EQUILIBRIUM GAS-PHASE COMPOSITIONS AND CARBON DEPOSITION BOUNDARIES IN THE CHO-INERT SYSTEM

by

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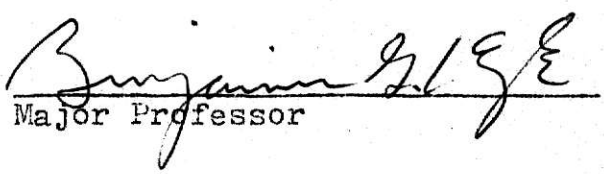

Major Professor

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CHAPTER I

INTRODUCTION

1.1 FIELDS OF APPLICATION

Chemically reacting systems comprised of the elements carbon, hydrogen, oxygen, and nitrogen are encountered in many industrial processes. In some processes solid carbon is present and the gas phase may be comprised of some or all of the elements C, H, O, and N, and in some other processes it is important to determine whether or not solid carbon will be present. Therefore, in such processes we confront a heterogeneous CHON system at a wide range of temperatures and pressures. Under moderate conditions, nitrogen will be present as an inert component in the gas phase. For proper design of these industrial processes and analysis of experimental data, engineers require knowledge of the limits set by equilibrium, though equilibrium is seldom achieved. Some of the important process areas in which CHON system is encountered are gasification, combustion of carbonaceous fuels, waste conversion, fuel cells, hydrogen production, and chemical synthesis processes (3, 4).

1.2 LITERATURE REVIEW

Cairns and Tevebaugh (4) considered, the simpler, CHO system, at atmospheric pressure and for a wide range of temperatures from 298° K to 1500° K. They showed that the six species of prime importance (thermodynamically more stable) are solid C, H_2, CO, CH_4, H_2O, and CO_2. This system has three degrees of freedom and

therefore three intensive variables must be specified. They chose temperature, pressure, and the elemental ratio O/H of the system under consideration. For this system, they presented gas phase compositions in equilibrium with solid carbon for O/H ratios ranging from 0.026 to 4.5, and carbon deposition boundaries. The carbon deposition boundaries were presented on triangular coordinates in terms of atom percent of the elements in the gas phase and are very informative and easy to use for practical design calculations. They also presented log-log plots of equilibrium compositions against O/H ratio for several temperatures which illustrate the trends. The method of calculation employed by them was algebraic solution of nonlinear equilibrium constant and material balance equations.

After this present study was initiated, Baron et al. (3) published the results of their investigation of the basic gasification system consisting of water, hydrogen, and oxygen in the presence of excess solid carbon. Their results include equilibrium gas composition, gas heating value, reactor energy balance, and moles of product gas per mole of carbon reacted. The results are tabulated for temperatures ranging from 76.4° F to 2500° F, pressures ranging from 1 to 100 atmospheres, and for H/O ratios of 1, 2, and 3. They have also presented rectangular and semi-logarithmic plots of equilibrium compositions as functions of pressure, temperature and H/O ratio which are illustrative of trends. They have also considered equilibrium of a coal gasification system in which H_2O and a nitrogen-oxygen mixture are used. For this system, their results are included for N/O

ratios of gaseous reactant ranging from 0.25 to 3.76 for a specific case of overall O/H ratio of unity. Their method of calculation applies trial and error solution of equilibrium constant equations and material balance equations.

1.3 OBJECTIVES

Thus the CHON system has not been studied over the full range of values of the parameters. Carbon deposition boundaries are available only for atmospheric pressure and in the absence of nitrogen.

The objectives of this work have been:

(1) to derive and use the general technique of heterogeneous complex chemical equilibrium calculations based on free energy minimization, and

(2) to provide equilibrium compositions and carbon deposition boundaries for the CHON system, for a wide range of parameter values. For the results presented, temperatures range from 500 to 1500° K, pressures range from 1 to 25 atm., overall H/O elemental ratios range from 0.01 to 10, and overall N/O elemental ratios range from 0 to 20.

1.4 CARBON DEPOSITION BOUNDARIES

The purpose of the carbon deposition boundaries is to enable one to predict whether or not solid carbon will form in a given system, at equilibrium. The convenient and informative way to present these for the ternary CHO system is a set of triangular coordinates, first used by Cairns and Tevebaugh (4). For the

CHON system at the pressure, P, and temperature, T, the knowledge of ratios of C, H, O, and N in the system is sufficient to determine whether or not carbon will form from the given reactants. Since N_2 is considered to be present as an inert, its amount in the system can be used as a parameter, and the CHO triangular coordinates can be used also for the CHON system.

CHO triangular plots require inert-free percentages of the atoms of C, H, and O. To prepare a carbon deposition boundary, the gas-phase compositions in equilibrium with carbon should be converted to elemental percentages and plotted for various O/H ratios for a particular set of values of P, T, and η, N/O ratio. (The four variables namely P, T, O/H, and N/O are the degrees of freedom chosen for this system and shall be discussed in section 2-2.) The resulting plot is the carbon deposition boundary corresponding to P, T, and η. Above the carbon deposition boundary, solid carbon is present and below the boundary, solid carbon is absent. Carbon deposition boundaries shall be presented for various values of the parameters P, T, and η.

In order to utilize these boundaries, the inert-free C, H, and O atomic percentages of the total reactant mixture of the given CHON system should be plotted as a point on the triangular diagram of the corresponding P, T, and η. If this point is above the carbon deposition boundary, e.g., the point U in the Plate 1, then the system at equilibrium shall contain solid carbon and the gas phase of inert-free composition corresponding to the point V. The relative amounts of the solid carbon and the gas phase atoms are given by the lever arm rule. This is

valid because any point, such as U, can be considered a mixture of solid carbon and a gas-phase whose C, H, and O percentages are represented by the carbon deposition boundary. It should be remembered that the triangular CHO plots are prepared on the basis of atom percentages, hence the lever arm rule provides the ratio of numbers of atoms.

The following additional information can be obtained from such plots:

The effect of varying the hydrogen or oxygen content of any system containing carbon as in hydrogenation or oxidation can also be determined by the use of triangular CHO diagram. For example, if a hydrocarbon whose composition is given by the point HC in Plate 1 is oxidized, the overall composition of the reaction mixture moves from HC towards O, the exact coordinates depend upon the amount of oxygen (or air) added. At W, the system has solid carbon and gas phase of CHO composition given by X. The point Y represents the minimum amount of oxygen which must be added to the system so that solid carbon does not form at equilibrium. Position Z corresponds to state of complete oxidation or combustion when only CO_2 and H_2O are present, at equilibrium.

The triangular diagram may also be used to show those CHO composition regions where free oxygen, free hydrogen, and solid carbon are present as major species at equilibrium, as shown in the Plate 2. In the central region bounded by the above areas, the five most important gaseous species, H_2, CO, CH_4, H_2O, and CO_2, are present in varying amounts, and solid carbon

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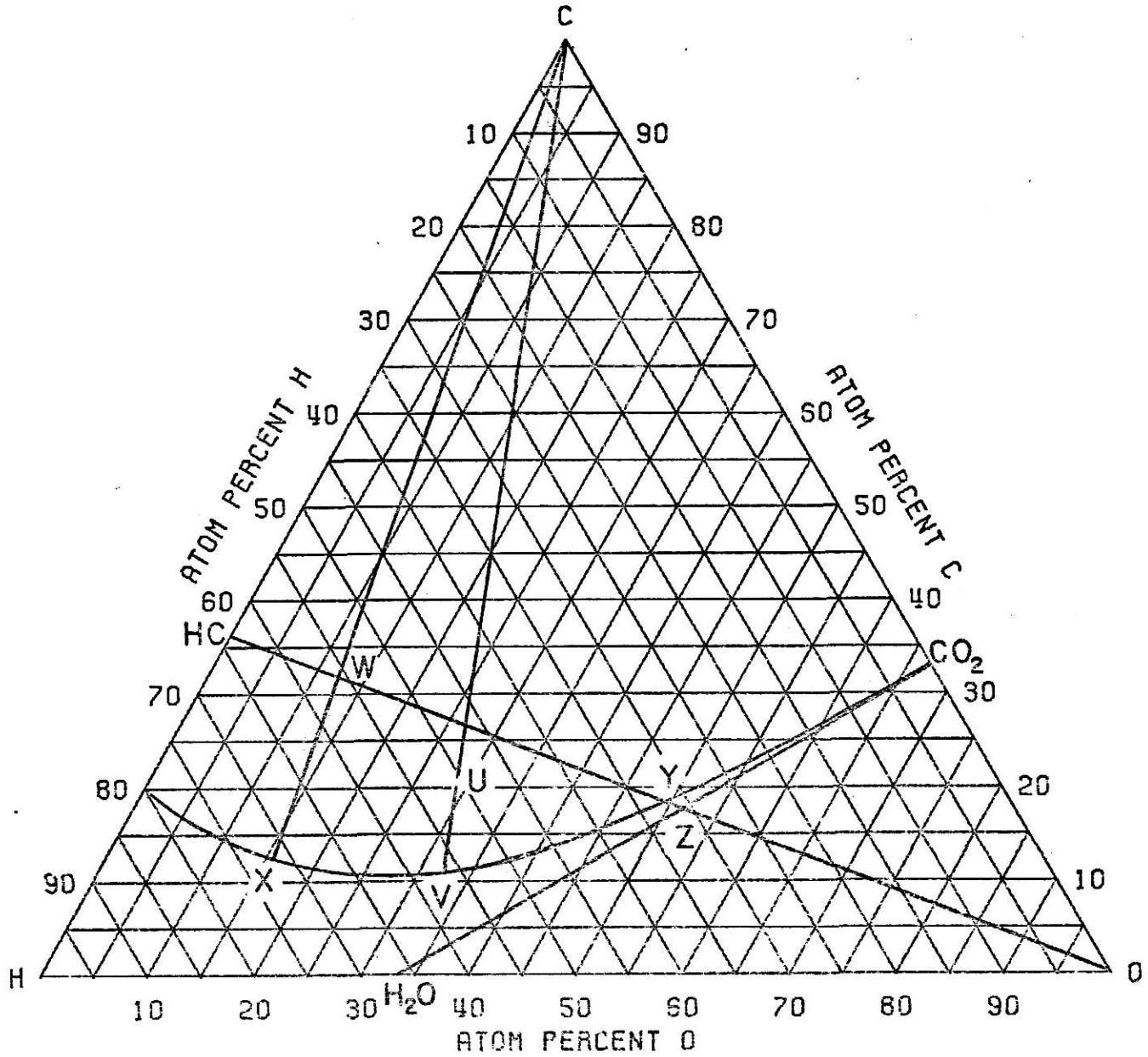

