1	1038.700	1100.525	61.825	5.952	1
100.00	1.090	1	1030.800	1090.809	60.009	5.822	1
120.00	2.720	1	1014.800	1071.736	56.936	5.611	1
140.00	6.048	1	998.600	1053.048	54.448	5.452	1
160.00	12.266	1	982.300	1034.640	52.340	5.328	1
180.00	23.027	1	965.700	1016.404	50.704	5.251	1
200.00	40.500	1	949.000	998.234	49.234	5.188	1
220.00	67.370	1	931.800	980.019	48.219	5.175	1
237.60	101.325	1	916.500	963.859	47.359	5.167	1
240.00	106.850	1	914.300	961.641	47.341	5.178	1
30.00		4	0.012	0.013	0.001	5.405	1
40.00		4	0.027	0.027	-0.000	-0.408	1
220.00		4	67.370	64.905	-2.465	-3.659	1
237.60		4	101.325	98.751	-2.574	-2.541	1
240.00		4	106.850	104.285	-2.565	-2.401	1
260.00		4	162.900	160.566	-2.334	-1.433	1
280.00		4	240.400	238.256	-2.144	-0.892	1
300.00		4	344.500	342.336	-2.164	-0.628	1
320.00		4	481.000	478.261	-2.739	-0.569	1
340.00		4	655.900	651.949	-3.951	-0.602	1
360.00		4	876.000	869.827	-6.173	-0.705	1
380.00		4	1148.000	1138.884	-9.116	-0.794	1
400.00		4	1479.000	1466.819	-12.181	-0.824	1
420.00		4	1875.000	1862.246	-12.754	-0.680	1
440.00		4	2345.000	2335.107	-9.893	-0.422	1
460.00		4	2895.000	2897.012	2.012	0.069	1
480.00		4	3531.000	3559.475	28.475	0.806	1
70.00	0.213	5	460.665	447.510	-13.155	-2.856	1
80.00	0.383	5	452.149	445.497	-6.652	-1.471	1
90.00	0.660	5	443.632	442.716	-0.916	-0.207	1
100.00	1.090	5	436.664	439.329	2.665	0.610	1

Q0034 C9H7N QUINOLINE. 1-BENZAZINE. BENZO(B) PYRIDINE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
120.00	2.720	5	422.728	431.224	8.495	2.010	1
140.00	6.048	5	410.341	421.936	11.596	2.826	1
160.00	12.266	5	398.727	411.940	13.213	3.314	1
180.00	23.027	5	387.888	401.522	13.634	3.515	1
200.00	40.500	5	377.823	390.839	13.015	3.445	1
220.00	67.370	5	368.532	379.959	11.427	3.101	1
237.60	101.325	5	360.016	370.233	10.217	2.838	1
240.00	106.850	5	358.467	368.894	10.427	2.909	1
260.00	162.900	5	352.274	357.598	5.325	1.511	1
280.00	240.400	5	345.305	345.981	0.676	0.196	1
300.00	344.500	5	336.789	333.935	-2.854	-0.847	1
320.00	481.000	5	329.047	321.314	-7.732	-2.350	1
340.00	655.900	5	317.433	307.948	-9.485	-2.988	1
360.00	876.000	5	309.691	293.609	-16.082	-5.193	1
114.82		4	1.743	1.864	0.122	6.976	2
200.56		4	41.240	39.055	-2.186	-5.300	2
274.87		4	230.730	216.408	-14.321	-6.207	2
323.10		4	515.852	502.795	-13.057	-2.531	2
328.14		4	555.819	544.238	-11.582	-2.084	2
260.00		4	164.095	160.605	-3.490	-2.127	3
343.33		4	730.844	685.760	-45.084	-6.169	3
371.11		4	1048.003	1012.935	-35.068	-3.346	3
398.89		4	1503.057	1447.479	-55.578	-3.698	3
426.66		4	2054.638	2011.064	-43.574	-2.121	3
454.44		4	2806.166	2731.968	-74.198	-2.644	3

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	5.83 %AARD FOR 16 POINTS
4	VAPOR PRESSURE	KPA	2.36 %AARD FOR 28 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	2.34 %AARD FOR 18 POINTS

I0049 C9H8 INDENE

CONST: KUDCHADKER ET AL 1980
PROP.: 1. KUDCHADKER ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	116.162	702.49	557.84	370.96	5.813	0.26200
FITTED:				368.34	5.799	0.27650

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
100.00		4	7.765	7.881	0.116	1.499	1
120.00		4	16.360	16.473	0.113	0.693	1
140.00		4	31.530	31.592	0.062	0.197	1
160.00		4	56.460	56.365	-0.095	-0.168	1
180.00		4	95.030	94.614	-0.416	-0.437	1
182.08		4	100.000	99.541	-0.459	-0.459	1
182.62		4	101.325	100.852	-0.473	-0.467	1
200.00		4	151.800	150.818	-0.982	-0.647	1
220.00		4	232.000	230.058	-1.942	-0.837	1
240.00		4	340.000	337.922	-2.078	-0.611	1
420.00		4	3770.000	3786.078	16.078	0.426	1
422.00		4	3800.000	3874.865	74.865	1.970	1
100.00	7.765	1	922.000	906.762	-15.238	-1.653	1
120.00	16.360	1	900.000	889.110	-10.890	-1.210	1
140.00	31.530	1	880.000	871.612	-8.388	-0.953	1
160.00	56.460	1	860.000	854.133	-5.867	-0.682	1
180.00	95.030	1	840.000	836.534	-3.466	-0.413	1
182.08	100.000	1	840.000	834.691	-5.309	-0.632	1
182.62	101.325	1	830.000	834.211	4.211	0.507	1
200.00	151.800	1	810.000	818.663	8.663	1.070	1
220.00	232.000	1	790.000	800.355	10.355	1.311	1
240.00	340.000	1	760.000	781.409	21.409	2.817	1
260.00	520.000	1	730.000	761.680	31.680	4.340	1
280.00	760.000	1	700.000	740.857	40.857	5.837	1
422.00	3800.000	1	310.000	283.721	-26.279	-8.477	1
100.00	7.765	5	393.416	388.052	-5.364	-1.363	1
120.00	16.360	5	381.278	378.023	-3.255	-0.854	1
140.00	31.530	5	369.828	367.673	-2.156	-0.583	1
160.00	56.460	5	358.637	357.084	-1.553	-0.433	1
180.00	95.030	5	347.532	346.257	-1.275	-0.367	1
182.08	100.000	5	346.413	345.115	-1.298	-0.375	1
182.62	101.325	5	346.327	344.818	-1.509	-0.436	1
200.00	151.800	5	336.255	335.131	-1.124	-0.334	1
220.00	232.000	5	324.547	323.603	-0.943	-0.291	1
240.00	340.000	5	311.634	311.587	-0.047	-0.015	1
260.00	520.000	5	298.721	297.576	-1.145	-0.383	1
280.00	760.000	5	284.086	282.040	-2.046	-0.720	1

I0049 C9H8 INDENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
300.00	1060.000	5	268.590	264.839	-3.751	-1.397	1
320.00	1440.000	5	250.512	244.840	-5.673	-2.264	1
70.00	101.325	21	0.844	0.761	-0.083	-9.836	1
80.00	101.325	21	0.741	0.682	-0.059	-7.994	1
90.00	101.325	21	0.653	0.615	-0.038	-5.792	1
100.00	101.325	21	0.578	0.559	-0.019	-3.350	1
110.00	101.325	21	0.513	0.510	-0.003	-0.555	1
120.00	101.325	21	0.457	0.468	0.011	2.454	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	2.30 %AARD FOR 13 POINTS
4	VAPOR PRESSURE	KPA	0.70 %AARD FOR 12 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.70 %AARD FOR 14 POINTS
21	LIQUID VISCOSITY	CP	5.00 %AARD FOR 6 POINTS

I0016 C9H10 INDAN (2,3-DIHYDROINDENE)

CONST: KUDCHADKER AND KUDCHADKER 1980
PROP.: 1. KUDCHADKER AND KUDCHADKER 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	118.178	685.61	544.44	382.16	5.871	0.30700
FITTED:				381.66	5.868	0.30130

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
100.00		4	9.206	9.144	-0.062	-0.679	1
120.00		4	19.010	18.976	-0.034	-0.178	1
140.00		4	36.120	36.179	0.059	0.164	1
160.00		4	64.010	64.217	0.207	0.323	1
177.27		4	100.000	100.357	0.357	0.357	1
177.80		4	101.325	101.676	0.351	0.347	1
180.00		4	106.930	107.297	0.367	0.343	1
200.00		4	169.840	170.316	0.476	0.280	1
220.00		4	258.400	258.813	0.413	0.160	1
240.00		4	379.000	378.919	-0.081	-0.021	1
260.00		4	538.000	537.323	-0.677	-0.126	1
280.00		4	742.000	741.316	-0.684	-0.092	1
300.00		4	1000.000	998.915	-1.085	-0.109	1
320.00		4	1320.000	1318.949	-1.051	-0.080	1
340.00		4	1720.000	1711.563	-8.437	-0.491	1
360.00		4	2190.000	2188.081	-1.919	-0.088	1
380.00		4	2770.000	2762.380	-7.620	-0.275	1
400.00		4	3470.000	3431.863	-38.137	-1.099	1
411.80		4	3950.000	3936.487	-13.513	-0.342	1
-0.00	0.032	1	977.500	980.836	3.336	0.341	1
10.00	0.071	1	971.100	970.535	-0.565	-0.058	1
20.00	0.147	1	964.000	960.464	-3.536	-0.367	1
30.00	0.285	1	955.700	950.603	-5.097	-0.533	1
40.00	0.526	1	947.600	940.929	-6.671	-0.704	1
50.00	0.927	1	940.000	931.422	-8.578	-0.913	1
60.00	1.570	1	931.000	922.064	-8.936	-0.960	1
70.00	2.560	1	922.000	912.835	-9.165	-0.994	1
80.00	4.040	1	912.000	903.718	-8.282	-0.908	1
90.00	6.179	1	903.000	894.694	-8.306	-0.920	1
100.00	9.206	1	893.000	885.746	-7.254	-0.812	1
120.00	19.010	1	872.000	868.007	-3.993	-0.458	1
140.00	36.120	1	851.000	850.363	-0.637	-0.075	1
160.00	64.010	1	829.000	832.672	3.672	0.443	1
177.27	100.000	1	809.000	817.240	8.240	1.019	1
177.80	101.325	1	808.000	816.763	8.763	1.085	1
180.00	106.930	1	806.000	814.780	8.780	1.089	1
200.00	169.840	1	781.000	796.523	15.523	1.988	1

I0016 C9H10 INDAN (2,3-DIHYDROINDENE)

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
220.00	258.400	1	754.000	777.706	23.706	3.144	1
240.00	379.000	1	727.000	758.099	31.099	4.278	1
400.00	3470.000	1	406.000	400.557	-5.443	-1.341	1
411.80	3950.000	1	300.000	301.018	1.018	0.339	1
10.00	0.071	5	424.783	410.759	-14.024	-3.301	1
20.00	0.147	5	418.014	410.005	-8.009	-1.916	1
30.00	0.285	5	410.059	408.090	-1.969	-0.480	1
40.00	0.526	5	405.998	405.285	-0.712	-0.175	1
50.00	0.927	5	400.328	401.801	1.472	0.368	1
60.00	1.570	5	394.913	397.799	2.887	0.731	1
70.00	2.560	5	389.666	393.410	3.743	0.961	1
80.00	4.040	5	384.589	388.729	4.139	1.076	1
90.00	6.179	5	379.597	383.831	4.235	1.116	1
100.00	9.206	5	374.604	378.773	4.168	1.113	1
120.00	19.010	5	365.973	368.322	2.349	0.642	1
140.00	36.120	5	355.904	357.569	1.665	0.468	1
160.00	64.010	5	344.650	346.577	1.927	0.559	1
177.27	100.000	5	333.988	336.879	2.892	0.866	1
177.80	101.325	5	333.734	336.578	2.844	0.852	1
180.00	106.930	5	332.295	335.325	3.030	0.912	1
200.00	169.840	5	319.010	323.735	4.725	1.481	1
220.00	258.400	5	303.779	311.680	7.901	2.601	1
240.00	379.000	5	287.702	298.988	11.287	3.923	1
30.00	101.325	21	1.250	1.201	-0.049	-3.901	1
40.00	101.325	21	1.070	1.037	-0.033	-3.122	1
50.00	101.325	21	0.929	0.905	-0.024	-2.598	1
60.00	101.325	21	0.818	0.798	-0.020	-2.456	1
70.00	101.325	21	0.728	0.710	-0.018	-2.485	1
80.00	101.325	21	0.656	0.637	-0.019	-2.957	1
90.00	101.325	21	0.595	0.575	-0.020	-3.384	1
100.00	101.325	21	0.545	0.522	-0.023	-4.161	1
110.00	101.325	21	0.502	0.477	-0.025	-4.944	1
120.00	101.325	21	0.466	0.438	-0.028	-5.997	1

I0016 C9H10 INDAN (2,3-DIHYDROINDENE)

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.03 %AARD FOR 22 POINTS
4	VAPOR PRESSURE	KPA	0.29 %AARD FOR 19 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.24 %AARD FOR 19 POINTS
21	LIQUID VISCOSITY	CP	3.60 %AARD FOR 10 POINTS

N0014 C10H8 NAPHTHALENE

CONST: KUDCHADKER ET AL 1978F
PROP.: 1. KUDCHADKER ET AL 1978F, 2. KOBAYASHI 1979,
3. WILSON ET AL 1981

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	128.173	748.35	594.26	413.00	6.025	0.30200
FITTED:				401.29	5.967	0.30103

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
100.00	2.490	1	962.200	942.717	-19.483	-2.025	1
110.00	3.797	1	954.160	934.085	-20.075	-2.104	1
120.00	5.642	1	946.060	925.537	-20.523	-2.169	1
130.00	8.186	1	937.910	917.060	-20.850	-2.223	1
140.00	11.620	1	929.700	908.638	-21.062	-2.265	1
150.00	13.750	1	921.430	900.257	-21.173	-2.298	1
160.00	22.120	1	913.080	891.909	-21.171	-2.319	1
170.00	29.750	1	904.640	883.574	-21.066	-2.329	1
180.00	39.380	1	896.110	875.240	-20.870	-2.329	1
190.00	51.400	1	887.470	866.892	-20.578	-2.319	1
200.00	66.220	1	878.720	858.515	-20.205	-2.299	1
217.41	100.000	1	862.810	843.819	-18.991	-2.201	1
217.99	101.325	1	862.360	843.324	-19.036	-2.207	1
220.00	106.000	1	860.820	841.616	-19.204	-2.231	1
240.00	162.700	1	842.280	824.410	-17.870	-2.122	1
260.00	241.000	1	823.000	806.747	-16.253	-1.975	1
280.00	345.000	1	802.800	788.449	-14.351	-1.788	1
300.00	481.000	1	781.400	769.298	-12.102	-1.549	1
320.00	655.000	1	758.600	749.012	-9.588	-1.264	1
340.00	871.000	1	734.100	727.194	-6.906	-0.941	1
360.00	1136.000	1	707.300	703.270	-4.030	-0.570	1
380.00	1450.000	1	678.000	676.270	-1.730	-0.255	1
400.00	1820.000	1	644.000	644.452	0.452	0.070	1
420.00	2250.000	1	604.000	603.829	-0.171	-0.028	1
440.00	2730.000	1	555.000	539.913	-15.087	-2.718	1
100.00		4	2.490	2.459	-0.031	-1.232	1
110.00		4	3.797	3.764	-0.033	-0.881	1
120.00		4	5.642	5.614	-0.028	-0.499	1
130.00		4	8.186	8.178	-0.008	-0.097	1
140.00		4	11.620	11.656	0.036	0.311	1
160.00		4	22.120	22.327	0.207	0.936	1
170.00		4	29.750	30.093	0.343	1.153	1
180.00		4	39.380	39.919	0.539	1.368	1
190.00		4	51.400	52.179	0.779	1.516	1
200.00		4	66.220	67.283	1.063	1.606	1
217.41		4	100.000	101.691	1.691	1.691	1
217.99		4	101.325	103.045	1.720	1.697	1

N0014 C10H8 NAPHTHALENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
220.00		4	106.000	107.813	1.813	1.711	1
240.00		4	162.700	165.410	2.710	1.666	1
260.00		4	241.000	244.448	3.448	1.431	1
280.00		4	345.000	349.703	4.703	1.363	1
300.00		4	481.000	486.431	5.431	1.129	1
320.00		4	655.000	660.281	5.281	0.806	1
340.00		4	871.000	877.324	6.324	0.726	1
360.00		4	1136.000	1144.248	8.248	0.726	1
380.00		4	1450.000	1468.324	18.324	1.264	1
400.00		4	1820.000	1857.902	37.902	2.083	1
420.00		4	2250.000	2322.575	72.575	3.226	1
460.00		4	3340.000	3411.872	71.872	2.152	1
470.00		4	3770.000	3689.409	-80.591	-2.138	1
475.20		4	4050.000	4048.343	-1.657	-0.041	1
100.00	2.490	5	392.438	396.376	3.939	1.004	1
110.00	3.797	5	386.976	392.102	5.126	1.325	1
120.00	5.642	5	382.529	387.634	5.105	1.335	1
130.00	8.186	5	377.848	383.019	5.171	1.369	1
140.00	11.620	5	373.401	378.291	4.890	1.310	1
160.00	22.120	5	364.351	368.593	4.242	1.164	1
170.00	29.750	5	361.230	363.652	2.422	0.670	1
180.00	39.380	5	357.329	358.662	1.333	0.373	1
190.00	51.400	5	352.648	353.623	0.976	0.277	1
200.00	66.220	5	347.967	348.536	0.569	0.164	1
217.41	100.000	5	339.385	339.550	0.165	0.049	1
217.99	101.325	5	338.604	339.246	0.641	0.189	1
220.00	106.000	5	337.824	338.198	0.373	0.111	1
240.00	162.700	5	326.121	327.584	1.463	0.448	1
260.00	241.000	5	313.638	316.592	2.954	0.942	1
280.00	345.000	5	299.595	305.131	5.536	1.848	1
300.00	481.000	5	283.991	293.006	9.016	3.175	1
320.00	655.000	5	267.607	280.013	12.406	4.636	1
340.00	871.000	5	249.662	265.956	16.294	6.526	1
460.00	3340.000	5	91.283	84.360	-6.922	-7.583	1
91.45		4	1.725	1.677	-0.048	-2.804	2
100.30		4	2.596	2.503	-0.093	-3.586	2
121.08		4	6.113	5.881	-0.232	-3.793	2
129.17		4	8.255	7.968	-0.287	-3.480	2
139.54		4	11.888	11.518	-0.370	-3.113	2
150.19		4	16.445	16.400	-0.046	-0.277	2
158.79		4	21.436	21.521	0.085	0.399	2
173.42		4	33.001	33.219	0.218	0.660	2
191.43		4	54.143	54.207	0.064	0.118	2
211.09		4	87.735	87.963	0.227	0.259	2

N0014 C10H8 NAPHTHALENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
229.18		4	131.635	131.968	0.332	0.253	2
253.27		4	218.504	215.404	-3.100	-1.419	2
278.02		4	327.003	337.766	10.763	3.291	2
168.16		4	28.820	28.572	-0.248	-0.860	3
189.05		4	49.642	50.868	1.226	2.470	3
210.39		4	83.427	86.361	2.935	3.518	3
219.22		4	102.042	105.827	3.784	3.709	3
235.33		4	145.479	150.112	4.633	3.184	3
253.83		4	211.669	217.403	5.734	2.709	3
281.05		4	348.875	355.998	7.124	2.042	3
371.11		4	1316.899	1316.892	-0.007	-0.001	3
398.89		4	1868.479	1835.263	-33.216	-1.778	3
426.66		4	2551.060	2497.658	-53.402	-2.093	3
454.44		4	3378.431	3329.221	-49.210	-1.457	3
90.00	101.325	21	0.846	0.844	-0.002	-0.287	1
100.00	101.325	21	0.754	0.757	0.003	0.456	1
110.00	101.325	21	0.678	0.685	0.007	0.986	1
120.00	101.325	21	0.616	0.623	0.007	1.079	1
130.00	101.325	21	0.564	0.569	0.005	0.935	1
140.00	101.325	21	0.520	0.523	0.003	0.573	1
150.00	101.325	21	0.482	0.483	0.001	0.107	1
160.00	101.325	21	0.448	0.447	-0.001	-0.247	1
170.00	101.325	21	0.420	0.415	-0.005	-1.113	1
180.00	101.325	21	0.394	0.387	-0.007	-1.735	1
190.00	101.325	21	0.372	0.362	-0.010	-2.717	1
200.00	101.325	21	0.351	0.339	-0.012	-3.394	1
220.00	106.000	21	0.320	0.300	-0.020	-6.401	1
240.00	162.700	21	0.290	0.266	-0.024	-8.146	1
260.00	241.000	21	0.260	0.238	-0.022	-8.445	1
280.00	345.000	21	0.240	0.213	-0.027	-11.088	1

NOC14 C10H8 NAPHTHALENE

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.78 %AARD FOR 25 POINTS
4	VAPOR PRESSURE	KPA	1.61 %AARD FOR 50 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.72 %AARD FOR 20 POINTS
21	LIQUID VISCOSITY	CP	2.98 %AARD FOR 16 POINTS

T0098 C10H12 TETRALIN (1,2,3,4-TETRAHYDRONAPHTHALENE)

CONST: CHAO ET AL 1980, KUDCHADKER ET AL 1978D
PROP.: 1. KUDCHADKER ET AL 1978D, 2. KOBAYASHI 1979,
3. WILSON ET AL 1981

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	132.205	716.50	568.97	430.73	6.110	0.31550
FITTED:				430.54	6.109	0.34552

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
100.00		4	3.420	3.283	-0.137	-3.991	1
120.00		4	7.620	7.414	-0.206	-2.700	1
140.00		4	15.450	15.229	-0.221	-1.433	1
160.00		4	28.970	28.862	-0.108	-0.373	1
180.00		4	50.930	51.087	0.157	0.307	1
200.00		4	84.620	85.293	0.673	0.796	1
207.05		4	100.000	100.934	0.934	0.934	1
220.00		4	133.900	135.470	1.570	1.173	1
240.00		4	205.000	206.235	1.235	0.603	1
260.00		4	303.000	302.628	-0.372	-0.123	1
280.00		4	432.000	430.166	-1.834	-0.424	1
300.00		4	597.000	594.929	-2.071	-0.347	1
320.00		4	803.000	803.574	0.574	0.072	1
340.00		4	1057.000	1063.498	6.498	0.615	1
447.00		4	3300.000	3300.000	-0.000	-0.000	1
100.00	3.420	1	909.200	899.377	-9.823	-1.080	1
120.00	7.620	1	894.200	882.247	-11.953	-1.337	1
140.00	15.450	1	879.200	865.313	-13.887	-1.580	1
160.00	28.970	1	864.300	848.456	-15.844	-1.833	1
180.00	50.930	1	849.300	831.556	-17.744	-2.089	1
200.00	84.620	1	832.000	814.480	-17.520	-2.106	1
207.05	100.000	1	826.000	808.394	-17.606	-2.131	1
220.00	133.900	1	810.000	797.087	-12.913	-1.594	1
240.00	205.000	1	790.000	779.212	-10.788	-1.366	1
260.00	303.000	1	770.000	760.661	-9.339	-1.213	1
280.00	432.000	1	750.000	741.181	-8.819	-1.176	1
300.00	597.000	1	730.000	720.438	-9.562	-1.310	1
320.00	803.000	1	700.000	697.952	-2.048	-0.293	1
340.00	1057.000	1	670.000	672.989	2.989	0.446	1
360.00	1364.000	1	640.000	644.265	4.265	0.666	1
380.00	1732.000	1	610.000	609.180	-0.820	-0.134	1
400.00	2169.000	1	570.000	560.487	-9.513	-1.669	1
100.00	3.420	5	371.318	380.241	8.923	2.403	1
120.00	7.620	5	362.090	370.628	8.538	2.358	1
140.00	15.450	5	353.240	360.520	7.280	2.061	1
160.00	28.970	5	344.466	350.118	5.653	1.641	1
180.00	50.930	5	335.540	339.504	3.964	1.181	1

T0098 C10H12 TETRALIN (1,2,3,4-TETRAHYDRONAPHTHALENE)

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
200.00	84.620	5	326.312	328.682	2.370	0.726	1
207.05	100.000	5	322.984	324.811	1.827	0.566	1
220.00	133.900	5	316.933	317.604	0.671	0.212	1
240.00	205.000	5	304.830	306.105	1.275	0.418	1
260.00	303.000	5	291.971	294.061	2.090	0.716	1
280.00	432.000	5	277.600	281.359	3.760	1.354	1
300.00	597.000	5	261.715	267.806	6.091	2.327	1
320.00	803.000	5	244.318	253.144	8.826	3.613	1
340.00	1057.000	5	225.408	236.929	11.521	5.111	1
177.00		4	46.471	47.040	0.569	1.225	2
205.28		4	95.148	96.758	1.611	1.693	2
231.83		4	173.058	174.536	1.477	0.854	2
259.55		4	297.164	300.047	2.883	0.970	2
289.89		4	495.044	506.199	11.155	2.253	2
318.16		4	765.318	782.040	16.722	2.185	2
340.16		4	1038.350	1065.470	27.120	2.612	2
318.55		4	768.076	786.453	18.377	2.393	2
290.78		4	500.559	513.491	12.931	2.583	2
259.55		4	296.475	300.024	3.549	1.197	2
231.78		4	170.990	174.252	3.262	1.908	2
315.55		4	765.318	753.273	-12.045	-1.574	2
371.11		4	1599.584	1590.240	-9.343	-0.584	2
398.89		4	2247.691	2213.876	-33.814	-1.504	2
426.66		4	3040.588	3003.467	-37.121	-1.221	2
437.78		4	3364.641	3351.432	-13.210	-0.393	2
200.10		4	84.002	85.453	1.451	1.727	3
250.65		4	257.306	254.165	-3.141	-1.221	3
267.20		4	348.090	344.722	-3.368	-0.968	3
40.00	101.325	21	1.527	1.416	-0.111	-7.299	1
50.00	101.325	21	1.299	1.217	-0.082	-6.343	1
60.00	101.325	21	1.122	1.058	-0.064	-5.726	1
70.00	101.325	21	0.981	0.929	-0.052	-5.292	1
80.00	101.325	21	0.867	0.823	-0.044	-5.018	1
90.00	101.325	21	0.774	0.736	-0.038	-4.937	1
100.00	101.325	21	0.696	0.662	-0.034	-4.865	1
120.00	101.325	21	0.576	0.546	-0.030	-5.179	1
140.00	101.325	21	0.490	0.460	-0.030	-6.177	1

T0098 C10H12 TETRALIN (1,2,3,4-TETRAHYDRONAPHTHALENE)

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.30 %AARD FOR 17 POINTS
4	VAPOR PRESSURE	KPA	1.26 %AARD FOR 34 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.76 %AARD FOR 14 POINTS
21	LIQUID VISCOSITY	CP	5.65 %AARD FOR 9 POINTS

N0217 C11H10 1-METHYLNAPHTHALENE

CONST: REID ET AL 1977
PROP.: 1. WILSON ET AL 1981; 2. CAMIN & ROSSINI 1955
3. API-44 1967, 4. API-42 1966

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	142.201	772.00	613.04	445.00	6.177	0.33400
FITTED:				453.03	6.213	0.35191

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
173.89		4	15.582	15.971	0.389	2.494	1
202.22		4	35.991	36.474	0.484	1.344	1
232.33		4	75.842	77.417	1.575	2.077	1
248.61		4	111.006	111.414	0.408	0.368	1
287.22		4	239.938	238.562	-1.375	-0.573	1
314.55		4	391.622	381.322	-10.300	-2.630	1
352.89		4	672.928	680.445	7.517	1.117	1
316.05		4	390.933	390.442	-0.491	-0.126	1
287.66		4	242.006	240.492	-1.514	-0.625	1
248.05		4	111.006	110.149	-0.856	-0.771	1
315.55		4	388.175	387.311	-0.864	-0.223	1
371.11		4	868.739	873.507	4.767	0.549	1
398.89		4	1220.372	1244.150	23.778	1.948	1
426.66		4	1654.742	1724.618	69.877	4.223	1
454.44		4	2309.744	2340.460	30.717	1.330	1
471.11		4	2675.166	2783.378	108.213	4.045	1
482.22		4	3026.798	3014.561	-12.237	-0.404	1
142.14		4	5.524	5.393	-0.131	-2.369	2
153.60		4	8.314	8.174	-0.140	-1.688	2
157.54		4	9.510	9.371	-0.139	-1.457	2
161.69		4	10.942	10.790	-0.152	-1.386	2
167.21		4	13.088	12.948	-0.140	-1.070	2
179.97		4	19.442	19.329	-0.113	-0.582	2
185.50		4	22.881	22.802	-0.079	-0.344	2
193.28		4	28.542	28.528	-0.013	-0.047	2
200.54		4	34.832	34.879	0.048	0.137	2
208.68		4	43.162	43.317	0.156	0.360	2
217.37		4	53.762	54.071	0.309	0.575	2
226.50		4	67.057	67.544	0.487	0.727	2
236.24		4	84.026	84.752	0.726	0.864	2
243.18		4	98.081	98.978	0.897	0.915	2
243.95		4	99.656	100.667	1.012	1.015	2
244.55		4	101.030	102.014	0.984	0.974	2
245.33		4	102.757	103.747	0.990	0.964	2
-0.00	101.325	1	1034.000	1035.145	1.145	0.111	3
10.00	101.325	1	1027.300	1025.102	-2.198	-0.214	3
30.00	101.325	1	1020.280	1005.700	-14.580	-1.429	3

N0217 C11H10 1-METHYLNAPHTHALENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
30.00	101.325	1	1013.210	1005.700	-7.510	-0.741	3
40.00	101.325	1	1006.100	996.307	-9.793	-0.973	3
50.00	101.325	1	998.900	987.100	-11.800	-1.181	3
60.00	101.325	1	991.600	978.063	-13.537	-1.365	3
70.00	101.325	1	984.300	969.184	-15.116	-1.536	3
80.00	101.325	1	977.000	960.447	-16.553	-1.694	3
90.00	101.325	1	969.400	951.840	-17.560	-1.811	3
100.00	101.325	1	961.900	943.349	-18.551	-1.929	3
110.00	101.325	1	954.200	934.963	-19.237	-2.016	3
120.00	101.325	1	947.000	926.669	-20.331	-2.147	3
130.00	101.325	1	939.000	918.454	-20.546	-2.188	3
140.00	101.325	1	931.000	910.306	-20.694	-2.223	3
150.00	101.325	1	923.000	902.214	-20.786	-2.252	3
37.78	101.325	21	2.226	2.304	0.078	3.526	4
60.00	101.325	21	1.494	1.592	0.098	6.549	4
98.89	101.325	21	0.882	0.953	0.071	8.038	4
-0.00	101.325	1	1035.700	1035.148	-0.552	-0.053	4
20.00	101.325	1	1021.100	1015.295	-5.805	-0.569	4
37.78	101.325	1	1007.900	998.380	-9.520	-0.945	4
60.00	101.325	1	991.400	978.065	-13.335	-1.345	4
98.89	101.325	1	962.400	944.289	-18.111	-1.882	4

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.36 %AARD FOR 21 POINTS
4	VAPOR PRESSURE	KPA	1.19 %AARD FOR 34 POINTS
21	LIQUID VISCOSITY	CP	6.04 %AARD FOR 3 POINTS

N0218 C11H10 2-METHYLNAPHTHALENE

CONST: REID ET AL 1977
PROP.: 1. KOBAYASHI ET AL 1979, 2. CAMIN AND ROSSINI 1955,
3. HALES AND TOWNSEND 1972, 4. API-42

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	142.201	761.00	604.30	462.09	6.255	0.38200
FITTED:				462.27	6.255	0.36876

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
130.22		4	3.800	3.709	-0.090	-2.381	1
150.06		4	7.651	7.830	0.179	2.334	1
163.34		4	11.874	12.357	0.483	4.069	1
174.18		4	16.945	17.536	0.590	3.484	1
195.28		4	30.883	32.627	1.744	5.647	1
223.07		4	63.564	67.128	3.564	5.607	1
243.59		4	103.313	107.686	4.374	4.233	1
273.10		4	190.938	197.051	6.113	3.201	1
304.30		4	341.831	345.069	3.238	0.947	1
308.05		4	362.829	367.324	4.495	1.239	1
320.73		4	447.234	450.946	3.712	0.830	1
325.34		4	462.798	484.202	21.404	4.625	1
139.19		4	5.536	5.287	-0.248	-4.484	2
145.43		4	6.951	6.673	-0.278	-3.998	2
150.66		4	8.339	8.059	-0.280	-3.361	2
154.58		4	9.539	9.247	-0.292	-3.065	2
158.69		4	10.942	10.649	-0.292	-2.672	2
164.15		4	13.100	12.787	-0.314	-2.394	2
176.72		4	19.433	19.073	-0.360	-1.854	2
182.32		4	22.882	22.588	-0.294	-1.287	2
190.03		4	28.551	28.287	-0.264	-0.924	2
197.23		4	34.820	34.616	-0.204	-0.586	2
205.33		4	43.163	43.050	-0.113	-0.261	2
213.96		4	53.782	53.794	0.012	0.023	2
223.03		4	67.089	67.277	0.188	0.281	2
239.61		4	98.125	98.813	0.688	0.702	2
240.34		4	99.734	100.416	0.682	0.683	2
240.96		4	101.114	101.808	0.693	0.686	2
241.76		4	102.929	103.630	0.701	0.681	2
36.85	374.635	1	993.410	977.376	-16.034	-1.614	3
46.85	440.096	1	985.760	968.234	-17.526	-1.778	3
56.85	513.690	1	978.090	959.261	-18.829	-1.925	3
66.85	596.216	1	970.420	950.441	-19.979	-2.059	3
86.85	790.333	1	955.040	933.209	-21.831	-2.286	3
106.85	1027.379	1	939.600	916.435	-23.165	-2.465	3
126.85	1312.422	1	923.970	900.018	-23.952	-2.592	3
146.85	1650.260	1	908.140	883.861	-24.279	-2.673	3

N0218 C11H10 2-METHYLNAPHTHALENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
166.85	2045.293	1	892.000	867.868	-24.132	-2.705	3
186.85	2502.321	1	875.540	851.941	-23.599	-2.695	3
196.85	2755.232	1	867.190	843.971	-23.219	-2.677	3
206.85	3025.076	1	858.720	835.980	-22.740	-2.648	3
216.85	3312.385	1	850.110	827.953	-22.157	-2.606	3

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	2.36 %AARD FOR 13 POINTS
4	VAPOR PRESSURE	KPA	2.29 %AARD FOR 29 POINTS

H0009 C11H24 UNDECANE (HENDECANE)

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P282, 2. CAMIN AND ROSSINI 1955
3. REID ET AL 1977

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	156.313	638.80	507.27	660.00	7.044	0.53500
FITTED:						0.52914

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
30.00		4	0.077	0.078	0.001	1.570	1
40.00		4	0.160	0.160	-0.000	-0.143	1
50.00		4	0.311	0.309	-0.002	-0.624	1
60.00		4	0.575	0.569	-0.006	-1.034	1
70.00		4	1.013	1.002	-0.011	-1.124	1
80.00		4	1.713	1.695	-0.018	-1.042	1
90.00		4	2.786	2.765	-0.021	-0.766	1
100.00		4	4.381	4.362	-0.019	-0.435	1
110.00		4	6.682	6.675	-0.007	-0.108	1
120.00		4	9.916	9.935	0.018	0.184	1
130.00		4	14.355	14.416	0.062	0.429	1
140.00		4	20.314	20.440	0.126	0.618	1
150.00		4	28.162	28.372	0.210	0.747	1
160.00		4	38.313	38.625	0.313	0.816	1
170.00		4	51.233	51.659	0.426	0.831	1
180.00		4	67.434	67.975	0.541	0.803	1
190.00		4	87.477	88.123	0.646	0.739	1
200.00		4	111.930	112.691	0.761	0.680	1
210.00		4	141.480	142.317	0.837	0.591	1
220.00		4	176.810	177.679	0.869	0.492	1
230.00		4	218.600	219.501	0.901	0.412	1
367.00		4	1940.000	1934.564	-5.436	-0.280	3
25.00	0.052	5	360.700	360.255	-0.445	-0.123	1
195.90	101.325	5	265.760	266.635	0.875	0.329	1
-10.00	101.325	21	2.163	2.259	0.096	4.419	1
-0.00	101.325	21	1.742	1.811	0.069	3.942	1
10.00	101.325	21	1.425	1.482	0.057	3.972	1
20.00	101.325	21	1.182	1.234	0.052	4.402	1
30.00	101.325	21	1.010	1.044	0.034	3.351	1
40.00	101.325	21	0.871	0.895	0.024	2.749	1
50.00	101.325	21	0.759	0.776	0.017	2.292	1
60.00	101.325	21	0.671	0.681	0.010	1.426	1
70.00	101.325	21	0.597	0.602	0.005	0.841	1
80.00	101.325	21	0.535	0.537	0.002	0.340	1
90.00	101.325	21	0.482	0.482	0.000	0.015	1
100.00	101.325	21	0.437	0.436	-0.001	-0.319	1
120.00	101.325	21	0.365	0.361	-0.004	-1.008	1

H0009 C11H24 UNDECANE (HENDECANE)

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
140.00	101.325	21	0.311	0.305	-0.006	-1.996	1
160.00	101.325	21	0.268	0.260	-0.008	-2.847	1
180.00	101.325	21	0.233	0.224	-0.009	-3.683	1
20.00	101.325	1	740.240	739.807	-0.433	-0.058	2
25.00	101.325	1	736.520	735.814	-0.706	-0.096	2
30.00	101.325	1	732.840	731.852	-0.988	-0.135	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.10 %AARD FOR 3 POINTS
4	VAPOR PRESSURE	KPA	0.66 %AARD FOR 22 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.23 %AARD FOR 2 POINTS
21	LIQUID VISCOSITY	CP	2.35 %AARD FOR 16 POINTS

C1410 C12H9N CARBAZOLE. DIBENZOPYRROLE. DIPHENYLENIMINE.