PLATE 1 . CARBON DEPOSITION BOUNDARY FOR THE CHON SYSTEM AT P,T,AND η .

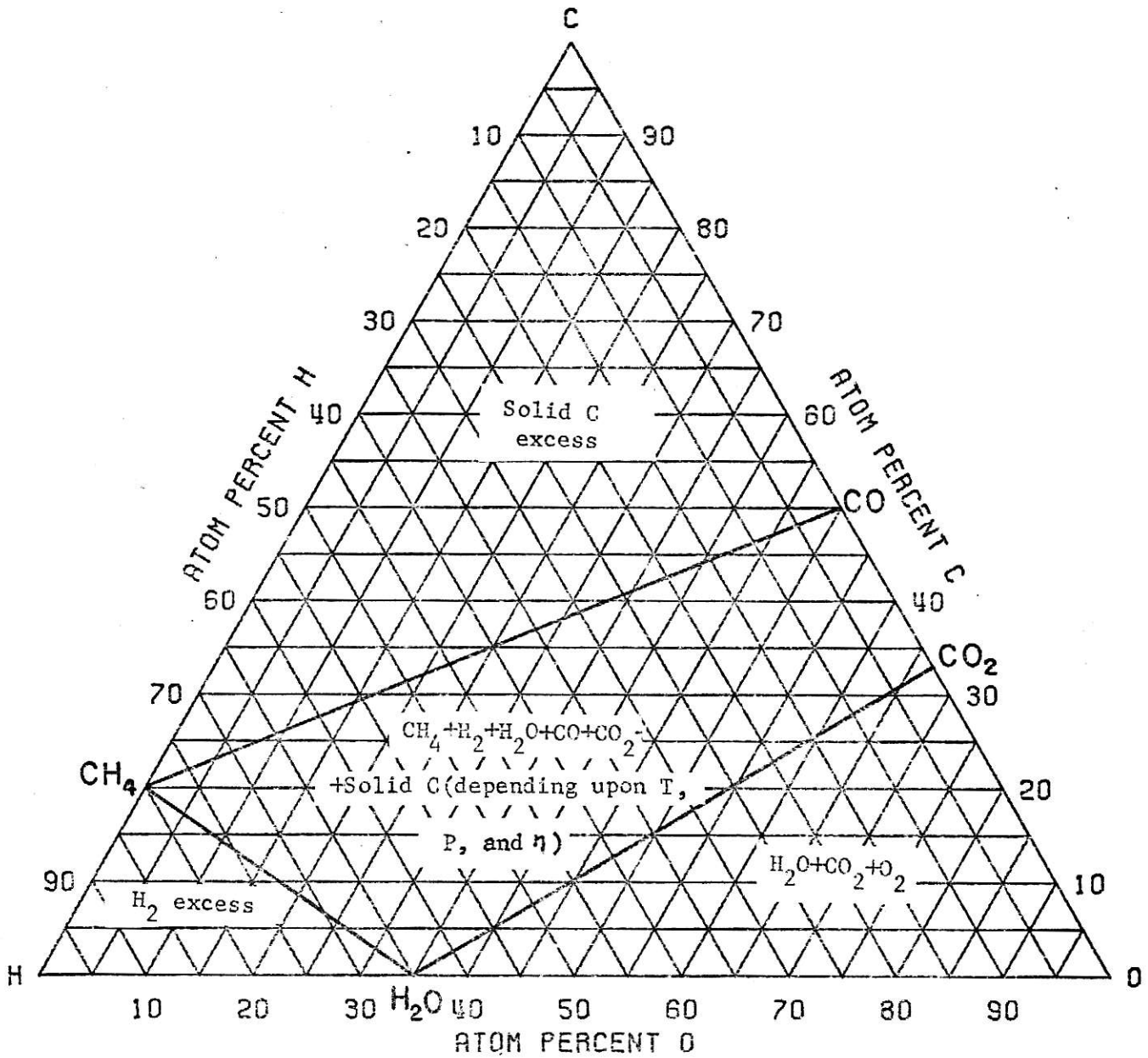

PLATE 2 . REGIONS OF THE CHO DIAGRAM

may or may not be present depending upon the location of the carbon deposition boundary. The zones are indicated in the plate. The central region is the most important and this work relates to that region.

CHAPTER II

THERMODYNAMIC CONSIDERATIONS

2.1 THE SYSTEM

This work is concerned with a system in which the feed is comprised of the elements Carbon, Hydrogen and Oxygen with Nitrogen, or any other inert gaseous species designated "I" ("I" may be composed of one or more elements). This system has been called CHON, or, in general CHOI. For this CHON system thermodynamic equilibrium shall be considered at the given conditions of temperature and pressure in the presence of excess solid carbon (assumed to be graphite). Approximate estimation of the relative abundance of various molecular species comprised of the elements C, H, O, and N at equilibrium can be obtained from the relative magnitudes of their equilibrium constants of formation. By consideration of these data, which indicate the relative importance of more stable species, Cairns and Tevebaugh have shown that only solid C and the gas phase consisting of H_2, CO, CH_4, H_2O, and CO_2 need to be considered for the CHO system. For the CHON system, the gas phase contains the additional inert species, N_2. The other species, e.g. O_2, Nitrogen compounds, and hydrocarbons of higher molecular weight are less abundant by about 5 to 6 significant figures at atmospheric pressure for a full range of temperatures. Higher pressures favor higher molecular weight hydrocarbons when the hydrogen partial pressure is high which occurs at high temperatures. Even then, their relative concentration is low enough so as not to warrant the need for

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their inclusion in equilibrium calculation, as shown in Chapter V. On this basis, only seven species were deemed to be important, namely, C (solid), N_2, H_2, CO, CH_4, H_2O, and CO_2; they are numbered 1 through 7 respectively.

2.2 PHASE RULE

The phase rule provides the information regarding the number of intensive variables (called variance or degrees of freedom) that need to be specified in order to find or fix the values of intensive state properties of the individual phases in equilibrium. The degrees of freedom, F, of a non-reactive system of P phases involving C components is given by Gibbs phase rule, Denbigh (10):

$$F = C + 2 - P$$

For a reactive system involving N total chemical species and having R independent reactions, the number of components, in the sense of phase rule, C, is given by:

$$C = N - R - S$$

where S is the number of additional restrictions (10). C can also be termed as the number of independent components of a reactive system and it is equal to the rank of the formula matrix of the system (1).

For the CHON system S=0, P=2, N=7, and C is found to be four from the following formula matrix $[a_{ji}]$:

Element		Formula	C	N_2	H_2	CO	CH_4	H_2O	CO_2
Subscripts j		i	1	2	3	4	5	6	7
C	1		1	0	0	1	1	0	1
H	2		0	0	2	0	4	2	0
O	3		0	0	0	1	0	1	2
N	4		0	2	0	0	0	0	0

The rank of this matrix is four, therefore C=4, R=3 and by the phase rule F=4. The CHO system, as considered by Cairns and Tevebaugh (4), possesses three degrees of freedom. They selected temperature, pressure, and overall elemental ratio O/H as variables to be specified. For the CHON system, for the additional degree of freedom, the elemental ratio N/O of the system was selected. The four degrees of freedom are designated by T (^{o}K), P (ATM), ω (O/H), and η (N/O). Therefore, at a given temperature and pressure, the gas-phase compositions of a CHON system containing solid carbon will be determined by the elemental ratios η and ω and will be independent of the chemical identity of the reactant materials.

2.3 PROBLEM AND METHODS OF SOLUTION

The problem here is to determine the gas-phase compositions of the CHON system under the given values of all the four degrees of freedom.