CONST: ESTIMATED USING LYDERSEN'S METHOD
PROP.: 1.COAL TAR DATA BOOK, 2. SENSEMAN AND NELSON 1923

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	167.210	900.00	714.68	624.30	6.914	0.46500
FITTED:				616.48	6.885	0.45685

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
244.80		4	7.386	7.409	0.023	0.307	1
252.40		4	9.333	9.299	-0.033	-0.356	1
252.60		4	9.373	9.353	-0.020	-0.211	1
266.20		4	13.812	13.749	-0.063	-0.458	1
266.60		4	13.932	13.898	-0.034	-0.245	1
267.30		4	14.012	14.153	0.141	1.005	1
289.60		4	25.051	25.223	0.172	0.687	1
290.00		4	25.398	25.478	0.080	0.316	1
290.60		4	25.744	25.854	0.110	0.425	1
308.30		4	39.437	39.234	-0.202	-0.513	1
309.00		4	39.730	39.843	0.114	0.286	1
336.80		4	72.487	71.989	-0.498	-0.687	1
336.90		4	72.980	72.147	-0.834	-1.142	1
337.50		4	73.540	73.006	-0.534	-0.726	1
351.80		4	99.192	96.437	-2.755	-2.777	1
352.00		4	99.192	96.789	-2.402	-2.422	1
252.61		4	9.346	9.353	0.007	0.078	2
258.28		4	11.052	11.019	-0.033	-0.301	2
259.43		4	11.372	11.381	0.009	0.079	2
261.99		4	12.372	12.242	-0.130	-1.053	2
266.13		4	13.785	13.722	-0.063	-0.457	2
270.15		4	15.319	15.302	-0.017	-0.112	2
274.04		4	17.145	16.983	-0.162	-0.944	2
276.31		4	18.025	18.016	-0.009	-0.050	2
281.93		4	20.878	20.830	-0.048	-0.232	2
288.02		4	24.131	24.261	0.130	0.537	2
290.09		4	25.465	25.535	0.071	0.277	2
291.25		4	26.291	26.276	-0.015	-0.058	2
292.65		4	26.958	27.172	0.215	0.796	2
294.40		4	28.371	28.360	-0.011	-0.039	2
298.16		4	30.864	31.013	0.149	0.482	2
302.71		4	34.744	34.522	-0.222	-0.639	2
307.18		4	38.197	38.238	0.041	0.108	2
309.85		4	40.490	40.613	0.123	0.304	2
310.81		4	41.010	41.479	0.469	1.144	2
311.83		4	42.370	42.455	0.085	0.201	2
315.77		4	46.449	46.326	-0.123	-0.265	2

C1410 C12H9N CARBAZOLE. DIBENZOPYRROLE. DIPHENYLENIMINE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
320.85		4	51.396	51.696	0.300	0.584	2
322.80		4	53.489	53.889	0.400	0.748	2
326.60		4	58.208	58.396	0.188	0.322	2
332.65		4	65.488	66.149	0.661	1.010	2
343.42		4	81.446	82.014	0.568	0.698	2
348.05		4	89.246	89.700	0.454	0.509	2
348.26		4	89.606	90.061	0.455	0.508	2
350.05		4	92.392	93.176	0.784	0.849	2
354.28		4	100.445	100.919	0.474	0.472	2
354.49		4	101.245	101.329	0.084	0.083	2
354.72		4	101.498	101.758	0.260	0.257	2
357.31		4	106.364	106.763	0.399	0.375	2
357.71		4	107.618	107.569	-0.049	-0.045	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	0.54 %AARD FOR 50 POINTS

A0004 C12H10 ACENAPHTHENE. NAPHTHYLENEETHYLENE.

CONST: COAL TAR DATA BOOK 1965
PROP.: 1. MORTIMER AND MURPHY 1922, 2. COAL TAR DATA BOOK 1965,
3. ANDERSON AND WU 1963

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	154.212	789.00	626.54	635.00	6.954	0.36400
FITTED:		824.13	654.43	460.05	6.245	0.35643

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
182.40		4	8.479	8.367	-0.112	-1.321	1
210.20		4	19.732	19.677	-0.054	-0.275	1
210.40		4	19.865	19.792	-0.073	-0.368	1
227.20		4	31.277	31.352	0.074	0.238	1
233.20		4	36.264	36.603	0.339	0.936	1
246.20		4	49.942	50.475	0.533	1.067	1
246.60		4	50.382	50.959	0.576	1.144	1
247.00		4	51.049	51.458	0.409	0.802	1
252.40		4	57.928	58.440	0.512	0.883	1
264.40		4	76.407	76.698	0.291	0.380	1
275.30		4	97.778	96.983	-0.796	-0.814	1
277.20		4	101.325	100.889	-0.436	-0.430	1
286.80		4	124.029	122.688	-1.341	-1.081	1
287.00		4	124.296	123.170	-1.127	-0.906	1
287.80		4	125.723	125.123	-0.600	-0.477	1
99.00	101.325	1	1024.000	1030.548	6.548	0.639	3
92.00	101.325	21	1.577	1.503	-0.074	-4.682	1
100.00	101.325	21	1.390	1.355	-0.035	-2.528	1
110.00	101.325	21	1.216	1.199	-0.017	-1.387	1
120.00	101.325	21	1.072	1.070	-0.002	-0.223	1
130.00	101.325	21	0.953	0.961	0.008	0.817	1
140.00	101.325	21	0.854	0.869	0.015	1.700	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.64 %AARD FOR 1 POINTS
4	VAPOR PRESSURE	KPA	0.74 %AARD FOR 15 POINTS
21	LIQUID VISCOSITY	CP	1.89 %AARD FOR 6 POINTS

B2214 C12H10 BIPHENYL. DIPHENYL. PHENYLBENZENE.

CONST: REID ET AL 1977
PROP : 1. VARGAFTIK 1975 P 356, 2. KOBAYASHI 1979
3. COAL TAR DATA BOOK 1965

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	154.212	789.00	626.54	478.80	6.329	0.32314
FITTED:				480.54	6.337	0.32215

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
100.00	0.573	1	970.000	967.242	-2.758	-0.284	1
160.00	7.253	1	922.000	917.841	-4.159	-0.451	1
180.00	13.999	1	905.000	901.831	-3.169	-0.350	1
200.00	25.331	1	889.000	885.894	-3.106	-0.349	1
220.00	43.596	1	872.000	869.934	-2.066	-0.237	1
240.00	71.194	1	855.000	853.850	-1.150	-0.135	1
260.00	108.000	1	838.000	837.527	-0.473	-0.056	1
280.00	174.000	1	820.000	820.876	0.876	0.107	1
300.00	238.000	1	801.000	803.687	2.687	0.335	1
320.00	338.000	1	782.000	785.861	3.861	0.494	1
340.00	447.000	1	762.000	767.104	5.104	0.670	1
360.00	655.000	1	740.000	747.430	7.430	1.004	1
380.00	880.000	1	717.000	726.215	9.215	1.285	1
240.00	71.194	5	316.000	306.400	-9.600	-3.038	1
260.00	108.000	5	305.000	297.475	-7.525	-2.467	1
280.00	174.000	5	294.000	287.740	-6.260	-2.129	1
300.00	238.000	5	283.000	278.483	-4.517	-1.596	1
320.00	338.000	5	272.000	268.283	-3.717	-1.367	1
340.00	447.000	5	261.000	258.132	-2.868	-1.099	1
360.00	655.000	5	249.000	244.948	-4.052	-1.627	1
380.00	880.000	5	237.000	231.455	-5.545	-2.340	1
75.00	101.325	21	1.349	1.343	-0.006	-0.450	3
90.00	101.325	21	1.084	1.106	0.022	1.984	3
105.00	101.325	21	0.900	0.928	0.028	3.060	3
110.50	101.325	21	0.844	0.874	0.029	3.472	3
139.50	101.325	21	0.618	0.657	0.039	6.312	3
154.50	101.325	21	0.537	0.577	0.040	7.433	3
170.00	101.325	21	0.467	0.510	0.043	9.290	3
182.00	101.325	21	0.424	0.466	0.043	10.038	3
193.30	101.325	21	0.387	0.430	0.043	11.143	3
210.00	101.325	21	0.342	0.385	0.042	12.279	3
122.99		4	2.040	2.068	0.028	1.394	2
143.80		4	4.773	4.729	-0.044	-0.912	2
164.68		4	9.962	9.836	-0.126	-1.267	2
181.26		4	16.447	16.566	0.119	0.724	2
200.86		4	28.599	29.025	0.427	1.491	2
223.65		4	51.518	52.128	0.609	1.183	2

B2214 C12H10 BIPHENYL. DIPHENYL. PHENYLBENZENE.

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
245.64		4	86.254	86.491	0.237	0.275	2
257.90		4	111.343	112.171	0.829	0.744	2
274.08		4	154.492	154.846	0.354	0.229	2
296.13		4	235.344	232.164	-3.180	-1.351	2
315.18		4	329.299	320.251	-9.048	-2.748	2
327.54		4	400.174	389.620	-10.554	-2.637	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.44 %AARD FOR 13 POINTS
4	VAPOR PRESSURE	KPA	1.25 %AARD FOR 12 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.96 %AARD FOR 8 POINTS
21	LIQUID VISCOSITY	CP	6.55 %AARD FOR 10 POINTS

B2186 C12H22 BICYCLOHEXYL. DODECAHYDRO BIPHENYL.
(CIS,CIS) AND (TRANS,TRANS) CONFORMATIONS EXIST.
CONST: CHAO ET AL 1980
PROP.: 1. KOBAYASHI ET AL 1979

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	166.310	731.40	580.80	577.00	6.735	0.38800
FITTED:				626.14	6.921	0.38296

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
151.10		4	9.591	9.648	0.057	0.593	1
157.94		4	12.058	12.125	0.067	0.556	1
163.83		4	14.596	14.658	0.062	0.422	1
170.29		4	17.880	17.919	0.039	0.219	1
176.33		4	21.562	21.488	-0.074	-0.345	1
182.17		4	25.406	25.445	0.039	0.153	1
189.41		4	31.123	31.163	0.040	0.128	1
189.42		4	31.128	31.171	0.043	0.138	1
196.03		4	37.603	37.280	-0.324	-0.861	1
202.67		4	44.731	44.316	-0.414	-0.927	1
210.00		4	53.518	53.256	-0.262	-0.489	1
217.59		4	64.483	63.990	-0.492	-0.764	1
226.13		4	77.731	77.979	0.248	0.319	1
233.18		4	92.404	91.352	-1.052	-1.138	1
240.06		4	106.548	105.970	-0.578	-0.543	1
248.26		4	125.845	125.722	-0.123	-0.098	1
255.52		4	144.830	145.485	0.655	0.452	1
263.89		4	170.547	171.209	0.662	0.388	1
272.07		4	198.480	199.588	1.108	0.558	1
280.03		4	229.391	230.562	1.171	0.511	1
288.21		4	265.261	266.111	0.850	0.320	1
295.64		4	301.060	301.888	0.828	0.275	1
304.10		4	346.747	346.983	0.237	0.068	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	0.45 %AARD FOR 23 POINTS

D0284 C12H26 DODECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 284, 2. COAL TAR DATA BOOK 1965
3. REID ET AL 1977

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	170.340	658.30	522.75	713.00	7.228	0.56200
FITTED:				723.26	7.262	0.56895

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
40.00		4	0.053	0.055	0.001	2.512	1
50.00		4	0.111	0.112	0.001	0.857	1
60.00		4	0.219	0.218	-0.001	-0.315	1
70.00		4	0.407	0.403	-0.003	-0.773	1
80.00		4	0.724	0.715	-0.009	-1.179	1
90.00		4	1.232	1.218	-0.014	-1.139	1
100.00		4	2.018	1.999	-0.019	-0.955	1
110.00		4	3.198	3.175	-0.023	-0.733	1
120.00		4	4.913	4.891	-0.022	-0.445	1
130.00		4	7.342	7.329	-0.013	-0.182	1
140.00		4	10.700	10.705	0.005	0.047	1
150.00		4	15.243	15.278	0.035	0.230	1
160.00		4	21.268	21.343	0.075	0.353	1
170.00		4	29.115	29.236	0.122	0.418	1
180.00		4	39.167	39.337	0.169	0.432	1
190.00		4	51.854	52.061	0.207	0.398	1
200.00		4	67.645	67.866	0.221	0.327	1
210.00		4	87.050	87.248	0.198	0.227	1
220.00		4	110.590	110.741	0.151	0.136	1
230.00		4	138.900	138.921	0.021	0.015	1
240.00		4	172.580	172.403	-0.177	-0.102	1
250.00		4	212.270	211.844	-0.426	-0.201	1
386.00		4	1810.000	1806.283	-3.717	-0.205	1
-0.00	101.325	1	763.300	761.590	-1.710	-0.224	1
10.00	101.325	1	756.100	753.501	-2.599	-0.344	1
20.00	101.325	1	748.800	745.559	-3.241	-0.433	1
25.00	101.325	1	745.200	741.638	-3.562	-0.478	1
30.00	101.325	1	741.500	737.750	-3.750	-0.506	1
40.00	101.325	1	734.200	730.062	-4.138	-0.564	1
50.00	101.325	1	726.800	722.483	-4.317	-0.594	1
60.00	101.325	1	719.400	715.001	-4.399	-0.612	1
70.00	101.325	1	711.900	707.603	-4.297	-0.604	1
80.00	101.325	1	704.400	700.277	-4.123	-0.585	1
90.00	101.325	1	696.800	693.011	-3.789	-0.544	1
100.00	101.325	1	689.200	685.791	-3.409	-0.495	1
110.00	101.325	1	681.500	678.605	-2.895	-0.425	1
120.00	101.325	1	673.800	671.439	-2.361	-0.350	1

D0284 C12H26 DODECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
130.00	101.325	1	666.000	664.279	-1.721	-0.258	1
140.00	101.325	1	658.200	657.111	-1.089	-0.166	1
150.00	101.325	1	650.200	649.918	-0.282	-0.043	1
160.00	101.325	1	642.100	642.684	0.584	0.091	1
170.00	101.325	1	633.900	635.392	1.492	0.235	1
180.00	101.325	1	625.600	628.021	2.421	0.387	1
190.00	101.325	1	617.200	620.550	3.350	0.543	1
200.00	101.325	1	608.500	612.954	4.454	0.732	1
210.00	101.325	1	599.000	605.205	6.205	1.036	1
25.00	0.016	5	360.020	355.199	-4.821	-1.339	1
216.28	101.325	5	256.630	257.017	0.387	0.151	1
10.00	101.325	21	1.827	1.874	0.047	2.567	1
20.00	101.325	21	1.492	1.541	0.049	3.290	1
40.00	101.325	21	1.064	1.094	0.030	2.811	1
60.00	101.325	21	0.803	0.818	0.015	1.837	1
70.00	101.325	21	0.709	0.718	0.009	1.293	1
80.00	101.325	21	0.632	0.636	0.004	0.678	1
90.00	101.325	21	0.566	0.568	0.002	0.377	1
100.00	101.325	21	0.510	0.511	0.001	0.153	1
91.60		4	1.333	1.321	-0.012	-0.927	2
106.00		4	2.666	2.648	-0.018	-0.693	2
115.13		4	4.000	3.977	-0.023	-0.564	2
121.99		4	5.333	5.312	-0.021	-0.387	2
127.54		4	6.666	6.651	-0.015	-0.229	2
132.22		4	7.999	7.989	-0.010	-0.131	2
139.91		4	10.666	10.670	0.004	0.041	2
146.14		4	13.332	13.353	0.021	0.158	2
158.11		4	19.998	20.067	0.068	0.342	2
167.14		4	26.664	26.771	0.107	0.399	2
174.49		4	33.330	33.474	0.144	0.432	2
180.73		4	39.997	40.171	0.175	0.437	2
191.03		4	53.329	53.538	0.210	0.393	2
199.43		4	66.661	66.874	0.213	0.320	2
206.59		4	79.993	80.204	0.211	0.264	2
212.85		4	93.325	93.501	0.175	0.188	2
213.44		4	94.659	94.838	0.179	0.189	2
214.02		4	95.992	96.167	0.175	0.182	2
214.59		4	97.325	97.488	0.163	0.167	2
215.16		4	98.658	98.822	0.164	0.166	2
215.72		4	99.991	100.148	0.156	0.156	2
216.28		4	101.325	101.486	0.161	0.159	2
216.83		4	102.658	102.815	0.157	0.153	2
217.37		4	103.991	104.133	0.142	0.137	2
217.91		4	105.324	105.464	0.140	0.133	2

D0284 C12H26 DODECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
218.44		4	106.658	106.784	0.126	0.119	2
223.51		4	119.990	120.069	0.079	0.066	2
228.15		4	133.322	133.329	0.007	0.005	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.45 %AARD FOR 23 POINTS
4	VAPOR PRESSURE	KPA	0.39 %AARD FOR 51 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.74 %AARD FOR 2 POINTS
21	LIQUID VISCOSITY	CP	1.63 %AARD FOR 8 POINTS

F0045 C13H10 FLUORENE. 2,3-BENZINDENE. DIPHENYLENEMETHANE.

CONST: ESTIMATED
PROP.: 1. COAL TAR DATA BOOK, 2. MORTIMER AND MURPHY 1923

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	166.225	841.81	668.47	546.98	6.616	0.36417
FITTED:		843.54	669.85	542.23	6.597	0.36037

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
161.00		4	2.400	2.285	-0.115	-4.789	2
202.50		4	9.266	9.526	0.261	2.812	2
203.00		4	9.399	9.674	0.275	2.922	2
240.40		4	27.398	27.745	0.347	1.268	2
241.40		4	27.784	28.442	0.657	2.366	2
276.60		4	64.994	65.079	0.084	0.130	2
277.10		4	65.421	65.773	0.352	0.538	2
295.60		4	98.498	96.610	-1.889	-1.918	2
299.80		4	107.231	104.962	-2.269	-2.116	2
300.40		4	108.297	106.192	-2.105	-1.944	2
113.70	101.325	21	1.206	1.212	0.006	0.500	1
120.20	101.325	21	1.105	1.123	0.018	1.635	1
127.20	101.325	21	1.024	1.038	0.014	1.383	1
133.70	101.325	21	0.954	0.968	0.014	1.466	1
140.20	101.325	21	0.891	0.905	0.014	1.571	1
147.30	101.325	21	0.828	0.843	0.015	1.850	1
152.70	101.325	21	0.791	0.801	0.010	1.233	1
167.10	101.325	21	0.706	0.703	-0.003	-0.480	1
177.60	101.325	21	0.646	0.643	-0.003	-0.523	1
187.30	101.325	21	0.600	0.594	-0.006	-0.968	1
202.20	101.325	21	0.544	0.530	-0.014	-2.499	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	2.08 %AARD FOR 10 POINTS
21	LIQUID VISCOSITY	CP	1.28 %AARD FOR 11 POINTS

M0271 C13H12 DIPHENYLMETHANE

CONST: REID ET AL 1977
PROP.: 1. KOBAYASHI 1979, 2. WILSON ET AL 1981
3. CHAO ET AL 1980, 4. API-42 1966

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	168.241	775.34	615.69	543.27	6.601	0.47100
FITTED:				543.25	6.601	0.42576

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
151.49		4	3.904	3.871	-0.033	-0.841	1
151.76		4	3.929	3.910	-0.019	-0.496	1
158.06		4	4.942	4.960	0.018	0.359	1
164.06		4	6.182	6.183	0.001	0.008	1
170.31		4	7.799	7.722	-0.077	-0.994	1
176.25		4	9.487	9.452	-0.035	-0.367	1
182.32		4	11.487	11.541	0.054	0.471	1
189.57		4	14.279	14.521	0.242	1.697	1
196.01		4	17.435	17.698	0.263	1.509	1
202.69		4	21.342	21.577	0.235	1.102	1
209.70		4	26.436	26.387	-0.050	-0.189	1
217.16		4	32.381	32.387	0.005	0.016	1
225.99		4	41.037	40.884	-0.152	-0.370	1
232.67		4	48.733	48.433	-0.300	-0.615	1
240.33		4	58.832	58.415	-0.417	-0.709	1
247.79		4	70.499	69.663	-0.837	-1.187	1
255.23		4	83.501	82.506	-0.994	-1.191	1
263.79		4	100.021	99.494	-0.527	-0.527	1
264.36		4	100.938	100.705	-0.233	-0.231	1
272.29		4	119.269	118.992	-0.276	-0.232	1
280.28		4	137.736	139.851	2.115	1.535	1
288.00		4	162.025	162.790	0.765	0.472	1
295.97		4	186.463	189.288	2.825	1.515	1
303.88		4	218.740	218.957	0.216	0.099	1
311.45		4	253.089	250.567	-2.523	-0.997	1
320.63		4	298.025	293.417	-4.608	-1.546	1
349.23		4	458.892	463.239	4.348	0.947	1
357.08		4	513.482	520.884	7.402	1.442	1
364.42		4	576.755	579.769	3.014	0.523	1
374.10		4	670.228	665.052	-5.176	-0.772	1
343.33		4	420.580	423.231	2.651	0.630	2
454.44		4	1827.111	1803.052	-24.059	-1.317	2
37.80	101.325	1	992.900	995.741	2.841	0.286	4
60.00	101.325	1	975.600	975.661	0.061	0.006	4
98.90	101.325	1	945.300	942.158	-3.142	-0.332	4