The two standard methods of calculation of chemical equilibria are:

(1) solution of equilibrium constant and material balance

equations, by reducing them to a single polynomial equation as used by Cairns and Tevebaugh (4) or by a trial and error method without reducing to a single polynomial, as used by Baron et al. (3);

(2) Minimization of free energy of the system. This method is very general and can be applied to homogeneous as well as to heterogeneous complex chemical equilibrium problems. The free energy of the system needs to be minimized with material balance constraints. White, Johnson, and Dantzig (11) have explained this method for a homogeneous gas phase equilibrium problem.

In this work, the second method has been used to find the state of minimum free energy.

2.4 FREE ENERGY MINIMIZATION

The state of thermodynamic equilibrium of a system is one that has the minimum Gibbs free energy, G, which is a nonlinear function of mole fractions in a mixture. Thus, for the given input materials in the system, the problem of determining equilibrium state reduces to a nonlinear optimization problem with atomic balance (mass balance) constraints. The computational method of locating the state of minimum G is based on an iterative procedure which is generated by applying the method of steepest descent, first described by White, Johnson and Dantzig (11).

For the CHON system consisting of solid C, N_2, H_2, CO, CH_4, H_2O, and CO_2 at given values of the four degrees of freedom, let $n_1, n_2, \ldots, n_7$ be the mole numbers of the species respectively.

The total Gibbs Free energy of the system can be written as

$$G = \sum_{i=1}^{7} n_i \mu_i \qquad (2\text{-}1)$$

$$= n_1 \mu_1 + \sum_{i=2}^{7} n_i \left(\mu_i^{\circ} + R\,T \ln \hat{f}_i\right) \qquad (2\text{-}2)$$

where,

$$\mu_1 = \mu_1^{\circ} + v_s\,(P - 1) \qquad (2\text{-}3)$$

Even at very high pressures, the product $v_s\,(P\text{-}1)$ is negligibly small compared to other terms in the expression for G and can be neglected and thus the chemical potential of solid carbon may be regarded as constant. Secondly, if the gas mixture is assumed to be an ideal solution, i.e. where the Lewis and Randall Rule applies, the fugacity of a component in the mixture can be written as

$$\hat{f}_i = f_i y_i = f_i \frac{n_i}{n}\,; \quad 2 \le i \le 7 \qquad (2\text{-}4)$$

Thus,

$$g = \frac{G}{RT} = \frac{n_1 \mu_1^{\circ}}{RT} + \sum_{i=2}^{7} n_i \left(c_i + \ln \frac{n_i}{n}\right) \qquad (2\text{-}5)$$

where,

$$n = \sum_{i=2}^{7} n_i \qquad (2\text{-}6)$$

And,

$$c_i = \frac{\mu_i^{\circ}}{RT} + \ln f_i\,; \quad 2 \le i \le 7 \qquad (2\text{-}7)$$

For the CHON system, some simplification can be made in the

objective function. It can be shown (Appendix B) that the position of the minimum in G or g is unaffected by the choice of reference state for μ_i^o. However, it is convenient to choose the elements in their standard states at the temperature of the system as the reference state. Then, at moderate pressures

$$\mu_1 \doteq \mu_1^o = 0 \tag{2-8}$$

And,

$$\mu_i^o = \Delta G_{fi}^o = -RT \ln K_i^f \; ; \quad 2 \leq i \leq 7 \tag{2-9}$$

Therefore,

$$g = \sum_{i=2}^{7} n_i \left(c_i + \ln \frac{n_i}{n}\right) \tag{2-10}$$

where

$$c_i = -\ln K_i^f + \ln f_i \; ; \quad 2 \leq i \leq 7 \tag{2-11}$$

The concomitant mass balance constraints can be described as

$$\sum_{i=1}^{7} a_{ji} \, n_i = b_j \tag{2-12}$$

Where j=1, 2, 3, and 4 for the elements C, H, O, and N respectively. The symbol a_{ji} is the chemical formula coefficient of the jth element in the ith chemical specie. For the system under study the $[a_{ji}]$ matrix has been written in section 2-2. And, b_j is the total number of atoms of jth element, irrespective of the identity of the species in the input to the reactive system. The case of j=4, i.e. nitrogen, is trivial since nitrogen is not a part of the reactive system. The nitrogen atomic balance is simply $n_2 = \frac{b_4}{2}$ = constant. In terms of b_1, b_2, b_3, and n_2, the

values of the O/H ratio, ω , and the N/O ratio, η , are:

$$\omega = \frac{O}{H} = \frac{b_3}{b_2} \tag{2-13}$$

$$\eta = \frac{N}{O} = \frac{n_2}{b_3/2} = \frac{2n_2}{b_3} \tag{2-14}$$

If the inert species (i=2) is other than N_2, then the expression written above can be used to find η from a known mole number n_2 which is fixed. In fact, any number of such inert species can be handled in this manner by simply classifying all inerts as a single pseudo-element. If the inert specie involves one or more of the elements from C, H, and O, then b_1, b_2, and b_3 are not the total number of the atoms of the respective elements in the system, but are only those atoms which are commutable in the reactive system.

The objective function to be minimized can be modified by incorporating Lagragian multipliers, π_j's, with the mass balance constraints

$$F = g + \sum_{j=1}^{3} \pi_j \left(- \sum_{i=1}^{7} a_{ji}\, n_i + b_j \right) \tag{2-15}$$

or,

$$F = \sum_{i=2}^{7} n_i \left(-\ln K_i^f + \ln f_i + \ln \frac{n_i}{n} \right) + \sum_{j=1}^{3} \pi_j \left(- \sum_{i=1}^{7} a_{ji}\, n_i + b_j \right) \tag{2-15a}$$

The minimum in F is found by setting the partial derivatives of F with respect to the n_i's equal to zero. Since n_2 = constant, we get 6 implicit transcendental equations from the relations:

$$\frac{\partial F}{\partial n_i} = 0 \; ; \quad 1 \leq \underset{i \neq 2}{i} \leq 7 \qquad (2\text{-}16)$$

And, there are 3 linear equations from the mass balance constraints. Thus, 6 mole numbers and 3 Lagrangian multipliers, a total of 9 unknowns can be uniquely determined by the 9 available equations. If n is treated as an additional unknown, the relation $n = \sum_{i=2}^{7} n_i$ must be considered as the tenth equation. A set of implicit transcendental equations can not be solved easily. Therefore, a different technique is necessary for calculation. An iterative procedure based on the method of steepest descent (11) can be used with a digital computer. The physical constraints that all $n_i > 0$ must be borne in mind while calculating.

Although, the relation $\frac{\partial F}{\partial n_i} = 0$ can not be used directly to compute equilibrium mole numbers or concentrations, it can, however, be used to obtain a good estimate of mole number or mole fraction of trace gaseous species. The condition $\frac{\partial F}{\partial n_i} = 0$ provides,

$$0 = c_i + \ln \frac{n_i}{n} - \sum_{j=1}^{3} \pi_j \, a_{ji} \qquad (2\text{-}17)$$

Therefore, after n and π_j's have been found for a system comprised of the major species, the mole number of any trace specie i, is given by:

$$n_i = n \exp \left(\sum_{j=1}^{3} \pi_j \, a_{ji} - c_i \right)$$

2.5 RELATION BETWEEN CHO AND CHOI SYSTEMS

Under most of the usual conditions of temperature and pressure, the effect of non-ideality of gas mixture is found to be negligible (discussed in Chapter V). Thus we can replace f_i by P for all gaseous species. Then, the modified objective function F can be written as

$$F = \sum_{i=2}^{7} n_i \left(-\ln K_i^f + \ln P + \ln \frac{n_i}{n}\right) + \sum_{j=1}^{3} \pi_j \left(-\sum_{j=1}^{7} a_{ji}\, n_i + b_j\right) \tag{2-18}$$

Considering first carbon, i=1, the condition $\frac{\partial F}{\partial n_i}=0$ provides $\pi_1=0$ since

$$a_{ji} = 0 \quad \text{if} \quad j \neq 1 \,. \tag{2-19}$$

For $3 \leq i \leq 7$, the conditions $\frac{\partial F}{\partial n_i} = 0$ and $\pi_1 = 0$ provide,

$$-\ln K_i^f + \ln \frac{P}{n} + \ln n_i - \pi_2\, a_{2i} - \pi_3\, a_{3i} = 0 \tag{2-20}$$

Unknowns: n_1, n_3, n_4, n_5, n_6, n_7, n, π_2, π_3; total 9.
Equations: 5 from equation (2-20), 3 mass balances, 1 from equation (2-6); total 9.

Thus the system has a unique solution. The inspection of equation (2-20) suggests that the effects of the amount of inert and the pressure can be combined in the term P/n, even though, as required by the phase rule, the CHON system has four independent variables. Equation (2-20) and mass balance equations reveal that the mole numbers of the non-inerts are fixed, when values of b_j's, T and P/n are specified. Therefore, if N_o is the total

number of moles of the CHO system (n_2=0) at P_o, then the mole numbers, for all CHON systems at T, having the same atomic inputs b_1, b_2, and b_3, and having inert moles n_2 such that the total pressure P satisfies the relation,

$$\frac{P}{N_o + n_2} = \frac{P_o}{N_o} \qquad (2\text{-}21)$$

shall be the same for all species except the inert.

Although, this relation exists, by which the effects of the two variables can be combined, a quantitative relation between the total number of gas phase moles, n, and the moles of inert cannot be determined a priori, otherwise the degrees of freedom of the CHON system would be reduced by one. In other words, the equation (2-21) cannot be used to generate data for any arbitrarily chosen values of P and n although it may be useful, in predicting the behavior of the CHON system in a qualitative manner.

CHAPTER III

MATHEMATICAL AND COMPUTATIONAL ASPECTS

3.1 GENERAL

In this chapter a general derivation of the method of equilibrium calculations for a heterogeneous system consisting of solid and gas phases is provided, using the method of steepest descent. Then, the simplifications for the CHON system are made and the computational aspects are discussed.

3.2 GENERAL MATHEMATICAL DERIVATION

Here, a general derivation shall be given for the iterative procedure of locating the state of minimum G of a heterogeneous system in which there are s pure solid phases in equilibrium with (c-s) gaseous components (including one inert species), where c is total number of components and m is total number of reactive atomic species in the system. No component is assumed to exist in both the phases.

The subscripts used are: i=1 to s for solids and i=s+1 to c for gaseous components. Let the (s+1)th component be inert. Since, in general, each solid phase may be composed of more than one element let

$$d_i = \frac{\mu_i}{RT} \pm \frac{\mu_i^o}{RT} = -\ln K_i^f \; ; \quad 1 \leq i \leq s \qquad (3\text{-}1)$$

Similarly, for gas phase components, recalling (2-11),

$$c_i = \frac{\mu_i^o}{RT} + \ln f_i = -\ln K_i^f + \ln f_i \; ; \quad s+1 \leq i \leq c \qquad (2\text{-}11)$$

The Gibbs Free Energy expression (like equation 2-5) can be written as:

$$g = \frac{G}{RT} = \sum_{i=1}^{s} n_i d_i + \sum_{i=s+1}^{c} n_i \left(c_i + \ln \frac{n_i}{n}\right) \qquad (3\text{-}2)$$

where

$$n = \sum_{i=s+1}^{c} n_i \qquad (3\text{-}3)$$

and the corresponding mass-balance constraints are

$$\sum_{i=1}^{c} a_{ji} n_i = b_j \; ; \quad 1 \leq j \leq m \qquad (3\text{-}4)$$

$[a_{ji}]$ is an m by c formula matrix for the system. $n_{(s+1)}$ is fixed.

The superscript ν, number of iteration, applies to all terms which change every iteration, e.g., n_i, n, g, G, $(\frac{\partial g}{\partial n_i})$, $(\frac{\partial^2 g}{\partial n_i \partial n_l})$, Δ_i, Δ_l, etc. The Taylor series expansion of g about νth iteration can be written as:

$$g^{\nu+1} = g^{\nu} + \sum_{\substack{i=1 \\ i \neq s+1}}^{c} \Delta_i^{\nu} \left(\frac{\partial g}{\partial n_i}\right)^{\nu} + \frac{1}{2} \sum_{\substack{i=1 \\ i \neq s+1}}^{c} \sum_{\substack{l=1 \\ l \neq s+1}}^{c} \Delta_i^{\nu} \Delta_l^{\nu} \left(\frac{\partial^2 g}{\partial n_i \partial n_l}\right)^{\nu} \qquad (3\text{-}5)$$

where

$$\Delta_i^{\nu} = n_i^{\nu+1} - n_i^{\nu} \qquad (3\text{-}6)$$

Therefore, the total change

$$\Delta^{\nu} = n^{\nu+1} - n^{\nu} = \sum_{i=s+2}^{c} \Delta_i^{\nu} \qquad (3\text{-}7)$$

The partial derivatives can be derived from (3-2) remembering that c_i is a function of T and P and d_i is a function of T only. The superscript is removed temporarily for simplicity and generality of the expressions.

For $1 \leq i \leq s$,

$$\frac{\partial g}{\partial n_i} = 0 \tag{3-8}$$

And, therefore,

$$\frac{\partial^2 g}{\partial n_i \partial n_\ell} = 0 \tag{3-9}$$

For $s+2 < i < c$,

$$\frac{\partial g}{\partial n_i} = \frac{\partial}{\partial n_i} \left[\sum_{i=s+1}^{c} n_i \left(c_i + \ln \frac{n_i}{n} \right) \right]$$

$$= \frac{\partial}{\partial n_i} \left[\sum_{k=s+1}^{c} n_k \left(c_k + \ln \frac{n_k}{n} \right) \right]$$

$$= \frac{\partial}{\partial n_i} \left[\left(c_i n_i + n_i \ln n_i - n_i \ln n \right) \right.$$

$$\left. + \sum_{\substack{k=s+1 \\ k \neq i}}^{c} \left(c_k n_k + n_k \ln n_k - n_k \ln n \right) \right]$$

$$= c_i + \frac{n_i}{n_i} \cdot 1 + \ln n_i - \ln n - \frac{n_i}{n} + \sum_{\substack{k=s+1 \\ k \neq i}}^{c} n_k \left(-\frac{1}{n} \right)$$

$$= c_i + \ln \frac{n_i}{n} + 1 - \left(n_i + \sum_{\substack{j=s+1 \\ j \neq i}}^{c} n_j \right) / n$$

$$= c_i + \ln \frac{n_i}{n} = A_i \qquad (3\text{-}10)$$

Therefore,

$$\frac{\partial^2 g}{\partial n_i^2} = \frac{\partial A_i}{\partial n_i} = \frac{\partial}{\partial n_i} \left(\ell n \frac{n_i}{n} \right) = \frac{1}{n_i} - \frac{1}{n} \qquad (3\text{-}11)$$

$$\frac{\partial^2 g}{\partial n_i \partial n_\ell} = 0 \quad \text{for} \quad 1 \leq \ell \leq s \qquad (3\text{-}12)$$

and for $s+2 \leq 1 \leq c$

$$\frac{\partial^2 g}{\partial n_i \partial n_1} = \frac{\partial}{\partial n_1} (\ln n_i - \ln n) = - \frac{1}{n} \qquad (3\text{-}13)$$

Using these expressions of second partial derivatives, the last term in (3-5) becomes:

$$\sum_{\substack{i=1 \\ i \neq s+1}}^{c} \sum_{\substack{\ell=1 \\ \ell \neq s+1}}^{c} \Delta_i \Delta_1 \frac{\partial^2 g}{\partial n_i \partial n_1} = \sum_{s+2}^{c} \sum_{s+2}^{c} \Delta_i \Delta_1 \frac{\partial^2 g}{\partial n_i \partial n_1}$$

$$= \sum_{i=s+2}^{c} \Delta_i \left(\sum_{1=s+2}^{c} \Delta_1 \frac{\partial^2 g}{\partial n_i \partial n_1} \right)$$

$$= \sum_{i=s+2}^{c} \Delta_i \left[\Delta_i \left(\frac{1}{n_i} - \frac{1}{n} \right) + \sum_{\substack{1=s+2 \\ 1 \neq i}}^{c} \Delta_1 \left(- \frac{1}{n} \right) \right]$$

$$= \sum_{i=s+2}^{c} \left(\frac{\Delta_i^2}{n_i} - \frac{\Delta_i}{n} \sum_{1=s+2}^{c} \Delta_1 \right) \qquad (3\text{-}14)$$

But,

$$\sum_{l=s+2}^{c} \Delta_l^{\nu} = \sum_{l=s+2}^{c} n_i^{\nu+1} - \sum_{l=s+2}^{c} n_i^{\nu}$$

$$= n^{\nu+1} - n_{(s+1)} - n^{\nu} + n_{(s+1)}$$

$$= \Delta^{\nu} = \Delta \qquad (3\text{-}15)$$

Therefore, (3-14) becomes

$$= \sum_{i=s+2}^{c} \frac{\Delta_i^2}{n_i} - \frac{\Delta}{n} \sum_{i=s+2}^{c} \Delta_i$$

$$= \sum_{i=s+2}^{c} \frac{\Delta_i^2}{n_i} - \frac{\Delta^2}{n} \qquad (3\text{-}16)$$

Now, using equations (3-2), (3-8), (3-10), and (3-16), (3-5) changes to

$$g^{\nu+1} = \sum_{i=1}^{s} d_i n_i^{\nu} + \sum_{i=s+1}^{c} A_i^{\nu} n_i^{\nu} + \sum_{i=1}^{s} d_i \Delta_i^{\nu} +$$

$$\sum_{i=s+2}^{c} A_i^{\nu} \Delta_i^{\nu} + \frac{1}{2} \left[- \frac{(\Delta^{\nu})^2}{n^{\nu}} + \sum_{i=s+2}^{c} \frac{(\Delta_i^{\nu})^2}{n_i^{\nu}} \right] \qquad (3\text{-}17)$$

Introducing Lagrangian multipliers and including mass balance constraints in the objective function, (3-17) is modified to

$$F^{\nu+1} = g^{\nu+1} + \sum_{j=1}^{m} \pi_j \left(b_j - \sum_{i=1}^{c} a_{ji} n_i^{\nu+1} \right) \qquad (3\text{-}18)$$