M0271 C13H12 DIPHENYLMETHANE

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.21 %AARD FOR 3 POINTS
4	VAPOR PRESSURE	KPA	0.78 %AARD FOR 32 POINTS

T0716 C13H28 TRIDECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 284, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	184.367	675.80	536.65	780.00	7.447	0.62300
FITTED:				786.31	7.467	0.60703

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
70.00		4	0.167	0.167	0.000	0.030	1
80.00		4	0.311	0.309	-0.002	-0.519	1
90.00		4	0.555	0.549	-0.006	-0.996	1
100.00		4	0.947	0.937	-0.009	-0.986	1
110.00		4	1.556	1.543	-0.012	-0.802	1
120.00		4	2.473	2.460	-0.013	-0.545	1
130.00		4	3.813	3.804	-0.009	-0.242	1
140.00		4	5.721	5.723	0.002	0.035	1
150.00		4	8.369	8.395	0.026	0.311	1
160.00		4	11.967	12.031	0.064	0.537	1
170.00		4	16.760	16.879	0.119	0.712	1
180.00		4	23.018	23.220	0.202	0.876	1
190.00		4	31.100	31.375	0.275	0.883	1
200.00		4	41.328	41.695	0.366	0.886	1
210.00		4	54.111	54.571	0.459	0.849	1
220.00		4	69.887	70.429	0.541	0.775	1
230.00		4	89.126	89.730	0.604	0.678	1
240.00		4	112.300	112.968	0.668	0.595	1
402.65		4	1722.525	1750.012	27.487	1.596	2
25.00	0.004	5	359.500	348.968	-10.532	-2.929	1
235.40	101.325	5	247.540	247.877	0.337	0.136	1
-0.00	101.325	1	770.400	766.926	-3.474	-0.451	1
10.00	101.325	1	763.300	758.959	-4.341	-0.569	1
20.00	101.325	1	756.200	751.134	-5.066	-0.670	1
25.00	101.325	1	752.700	747.273	-5.427	-0.721	1
30.00	101.325	1	749.100	743.443	-5.657	-0.755	1
40.00	101.325	1	741.800	735.874	-5.926	-0.799	1
50.00	101.325	1	734.600	728.416	-6.184	-0.842	1
60.00	101.325	1	727.300	721.059	-6.241	-0.858	1
70.00	101.325	1	720.000	713.791	-6.209	-0.862	1
80.00	101.325	1	712.700	706.603	-6.097	-0.856	1
90.00	101.325	1	705.300	699.481	-5.819	-0.825	1
100.00	101.325	1	697.800	692.416	-5.384	-0.772	1
110.00	101.325	1	690.300	685.395	-4.905	-0.710	1
120.00	101.325	1	682.800	678.408	-4.392	-0.643	1
130.00	101.325	1	675.200	671.440	-3.760	-0.557	1
140.00	101.325	1	667.600	664.481	-3.119	-0.467	1

T0716 C13H28 TRIDECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
150.00	101.325	1	659.900	657.516	-2.384	-0.361	1
160.00	101.325	1	652.100	650.532	-1.568	-0.241	1
170.00	101.325	1	644.100	643.513	-0.587	-0.091	1
180.00	101.325	1	636.200	636.445	0.245	0.038	1
190.00	101.325	1	628.100	629.308	1.208	0.192	1
200.00	101.325	1	619.800	622.084	2.284	0.369	1
210.00	101.325	1	611.000	614.752	3.752	0.614	1
220.00	101.325	1	601.000	607.286	6.286	1.046	1
230.00	101.325	1	592.000	599.658	7.658	1.294	1
-0.00	101.325	21	2.962	2.933	-0.029	-0.966	1
10.00	101.325	21	2.339	2.334	-0.005	-0.212	1
20.00	101.325	21	1.878	1.896	0.018	0.974	1
30.00	101.325	21	1.561	1.569	0.008	0.504	1
40.00	101.325	21	1.312	1.319	0.007	0.512	1
50.00	101.325	21	1.114	1.124	0.010	0.895	1
60.00	101.325	21	0.969	0.970	0.001	0.080	1
70.00	101.325	21	0.849	0.846	-0.003	-0.377	1
80.00	101.325	21	0.751	0.745	-0.006	-0.833	1
90.00	101.325	21	0.668	0.661	-0.007	-1.001	1
100.00	101.325	21	0.598	0.592	-0.006	-1.063	1
120.00	101.325	21	0.489	0.483	-0.006	-1.289	1
140.00	101.325	21	0.408	0.402	-0.006	-1.433	1
160.00	101.325	21	0.347	0.341	-0.006	-1.849	1
180.00	101.325	21	0.299	0.292	-0.007	-2.311	1
200.00	101.325	21	0.260	0.253	-0.007	-2.755	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.62 %AARD FOR 25 POINTS
4	VAPOR PRESSURE	KPA	0.68 %AARD FOR 19 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	1.53 %AARD FOR 2 POINTS
21	LIQUID VISCOSITY	CP	1.07 %AARD FOR 16 POINTS

A1193 C14H10 ANTHRACENE

CONST: KUDCHADKER 1979A
PROP.: 1. KUDCHADKER 1979A

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	178.233	886.09	703.64	554.80	6.648	0.43901
FITTED:		889.19	706.10	553.07	6.641	

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
215.78		4	4.900	4.354	-0.546	-11.137	1
220.00		4	5.600	5.011	-0.589	-10.516	1
240.00		4	10.100	9.379	-0.721	-7.137	1
260.00		4	17.300	16.568	-0.732	-4.230	1
280.00		4	28.000	27.796	-0.204	-0.730	1
300.00		4	44.000	44.613	0.613	1.393	1
320.00		4	67.000	68.839	1.839	2.745	1
340.00		4	98.000	102.537	4.537	4.630	1
341.30		4	100.000	105.096	5.096	5.096	1
342.03		4	101.325	106.563	5.238	5.170	1
360.00		4	139.000	148.088	9.088	6.538	1
380.00		4	193.000	208.164	15.164	7.857	1
400.00		4	261.000	285.619	24.619	9.432	1
215.78	4.900	1	975.000	935.760	-39.240	-4.025	1
220.00	5.600	1	972.000	932.698	-39.302	-4.043	1
240.00	10.100	1	958.000	918.251	-39.749	-4.149	1
260.00	17.300	1	944.000	903.864	-40.136	-4.252	1
280.00	28.000	1	929.000	889.473	-39.527	-4.255	1
300.00	44.000	1	915.000	875.011	-39.989	-4.370	1
320.00	67.000	1	901.000	860.405	-40.595	-4.506	1
215.78	4.900	5	352.348	376.410	24.062	6.829	1
220.00	5.600	5	348.420	374.610	26.190	7.517	1
240.00	10.100	5	341.688	365.888	24.200	7.083	1
260.00	17.300	5	334.394	356.941	22.547	6.743	1
280.00	28.000	5	327.661	347.872	20.211	6.168	1
300.00	44.000	5	320.928	338.694	17.765	5.536	1
320.00	67.000	5	314.195	329.411	15.216	4.843	1
340.00	98.000	5	307.463	320.045	12.583	4.092	1
341.30	100.000	5	307.463	319.448	11.985	3.898	1
342.03	101.325	5	306.902	319.104	12.202	3.976	1
360.00	139.000	5	301.291	310.557	9.266	3.075	1
380.00	193.000	5	294.558	300.860	6.301	2.139	1
400.00	261.000	5	287.825	290.940	3.115	1.082	1
220.00	101.325	21	0.725	0.663	-0.062	-8.520	1
230.00	101.325	21	0.617	0.616	-0.001	-0.209	1
240.00	101.325	21	0.556	0.573	0.017	3.122	1
250.00	101.325	21	0.518	0.535	0.017	3.364	1

A1193 C14H10 ANTHRACENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
260.00	101.325	21	0.490	0.501	0.011	2.302	1
270.00	101.325	21	0.470	0.470	0.000	0.087	1
280.00	101.325	21	0.454	0.442	-0.012	-2.562	1
290.00	101.325	21	0.441	0.417	-0.024	-5.489	1
300.00	101.325	21	0.430	0.393	-0.037	-8.518	1
310.00	101.325	21	0.420	0.372	-0.048	-11.467	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	4.23 %AARD FOR 7 POINTS
4	VAPOR PRESSURE	KPA	5.89 %AARD FOR 13 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	4.84 %AARD FOR 13 POINTS
21	LIQUID VISCOSITY	CP	4.56 %AARD FOR 10 POINTS

P0484 C14H10 PHENANTHRENE

CONST: KUDCHADKER ET AL 1979A
PROP.: 1. KUDCHADKER ET AL 1979A, 2. WILSON ET AL 1981
3. COAL TAR DATA BOOK 1965

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	178.233	890.00	706.74	541.50	6.594	0.54000
FITTED:				540.23	6.589	0.41230

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
200.00	3.014	1	997.000	966.838	-30.162	-3.025	1
220.00	5.810	1	982.000	951.975	-30.025	-3.058	1
240.00	10.500	1	968.000	937.236	-30.764	-3.178	1
260.00	18.000	1	954.000	922.559	-31.441	-3.296	1
280.00	29.300	1	939.000	907.875	-31.125	-3.315	1
300.00	45.800	1	925.000	893.115	-31.885	-3.447	1
320.00	69.100	1	910.000	878.205	-31.795	-3.494	1
180.00		4	1.456	1.394	-0.062	-4.258	1
200.00		4	3.014	2.955	-0.059	-1.969	1
220.00		4	5.810	5.821	0.011	0.192	1
240.00		4	10.500	10.751	0.251	2.391	1
260.00		4	18.000	18.765	0.765	4.247	1
286.94		4	36.335	36.873	0.538	1.479	2
314.44		4	65.638	67.693	2.054	3.130	2
317.55		4	69.637	72.178	2.541	3.649	2
293.50		4	41.506	42.872	1.366	3.290	2
371.11		4	199.948	194.577	-5.371	-2.686	2
426.66		4	448.159	449.301	1.142	0.255	2
454.44		4	682.581	647.393	-35.188	-5.155	2
200.00	3.014	5	357.958	372.979	15.021	4.196	1
220.00	5.810	5	350.104	364.969	14.866	4.246	1
240.00	10.500	5	342.810	356.620	13.811	4.029	1
260.00	18.000	5	335.516	348.065	12.550	3.740	1
280.00	29.300	5	327.661	339.387	11.726	3.579	1
300.00	45.800	5	320.367	330.618	10.251	3.200	1
320.00	69.100	5	313.073	321.760	8.687	2.775	1
339.56	100.000	5	305.218	313.003	7.784	2.550	1
340.00	100.800	5	305.218	312.804	7.586	2.485	1
340.30	101.325	5	305.218	312.670	7.452	2.441	1
360.00	142.900	5	297.364	303.714	6.350	2.135	1
100.00	101.325	21	1.890	2.288	0.398	21.036	1
110.00	101.325	21	1.660	1.982	0.322	19.377	1
120.00	101.325	21	1.460	1.733	0.273	18.695	1
130.00	101.325	21	1.290	1.528	0.238	18.484	1
140.00	101.325	21	1.150	1.359	0.209	18.135	1
150.00	101.325	21	1.030	1.216	0.186	18.062	1
160.00	101.325	21	0.920	1.095	0.175	19.068	1

P0484 C14H10 PHENANTHRENE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
170.00	101.325	21	0.830	0.993	0.163	19.579	1
180.00	101.325	21	0.750	0.904	0.154	20.534	1
315.55	69.637	21	0.450	0.356	-0.094	-20.835	3

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	3.26 %AARD FOR 7 POINTS
4	VAPOR PRESSURE	KPA	2.73 %AARD FOR 12 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	3.22 %AARD FOR 11 POINTS
21	LIQUID VISCOSITY	CP	19.38 %AARD FOR 10 POINTS

P0510 C14H18 OCTANTHRENE.
1,2,3,4,5,6,7,8-OCTAHYDROPHENANTHRENE.
CONST: ESTIMATED USING LYDERSEN'S METHOD
PROP.: 1. API-42 1966

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	186.300	849.28	674.41	597.75	6.815	0.41058
FITTED:				609.42	6.859	0.52014

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
60.00	101.325	1	997.300	999.786	2.486	0.249	1
98.90	101.325	1	970.900	967.890	-3.010	-0.310	1
60.00	101.325	21	4.260	4.017	-0.243	-5.699	1
98.90	101.325	21	1.945	2.063	0.118	6.072	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.28 %AARD FOR 2 POINTS
21	LIQUID VISCOSITY	CP	5.89 %AARD FOR 2 POINTS

T0067 C14H30 TETRADECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P287, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	198.394	694.00	551.10	830.00	7.603	0.67900
FITTED:				846.16	7.652	0.63651

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
120.00		4	1.241	1.236	-0.005	-0.429	1
130.00		4	1.980	1.972	-0.008	-0.383	1
140.00		4	3.062	3.055	-0.007	-0.239	1
150.00		4	4.609	4.605	-0.004	-0.078	1
160.00		4	6.763	6.770	0.007	0.103	1
170.00		4	9.705	9.727	0.022	0.231	1
180.00		4	13.636	13.681	0.045	0.331	1
190.00		4	18.797	18.871	0.074	0.395	1
200.00		4	25.463	25.567	0.104	0.407	1
210.00		4	33.941	34.069	0.128	0.378	1
220.00		4	44.575	44.713	0.138	0.309	1
230.00		4	57.742	57.862	0.120	0.208	1
240.00		4	73.847	73.915	0.068	0.092	1
250.00		4	93.352	93.301	-0.051	-0.055	1
260.00		4	116.700	116.480	-0.220	-0.188	1
420.85		4	1621.200	1616.137	-5.063	-0.312	2
253.60	101.325	5	240.600	239.558	-1.042	-0.433	1
10.00	101.325	1	769.700	766.974	-2.726	-0.354	1
20.00	101.325	1	772.700	759.239	-13.461	-1.742	1
25.00	101.325	1	759.200	755.422	-3.778	-0.498	1
30.00	101.325	1	755.700	751.636	-4.064	-0.538	1
40.00	101.325	1	748.600	744.156	-4.444	-0.594	1
50.00	101.325	1	741.500	736.790	-4.710	-0.635	1
60.00	101.325	1	734.300	729.527	-4.773	-0.650	1
70.00	101.325	1	727.200	722.358	-4.842	-0.666	1
80.00	101.325	1	720.000	715.273	-4.727	-0.656	1
90.00	101.325	1	712.700	708.262	-4.438	-0.623	1
100.00	101.325	1	705.500	701.315	-4.185	-0.593	1
110.00	101.325	1	698.100	694.421	-3.679	-0.527	1
120.00	101.325	1	690.800	687.570	-3.230	-0.468	1
130.00	101.325	1	683.400	680.752	-2.648	-0.387	1
140.00	101.325	1	675.900	673.954	-1.946	-0.288	1
150.00	101.325	1	668.400	667.167	-1.233	-0.185	1
160.00	101.325	1	660.700	660.376	-0.324	-0.049	1
170.00	101.325	1	653.000	653.571	0.571	0.087	1
180.00	101.325	1	645.200	646.737	1.537	0.238	1
190.00	101.325	1	637.300	639.861	2.561	0.402	1

T0067 C14H30 TETRADECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
200.00	101.325	1	629.300	632.926	3.626	0.576	1
210.00	101.325	1	621.000	625.915	4.915	0.791	1
220.00	101.325	1	613.000	618.809	5.809	0.948	1
230.00	101.325	1	605.000	611.586	6.586	1.089	1
240.00	101.325	1	595.000	604.223	9.223	1.550	1
250.00	101.325	1	585.000	596.690	11.690	1.998	1
10.00	101.325	21	2.960	2.909	-0.051	-1.725	1
20.00	101.325	21	2.322	2.334	0.012	0.528	1
30.00	101.325	21	1.889	1.910	0.021	1.113	1
40.00	101.325	21	1.560	1.590	0.030	1.906	1
50.00	101.325	21	1.323	1.343	0.020	1.518	1
60.00	101.325	21	1.135	1.150	0.015	1.296	1
70.00	101.325	21	0.988	0.996	0.008	0.776	1
80.00	101.325	21	0.868	0.871	0.003	0.363	1
90.00	101.325	21	0.769	0.769	0.000	0.024	1
100.00	101.325	21	0.685	0.685	-0.000	-0.050	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.66 %AARD FOR 26 POINTS
4	VAPOR PRESSURE	KPA	0.26 %AARD FOR 16 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.43 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	0.93 %AARD FOR 10 POINTS

P0032 C15H32 PENTADECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P288, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	212.421	707.00	561.42	880.00	7.753	0.70600
FITTED:				911.22	7.843	0.68688

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
140.00		4	1.644	1.624	-0.020	-1.235	1
150.00		4	2.546	2.522	-0.024	-0.943	1
160.00		4	3.838	3.815	-0.024	-0.621	1
170.00		4	5.644	5.627	-0.017	-0.299	1
180.00		4	8.111	8.111	0.000	0.001	1
190.00		4	11.420	11.449	0.029	0.250	1
200.00		4	15.776	15.848	0.072	0.454	1
210.00		4	21.418	21.546	0.127	0.595	1
220.00		4	28.616	28.810	0.194	0.678	1
230.00		4	37.669	37.939	0.270	0.718	1
240.00		4	48.911	49.260	0.349	0.714	1
250.00		4	62.705	63.129	0.424	0.676	1
260.00		4	79.447	79.935	0.489	0.615	1
270.00		4	99.565	100.097	0.532	0.535	1
280.00		4	123.460	124.062	0.602	0.488	1
433.85		4	1519.875	1569.819	49.944	3.286	2
10.00	101.325	1	775.200	770.158	-5.042	-0.650	1
20.00	101.325	1	768.300	762.521	-5.779	-0.752	1
25.00	101.325	1	764.900	758.750	-6.150	-0.804	1
30.00	101.325	1	761.400	755.011	-6.389	-0.839	1
40.00	101.325	1	754.400	747.623	-6.777	-0.898	1
50.00	101.325	1	747.400	740.346	-7.054	-0.944	1
60.00	101.325	1	740.400	733.174	-7.226	-0.976	1
70.00	101.325	1	733.300	726.096	-7.204	-0.982	1
80.00	101.325	1	726.200	719.105	-7.095	-0.977	1
90.00	101.325	1	719.100	712.191	-6.909	-0.961	1
100.00	101.325	1	712.000	705.345	-6.655	-0.935	1
110.00	101.325	1	704.900	698.558	-6.342	-0.900	1
120.00	101.325	1	697.700	691.820	-5.880	-0.843	1
130.00	101.325	1	690.400	685.122	-5.278	-0.765	1
140.00	101.325	1	683.100	678.453	-4.647	-0.680	1
150.00	101.325	1	675.700	671.803	-3.897	-0.577	1
160.00	101.325	1	668.300	665.162	-3.138	-0.470	1
170.00	101.325	1	660.800	658.518	-2.282	-0.345	1
180.00	101.325	1	653.200	651.860	-1.340	-0.205	1
190.00	101.325	1	645.500	645.175	-0.325	-0.050	1
200.00	101.325	1	637.700	638.449	0.749	0.117	1

P0C32 C15H32 PENTADECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
210.00	101.325	1	630.000	631.669	1.669	0.265	1
220.00	101.325	1	622.000	624.817	2.817	0.453	1
230.00	101.325	1	614.000	617.877	3.877	0.631	1
240.00	101.325	1	605.000	610.828	5.828	0.963	1
250.00	101.325	1	596.000	603.647	7.647	1.283	1
260.00	101.325	1	587.000	596.309	9.309	1.586	1
270.60	101.325	5	232.580	232.915	0.335	0.144	1
20.00	101.325	21	2.841	2.826	-0.015	-0.516	1
30.00	101.325	21	2.291	2.288	-0.003	-0.114	1
40.00	101.325	21	1.873	1.887	0.014	0.740	1
50.00	101.325	21	1.570	1.581	0.011	0.692	1
60.00	101.325	21	1.335	1.343	0.008	0.616	1
70.00	101.325	21	1.155	1.156	0.001	0.048	1
80.00	101.325	21	1.010	1.005	-0.005	-0.486	1
90.00	101.325	21	0.888	0.883	-0.005	-0.590	1
100.00	101.325	21	0.786	0.782	-0.004	-0.501	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.74 %AARD FOR 27 POINTS
4	VAPOR PRESSURE	KPA	0.76 %AARD FOR 16 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.14 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	0.48 %AARD FOR 9 POINTS

P1930 C16H10 PYRENE. BENZO(D,E,F)PHENANTHRENE.