To minimize $F^{\nu+1}$,

$$\frac{\partial F^{\nu+1}}{\partial n_i^{\nu+1}} = 0 \quad ; \quad 1 \leq i \leq c \quad (i \neq s+1) \tag{3-19}$$

Therefore, the following s relations hold for $1 \leq i \leq s$,

$$d_i - \sum_{j=1}^{m} \pi_j \, a_{ji} = 0 \tag{3-20}$$

and (c - s - 1) equations for the reactive gas phase components become, for

$$s+2 \leq i \leq c \quad ,$$

$$A_i^{\nu} + \left(\frac{n_i^{\nu+1}}{n_i^{\nu}} - \frac{n^{\nu+1}}{n^{\nu}} \right) + \sum_{j=1}^{m} \pi_j \, a_{ji} = 0 \tag{3-21}$$

Since atomic balance equations should be followed at all times, there are m equations, for $1 \leq j \leq m$

$$\sum_{i=1}^{c} a_{ji} \, n_i^{\nu+1} = b_j \tag{3-22}$$

and, also

$$n^{\nu+1} = n_{(s+1)} + \sum_{i=s+2}^{c} n_i^{\nu+1} \tag{3-23}$$

Thus, equations (3-20) to (3-23) provide s + (c - s - 1) + m + 1 = c + m, linear equations in (c+m) unknowns which are:

$n_i^{\nu+1}$ $\quad 1 \leq i \leq c \quad (i \neq s+1)$,

$n^{\nu+1}$, and

π_j $\quad 1 \leq j \leq m$

By further algebraic manipulation, the size of the system of linear equations required to be solved can be reduced, from (c+m) to (m+s+1). The (m+s+1) unknowns are:

$$n_i^{\nu+1} \qquad 1 \le i \le s \quad ,$$

$$n^{\nu+1} \quad , \text{ and}$$

$$\pi_j \qquad 1 \le j \le m$$

From (3-21), solving for $n_i^{\nu+1}$, for $s+2 \le i \le c$,

$$n_i^{\nu+1} = n_i^{\nu} \left(\frac{n^{\nu+1}}{n^{\nu}} + \sum_{j=1}^{m} \pi_j a_{ji} - A_i^{\nu} \right) \qquad (3\text{-}24)$$

summing these over all i, $s+2 \le i \le c$, and using relation (3-3) for iterations ν and $\nu+1$, we have

$$\left(n^{\nu+1} - n_{(s+1)} \right) = \left(n^{\nu} - n_{(s+1)} \right) \frac{n^{\nu+1}}{n^{\nu}}$$

$$+ \sum_{i=s+2}^{c} n_i^{\nu} \left(\sum_{j=1}^{m} \pi_j a_{ji} \right) - \sum_{i=s+2}^{c} B_i^{\nu} \qquad (3\text{-}25)$$

where

$$B_i = n_i A_i$$

$$= n_i \left(c_i + \ln \frac{n_i}{n} \right) \qquad (3\text{-}26)$$

multiplying (3-20) by n_i^{ν} and summing over all i, $1 \le i \le s$,

$$\sum_{i=1}^{s} n_i^{\nu} d_i = \sum_{i=1}^{s} n_i^{\nu} \left(\sum_{j=1}^{m} \pi_j a_{ji} \right) = \sum_{j=1}^{s} \pi_j \left(\sum_{i=1}^{s} a_{ji} n_i^{\nu} \right)$$

(3-27)

similarly interchanging the order of summation of 2nd term on right hand side of equation (3-25),

$$\sum_{i=s+2}^{c} n_i^{\nu} \left(\sum_{j=1}^{m} \pi_j a_{ji} \right) = \sum_{j}^{m} \pi_j \left(\sum_{i=s+2}^{c} a_{ji} n_i^{\nu} \right) \tag{3-28}$$

Since $i = s+1$ is the inert species, either $a_{j,(s+1)} = 0$ for all j, or, b_j excludes the fixed number of atoms of all m atomic species that appear in the inert. Thus, the mass balance constraints, for $1 \leq j \leq m$, can be written as:

$$b_j = \sum_{i=1}^{c} a_{ji} n_i = \sum_{i=1}^{s} a_{ji} n_i + \sum_{i=s+2}^{c} a_{ji} n_i \tag{3-29}$$

Addition of (3-25) and (3-27), and use of (3-28) and (3-29) provides:

$$n_{(s+1)} + \sum_{i=1}^{s} n_i^{\nu} d_i = n_{(s+1)} \frac{n^{\nu+1}}{n^{\nu}} + \sum_{j=1}^{m} \pi_j b_j - \sum_{i=s+2}^{c} B_i^{\nu} \tag{3-30}$$

Using (3-24) and remembering (3-29), (3-22) can be expanded for $1 \leq j \leq m$, as

$$\sum_{i=1}^{s} a_{ji} n_i^{\nu+1} + \sum_{i=s+2}^{c} a_{ji} \left(n_i^{\nu} \frac{n^{\nu+1}}{n^{\nu}} + n_i^{\nu} \sum_{l=1}^{m} \pi_l a_{li} - A_i^{\nu} n_i^{\mu} \right) = b_j \tag{3-31}$$

Using (3-26) and,

$$r_{jl} = \sum_{i=s+2}^{c} a_{ji} a_{li} n_i^{\nu} \tag{3-32}$$

(3-31) can be written as; for $1 \leq j \leq m$,

$$\sum_{i=1}^{s} a_{ji}\, n_i^{\nu+1} + n^{\nu+1} \left(\frac{1}{n^{\nu}} \sum_{i=s+2}^{c} a_{ji}\, n_i \right) + \sum_{l=1}^{m} r_{jl}\, \pi_l$$

$$= b_j + \sum_{i=s+2}^{c} a_{ji}\, B_i^{\nu} \qquad (3\text{-}33)$$

(3-20) and (3-30) can be rearranged to contain unknown terms on the left hand side:

$$\sum_{j=1}^{m} \pi_j\, b_j - \frac{n_{(s+1)}}{n^{\nu}}\, n^{\nu+1} = -n_{(s+1)} + \sum_{i=1}^{s} d_i\, n_i^{\nu} + \sum_{i=s+2}^{c} B_i^{\nu} \qquad (3\text{-}30a)$$

$$\sum_{j=1}^{m} \pi_j\, a_{ji} = d_i \qquad 1 \le i \le s \qquad (3\text{-}20a)$$

This forms the desired system of linear equations. The $(m + 1 + s)$ equations are (3-33), (3-30a) and (3-20a). Therefore, if the mole numbers of all the components of the system in the input to the system or the initial guesses (satisfying the mass balance constraints) are known, the values of π_j, $1 \le j \le m$; $n^{\nu+1}$; and $n_i^{\nu+1}$, $1 \le i \le s$ can be found from the $(m + s + 1)$ linear equations mentioned above. Then the use of (3-24) shall enable finding the values of new mole numbers in the gas-phase $n_i^{\nu+1}$, $s+2 \le i \le c$.

By this step, new mole numbers are obtained such that the total free energy of the system is reduced. Before, proceeding to next iteration, it is necessary to check to prevent the possibility of negative n_i's and to guarantee convergence of the iteration scheme. Let the computed changes in mole numbers, $\Delta_i = n_i^{\nu+1} - n_i^{\nu}$, be direction numbers which indicate the "best" direction of travel but not necessarily the "best" length of

travel. Rather the distance traveled should be restricted to some fraction λ of the calculated travel. The value of λ will be chosen as the largest value that satisfies the two conditions:

(1) All $n_i^{\nu+1}$ are positive, and

(2) The derivative $\frac{\partial g}{\partial \lambda}$ does not become positive, that is, the minimum is not passed.

The derivation for the expression of $\frac{\partial g}{\partial \lambda}$ is given below:

From the method of steepest descent, the Δ_i's and Δ are found, and thus n_i^{ν}, Δ_i, n^{ν}, and Δ shall be treated as constants during the process of obtaining the derivative $\frac{\partial g}{\partial \lambda}$. Starting with equation (3-2) for $\nu+1$ iteration, and expanding it in terms of ν-th iteration and λ, the following expression results:

$$g^{\nu+1} = \sum_{i=1}^{s} d_i\, n_i^{\nu+1} + \sum_{i=s+1}^{c} n_i^{\nu+1} \left(c_i + \ln \frac{n_i^{\nu+1}}{n^{\nu+1}} \right)$$

$$= \sum_{i=1}^{s} d_i\, (n_i^{\nu} + \lambda\, \Delta_i) + \sum_{i=s+2}^{c} \Big[n_i^{\nu} c_i + (n_i^{\nu} + \lambda\, \Delta_i) \ln \frac{n_i^{\nu} + \lambda\, \Delta_i}{n^{\nu} + \lambda\, \Delta} + \lambda\, \Delta_i\, c_i \Big] + n_{(s+1)} \left(c_{(s+1)} + \ln \frac{n_{(s+1)}}{n^{\nu} + \lambda\, \Delta} \right)$$