CONST: ESTIMATED
PROP.: 1. KUDCHADKER ET AL 1979B

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	202.258	982.05	779.84	600.88	6.827	0.34400
FITTED:		985.00	782.18	590.14	6.786	0.38040

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
260.00		4	4.600	4.860	0.260	5.653	1
280.00		4	8.700	8.664	-0.036	-0.417	1
300.00		4	15.200	14.648	-0.552	-3.630	1
320.00		4	24.800	23.667	-1.133	-4.568	1
340.00		4	38.300	36.761	-1.539	-4.019	1
360.00		4	56.500	55.151	-1.349	-2.388	1
393.90		4	100.000	102.440	2.440	2.440	1
394.80		4	101.325	104.026	2.701	2.666	1
400.00		4	110.000	113.598	3.598	3.271	1
157.50	101.325	21	1.919	1.800	-0.119	-6.226	2
162.90	101.325	21	1.778	1.690	-0.088	-4.928	2
170.40	101.325	21	1.603	1.555	-0.048	-3.012	2
177.30	101.325	21	1.448	1.444	-0.004	-0.271	2
185.60	101.325	21	1.306	1.326	0.020	1.556	2
197.00	101.325	21	1.160	1.187	0.027	2.356	2
213.30	101.325	21	0.978	1.025	0.047	4.792	2

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	3.23 %AARD FOR 9 POINTS
21	LIQUID VISCOSITY	CP	3.31 %AARD FOR 7 POINTS

PSU641 C16H16 1,2,2A,3,4,5-HEXAHYDROPYRENE

CONST: ESTIMATED USING LYDERSEN'S METHOD
PROP.: API-42

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	208.300	987.57	784.22	609.23	6.858	0.30000
FITTED:		987.67	784.30	608.17	6.854	

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
137.50		4	0.067	0.073	0.007	10.053	1
150.50		4	0.133	0.140	0.006	4.758	1
164.50		4	0.267	0.266	-0.001	-0.347	1
184.50		4	0.667	0.615	-0.051	-7.687	1
201.00		4	1.333	1.155	-0.178	-13.382	1
115.00	101.325	1	1039.500	1089.045	49.545	4.766	1
135.00	101.325	1	1026.100	1073.164	47.064	4.587	1
115.00	101.325	21	3.299	2.559	-0.740	-22.435	1
135.00	101.325	21	2.296	1.950	-0.346	-15.075	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	4.68 %AARD FOR 2 POINTS
4	VAPOR PRESSURE	KPA	7.25 %AARD FOR 5 POINTS
21	LIQUID VISCOSITY	CP	18.75 %AARD FOR 2 POINTS

F0044 C16H10 FLUORANTHENE. 1,2-BENZACENAPHTHENE. IDRYL.

CONST: ESTIMATED
PROP.: 1. COAL TAR DATA BOOK 1965

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	202.258	956.60	759.63	652.32	7.016	0.37000
FITTED:		956.74	759.74	652.97	7.019	

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
228.50		4	2.586	2.716	0.129	4.997	1
238.10		4	3.800	3.728	-0.072	-1.898	1
255.00		4	6.586	6.230	-0.357	-5.414	1
261.30		4	7.919	7.461	-0.458	-5.787	1
270.90		4	10.319	9.721	-0.598	-5.796	1
281.50		4	13.386	12.837	-0.549	-4.099	1
314.50		4	27.384	28.180	0.796	2.907	1
382.90		4	99.058	106.581	7.523	7.594	1
384.20		4	101.325	108.961	7.636	7.536	1
119.80	101.325	21	3.218	2.254	-0.964	-29.948	1
130.10	101.325	21	2.711	1.958	-0.753	-27.787	1
145.00	101.325	21	2.237	1.622	-0.615	-27.490	1
160.00	101.325	21	1.902	1.365	-0.537	-28.237	1
179.10	101.325	21	1.528	1.119	-0.409	-26.778	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	5.11 %AARD FOR 9 POINTS
21	LIQUID VISCOSITY	CP	28.05 %AARD FOR 5 POINTS

H0243 C16H34 HEXADECANE

CONST: REID ET AL 1977
PROP.: 1. VARGAFTIK 1975, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	226.448	717.00	569.36	973.12	8.017	0.74200
FITTED:				973.42	8.018	0.75477

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
190.00		4	6.917	6.845	-0.072	-1.042	1
200.00		4	9.769	9.709	-0.059	-0.604	1
210.00		4	13.551	13.507	-0.044	-0.323	1
220.00		4	18.564	18.460	-0.104	-0.559	1
230.00		4	24.707	24.784	0.077	0.310	1
240.00		4	32.632	32.783	0.151	0.463	1
250.00		4	42.491	42.747	0.256	0.603	1
260.00		4	54.639	55.010	0.371	0.679	1
270.00		4	69.594	69.941	0.347	0.498	1
280.00		4	87.282	87.906	0.624	0.715	1
443.85		4	1418.550	1487.506	68.956	4.861	2
286.80	101.325	5	227.430	228.093	0.663	0.292	1
20.00	101.325	1	773.400	768.125	-5.275	-0.682	1
25.00	101.325	1	770.000	764.379	-5.621	-0.730	1
30.00	101.325	1	766.500	760.663	-5.837	-0.761	1
40.00	101.325	1	759.700	753.320	-6.380	-0.840	1
50.00	101.325	1	752.800	746.087	-6.713	-0.892	1
60.00	101.325	1	745.900	738.957	-6.943	-0.931	1
70.00	101.325	1	738.900	731.922	-6.978	-0.944	1
80.00	101.325	1	731.900	724.975	-6.925	-0.946	1
90.00	101.325	1	724.900	718.107	-6.793	-0.937	1
100.00	101.325	1	717.900	711.311	-6.589	-0.918	1
110.00	101.325	1	710.800	704.576	-6.224	-0.876	1
120.00	101.325	1	703.700	697.896	-5.804	-0.825	1
130.00	101.325	1	696.500	691.260	-5.240	-0.752	1
140.00	101.325	1	689.200	684.660	-4.540	-0.659	1
150.00	101.325	1	682.000	678.086	-3.914	-0.574	1
160.00	101.325	1	674.700	671.528	-3.172	-0.470	1
170.00	101.325	1	667.400	664.978	-2.422	-0.363	1
180.00	101.325	1	659.900	658.422	-1.478	-0.224	1
190.00	101.325	1	652.200	651.852	-0.348	-0.053	1
200.00	101.325	1	644.700	645.254	0.554	0.086	1
210.00	101.325	1	637.000	638.616	1.616	0.254	1
220.00	101.325	1	629.000	631.924	2.924	0.465	1
230.00	101.325	1	621.000	625.162	4.162	0.670	1
240.00	101.325	1	612.000	618.313	6.313	1.032	1
250.00	101.325	1	604.000	611.359	7.359	1.218	1

H0243 C16H34 HEXADECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
260.00	101.325	1	596.000	604.278	8.278	1.389	1
270.00	101.325	1	587.000	597.044	10.044	1.711	1
280.00	101.325	1	578.000	589.629	11.629	2.012	1
20.00	101.325	21	3.451	3.418	-0.033	-0.948	1
30.00	101.325	21	2.754	2.738	-0.016	-0.570	1
40.00	101.325	21	2.232	2.237	0.005	0.213	1
50.00	101.325	21	1.852	1.859	0.007	0.355	1
60.00	101.325	21	1.560	1.568	0.008	0.494	1
70.00	101.325	21	1.338	1.340	0.002	0.151	1
80.00	101.325	21	1.161	1.159	-0.002	-0.181	1
90.00	101.325	21	1.014	1.013	-0.001	-0.125	1
100.00	101.325	21	0.892	0.893	0.001	0.137	1
120.00	101.325	21	0.716	0.712	-0.004	-0.615	1
140.00	101.325	21	0.584	0.582	-0.002	-0.337	1
160.00	101.325	21	0.486	0.486	0.000	0.037	1
180.00	101.325	21	0.409	0.413	0.004	0.974	1
200.00	101.325	21	0.349	0.355	0.006	1.858	1
220.00	101.325	21	0.299	0.309	0.010	3.387	1
240.00	101.325	21	0.259	0.271	0.012	4.571	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.79 %AARD FOR 28 POINTS
4	VAPOR PRESSURE	KPA	0.97 %AARD FOR 11 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.29 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	0.93 %AARD FOR 16 POINTS

H0066 C17H36 HEPTADECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P291, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	240.475	733.00	582.07	1000.00	8.090	0.77000
FITTED:				1038.75	8.193	0.76871

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
160.00		4	1.249	1.229	-0.020	-1.613	1
170.00		4	1.933	1.909	-0.025	-1.267	1
180.00		4	2.912	2.887	-0.025	-0.846	1
190.00		4	4.284	4.263	-0.021	-0.482	1
200.00		4	6.161	6.155	-0.006	-0.097	1
210.00		4	8.685	8.704	0.020	0.228	1
220.00		4	12.016	12.077	0.060	0.502	1
230.00		4	16.341	16.461	0.120	0.732	1
240.00		4	21.875	22.072	0.197	0.900	1
250.00		4	28.856	29.151	0.295	1.023	1
260.00		4	37.554	37.965	0.411	1.094	1
270.00		4	48.260	48.805	0.545	1.129	1
280.00		4	61.301	61.991	0.690	1.125	1
300.00		4	95.765	96.814	1.049	1.095	1
310.00		4	117.940	119.227	1.287	1.091	1
459.85		4	1317.225	1319.879	2.654	0.202	2
30.00	101.325	1	771.100	762.702	-8.398	-1.089	1
40.00	101.325	1	764.300	755.472	-8.828	-1.155	1
50.00	101.325	1	757.500	748.353	-9.147	-1.208	1
60.00	101.325	1	750.700	741.336	-9.364	-1.247	1
70.00	101.325	1	743.900	734.416	-9.484	-1.275	1
80.00	101.325	1	737.000	727.584	-9.416	-1.278	1
90.00	101.325	1	730.100	720.834	-9.266	-1.269	1
100.00	101.325	1	723.100	714.157	-8.943	-1.237	1
110.00	101.325	1	716.200	707.547	-8.653	-1.208	1
120.00	101.325	1	709.200	700.995	-8.205	-1.157	1
130.00	101.325	1	702.200	694.494	-7.706	-1.097	1
140.00	101.325	1	695.100	688.034	-7.066	-1.017	1
150.00	101.325	1	687.900	681.607	-6.293	-0.915	1
160.00	101.325	1	680.700	675.206	-5.494	-0.807	1
170.00	101.325	1	673.500	668.820	-4.680	-0.695	1
180.00	101.325	1	666.200	662.440	-3.760	-0.564	1
190.00	101.325	1	658.800	656.057	-2.743	-0.416	1
200.00	101.325	1	651.400	649.659	-1.741	-0.267	1
210.00	101.325	1	643.800	643.237	-0.563	-0.087	1
220.00	101.325	1	636.100	636.778	0.678	0.107	1
230.00	101.325	1	628.300	630.269	1.969	0.313	1

H0066 C17H36 HEPTADECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
240.0C	101.325	1	620.400	623.696	3.296	0.531	1
250.0C	101.325	1	612.300	617.044	4.744	0.775	1
260.00	101.325	1	604.100	610.295	6.195	1.025	1
270.00	101.325	1	595.700	603.430	7.730	1.298	1
280.00	101.325	1	587.100	596.426	9.326	1.588	1
290.00	101.325	1	578.200	589.256	11.056	1.912	1
300.00	101.325	1	568.900	581.890	12.990	2.283	1
301.80	101.325	5	221.110	220.367	-0.743	-0.336	1
30.00	101.325	21	3.291	3.220	-0.071	-2.165	1
40.00	101.325	21	2.652	2.606	-0.046	-1.728	1
50.00	101.325	21	2.169	2.148	-0.021	-0.974	1
60.0C	101.325	21	1.829	1.799	-0.030	-1.667	1
70.0C	101.325	21	1.557	1.527	-0.030	-1.916	1
80.00	101.325	21	1.340	1.313	-0.027	-2.021	1
90.00	101.325	21	1.161	1.141	-0.020	-1.706	1
100.00	101.325	21	1.014	1.002	-0.012	-1.215	1
120.00	101.325	21	0.794	0.791	-0.003	-0.321	1
140.C0	101.325	21	0.655	0.643	-0.012	-1.821	1
160.00	101.325	21	0.546	0.534	-0.012	-2.132	1
180.00	101.325	21	0.460	0.452	-0.008	-1.720	1
200.00	101.325	21	0.392	0.388	-0.004	-1.015	1
220.00	101.325	21	0.339	0.337	-0.002	-0.643	1
240.00	101.325	21	0.296	0.295	-0.001	-0.369	1
260.00	101.325	21	0.260	0.260	-0.000	-0.075	1
280.00	101.325	21	0.229	0.230	0.001	0.326	1
300.00	101.325	21	0.203	0.203	0.000	0.216	1

H0066 C17H36 HEPTADECANE

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.99 %AARD FOR 28 POINTS
4	VAPOR PRESSURE	KPA	0.84 %AARD FOR 16 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.34 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	1.22 %AARD FOR 18 POINTS

B1957 C18H12 TRIPHENYLENE. 9,10-BENZOPHENANTHRENE.

CONST: ESTIMATED
PROP.: 1. KUDCHADKER ET AL 1979B

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	228.296	1065.08	845.77	801.73	7.516	0.30900
FITTED:		1083.18	860.14	749.14	7.348	0.28040

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
260.00		4	1.900	1.804	-0.096	-5.052	1
280.00		4	3.300	3.232	-0.068	-2.074	1
300.00		4	5.500	5.522	0.022	0.392	1
320.00		4	8.800	9.040	0.240	2.728	1
340.00		4	13.800	14.257	0.457	3.311	1
360.00		4	21.000	21.724	0.724	3.448	1
380.00		4	31.200	32.099	0.899	2.883	1
400.00		4	45.100	46.125	1.025	2.273	1
420.00		4	63.900	64.649	0.749	1.173	1
440.00		4	88.800	88.599	-0.201	-0.227	1
447.50		4	100.000	99.183	-0.817	-0.817	1
448.40		4	101.325	100.514	-0.811	-0.800	1
460.00		4	121.000	118.980	-2.020	-1.669	1
480.00		4	163.000	156.898	-6.102	-3.744	1
500.00		4	210.000	203.422	-6.578	-3.133	1
200.00	101.325	21	1.370	1.341	-0.029	-2.094	1
210.00	101.325	21	1.210	1.219	0.009	0.742	1
220.00	101.325	21	1.090	1.113	0.023	2.139	1
230.00	101.325	21	1.000	1.021	0.021	2.145	1
240.00	101.325	21	0.910	0.941	0.031	3.420	1
250.00	101.325	21	0.840	0.870	0.030	3.628	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	2.25 %AARD FOR 15 POINTS
21	LIQUID VISCOSITY	CP	2.36 %AARD FOR 6 POINTS

00011 C18H38 OCTADECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P292, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	254.502	745.00	591.60	1100.92	8.354	0.79000
FITTED:				1101.09	8.354	0.80940

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
190.00		4	2.638	2.595	-0.044	-1.659	1
200.00		4	3.876	3.829	-0.047	-1.216	1
210.00		4	5.570	5.526	-0.044	-0.794	1
220.00		4	7.847	7.815	-0.033	-0.415	1
230.00		4	10.852	10.844	-0.008	-0.074	1
240.00		4	14.755	14.787	0.032	0.219	1
250.00		4	19.749	19.839	0.090	0.455	1
260.00		4	26.051	26.219	0.168	0.645	1
270.00		4	33.905	34.172	0.267	0.788	1
280.00		4	43.583	43.967	0.384	0.882	1
290.00		4	55.369	55.898	0.529	0.956	1
300.00		4	69.581	70.283	0.702	1.009	1
310.00		4	86.566	87.470	0.904	1.044	1
320.00		4	106.650	107.829	1.179	1.105	1
471.85		4	1205.767	1205.817	0.050	0.004	2
316.10	101.325	5	215.490	215.111	-0.379	-0.176	1
30.00	101.325	1	775.300	767.738	-7.562	-0.975	1
40.00	101.325	1	768.600	760.566	-8.034	-1.045	1
50.00	101.325	1	761.800	753.502	-8.298	-1.089	1
60.00	101.325	1	755.100	746.539	-8.561	-1.134	1
70.00	101.325	1	748.300	739.673	-8.627	-1.153	1
80.00	101.325	1	741.500	732.896	-8.604	-1.160	1
90.00	101.325	1	734.700	726.202	-8.498	-1.157	1
100.00	101.325	1	727.900	719.583	-8.317	-1.143	1
110.00	101.325	1	721.000	713.034	-7.966	-1.105	1
120.00	101.325	1	714.000	706.545	-7.455	-1.044	1
130.00	101.325	1	707.100	700.111	-6.989	-0.988	1
140.00	101.325	1	700.100	693.723	-6.377	-0.911	1
150.00	101.325	1	693.100	687.373	-5.727	-0.826	1
160.00	101.325	1	686.100	681.054	-5.046	-0.735	1
170.00	101.325	1	679.000	674.758	-4.242	-0.625	1
180.00	101.325	1	671.800	668.475	-3.325	-0.495	1
190.00	101.325	1	664.500	662.197	-2.303	-0.347	1
200.00	101.325	1	657.200	655.915	-1.285	-0.196	1
210.00	101.325	1	649.800	649.618	-0.182	-0.028	1
220.00	101.325	1	642.300	643.296	0.996	0.155	1
230.00	101.325	1	634.700	636.938	2.238	0.353	1

00011 C18H38 OCTADECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
240.00	101.325	1	627.000	630.531	3.531	0.563	1
250.00	101.325	1	619.200	624.063	4.863	0.785	1
260.00	101.325	1	611.300	617.518	6.218	1.017	1
270.00	101.325	1	603.200	610.880	7.680	1.273	1
280.00	101.325	1	594.800	604.131	9.331	1.569	1
290.00	101.325	1	586.100	597.248	11.148	1.902	1
300.00	101.325	1	577.000	590.208	13.208	2.289	1
30.00	101.325	21	3.813	3.801	-0.012	-0.316	1
40.00	101.325	21	3.060	3.048	-0.012	-0.388	1
50.00	101.325	21	2.491	2.491	0.000	0.020	1
60.00	101.325	21	2.060	2.071	0.011	0.533	1
70.00	101.325	21	1.748	1.747	-0.001	-0.051	1
80.00	101.325	21	1.484	1.493	0.009	0.627	1
90.00	101.325	21	1.297	1.291	-0.006	-0.439	1
100.00	101.325	21	1.131	1.128	-0.003	-0.245	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.93 %AARD FOR 28 POINTS
4	VAPOR PRESSURE	KPA	0.75 %AARD FOR 15 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.18 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	0.33 %AARD FOR 8 POINTS

NC505 C19H40 NONADECANE

CONST: VARGAFTIK 1975, REID ET AL 1977
PROP.: 1. VARGAFTIK 1975 P 294, 2. REID ET AL

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	268.529	756.00	600.33	1166.90	8.517	0.82700
FITTED:				1166.43	8.516	0.84882

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
190.00		4	1.625	1.594	-0.031	-1.901	1
200.00		4	2.441	2.404	-0.037	-1.531	1
210.00		4	3.578	3.540	-0.038	-1.076	1
220.00		4	5.136	5.101	-0.034	-0.665	1
230.00		4	7.225	7.205	-0.019	-0.269	1
240.00		4	9.982	9.989	0.007	0.074	1
250.00		4	13.560	13.611	0.051	0.378	1
260.00		4	18.140	18.253	0.113	0.622	1
270.00		4	23.918	24.115	0.197	0.825	1
280.00		4	31.117	31.425	0.308	0.990	1
290.00		4	39.983	40.432	0.449	1.122	1
300.00		4	50.796	51.408	0.612	1.205	1
310.00		4	63.848	64.650	0.802	1.257	1
320.00		4	79.433	80.480	1.047	1.318	1
330.00		4	97.898	99.246	1.348	1.377	1
340.00		4	119.500	121.320	1.820	1.523	1
487.00		4	1215.600	1224.486	8.886	0.731	1
329.70	101.325	5	210.500	209.818	-0.682	-0.324	1
40.00	101.325	1	772.300	762.294	-10.006	-1.296	1
50.00	101.325	1	765.700	755.307	-10.393	-1.357	1
60.00	101.325	1	759.000	748.420	-10.580	-1.394	1
70.00	101.325	1	752.300	741.627	-10.673	-1.419	1
80.00	101.325	1	745.600	734.924	-10.676	-1.432	1
90.00	101.325	1	738.800	728.304	-10.496	-1.421	1
100.00	101.325	1	732.100	721.760	-10.340	-1.412	1
110.00	101.325	1	725.400	715.287	-10.113	-1.394	1
120.00	101.325	1	718.600	708.878	-9.722	-1.353	1
130.00	101.325	1	711.600	702.525	-9.075	-1.275	1
140.00	101.325	1	704.600	696.221	-8.379	-1.189	1
150.00	101.325	1	697.600	689.961	-7.639	-1.095	1
160.00	101.325	1	690.600	683.735	-6.865	-0.994	1
170.00	101.325	1	683.600	677.537	-6.063	-0.887	1
180.00	101.325	1	676.600	671.358	-5.242	-0.775	1
190.00	101.325	1	669.500	665.191	-4.309	-0.644	1
200.00	101.325	1	662.400	659.027	-3.373	-0.509	1
210.00	101.325	1	655.100	652.857	-2.243	-0.342	1
220.00	101.325	1	647.800	646.671	-1.129	-0.174	1

N0505 C19H40 NONADECANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
230.00	101.325	1	640.400	640.460	0.060	0.009	1
240.00	101.325	1	632.800	634.213	1.413	0.223	1
250.00	101.325	1	625.000	627.917	2.917	0.467	1
260.00	101.325	1	617.000	621.561	4.561	0.739	1
270.00	101.325	1	608.900	615.130	6.230	1.023	1
280.00	101.325	1	600.700	608.608	7.908	1.316	1
290.00	101.325	1	592.400	601.977	9.577	1.617	1
300.00	101.325	1	584.000	595.218	11.218	1.921	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.03 %AARD FOR 27 POINTS
4	VAPOR PRESSURE	KPA	0.99 %AARD FOR 17 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.32 %AARD FOR 1 POINTS

PSU635 C20H26 1,2,3,3A,4,5,6,7,8,9,9A,10,11,12-
TETRADECAHYDROPERYLENE
CONST: ESTIMATED USING LYDERSEN'S METHOD
PROP.: 1. API-42

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	266.400	929.40	738.03	889.30	7.780	0.65910
FITTED:		976.03	775.06	564.81	6.687	0.57988

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
184.00		4	0.067	0.066	-0.000	-0.445	1
198.00		4	0.133	0.134	0.000	0.309	1
213.50		4	0.267	0.274	0.008	2.902	1
234.50		4	0.667	0.676	0.009	1.359	1
251.50		4	1.333	1.316	-0.018	-1.318	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	1.27 %AARD FOR 5 POINTS

E0016 C20H42 EICOSANE

VARGAFTIK 1975, REID ET AL 1977
1. VARGAFTIK 1975, 2. REID ET AL 1977

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	282.556	767.00	609.07	1225.11	8.657	0.90700
FITTED:				1228.20	8.664	0.88511

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
200.00		4	1.533	1.508	-0.026	-1.674	1
210.00		4	2.306	2.267	-0.039	-1.699	1
220.00		4	3.360	3.329	-0.031	-0.926	1
230.00		4	4.813	4.787	-0.026	-0.548	1
240.00		4	6.773	6.750	-0.023	-0.341	1
250.00		4	9.333	9.342	0.010	0.105	1
260.00		4	12.666	12.715	0.049	0.386	1
270.00		4	16.919	17.032	0.114	0.673	1
280.00		4	22.265	22.484	0.219	0.985	1
290.00		4	28.931	29.281	0.350	1.211	1
300.00		4	37.224	37.661	0.438	1.176	1
320.00		4	59.395	60.191	0.796	1.340	1
330.00		4	73.887	74.923	1.036	1.402	1
340.00		4	91.059	92.393	1.334	1.465	1
350.00		4	111.000	112.945	1.945	1.753	1
502.00		4	1114.000	1096.763	-17.237	-1.547	1
40.00	101.325	1	775.600	767.121	-8.479	-1.093	1
50.00	101.325	1	769.000	760.180	-8.820	-1.147	1
60.00	101.325	1	762.400	753.338	-9.062	-1.189	1
70.00	101.325	1	755.800	746.589	-9.211	-1.219	1
80.00	101.325	1	749.100	739.929	-9.171	-1.224	1
90.00	101.325	1	742.400	733.353	-9.047	-1.219	1
100.00	101.325	1	735.700	726.855	-8.845	-1.202	1
110.00	101.325	1	729.000	720.428	-8.572	-1.176	1
120.00	101.325	1	722.200	714.067	-8.133	-1.126	1
130.00	101.325	1	715.400	707.765	-7.635	-1.067	1
140.00	101.325	1	708.700	701.515	-7.185	-1.014	1
150.00	101.325	1	701.800	695.312	-6.488	-0.925	1
160.00	101.325	1	694.800	689.147	-5.653	-0.814	1
170.00	101.325	1	687.800	683.015	-4.785	-0.696	1
180.00	101.325	1	680.800	676.907	-3.893	-0.572	1
190.00	101.325	1	673.800	670.816	-2.984	-0.443	1
200.00	101.325	1	666.800	664.735	-2.065	-0.310	1
210.00	101.325	1	659.700	658.655	-1.045	-0.158	1
220.00	101.325	1	652.500	652.568	0.068	0.010	1
230.00	101.325	1	645.200	646.464	1.264	0.196	1
240.00	101.325	1	637.800	640.334	2.534	0.397	1

E0016 C20H42 EICOSANE

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
250.00	101.325	1	630.200	634.167	3.967	0.630	1
260.00	101.325	1	622.500	627.953	5.453	0.876	1
270.00	101.325	1	614.700	621.678	6.978	1.135	1
280.00	101.325	1	606.800	615.329	8.529	1.406	1
290.00	101.325	1	598.700	608.891	10.191	1.702	1
300.00	101.325	1	590.300	602.347	12.047	2.041	1
342.70	101.325	5	204.500	205.008	0.508	0.248	1
40.00	101.325	21	4.072	4.070	-0.002	-0.056	1
50.00	101.325	21	3.259	3.273	0.014	0.444	1
60.00	101.325	21	2.665	2.682	0.017	0.654	1
70.00	101.325	21	2.220	2.234	0.014	0.651	1
90.00	101.325	21	1.614	1.617	0.003	0.168	1
100.00	101.325	21	1.403	1.400	-0.003	-0.215	1
120.00	101.325	21	1.094	1.081	-0.013	-1.164	1
140.00	101.325	21	0.876	0.863	-0.013	-1.489	1
160.00	101.325	21	0.717	0.707	-0.010	-1.370	1
180.00	101.325	21	0.598	0.592	-0.006	-0.989	1
200.00	101.325	21	0.505	0.504	-0.001	-0.114	1
220.00	101.325	21	0.432	0.436	0.004	0.889	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.93 %AARD FOR 27 POINTS
4	VAPOR PRESSURE	KPA	1.08 %AARD FOR 16 POINTS
5	HEAT OF VAPORIZATION	KJ/KG	0.25 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	0.68 %AARD FOR 12 POINTS

Appendix *B*.

DETAILED LISTINGS OF CALCULATIONS FOR COMPLEX COAL FLUIDS

The Exxon Data

The only substantial collection of data for full-range coal fluids has been reported by Wilson et al (1980) and Hwang et al (1981). Measurements were made on Exxon coal fluids under contract to Wiltech Research Company, Provo, UT. No other data are available in the open literature, and it is doubtful that more data is under proprietary wraps. Fortunately, these data were available to test Therm-Trans.

The output is in the same format as given in the preface to Appenix A, except that empirical formula, etc... are not given. Descriptions of the calculation methods are given in Chapter 5.

EXXON COAL LIQUID: NARROW-BOILING FRACTION N-1
VOLATILITY MEASUREMENTS
CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	164.000	749.00	594.77	555.00	6.648	0.38400
FITTED:						0.38469

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
181.89		4	20.615	21.085	0.469	2.277	1
193.11		4	31.371	29.326	-2.046	-6.521	1
215.55		4	49.987	52.544	2.557	5.116	1
234.28		4	75.842	81.839	5.997	7.907	1
258.66		4	137.895	138.492	0.597	0.433	1
286.78		4	239.938	236.534	-3.403	-1.418	1
308.78		4	354.391	344.841	-9.550	-2.695	1
314.94		4	395.070	381.120	-13.949	-3.531	1
329.00		4	495.044	474.512	-20.532	-4.147	1
337.16		4	593.639	536.733	-56.906	-9.586	1
315.55		4	386.106	384.565	-1.541	-0.399	1
343.33		4	613.633	586.685	-26.948	-4.392	1
371.11		4	854.950	859.705	4.755	0.556	1
398.89		4	1213.477	1221.929	8.452	0.697	1
426.66		4	1558.215	1691.633	133.418	8.562	1
454.44		4	2096.006	2129.651	33.645	1.605	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	3.74 %AARD FOR 16 POINTS

EXXON COAL LIQUID: NARROW-BOILING FRACTION N-2
VOLATILITY MEASUREMENTS
CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	205.000	893.00	709.12	700.00	7.183	0.38500
FITTED:						0.38414

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
200.11		4	3.034	2.627	-0.407	-13.416	1
223.50		4	5.792	5.610	-0.182	-3.137	1
243.66		4	9.928	10.128	0.200	2.014	1
263.44		4	16.478	17.188	0.709	4.304	1
277.94		4	23.028	24.575	1.546	6.714	1
293.00		4	33.371	34.875	1.505	4.509	1
296.78		4	36.266	37.926	1.660	4.576	1
313.89		4	53.090	54.582	1.492	2.811	1
315.39		4	53.917	56.240	2.323	4.309	1
338.22		4	86.184	87.679	1.495	1.734	1
371.11		4	158.579	155.438	-3.141	-1.981	1
398.89		4	246.832	239.279	-7.554	-3.060	1
426.66		4	372.317	354.152	-18.165	-4.879	1
454.44		4	566.749	507.184	-59.565	-10.510	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	4.85 %AARD FOR 14 POINTS

EXXON COAL LIQUID: NARROW-BOILING FRACTION S-1
VOLATILITY MEASUREMENTS
CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	134.000	715.00	567.78	435.00	6.130	0.33500
FITTED:						0.33438

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
174.94		4	47.091	47.074	-0.017	-0.037	1
201.78		4	93.079	93.343	0.264	0.284	1
231.66		4	177.885	180.626	2.741	1.541	1
257.44		4	294.406	297.880	3.473	1.180	1
289.33		4	508.144	514.659	6.515	1.282	1
317.83		4	783.934	794.548	10.614	1.354	1
345.78		4	1154.872	1168.384	13.513	1.170	1
232.22		4	186.158	182.949	-3.210	-1.724	1
260.00		4	317.159	312.348	-4.811	-1.517	1
287.78		4	503.317	502.117	-1.201	-0.239	1
315.55		4	799.792	769.519	-30.273	-3.785	1
343.33		4	1123.845	1131.309	7.463	0.664	1
371.11		4	1606.478	1611.564	5.086	0.317	1
398.89		4	2275.270	2237.137	-38.133	-1.676	1
426.66		4	3006.114	3023.744	17.630	0.586	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	1.16 %AARD FOR 15 POINTS

EXXON COAL LIQUID: NARROW-BOILING FRACTION S-2
VOLATILITY MEASUREMENTS
CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	179.000	803.00	637.66	606.00	6.846	0.42000
FITTED:						0.41909

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
173.83		4	5.171	4.882	-0.289	-5.597	1
203.78		4	12.962	12.984	0.022	0.167	1
226.66		4	26.062	25.042	-1.020	-3.915	1
259.55		4	57.985	56.628	-1.357	-2.340	1
286.83		4	102.732	101.893	-0.839	-0.817	1
264.28		4	65.018	63.050	-1.967	-3.026	1
289.78		4	110.316	108.167	-2.150	-1.949	1
226.55		4	25.511	24.939	-0.572	-2.242	1
232.22		4	24.614	28.574	3.959	16.086	1
260.00		4	52.883	56.895	4.012	7.587	1
287.78		4	117.211	104.241	-12.970	-11.065	1
315.55		4	174.437	176.151	1.713	0.982	1
343.33		4	272.343	282.377	10.034	3.684	1
371.11		4	427.475	432.592	5.117	1.197	1
398.89		4	655.002	637.450	-17.551	-2.680	1
426.66		4	958.371	909.121	-49.250	-5.139	1
482.22		4	1668.531	1714.131	45.600	2.733	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	4.19 %AARD FOR 17 POINTS

EXXON COAL LIQUID: NARROW-BOILING FRACTION U-1
VOLATILITY MEASUREMENTS
CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	158.000	747.00	593.19	534.00	6.564	0.42600
FITTED:						0.42286

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
214.33		4	48.884	48.157	-0.727	-1.487	1
244.50		4	99.285	99.028	-0.256	-0.258	1
271.66		4	173.748	174.503	0.755	0.435	1
300.61		4	298.543	297.692	-0.851	-0.285	1
333.22		4	515.038	506.699	-8.339	-1.619	1
313.66		4	380.591	371.459	-9.132	-2.399	1
300.83		4	299.232	298.828	-0.404	-0.135	1
270.89		4	172.369	171.904	-0.465	-0.270	1
247.55		4	104.800	105.864	1.063	1.015	1
260.00		4	131.000	137.688	6.687	5.105	1
287.78		4	241.316	236.955	-4.361	-1.807	1
315.55		4	386.106	383.002	-3.104	-0.804	1
343.33		4	586.054	589.673	3.619	0.617	1
371.11		4	868.739	872.745	4.005	0.461	1
398.89		4	1261.741	1250.753	-10.988	-0.871	1
426.66		4	1703.005	1745.732	42.727	2.509	1
454.44		4	2420.060	2375.224	-44.836	-1.853	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	1.29 %AARD FOR 17 POINTS

EXXON COAL LIQUID: NARROW-BOILING FRACTION U-2
VOLATILITY MEASUREMENTS
CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. WILSON ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	225.000	874.00	694.04	766.00	7.402	0.42800
FITTED:						0.42735

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
219.11		4	5.309	4.849	-0.460	-8.660	1
239.61		4	9.584	9.028	-0.556	-5.800	1
268.33		4	20.133	19.568	-0.564	-2.803	1
293.66		4	35.991	35.723	-0.268	-0.744	1
319.44		4	62.949	61.814	-1.135	-1.804	1
343.33		4	99.974	97.675	-2.299	-2.300	1
315.89		4	58.468	57.515	-0.953	-1.629	1
288.55		4	32.061	31.806	-0.255	-0.795	1
260.00		4	16.065	15.784	-0.281	-1.750	1
239.55		4	9.446	9.006	-0.440	-4.660	1
287.78		4	25.511	30.812	5.301	20.780	1
315.55		4	47.574	56.552	8.978	18.873	1
343.33		4	97.216	97.589	0.373	0.384	1
371.11		4	158.579	157.805	-0.774	-0.488	1
398.89		4	262.001	243.714	-18.286	-6.979	1
426.66		4	372.317	360.999	-11.318	-3.040	1
454.44		4	579.160	518.113	-61.047	-10.541	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
4	VAPOR PRESSURE	KPA	5.41 %AARD FOR 17 POINTS

EXXON COAL LIQUID IHS FROM ILLINOIS NO. 6 COAL

CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. HWANG ET AL 1980
NOTES: 2 ROGUES ELIMINATED

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	179.000	762.06	605.15	608.05	6.854	0.49476
FITTED:		772.75	613.64	608.56	6.856	0.45086

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
271.11		4	101.325	100.487	-0.838	-0.827	1
23.89	689.476	1	951.000	960.291	9.291	0.977	1
23.89	3447.378	1	952.000	961.371	9.371	0.984	1
23.89	6894.757	1	954.000	962.705	8.705	0.912	1
23.89	10342.135	1	955.000	964.022	9.022	0.945	1
23.89	13789.514	1	957.000	965.322	8.322	0.870	1
37.78	689.476	1	943.000	947.945	4.945	0.524	1
37.78	3447.378	1	943.000	949.130	6.130	0.650	1
37.78	6894.757	1	943.000	950.592	7.592	0.805	1
37.78	10342.135	1	945.000	952.033	7.033	0.744	1
37.78	13789.514	1	946.000	953.454	7.454	0.788	1
93.33	689.476	1	904.000	901.434	-2.566	-0.284	1
93.33	3447.378	1	905.000	903.125	-1.875	-0.207	1
93.33	6894.757	1	907.000	905.197	-1.803	-0.199	1
93.33	10342.135	1	910.000	907.224	-2.776	-0.305	1
93.33	13789.514	1	913.000	909.209	-3.791	-0.415	1
176.66	689.476	1	847.000	837.123	-9.877	-1.166	1
176.66	3447.378	1	846.000	339.936	-6.064	-0.717	1
176.66	6894.757	1	847.000	843.325	-3.675	-0.434	1
176.66	10342.135	1	850.000	846.584	-3.416	-0.402	1
176.66	13789.514	1	857.000	849.725	-7.275	-0.849	1
260.00	689.476	1	789.000	773.826	-15.174	-1.923	1
260.00	3447.378	1	792.000	778.613	-13.387	-1.690	1
260.00	6894.757	1	800.000	784.200	-15.800	-1.975	1
260.00	10342.135	1	805.000	789.411	-15.589	-1.936	1
260.00	13789.514	1	794.000	794.300	0.300	0.038	1
371.11	3447.378	1	683.000	686.934	3.934	0.576	1
371.11	6894.757	1	709.000	699.530	-9.470	-1.336	1
371.11	10342.135	1	720.000	710.158	-9.842	-1.367	1
371.11	13789.514	1	711.000	719.406	8.406	1.182	1
454.44	3447.378	1	573.000	582.562	9.562	1.669	1
454.44	6894.757	1	602.000	617.618	15.618	2.594	1
454.44	10342.135	1	620.000	639.684	19.684	3.175	1
454.44	13789.514	1	631.000	656.306	25.306	4.010	1
37.78	689.476	21	2.710	2.749	0.039	1.431	1
37.78	3447.378	21	2.810	2.786	-0.024	-0.858	1
37.78	6894.757	21	2.990	2.833	-0.157	-5.263	1

EXXON COAL LIQUID IHS FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
37.78	10342.135	21	3.360	2.880	-0.480	-14.291	1
37.78	13789.514	21	3.230	2.927	-0.303	-9.386	1
93.33	689.476	21	1.090	1.143	0.053	4.899	1
93.33	3447.378	21	1.110	1.162	0.052	4.722	1
93.33	6894.757	21	1.150	1.186	0.036	3.157	1
93.33	10342.135	21	1.190	1.210	0.020	1.708	1
93.33	13789.514	21	1.230	1.234	0.004	0.365	1
176.66	689.476	21	0.482	0.498	0.016	3.259	1
176.66	3447.378	21	0.499	0.509	0.010	2.000	1
176.66	6894.757	21	0.513	0.523	0.010	1.958	1
176.66	10342.135	21	0.534	0.537	0.003	0.579	1
176.66	13789.514	21	0.572	0.551	-0.021	-3.644	1
260.00	3447.378	21	0.279	0.292	0.013	4.579	1
260.00	6894.757	21	0.269	0.303	0.034	12.662	1
260.00	10342.135	21	0.316	0.314	-0.002	-0.576	1
260.00	13789.514	21	0.318	0.325	0.007	2.241	1
371.11	3447.378	21	0.180	0.159	-0.021	-11.698	1
371.11	6894.757	21	0.185	0.171	-0.014	-7.745	1
371.11	13789.514	21	0.204	0.192	-0.012	-6.027	1
454.44	6894.757	21	0.143	0.110	-0.033	-23.218	1
454.44	10342.135	21	0.179	0.123	-0.056	-31.390	1
454.44	13789.514	21	0.196	0.134	-0.062	-31.619	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.11 %AARD FOR 33 POINTS
4	VAPOR PRESSURE	KPA	0.83 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	7.57 %AARD FOR 25 POINTS

EXXON COAL LIQUID IHS FROM ILLINOIS NO. 6 COAL

CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: 1. HWANG ET AL 1980
NOTES: 2 ROGUES ELIMINATED
Characterization parameters determined by Therm-Trans analysis of inspection data.