Differentiating with respect to λ, we have:

$$\frac{\partial g^{\nu+1}}{\partial \lambda} = \sum_{i=1}^{s} d_i\, \Delta_i + \sum_{i=s+2}^{c} \Big[\Delta_i \ln \frac{n_i^{\nu} + \lambda \Delta_i}{n^{\nu} + \lambda \Delta}$$

$$+ \left(n_i^{\nu} + \lambda \Delta_i \right) \frac{\partial}{\partial \lambda} \left(\ln \frac{n_i^{\nu} + \lambda \Delta_i}{n^{\nu} + \lambda \Delta} \right) + \Delta_i c_i \Big]$$

$$+ n_{(s+1)} \frac{\partial}{\partial \lambda} \left(\ln \frac{1}{n^{\nu} + \lambda \Delta} \right)$$

$$= \sum_{i=1}^{s} d_i \Delta_i + \sum_{i=s+2}^{c} \Delta_i \left(c_i + \ln \frac{n_i^{\nu} + \lambda \Delta_i}{n^{\nu} + \lambda \Delta} \right)$$

$$+ \sum_{i=s+2}^{c} \left(n_i^{\nu} + \lambda \Delta_i \right) \cdot \frac{\partial}{\partial \lambda} \left[\ln \left(n_i^{\nu} + \lambda \Delta_i \right) \right]$$

$$- \frac{\partial}{\partial \lambda} \left[\ln \left(n^{\nu} + \lambda \Delta \right) \right] \cdot \sum_{i=s+1}^{c} \left(n_i^{\nu} + \lambda \Delta_i \right) \qquad (3\text{-}34)$$

The last two terms in the above equation can be simplified to:

$$= \sum_{i=s+2}^{c} \frac{n_i^{\nu} + \lambda \Delta_i}{n_i^{\nu} + \lambda \Delta_i} \cdot \Delta_i - \frac{n^{\nu} + \lambda \Delta}{n^{\nu} + \lambda \Delta}$$

$$= \sum_{i=s+2}^{c} \Delta_i - \Delta = \Delta - \Delta = 0$$

Therefore:

$$\frac{\partial g}{\partial \lambda} = \sum_{i=1}^{s} d_i \Delta_i + \sum_{i=s+2}^{c} \Delta_i \left(c_i + \ln \frac{n_i^{\nu} + \lambda \Delta_i}{n^{\nu} + \lambda \Delta} \right) \qquad (3\text{-}35)$$

In the simplification of the expressions in the proof above, the following relations have been used:

$\Delta_{(s+1)} = 0$ and

$$\sum_{i=s+2}^{c} \Delta_i = \Delta = n^{\nu+1} - n^{\nu}$$

Thus, by meeting the conditions as explained before deriving the expression for $\frac{\partial g}{\partial \lambda}$, we can find λ, and thus $n_i^{\nu+1}$:

$$n_i^{\nu+1} = n_i^{\nu} + \lambda \Delta_i \qquad 1 \leq i \leq c \qquad (3\text{-}36)$$

The iteration will be repeated until the convergence is obtained, that is, e.g. the test of relative error is satisfied for all i:

$$\left| \frac{\lambda \Delta_i}{n_i^{\nu+1}} \right| < \delta \qquad 1 \leq i \leq c \qquad (3\text{-}37)$$

for a specified value of δ.

3.3 SIMPLIFICATIONS FOR THE CHON SYSTEM

The CHON system under study is a special case of the system considered for the preceding mathematical derivation. For the CHON system:

$$s = 1$$

$$c = 7$$

$$m = 3 \text{ (since N is not a reactive atomic species)}$$

$$d_1 = \frac{\mu_1^{\circ}}{RT} = 0 \qquad (3\text{-}38)$$

Therefore equation (3-20) yields:

$$\pi_1 = 0 \qquad (3\text{-}39)$$

Besides, equation (3-33), for j=1, can be directly used to find the value of $n_1^{\nu+1}$ explicitly, if π_2, π_3, and $n^{\nu+1}$ are known.

$$n_1^{\nu+1} = b_1 + \sum_{i=3}^{7} a_{1i} B_i^{\nu} - r_{12} \pi_2 - r_{23} \pi_3 - (b_1 - n_1^{\nu}) \frac{n^{\nu+1}}{n^{\nu}} \qquad (3\text{-}40)$$

Therefore, the size of system of linear equations reduces from $(s + m + 1) = 5$, as per general method, to 3 in this special case. The simplified form of the 3 equations in the three unknowns, π_2, π_3, and $n^{\nu+1}$, are written below:

for $j = 2$ *and* 3, *from* equation (3-33) -

$$r_{j2} \pi_2 + r_{j3} \pi_3 + \frac{b_j}{n^{\nu}} n^{\nu+1} = b_j + \sum_{i=3}^{7} a_{ji} B_i^{\nu} \qquad (3\text{-}41)$$

and, from (3-30a) -

$$b_2 \pi_2 + b_3 \pi_3 - \frac{n_2}{n^{\nu}} n^{\nu+1} = - n_2 + \sum_{i=3}^{7} B_i^{\nu} \qquad (3\text{-}42)$$

After obtaining π_2, π_3, and $n^{\nu+1}$ from these three equations, $n_1^{\nu+1}$ is found from (3-40) and $n_i^{\nu+1}$, $3 \leq i \leq 7$, are found from (3-24), rewritten below:

$$n_i^{\nu+1} = n_i^{\nu} \left(\frac{n^{\nu+1}}{n^{\nu}} + \sum_{j=2}^{3} \pi_j a_{ji} - A_i^{\nu} \right) \qquad (3\text{-}43)$$

The expression for $\frac{\partial g}{\partial \lambda}$, equation (3-35), used in the second condition to find the "best" length of travel during an iteration, gets simplified to:

$$\frac{\partial g}{\partial \lambda} = \sum_{i=3}^{7} \Delta_i \left(c_i + \ln \frac{n_i^{\nu} + \lambda \Delta_i}{n^{\nu} + \lambda \Delta} \right) \qquad (3\text{-}44)$$

3.4 COMPUTATIONAL ASPECTS

b_j and initial guess vectors

The execution of the iterative procedure, described in this chapter, to calculate the equilibrium state, requires the b_j vector and an initial guess of mole numbers of all species that are present in significant quantities, namely C, N_2, H_2, CO, CH_4, H_2O, and CO_2. We have to consider the following in choosing the values of b_j's and initial n_i's.

(a) Solid carbon must be present at equilibrium in the system. To make sure of this, the magnitude of b_1 should be large.

(b) Since the aim of this work is to generate a set of equilibrium data for the given values of the degrees of freedom, namely ω and η, the values of b_j's and n_2 must conform to the following:

$$\omega = \frac{O}{H} = \frac{b_3}{b_2} \tag{3-45}$$

Therefore, if b_3 is assumed, then b_2 is automatically found. Similarly, n_2 is easily found from b_3 and η:

$$\eta = \frac{N}{O} = \frac{2n_2}{b_3} \tag{3-46}$$

Thus b_1, b_2, b_3, and n_2 are fixed after assuming a reasonable value of b_3 (e.g., 50) and a large value of b_1 (e.g., 1×10^5).

(c) The initial guess for the other 6 components must satisfy the equations (2-12), which describe the conservation of the atomic species. Thus, there are 3 following relations for the 6 unknown mole numbers.

$$n_1 + n_4 + n_5 + n_7 = b_1$$

$$2n_3 + 4n_5 + 2n_6 = b_2 \qquad (3\text{-}47)$$

$$n_4 + n_6 + 2n_7 = b_3$$

Therefore, by assuming the guess for n_4, n_5, and n_6, the guess for the rest can be obtained, from (3-47),

$$n_7 = \frac{b_3 - n_4 - n_6}{2} \qquad (3\text{-}48)$$

$$n_3 = \frac{b_2 - 4n_5 - 2n_6}{2} \qquad (3\text{-}49)$$

$$n_1 = \frac{2b_1 - b_3 - n_4 - 2n_5 + n_6}{2} \qquad (3\text{-}50)$$

(d) The assumed guesses of n_4, n_5, and n_6 should be such that the calculated guesses n_3 or n_7 do not become zero or negative, for the complete range of values of ω, of interest.
As ω increases, b_2 decreases, therefore, if n_5 and n_6 are large, n_3 can become negative. Considering all these factors, the following values were assumed:

$$b_1 = 1 \times 10^5$$

$$b_3 = 50$$

$$n_4 = 0.1$$

If $\omega \leq 2$; $n_5 = n_6 = 0.1$

If $\omega > 2$; $n_5 = 0.004$ and $n_6 = 0.01$

These values do not create problems upto a value of ω about 1000.

Solution of Linear Algebraic Equations

For this purpose the standard library subprograms, e.g., SIMQ, LINEQ, etc. can be used. However due to the circumstances prevailing at the time this work was initiated, a subroutine had to be prepared to solve linear equations. This subroutine, called "DETSIM", is used all through the work and is very efficient.