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	179.000	764.06	606.73	606.20	6.847	0.49476

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
271.11		4	101.325	101.547	0.222	0.219	1
23.89	689.476	1	951.000	965.753	14.753	1.551	1
23.89	3447.378	1	952.000	966.813	14.813	1.556	1
23.89	6894.757	1	954.000	968.122	14.122	1.480	1
23.89	10342.135	1	955.000	969.414	14.414	1.509	1
23.89	13789.514	1	957.000	970.691	13.691	1.431	1
37.78	689.476	1	943.000	953.278	10.278	1.090	1
37.78	3447.378	1	943.000	954.441	11.441	1.213	1
37.78	6894.757	1	943.000	955.876	12.876	1.365	1
37.78	10342.135	1	945.000	957.291	12.291	1.301	1
37.78	13789.514	1	946.000	958.687	12.687	1.341	1
93.33	689.476	1	904.000	906.179	2.179	0.241	1
93.33	3447.378	1	905.000	907.842	2.842	0.314	1
93.33	6894.757	1	907.000	909.879	2.879	0.317	1
93.33	10342.135	1	910.000	911.873	1.873	0.206	1
93.33	13789.514	1	913.000	913.826	0.826	0.090	1
176.66	689.476	1	847.000	840.820	-6.180	-0.730	1
176.66	3447.378	1	846.000	843.601	-2.399	-0.284	1
176.66	6894.757	1	847.000	846.953	-0.047	-0.006	1
176.66	10342.135	1	850.000	850.178	0.178	0.021	1
176.66	13789.514	1	857.000	853.287	-3.713	-0.433	1
260.00	689.476	1	789.000	776.188	-12.812	-1.624	1
260.00	3447.378	1	792.000	780.972	-11.028	-1.392	1
260.00	6894.757	1	800.000	786.554	-13.446	-1.681	1
260.00	10342.135	1	805.000	791.762	-13.238	-1.645	1
260.00	13789.514	1	794.000	796.651	2.651	0.334	1
371.11	3447.378	1	683.000	686.313	3.313	0.485	1
371.11	6894.757	1	709.000	699.301	-9.699	-1.368	1
371.11	10342.135	1	720.000	710.194	-9.806	-1.362	1
371.11	13789.514	1	711.000	719.653	8.653	1.217	1
454.44	3447.378	1	573.000	572.980	-0.020	-0.003	1
454.44	6894.757	1	602.000	612.958	10.958	1.820	1
454.44	10342.135	1	620.000	636.675	16.675	2.689	1
454.44	13789.514	1	631.000	654.184	23.184	3.674	1
37.78	689.476	21	2.710	2.818	0.108	3.997	1
37.78	3447.378	21	2.810	2.856	0.046	1.628	1
37.78	6894.757	21	2.990	2.903	-0.087	-2.915	1

EXXON COAL LIQUID IHS FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
37.78	10342.135	21	3.360	2.950	-0.410	-12.196	1
37.78	13789.514	21	3.230	2.998	-0.232	-7.185	1
93.33	689.476	21	1.090	1.166	0.076	6.953	1
93.33	3447.378	21	1.110	1.185	0.075	6.757	1
93.33	6894.757	21	1.150	1.209	0.059	5.141	1
93.33	10342.135	21	1.190	1.233	0.043	3.646	1
93.33	13789.514	21	1.230	1.258	0.028	2.259	1
176.66	689.476	21	0.482	0.505	0.023	4.687	1
176.66	3447.378	21	0.499	0.516	0.017	3.409	1
176.66	6894.757	21	0.513	0.530	0.017	3.365	1
176.66	10342.135	21	0.534	0.545	0.011	1.968	1
176.66	13789.514	21	0.572	0.559	-0.013	-2.316	1
260.00	3447.378	21	0.279	0.294	0.015	5.446	1
260.00	6894.757	21	0.269	0.306	0.037	13.650	1
260.00	10342.135	21	0.316	0.317	0.001	0.331	1
260.00	13789.514	21	0.318	0.328	0.010	3.215	1
371.11	3447.378	21	0.180	0.158	-0.022	-12.213	1
371.11	6894.757	21	0.185	0.170	-0.015	-7.998	1
371.11	13789.514	21	0.204	0.192	-0.012	-5.900	1
454.44	6894.757	21	0.143	0.107	-0.036	-25.068	1
454.44	10342.135	21	0.179	0.121	-0.058	-32.439	1
454.44	13789.514	21	0.196	0.133	-0.063	-32.304	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.08 %AARD FOR 33 POINTS
4	VAPOR PRESSURE	KPA	0.22 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	8.28 %AARD FOR 25 POINTS

EXXON COAL LIQUID IA-3 FROM ILLINOIS NO. 6 COAL

CONST: ESIMATED USING METHODS OF BRULE' ET AL 1981
PROP.: 1. HWANG ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	167.000	760.09	603.58	535.16	6.568	0.36465
FITTED:						0.36629

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
246.11		4	101.325	100.430	-0.895	-0.884	1
44.16	2295.954	1	987.900	985.154	-2.746	-0.278	1
44.16	7011.968	1	990.800	987.450	-3.350	-0.338	1
44.16	13741.251	1	994.700	990.639	-4.061	-0.408	1
44.16	20477.428	1	998.500	993.737	-4.763	-0.477	1
90.44	2295.954	1	951.700	944.449	-7.251	-0.762	1
90.44	7011.968	1	955.000	947.531	-7.469	-0.782	1
90.44	13741.251	1	960.000	951.765	-8.235	-0.858	1
90.44	20477.428	1	964.700	955.830	-8.870	-0.919	1
151.05	2295.954	1	903.100	894.735	-8.365	-0.926	1
151.05	7011.968	1	907.900	899.179	-8.721	-0.961	1
151.05	13741.251	1	914.400	905.167	-9.233	-1.010	1
151.05	20477.428	1	920.500	910.801	-9.699	-1.054	1
206.28	2295.954	1	856.300	850.902	-5.398	-0.630	1
206.28	7011.968	1	863.000	857.093	-5.907	-0.684	1
206.28	13741.251	1	871.600	865.221	-6.379	-0.732	1
206.28	20477.428	1	879.500	872.677	-6.823	-0.776	1
256.39	2295.954	1	811.800	810.494	-1.306	-0.161	1
256.39	7011.968	1	820.600	818.984	-1.616	-0.197	1
256.39	13741.251	1	831.600	829.747	-1.853	-0.223	1
256.39	20477.428	1	841.800	839.320	-2.480	-0.295	1
313.22	2295.954	1	755.000	761.227	6.227	0.825	1
313.22	7011.968	1	768.600	773.919	5.319	0.692	1
313.22	13741.251	1	784.100	789.024	4.924	0.628	1
313.22	20477.428	1	797.700	801.795	4.095	0.513	1
368.16	7011.968	1	711.800	725.798	13.998	1.967	1
368.16	13741.251	1	734.800	747.657	12.857	1.750	1
368.16	20477.428	1	753.300	764.789	11.489	1.525	1
423.78	7011.968	1	636.400	667.541	31.141	4.893	1
423.78	13741.251	1	676.900	701.877	24.977	3.690	1
423.78	20477.428	1	704.700	725.546	20.846	2.958	1
176.66	1378.951	21	0.473	0.439	-0.035	-7.297	1
176.66	3447.378	21	0.495	0.446	-0.049	-9.841	1
176.66	13789.514	21	0.540	0.482	-0.059	-10.908	1
260.00	1378.951	21	0.282	0.257	-0.025	-8.766	1
260.00	3447.378	21	0.287	0.263	-0.024	-8.224	1
260.00	13789.514	21	0.324	0.293	-0.032	-9.755	1

EXXON COAL LIQUID IA-3 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
426.66	3447.378	21	0.103	0.102	-0.001	-0.779	1
426.66	6894.757	21	0.128	0.117	-0.012	-9.048	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.06 %AARD FOR 30 POINTS
4	VAPOR PRESSURE	KPA	0.88 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	8.08 %AARD FOR 8 POINTS

EXXON COAL LIQUID IA-3 FROM ILLINOIS NO. 6 COAL

CONST: ESIMATED USING METHODS OF BRULE' ET AL 1981
PROP.: 1. HWANG ET AL 1980
Characterization parameters determined by Therm-Trans analysis of inspection data.

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	167.000	760.60	603.99	530.67	6.550	0.36465

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
246.11		4	101.325	101.028	-0.297	-0.293	1
44.16	2295.954	1	987.900	993.459	5.559	0.563	1
44.16	7011.968	1	990.800	995.756	4.956	0.500	1
44.16	13741.251	1	994.700	998.946	4.246	0.427	1
44.16	20477.428	1	998.500	1002.046	3.546	0.355	1
90.44	2295.954	1	951.700	952.425	0.725	0.076	1
90.44	7011.968	1	955.000	955.508	0.508	0.053	1
90.44	13741.251	1	960.000	959.745	-0.255	-0.027	1
90.44	20477.428	1	964.700	963.813	-0.887	-0.092	1
151.05	2295.954	1	903.100	902.317	-0.783	-0.087	1
151.05	7011.968	1	907.900	906.762	-1.138	-0.125	1
151.05	13741.251	1	914.400	912.754	-1.646	-0.180	1
151.05	20477.428	1	920.500	918.393	-2.107	-0.229	1
206.28	2295.954	1	856.300	858.143	1.843	0.215	1
206.28	7011.968	1	863.000	864.335	1.335	0.155	1
206.28	13741.251	1	871.600	872.468	0.868	0.100	1
206.28	20477.428	1	879.500	879.933	0.433	0.049	1
256.39	2295.954	1	811.800	817.427	5.627	0.693	1
256.39	7011.968	1	820.600	825.916	5.316	0.648	1
256.39	13741.251	1	831.600	836.689	5.089	0.612	1
256.39	20477.428	1	841.800	846.277	4.477	0.532	1
313.22	2295.954	1	755.000	767.797	12.797	1.695	1
313.22	7011.968	1	768.600	780.486	11.886	1.546	1
313.22	13741.251	1	784.100	795.609	11.509	1.468	1
313.22	20477.428	1	797.700	808.409	10.709	1.342	1
368.16	7011.968	1	711.800	731.974	20.174	2.834	1
368.16	13741.251	1	734.800	753.873	19.073	2.596	1
368.16	20477.428	1	753.300	771.057	17.757	2.357	1
423.78	7011.968	1	636.400	673.269	36.869	5.793	1
423.78	13741.251	1	676.900	707.696	30.796	4.550	1
423.78	20477.428	1	704.700	731.456	26.756	3.797	1
176.66	1378.951	21	0.473	0.441	-0.032	-6.761	1
176.66	3447.378	21	0.495	0.449	-0.046	-9.333	1
176.66	13789.514	21	0.540	0.484	-0.057	-10.470	1
260.00	1378.951	21	0.282	0.259	-0.023	-8.208	1
260.00	3447.378	21	0.287	0.265	-0.022	-7.683	1
260.00	13789.514	21	0.324	0.294	-0.030	-9.312	1

EXXON COAL LIQUID IA-3 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
426.66	3447.378	21	0.103	0.103	-0.000	-0.076	1
426.66	6894.757	21	0.128	0.117	-0.011	-8.531	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.12 %AARD FOR 30 POINTS
4	VAPOR PRESSURE	KPA	0.29 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	7.55 %AARD FOR 8 POINTS

EXXON COAL LIQUID IA-6 FROM ILLINOIS NO. 6 COAL

CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: HWANG ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	172.000	754.92	599.48	583.40	6.760	0.46692
FITTED:						0.46107

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
260.00		4	101.325	102.775	1.450	1.431	1
22.05	2295.954	1	962.900	959.674	-3.226	-0.335	1
22.05	7011.968	1	965.800	961.513	-4.287	-0.444	1
22.05	13741.251	1	969.600	964.081	-5.519	-0.569	1
22.05	20477.428	1	973.600	966.589	-7.011	-0.720	1
46.16	2295.954	1	945.600	938.213	-7.387	-0.781	1
46.16	7011.968	1	948.600	940.372	-8.228	-0.867	1
46.16	13741.251	1	952.300	943.374	-8.926	-0.937	1
46.16	20477.428	1	956.500	946.291	-10.209	-1.067	1
107.33	2295.954	1	899.800	887.462	-12.338	-1.371	1
107.33	7011.968	1	904.000	890.638	-13.362	-1.478	1
107.33	13741.251	1	909.000	894.986	-14.014	-1.542	1
107.33	20477.428	1	914.200	899.145	-15.055	-1.647	1
159.61	2295.954	1	860.200	846.789	-13.411	-1.559	1
159.61	7011.968	1	865.400	851.146	-14.254	-1.647	1
159.61	13741.251	1	871.900	857.006	-14.894	-1.708	1
159.61	20477.428	1	878.600	862.508	-16.092	-1.831	1
201.72	2295.954	1	827.100	814.725	-12.375	-1.496	1
201.72	7011.968	1	833.400	820.353	-13.047	-1.565	1
201.72	13741.251	1	841.700	827.771	-13.929	-1.655	1
201.72	20477.428	1	849.600	834.604	-14.996	-1.765	1
261.94	2295.954	1	776.300	768.081	-8.219	-1.059	1
261.94	7011.968	1	785.400	776.356	-9.044	-1.152	1
261.94	13741.251	1	796.900	786.810	-10.090	-1.266	1
261.94	20477.428	1	807.100	796.079	-11.021	-1.365	1
312.61	2295.954	1	728.900	725.855	-3.045	-0.418	1
312.61	7011.968	1	742.200	737.787	-4.413	-0.595	1
312.61	13741.251	1	757.500	752.005	-5.495	-0.725	1
312.61	20477.428	1	771.000	764.040	-6.960	-0.903	1
368.22	2295.954	1	667.400	671.686	4.286	0.642	1
368.22	7011.968	1	689.300	691.300	2.000	0.290	1
368.22	13741.251	1	711.700	712.064	0.364	0.051	1
368.22	20477.428	1	729.900	728.318	-1.582	-0.217	1
428.05	2295.954	1	579.900	586.012	6.112	1.054	1
428.05	7011.968	1	616.900	630.986	14.086	2.283	1
428.05	13741.251	1	656.400	665.076	8.676	1.322	1
428.05	20477.428	1	682.300	688.165	5.865	0.860	1

EXXON COAL LIQUID IA-6 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
93.33	1378.951	21	1.028	1.046	0.018	1.743	1
93.33	3447.378	21	1.051	1.059	0.008	0.751	1
93.33	13789.514	21	1.183	1.125	-0.058	-4.879	1
260.00	13789.514	21	0.269	0.305	0.036	13.557	1
93.33	1378.951	21	1.045	1.046	0.001	0.118	1
93.33	3447.378	21	1.083	1.059	-0.024	-2.187	1
93.33	13789.514	21	1.206	1.125	-0.081	-6.693	1
176.66	2068.427	21	0.432	0.468	0.037	8.456	1
176.66	3447.378	21	0.435	0.474	0.038	8.733	1
176.66	13789.514	21	0.486	0.513	0.027	5.619	1
260.00	1378.951	21	0.247	0.266	0.019	7.728	1
260.00	3447.378	21	0.252	0.273	0.021	8.467	1
176.66	1378.951	21	0.424	0.466	0.041	9.771	1
176.66	3447.378	21	0.436	0.474	0.038	8.708	1
176.66	13789.514	21	0.487	0.513	0.027	5.489	1
260.00	1378.951	21	0.248	0.266	0.019	7.467	1
260.00	3447.378	21	0.254	0.273	0.020	7.697	1
260.00	13789.514	21	0.283	0.305	0.023	7.982	1
426.66	3447.378	21	0.084	0.101	0.018	20.968	1
426.66	13789.514	21	0.136	0.140	0.004	2.785	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.09 %AARD FOR 36 POINTS
4	VAPOR PRESSURE	KPA	1.43 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	6.99 %AARD FOR 20 POINTS

EXXON COAL LIQUID IA-6 FROM ILLINOIS NO. 6 COAL

CONST: ESTIMATED USING METHODS OF STARLING ET AL 1980
PROP.: HWANG ET AL 1980
Characterization parameters determined from Therm-Trans analysis of inspection data.

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	172.000	754.27	598.96	585.20	6.767	0.46692

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
260.00		4	101.325	101.906	0.581	0.574	1
22.05	2295.954	1	962.900	957.130	-5.770	-0.599	1
22.05	7011.968	1	965.800	958.960	-6.840	-0.708	1
22.05	13741.251	1	969.600	961.516	-8.084	-0.834	1
22.05	20477.428	1	973.600	964.013	-9.587	-0.985	1
46.16	2295.954	1	945.600	935.720	-9.880	-1.045	1
46.16	7011.968	1	948.600	937.869	-10.731	-1.131	1
46.16	13741.251	1	952.300	940.857	-11.443	-1.202	1
46.16	20477.428	1	956.500	943.761	-12.739	-1.332	1
107.33	2295.954	1	899.800	885.077	-14.723	-1.636	1
107.33	7011.968	1	904.000	888.238	-15.762	-1.744	1
107.33	13741.251	1	909.000	892.567	-16.433	-1.808	1
107.33	20477.428	1	914.200	896.707	-17.493	-1.913	1
159.61	2295.954	1	860.200	844.478	-15.722	-1.828	1
159.61	7011.968	1	865.400	848.818	-16.582	-1.916	1
159.61	13741.251	1	871.900	854.653	-17.247	-1.978	1
159.61	20477.428	1	878.600	860.132	-18.468	-2.102	1
201.72	2295.954	1	827.100	812.469	-14.631	-1.769	1
201.72	7011.968	1	833.400	818.076	-15.324	-1.839	1
201.72	13741.251	1	841.700	825.465	-16.235	-1.929	1
201.72	20477.428	1	849.600	832.270	-17.330	-2.040	1
261.94	2295.954	1	776.300	765.898	-10.402	-1.340	1
261.94	7011.968	1	785.400	774.146	-11.254	-1.433	1
261.94	13741.251	1	796.900	784.565	-12.335	-1.548	1
261.94	20477.428	1	807.100	793.803	-13.297	-1.647	1
312.61	2295.954	1	728.900	723.728	-5.172	-0.710	1
312.61	7011.968	1	742.200	735.631	-6.569	-0.885	1
312.61	13741.251	1	757.500	749.811	-7.689	-1.015	1
312.61	20477.428	1	771.000	761.811	-9.189	-1.192	1
368.22	2295.954	1	667.400	669.597	2.197	0.329	1
368.22	7011.968	1	689.300	689.196	-0.104	-0.015	1
368.22	13741.251	1	711.700	709.927	-1.773	-0.249	1
368.22	20477.428	1	729.900	726.146	-3.754	-0.514	1
428.05	2295.954	1	579.900	583.747	3.847	0.663	1
428.05	7011.968	1	616.900	628.936	12.036	1.951	1
428.05	13741.251	1	656.400	663.019	6.619	1.008	1
428.05	20477.428	1	682.300	686.074	3.774	0.553	1

EXXON COAL LIQUID IA-6 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
93.33	1378.951	21	1.028	1.050	0.022	2.104	1
93.33	3447.378	21	1.051	1.063	0.012	1.110	1
93.33	13789.514	21	1.183	1.129	-0.054	-4.540	1
260.00	13789.514	21	0.269	0.306	0.037	13.729	1
93.33	1378.951	21	1.045	1.050	0.005	0.472	1
93.33	3447.378	21	1.083	1.063	-0.020	-1.841	1
93.33	13789.514	21	1.206	1.129	-0.077	-6.361	1
176.66	2068.427	21	0.432	0.469	0.037	8.682	1
176.66	3447.378	21	0.435	0.475	0.039	8.961	1
176.66	13789.514	21	0.486	0.514	0.028	5.859	1
260.00	1378.951	21	0.247	0.267	0.019	7.837	1
260.00	3447.378	21	0.252	0.273	0.022	8.585	1
176.66	1378.951	21	0.424	0.467	0.042	9.999	1
176.66	3447.378	21	0.436	0.475	0.039	8.936	1
176.66	13789.514	21	0.487	0.514	0.028	5.728	1
260.00	1378.951	21	0.248	0.267	0.019	7.576	1
260.00	3447.378	21	0.254	0.273	0.020	7.814	1
260.00	13789.514	21	0.283	0.306	0.023	8.139	1
426.66	3447.378	21	0.084	0.101	0.017	20.713	1
426.66	13789.514	21	0.136	0.140	0.004	2.776	1

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.26 %AARD FOR 36 POINTS
4	VAPOR PRESSURE	KPA	0.57 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	7.09 %AARD FOR 20 POINTS

EXXON COAL LIQUID IA-10 FROM ILLINOIS NC. 6 COAL

CONST: ESTIMATED USING METHODS OF BRULE' ET AL 1981
PROP.: 1. HWANG ET AL 1980

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	164.000	733.25	582.27	556.67	6.655	0.46306
FITTED:		738.31	586.29	565.50	6.690	0.43177

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
243.89		4	101.325	101.721	0.396	0.391	1
42.50	2295.954	1	919.700	916.779	-2.921	-0.318	1
42.50	7011.968	1	922.800	919.012	-3.788	-0.410	1
42.50	13741.251	1	926.700	922.112	-4.588	-0.495	1
42.50	20477.428	1	930.800	925.119	-5.681	-0.610	1
102.61	2295.954	1	874.600	867.021	-7.579	-0.867	1
102.61	7011.968	1	878.900	870.307	-8.593	-0.978	1
102.61	13741.251	1	883.900	874.795	-9.105	-1.030	1
102.61	20477.428	1	889.300	879.077	-10.223	-1.150	1
171.72	2295.954	1	821.000	813.526	-7.474	-0.910	1
171.72	7011.968	1	826.500	818.560	-7.940	-0.961	1
171.72	13741.251	1	834.600	825.250	-9.350	-1.120	1
171.72	20477.428	1	841.700	831.459	-10.241	-1.217	1
206.50	2295.954	1	792.500	786.957	-5.543	-0.699	1
206.50	7011.968	1	799.900	793.219	-6.681	-0.835	1
206.50	13741.251	1	808.800	801.376	-7.424	-0.918	1
206.50	20477.428	1	817.400	808.809	-8.591	-1.051	1
264.61	2295.954	1	736.800	741.142	4.342	0.589	1
264.61	7011.968	1	752.600	750.384	-2.216	-0.294	1
264.61	13741.251	1	765.100	761.856	-3.244	-0.424	1
264.61	20477.428	1	776.200	771.880	-4.320	-0.557	1
314.44	2295.954	1	693.200	697.950	4.750	0.685	1
314.44	7011.968	1	708.800	711.542	2.742	0.387	1
314.44	13741.251	1	725.600	727.276	1.676	0.231	1
314.44	20477.428	1	740.100	740.316	0.216	0.029	1
373.05	2295.954	1	621.600	635.482	13.882	2.233	1
373.05	7011.968	1	647.800	660.054	12.254	1.892	1
373.05	13741.251	1	676.500	684.161	7.661	1.133	1
373.05	20477.428	1	696.100	702.264	6.164	0.886	1
429.16	2295.954	1	540.800	529.980	-10.820	-2.001	1
429.16	7011.968	1	578.300	598.210	19.910	3.443	1
429.16	13741.251	1	622.300	638.358	16.058	2.580	1
429.16	20477.428	1	651.400	663.877	12.477	1.915	1
93.33	1378.951	21	0.847	0.889	0.042	5.006	1
93.33	3447.378	21	0.872	0.901	0.028	3.253	1
93.33	13789.514	21	1.000	0.959	-0.041	-4.131	1
176.66	1378.951	21	0.382	0.410	0.027	7.114	1

EXXON COAL LIQUID IA-10 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
176.66	3447.378	21	0.397	0.417	0.020	5.117	1
176.66	13789.514	21	0.438	0.454	0.015	3.524	1
176.66	1378.951	21	0.369	0.410	0.041	11.032	1
176.66	2068.427	21	0.375	0.412	0.037	9.738	1
176.66	13789.514	21	0.419	0.454	0.034	8.187	1
176.66	1378.951	21	0.429	0.410	-0.019	-4.541	1
176.66	1378.951	21	0.391	0.410	0.018	4.705	1
176.66	3447.378	21	0.409	0.417	0.008	2.056	1
176.66	13789.514	21	0.454	0.454	-0.001	-0.164	1
260.00	1378.951	21	0.215	0.237	0.023	10.623	1
260.00	1378.951	21	0.236	0.237	0.002	0.808	1
260.00	3447.378	21	0.240	0.244	0.004	1.515	1
260.00	13789.514	21	0.267	0.274	0.007	2.637	1
260.00	1378.951	21	0.244	0.237	-0.007	-2.744	1
260.00	3447.378	21	0.251	0.244	-0.007	-2.736	1
260.00	13789.514	21	0.286	0.274	-0.012	-4.099	1
176.66	1378.951	21	0.444	0.410	-0.034	-7.682	1
176.66	3447.378	21	0.434	0.417	-0.017	-4.004	1
176.66	13789.514	21	0.493	0.454	-0.039	-7.939	1
176.66	1378.951	21	0.432	0.410	-0.023	-5.226	1
176.66	1378.951	21	0.425	0.410	-0.015	-3.643	1
176.66	1378.951	21	0.425	0.410	-0.015	-3.530	1
176.66	3447.378	21	0.434	0.417	-0.017	-4.004	1
260.00	1378.951	21	0.238	0.237	-0.001	-0.251	1
260.00	3447.378	21	0.252	0.244	-0.009	-3.429	1
426.66	13789.514	21	0.127	0.126	-0.001	-0.488	1

EXXON COAL LIQUID IA-10 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.03 %AARD FOR 32 POINTS
4	VAPOR PRESSURE	KPA	0.39 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	4.46 %AARD FOR 30 POINTS

EXXON COAL LIQUID IA-10 FROM ILLINOIS NO. 6 COAL

CONST: ESTIMATED USING METHODS OF BRULE' ET AL 1981
PROP.: 1. HWANG ET AL 1980
Characterization parameters determined by Therm-Trans analysis of inspection data.

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	164.000	732.44	581.62	567.12	6.697	0.46306

TEMP C	PRES KPA	PROPERTY CODE	EXPM	CALC	AAD	%AARD	REF
243.89		4	101.325	101.582	0.257	0.254	1
42.50	2295.954	1	919.700	915.354	-4.346	-0.473	1
42.50	7011.968	1	922.800	917.556	-5.244	-0.568	1
42.50	13741.251	1	926.700	920.612	-6.088	-0.657	1
42.50	20477.428	1	930.800	923.578	-7.222	-0.776	1
102.61	2295.954	1	874.600	865.379	-9.221	-1.054	1
102.61	7011.968	1	878.900	868.624	-10.276	-1.169	1
102.61	13741.251	1	883.900	873.058	-10.842	-1.227	1
102.61	20477.428	1	889.300	877.291	-12.009	-1.350	1
171.72	2295.954	1	821.000	811.517	-9.483	-1.155	1
171.72	7011.968	1	826.500	816.509	-9.991	-1.209	1
171.72	13741.251	1	834.600	823.144	-11.456	-1.373	1
171.72	20477.428	1	841.700	829.305	-12.395	-1.473	1
206.50	2295.954	1	792.500	784.710	-7.790	-0.983	1
206.50	7011.968	1	799.900	790.937	-8.963	-1.120	1
206.50	13741.251	1	808.800	799.051	-9.749	-1.205	1
206.50	20477.428	1	817.400	806.444	-10.956	-1.340	1
264.61	2295.954	1	736.800	738.367	1.567	0.213	1
264.61	7011.968	1	752.600	747.624	-4.976	-0.661	1
264.61	13741.251	1	765.100	759.102	-5.998	-0.784	1
264.61	20477.428	1	776.200	769.123	-7.077	-0.912	1
314.44	2295.954	1	693.200	694.458	1.258	0.181	1
314.44	7011.968	1	708.800	708.211	-0.589	-0.083	1
314.44	13741.251	1	725.600	724.067	-1.533	-0.211	1
314.44	20477.428	1	740.100	737.173	-2.927	-0.395	1
373.05	2295.954	1	621.600	630.150	8.550	1.375	1
373.05	7011.968	1	647.800	655.640	7.840	1.210	1
373.05	13741.251	1	676.500	680.252	3.752	0.555	1
373.05	20477.428	1	696.100	698.591	2.491	0.358	1
429.16	2295.954	1	540.800	511.123	-29.677	-5.488	1
429.16	7011.968	1	578.300	591.658	13.358	2.310	1
429.16	13741.251	1	622.300	633.519	11.219	1.803	1
429.16	20477.428	1	651.400	659.606	8.206	1.260	1
93.33	1378.951	21	0.847	0.900	0.053	6.254	1
93.33	3447.378	21	0.872	0.911	0.039	4.481	1
93.33	13789.514	21	1.000	0.970	-0.030	-2.990	1
176.66	1378.951	21	0.382	0.412	0.030	7.818	1

EXXON COAL LIQUID IA-10 FROM ILLINOIS NO. 6 COAL

(CONTINUED)

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
176.66	3447.378	21	0.397	0.420	0.023	5.821	1
176.66	13789.514	21	0.438	0.457	0.019	4.285	1
176.66	1378.951	21	0.369	0.412	0.043	11.763	1
176.66	2068.427	21	0.375	0.415	0.039	10.465	1
176.66	13789.514	21	0.419	0.457	0.038	8.985	1
176.66	1378.951	21	0.429	0.412	-0.017	-3.916	1
176.66	1378.951	21	0.391	0.412	0.021	5.392	1
176.66	3447.378	21	0.409	0.420	0.011	2.739	1
176.66	13789.514	21	0.454	0.457	0.003	0.567	1
260.00	1378.951	21	0.215	0.238	0.023	10.724	1
260.00	1378.951	21	0.236	0.238	0.002	0.897	1
260.00	3447.378	21	0.240	0.244	0.004	1.654	1
260.00	13789.514	21	0.267	0.275	0.008	2.977	1
260.00	1378.951	21	0.244	0.238	-0.006	-2.657	1
260.00	3447.378	21	0.251	0.244	-0.007	-2.604	1
260.00	13789.514	21	0.286	0.275	-0.011	-3.787	1
176.66	1378.951	21	0.444	0.412	-0.031	-7.078	1
176.66	3447.378	21	0.434	0.420	-0.015	-3.363	1
176.66	13789.514	21	0.493	0.457	-0.036	-7.270	1
176.66	1378.951	21	0.432	0.412	-0.020	-4.605	1
176.66	1378.951	21	0.425	0.412	-0.013	-3.012	1
176.66	1378.951	21	0.425	0.412	-0.012	-2.898	1
176.66	3447.378	21	0.434	0.420	-0.015	-3.363	1
260.00	1378.951	21	0.238	0.238	-0.000	-0.162	1
260.00	3447.378	21	0.252	0.244	-0.008	-3.298	1
426.66	13789.514	21	0.127	0.125	-0.002	-1.477	1

EXXON COAL LIQUID IA-10 FROM ILLINOIS NC. 6 COAL

(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.09 %AARD FOR 32 POINTS
4	VAPOR PRESSURE	KPA	0.25 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	4.58 %AARD FOR 30 POINTS

EXXON COAL LIQUID WV-1 FROM WYOMING WYODAK COAL
1 ROGUE ELIMINATED
CONST: ESTIMATED USING THE METHOD OF STARLING ET AL 1980
PROP.: 1. HWANG ET AL 1980

	CHARACTERIZATION PARAMETERS				
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	192.000	779.52	619.01	651.19	7.012	0.45875
FITTED:		777.00	617.01	620.26	6.899	0.45284

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
275.55		4	101.325	101.617	0.292	0.288	1
21.39	1378.951	1	1008.200	1015.038	6.838	0.678	1
21.39	3447.378	1	1009.200	1015.875	6.675	0.661	1
21.39	6894.757	1	1010.800	1017.256	6.456	0.639	1
21.39	10342.135	1	1012.400	1018.619	6.219	0.614	1
21.39	13789.514	1	1014.000	1019.965	5.965	0.588	1
21.39	20684.271	1	1017.100	1022.609	5.509	0.542	1
93.33	1378.951	1	954.100	951.039	-3.061	-0.321	1
93.33	3447.378	1	955.700	952.369	-3.331	-0.349	1
93.33	6894.757	1	958.300	954.546	-3.754	-0.392	1
93.33	10342.135	1	960.800	956.676	-4.124	-0.429	1
93.33	13789.514	1	963.100	958.762	-4.338	-0.450	1
93.33	17236.892	1	967.700	960.806	-6.894	-0.712	1
232.22	1378.951	1	845.800	840.393	-5.407	-0.639	1
232.22	3447.378	1	849.200	843.493	-5.707	-0.672	1
232.22	6894.757	1	854.300	848.414	-5.886	-0.689	1
232.22	10342.135	1	859.100	853.065	-6.035	-0.702	1
232.22	13789.514	1	863.600	857.479	-6.121	-0.709	1
232.22	20684.271	1	871.800	865.702	-6.098	-0.699	1
315.55	1378.951	1	772.500	771.547	-0.953	-0.123	1
315.55	3447.378	1	777.900	777.084	-0.816	-0.105	1
315.55	6894.757	1	786.300	785.483	-0.817	-0.104	1
315.55	10342.135	1	793.900	793.057	-0.843	-0.106	1
315.55	13789.514	1	800.700	799.980	-0.720	-0.090	1
315.55	20684.271	1	812.100	812.320	0.220	0.027	1
371.11	1378.951	1	712.200	717.674	5.474	0.769	1
371.11	3447.378	1	720.900	726.817	5.917	0.821	1
93.33	1378.951	21	1.320	1.213	-0.107	-8.141	1
93.33	13789.514	21	1.390	1.304	-0.086	-6.177	1
232.22	1378.951	21	0.316	0.354	0.038	11.925	1
232.22	13789.514	21	0.354	0.398	0.044	12.437	1
371.11	13789.514	21	0.175	0.200	0.025	14.524	1

EXXON COAL LIQUID WV-1 FROM WYOMING WYODAK COAL
1 ROGUE ELIMINATED
(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	0.49 %AARD FOR 26 POINTS
4	VAPOR PRESSURE	KPA	0.29 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	10.64 %AARD FOR 5 POINTS

EXXON COAL LIQUID WV-1 FROM WYOMING WYODAK COAL
1 ROGUE ELIMINATED
CONST: ESTIMATED USING THE METHOD OF STARLING ET AL 1980
PROP.: 1. HWANG ET AL 1980
Characterization parameters estimated by Therm-Trans analysis of inspection data.

	CHARACTERIZATION PARAMETERS					
	MW	TC K	E/K K	VC CC/MOL	SIG ANG	GMA
INPUT :	192.000	774.12	614.72	630.34	6.937	0.45875

TEMP	PRES	PROPERTY					
C	KPA	CODE	EXPM	CALC	AAD	%AARD	REF
275.55		4	101.325	102.390	1.065	1.052	1
21.39	1378.951	1	1008.200	998.466	-9.734	-0.965	1
21.39	3447.378	1	1009.200	999.306	-9.894	-0.980	1
21.39	6894.757	1	1010.800	1000.692	-10.108	-1.000	1
21.39	10342.135	1	1012.400	1002.059	-10.341	-1.021	1
21.39	13789.514	1	1014.000	1003.410	-10.590	-1.044	1
21.39	20684.271	1	1017.100	1006.061	-11.039	-1.085	1
93.33	1378.951	1	954.100	935.367	-18.733	-1.963	1
93.33	3447.378	1	955.700	936.703	-18.997	-1.988	1
93.33	6894.757	1	958.300	938.889	-19.411	-2.026	1
93.33	10342.135	1	960.800	941.027	-19.773	-2.058	1
93.33	13789.514	1	963.100	943.119	-19.981	-2.075	1
93.33	17236.892	1	967.700	945.168	-22.532	-2.328	1
232.22	1378.951	1	845.800	826.115	-19.685	-2.327	1
232.22	3447.378	1	849.200	829.238	-19.962	-2.351	1
232.22	6894.757	1	854.300	834.191	-20.109	-2.354	1
232.22	10342.135	1	859.100	838.865	-20.235	-2.355	1
232.22	13789.514	1	863.600	843.296	-20.304	-2.351	1
232.22	20684.271	1	871.800	851.540	-20.260	-2.324	1
315.55	1378.951	1	772.500	757.935	-14.565	-1.885	1
315.55	3447.378	1	777.900	763.540	-14.360	-1.846	1
315.55	6894.757	1	786.300	772.017	-14.283	-1.816	1
315.55	10342.135	1	793.900	779.643	-14.257	-1.796	1
315.55	13789.514	1	800.700	786.599	-14.101	-1.761	1
315.55	20684.271	1	812.100	798.972	-13.128	-1.617	1
371.11	1378.951	1	712.200	704.351	-7.849	-1.102	1
371.11	3447.378	1	720.900	713.669	-7.231	-1.003	1
93.33	1378.951	21	1.320	1.189	-0.131	-9.911	1
93.33	13789.514	21	1.390	1.281	-0.109	-7.850	1
232.22	1378.951	21	0.316	0.348	0.032	9.981	1
232.22	13789.514	21	0.354	0.392	0.038	10.789	1
371.11	13789.514	21	0.175	0.198	0.023	12.948	1

EXXON COAL LIQUID WV-1 FROM WYOMING WYODAK COAL
1 ROGUE ELIMINATED
(CONTINUED)

SUMMARY

CODE	PROPERTY	UNITS	PREDICTION DEVIATIONS
1	LIQUID DENSITY	KG/M3	1.75 %AARD FOR 26 POINTS
4	VAPOR PRESSURE	KPA	1.05 %AARD FOR 1 POINTS
21	LIQUID VISCOSITY	CP	10.30 %AARD FOR 5 POINTS