Positive Mole Numbers And Negative $\partial g/\partial \lambda$

Condition 1: All mole numbers must be positive. After calculating new mole numbers if any mole number $n_i^{\nu+1}$ is negative, then λ must be less than unity. However, since the magnitude of λ should be as big as possible, the value of $n_i^{\nu+1}$ should be very small, close to zero (it can't be zero, since the i-th species is significant and the expressions are logarithmic.). If more than one species has negative mole numbers, then the limiting value of λ for condition 1, denoted by λ_1, is determined by the species, i, whose mole number is such that it gives the lowest value of λ. As limited by this condition, let $n_i^{\nu+1} = 1 \times 10^{-5} n_i^{\nu}$. Then,

$$\left(n_i^{\nu+1} \right)_1 = n_i^{\nu} + \lambda_1^{\nu} \Delta_i^{\nu} = 1 \times 10^{-5} n_i$$

Therefore,

$$\lambda_1^{\nu} = -0.99999 \frac{n_i^{\nu}}{\Delta_i^{\nu}} \qquad (3\text{-}51)$$

where $\Delta_i^{\nu} < 0$. Therefore, the limiting value is determined by the specie whose $\left| \frac{n_i^{\nu}}{\Delta_i^{\nu}} \right|$ is minimum along among all those species whose mole numbers were negative as calculated by the method.

Using this value of λ_1, mole numbers of all other species (including those, whose mole numbers were positive as calculated by the method) are calculated. It should be noted that any value of λ will satisfy the mass balance constraints, since if n_i^{ν}'s and $n_i^{\nu+1}$'s follow constraints separately, a linear combination of those $= n_i^{\nu} + \lambda (n_i^{\nu+1} - n_i^{\nu})$

$$= (1 - \lambda)\, n_i^{\nu} + \lambda\, n_i^{\nu+1}$$

will also follow those constraints.

Condition 2: Now, it is to be ensured that $\left(\frac{\partial g}{\partial \lambda} \right)_{\lambda=\lambda_1}$ is negative so that the iteration is converging towards a minimum. If not, λ is decreased by 10% and checked if $\left(\frac{\partial g}{\partial \lambda} \right)_{\lambda=0.9\lambda_1} < 0$. If not, it is decreased by another 10%; this is continued until $\left(\frac{\partial g}{\partial \lambda} \right)_{\lambda=\lambda_2<\lambda_1} < 0$. Therefore, λ_2 is the fraction of travel, suggested by the method of steepest descent, to meet both these conditions, and $\lambda_2 \leq \lambda_1$.

Thus, now the iteration is complete in terms of approaching the minimum with meaningful values of the mole numbers. The new mole numbers are calculated by

$$n_i^{\nu+1} = n_i^{\nu} + \lambda_2\, \Delta_i \qquad 1 \leq i \leq 7$$

Convergence

Once the new mole numbers are calculated, the convergence of the solution should be checked, i.e., the following should be satisfied:

$$\left| \frac{n_i^{\nu+1} - n_i^{\nu}}{n_i^{\nu+1}} \right| = \left| \frac{\lambda_2 \Delta_i^{\nu}}{n_i^{\nu+1}} \right| < \delta \quad \text{for } 1 \leq i \leq 7$$

$\delta = 1 \times 10^{-8}$ was assumed. If the condition is not satisfied, the iteration is repeated until convergence is obtained. A maximum limit of 125 iterations was specified.

Computer Program

The source program is provided in appendix "A" along with the subroutine "DETSIM", used to solve a set of linear equations, and "TRIANG", used to prepare the triangular graph for plotting carbon deposition boundaries.

Precision

When the program was run with single precision, convergence could not be achieved even in 100 iterations in some cases. The problem was remedied by the use of double precision when convergence was achieved in less than 15 iterations in almost all cases.

CHAPTER IV

RESULTS

The computer program developed to perform chemical equilibrium calculations for the CHON system was run for the following range of parameter values:

T : 500 to 1500° K

P : 1 to 25 atm.

η : 0 to 40

ω : 10^{-3} to 10^{3}

The equilibrium constants of formation at various temperatures were taken from Zwolinski (12). The IBM 370/158 computer was used with double precision to execute the computations. The calculations were performed under the assumption of ideal gas behavior. The following relation was used in equation (2-11) under the ideality assumption:

$$f_i = P \qquad 2 \leq i \leq 7 \qquad (4\text{-}1)$$

The gas-phase ideality assumption was justified by redoing the calculations at the highest pressure and the lowest temperature. Also, the assumption of absence of compounds of nitrogen and of higher molecular weight hydrocarbons was tested. These results plus the trend in the carbon deposition boundaries and gas phase compositions are illustrated and discussed in the following chapter.

Gas-phase mole fractions, at equilibrium, are tabulated in Tables 1 through 40 for the following values of pressure and η :

P, atm : 1, 5, 10, 15, and 25

η : 0, 1, 2, 3, 3.76, 5, 10, and 20

The value of η = 3.76 corresponds to air being the sole source of N and O. Each table corresponds to a set of P and η values and includes mole fraction of all the six gas-phase components for the following sets of values of T and ω :

T, ^{o}K : 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, and 1500

ω : 0.01, 0.05, 0.1, 0.3, 0.5, 0.75, 1, 4, and 10

Thus, each table contains the data of mole fractions for 99 sets of T and ω values. In all, data have been tabulated for 3960 sets of parameter values of P, η , T, and ω , which cover a wide enough range to include almost all practical values of the parameters.

Figures 1 through 40 provide the carbon deposition boundaries, on triangular diagrams, obtained from equilibrium compositions. The set of parameter values of P and η for the figures correspond to those for the Tables 1 to 40. Each figure includes the boundaries for temperatures from 500 to 1500^{o} K, at intervals of 200^{o} K. To obtain smooth and accurate curves, the calculations were performed for 23 values of ω for each set of values of P, η , and T.

In the ranges where these results overlap those of Cairns and Tevebaugh and Baron et al., comparisons have shown excellent agreement. Also, several calculations were made using a newly developed random search technique (5). The results confirm that the minimum obtained by the method of steepest descent was the global minimum.

TABLE- 1 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O= 0.0

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.0	0.01877	0.00000	0.94251	0.03859	0.00013
	0.05	0.0	0.01735	0.00000	0.80549	0.17407	0.00308
	0.10	0.0	0.01577	0.00000	0.66517	0.30741	0.01164
	0.30	0.0	0.01106	0.00001	0.32690	0.57822	0.08381
	0.50	0.0	0.00817	0.00002	0.17852	0.63070	0.18259
	0.75	0.0	0.00603	0.00002	0.09737	0.59681	0.29977
	1.00	0.0	0.00475	0.00003	0.06036	0.53960	0.39526
	4.00	0.0	0.00132	0.00004	0.00468	0.21139	0.78257
	10.00	0.0	0.00054	0.00004	0.00078	0.09310	0.90553
600	0.01	0.0	0.09321	0.00002	0.86962	0.03694	0.00021
	0.05	0.0	0.08626	0.00010	0.74471	0.16400	0.00494
	0.10	0.0	0.07864	0.00018	0.61902	0.28431	0.01785
	0.30	0.0	0.05690	0.00045	0.32402	0.50921	0.10942
	0.50	0.0	0.04385	0.00063	0.19247	0.54896	0.21408
	0.75	0.0	0.03381	0.00078	0.11442	0.52350	0.32748
	1.00	0.0	0.02742	0.00088	0.07528	0.47925	0.41717
	4.00	0.0	0.00831	0.00121	0.00691	0.19905	0.78453
	10.00	0.0	0.00346	0.00130	0.00120	0.08915	0.90489
700	0.01	0.0	0.27718	0.00029	0.68935	0.03288	0.00031
	0.05	0.0	0.25679	0.00135	0.59163	0.14347	0.00677
	0.10	0.0	0.23485	0.00250	0.49485	0.24432	0.02347
	0.30	0.0	0.17383	0.00584	0.27112	0.42162	0.12758
	0.50	0.0	0.13738	0.00791	0.16933	0.45132	0.23406
	0.75	0.0	0.10863	0.00958	0.10587	0.43235	0.34357
	1.00	0.0	0.08975	0.01070	0.07227	0.39889	0.42839
	4.00	0.0	0.02898	0.01440	0.00754	0.17334	0.77574
	10.00	0.0	0.01230	0.01544	0.00136	0.07890	0.89200
800	0.01	0.0	0.54791	0.00206	0.42405	0.02560	0.00039
	0.05	0.0	0.50837	0.00943	0.36505	0.10899	0.00816
	0.10	0.0	0.46664	0.01713	0.30759	0.18171	0.02693
	0.30	0.0	0.35235	0.03783	0.17537	0.30305	0.13140
	0.50	0.0	0.28348	0.05008	0.11351	0.32272	0.23021
	0.75	0.0	0.22796	0.05984	0.07341	0.31010	0.32869
	1.00	0.0	0.19068	0.06634	0.05136	0.28758	0.40403
	4.00	0.0	0.06445	0.08810	0.00587	0.12908	0.71250
	10.00	0.0	0.02774	0.09436	0.00109	0.05951	0.81731
900	0.01	0.0	0.77922	0.00815	0.19734	0.01494	0.00034
	0.05	0.0	0.72392	0.03654	0.17033	0.06227	0.00693
	0.10	0.0	0.66632	0.06515	0.14430	0.10219	0.02204
	0.30	0.0	0.50933	0.13911	0.08431	0.16677	0.10048
	0.50	0.0	0.41380	0.18181	0.05565	0.17709	0.17164
	0.75	0.0	0.33573	0.21567	0.03663	0.17044	0.24152
	1.00	0.0	0.28263	0.23823	0.02596	0.15849	0.29469
	4.00	0.0	0.09785	0.31417	0.00311	0.07236	0.51250
	10.00	0.0	0.04244	0.33626	0.00059	0.03359	0.58712
1000	0.01	0.0	0.89936	0.01564	0.07950	0.00537	0.00013
	0.05	0.0	0.83475	0.07134	0.06849	0.02275	0.00268
	0.10	0.0	0.76689	0.12882	0.05780	0.03774	0.00874
	0.30	0.0	0.58181	0.28091	0.03327	0.06244	0.04156

TABLE- 1 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.0	0.47019	0.36968	0.02173	0.06641	0.07198
	0.75	0.0	0.37981	0.44012	0.01418	0.06386	0.10203
	1.00	0.0	0.31878	0.48700	0.00999	0.05931	0.12492
	4.00	0.0	0.10927	0.64413	0.00117	0.02689	0.21854
	10.00	0.0	0.04726	0.68959	0.00022	0.01245	0.25048
1100	0.01	0.0	0.94678	0.01870	0.03296	0.00153	0.00003
	0.05	0.0	0.87812	0.08637	0.02835	0.00655	0.00061
	0.10	0.0	0.80538	0.15776	0.02385	0.01097	0.00204
	0.30	0.0	0.60588	0.35205	0.01350	0.01842	0.01015
	0.50	0.0	0.48611	0.46765	0.00869	0.01963	0.01792
	0.75	0.0	0.39001	0.55986	0.00559	0.01886	0.02568
	1.00	0.0	0.32572	0.62128	0.00390	0.01748	0.03162
	4.00	0.0	0.10954	0.82627	0.00044	0.00782	0.05593
	10.00	0.0	0.04709	0.88506	0.00008	0.00360	0.06417
1200	0.01	0.0	0.96511	0.01943	0.01498	0.00047	0.00001
	0.05	0.0	0.89498	0.08998	0.01288	0.00202	0.00014
	0.10	0.0	0.82053	0.16478	0.01083	0.00338	0.00048
	0.30	0.0	0.61597	0.36982	0.00610	0.00570	0.00240
	0.50	0.0	0.49322	0.49253	0.00391	0.00608	0.00426
	0.75	0.0	0.39493	0.59060	0.00251	0.00584	0.00612
	1.00	0.0	0.32934	0.65596	0.00174	0.00541	0.00755
	4.00	0.0	0.11009	0.87390	0.00019	0.00241	0.01341
	10.00	0.0	0.04723	0.93624	0.00004	0.00111	0.01539
1300	0.01	0.0	0.97274	0.01959	0.00751	0.00017	0.00000
	0.05	0.0	0.90202	0.09077	0.00645	0.00072	0.00004
	0.10	0.0	0.82691	0.16632	0.00542	0.00121	0.00013
	0.30	0.0	0.62046	0.37378	0.00305	0.00203	0.00067
	0.50	0.0	0.49658	0.49811	0.00196	0.00217	0.00119
	0.75	0.0	0.39743	0.59752	0.00125	0.00208	0.00171
	1.00	0.0	0.33130	0.66378	0.00087	0.00193	0.00211
	4.00	0.0	0.11058	0.88471	0.00010	0.00086	0.00376
	10.00	0.0	0.04741	0.94786	0.00002	0.00039	0.00431
1400	0.01	0.0	0.97619	0.01962	0.00412	0.00007	0.00000
	0.05	0.0	0.90521	0.09094	0.00355	0.00029	0.00001
	0.10	0.0	0.82981	0.16667	0.00298	0.00049	0.00004
	0.30	0.0	0.62252	0.37474	0.00168	0.00083	0.00022
	0.50	0.0	0.49814	0.49950	0.00107	0.00089	0.00040
	0.75	0.0	0.39862	0.59927	0.00069	0.00085	0.00057
	1.00	0.0	0.33224	0.66578	0.00048	0.00079	0.00071
	4.00	0.0	0.11084	0.88750	0.00005	0.00035	0.00125
	10.00	0.0	0.04751	0.95088	0.00001	0.00016	0.00144
1500	0.01	0.0	0.97790	0.01962	0.00245	0.00003	0.00000
	0.05	0.0	0.90679	0.09097	0.00210	0.00014	0.00001
	0.10	0.0	0.83125	0.16674	0.00177	0.00023	0.00002
	0.30	0.0	0.62354	0.37499	0.00099	0.00038	0.00009
	0.50	0.0	0.49892	0.49988	0.00064	0.00041	0.00015
	0.75	0.0	0.39920	0.59978	0.00041	0.00039	0.00022
	1.00	0.0	0.33271	0.66637	0.00028	0.00036	0.00027
	4.00	0.0	0.11096	0.88836	0.00003	0.00016	0.00049
	10.00	0.0	0.04756	0.95180	0.00001	0.00007	0.00056

TABLE- 2 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O= 1.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.01905	0.01859	0.00000	0.92438	0.03785	0.00013
	0.05	0.08264	0.01661	0.00000	0.73829	0.15962	0.00283
	0.10	0.14181	0.01460	0.00000	0.56995	0.26364	0.00999
	0.30	0.27144	0.00942	0.00001	0.23735	0.42068	0.06110
	0.50	0.33222	0.00666	0.00001	0.11869	0.42039	0.12202
	0.75	0.37410	0.00476	0.00002	0.06065	0.37274	0.18772
	1.00	0.39926	0.00367	0.00002	0.03608	0.32342	0.23754
	4.00	0.47036	0.00096	0.00003	0.00247	0.11170	0.41449
	10.00	0.48770	0.00039	0.00003	0.00040	0.04758	0.46390
600	0.01	0.01834	0.09231	0.00002	0.85287	0.03624	0.00021
	0.05	0.07989	0.08256	0.00009	0.68231	0.15060	0.00454
	0.10	0.13765	0.07275	0.00017	0.52971	0.24431	0.01541
	0.30	0.26608	0.04834	0.00039	0.23385	0.37091	0.08044
	0.50	0.32732	0.03558	0.00052	0.12671	0.36562	0.14425
	0.75	0.36991	0.02651	0.00062	0.07034	0.32602	0.20659
	1.00	0.39565	0.02104	0.00069	0.04432	0.28598	0.25232
	4.00	0.46898	0.00597	0.00088	0.00356	0.10416	0.41646
	10.00	0.48698	0.00244	0.00093	0.00060	0.04506	0.46399
700	0.01	0.01659	0.27450	0.00028	0.67604	0.03229	0.00030
	0.05	0.07304	0.24567	0.00130	0.54149	0.13223	0.00628
	0.10	0.12720	0.21689	0.00234	0.42205	0.21100	0.02053
	0.30	0.25205	0.14661	0.00506	0.19286	0.30783	0.09560
	0.50	0.31388	0.11016	0.00655	0.10888	0.29985	0.16068
	0.75	0.35784	0.08382	0.00768	0.06304	0.26722	0.22040
	1.00	0.38481	0.06757	0.00838	0.04097	0.23530	0.26297
	4.00	0.46336	0.02021	0.01052	0.00366	0.08830	0.41395
	10.00	0.48306	0.00840	0.01107	0.00063	0.03863	0.45821
800	0.01	0.01399	0.54257	0.00204	0.41583	0.02518	0.00038
	0.05	0.06270	0.48596	0.00914	0.33359	0.10094	0.00766
	0.10	0.11100	0.42991	0.01616	0.26107	0.15791	0.02396
	0.30	0.22809	0.29421	0.03313	0.12227	0.22157	0.10074
	0.50	0.28907	0.22363	0.04194	0.07064	0.21323	0.16149
	0.75	0.33367	0.17205	0.04838	0.04181	0.18922	0.21487
	1.00	0.36156	0.13980	0.05240	0.02761	0.16654	0.25209
	4.00	0.44529	0.04303	0.06447	0.00262	0.06306	0.38153
	10.00	0.46692	0.01805	0.06758	0.00046	0.02773	0.41927
900	0.01	0.01173	0.77163	0.00809	0.19351	0.01470	0.00034
	0.05	0.05303	0.69185	0.03540	0.15557	0.05765	0.00651
	0.10	0.09466	0.61335	0.06143	0.12227	0.08869	0.01960
	0.30	0.19839	0.42345	0.12169	0.05828	0.12130	0.07690
	0.50	0.25401	0.32390	0.15204	0.03410	0.11592	0.12003
	0.75	0.29541	0.25051	0.17396	0.02040	0.10258	0.15714
	1.00	0.32162	0.20429	0.18759	0.01356	0.09021	0.18272
	4.00	0.40190	0.06364	0.22830	0.00132	0.03420	0.27064
	10.00	0.42303	0.02678	0.23880	0.00023	0.01505	0.29610
1000	0.01	0.01052	0.89061	0.01551	0.07796	0.00528	0.00013
	0.05	0.04722	0.79820	0.06857	0.06262	0.02091	0.00248
	0.10	0.08378	0.70710	0.11998	0.04914	0.03241	0.00758
	0.30	0.17348	0.48685	0.24097	0.02330	0.04482	0.03058

TABLE- 2 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.22095	0.37177	0.30252	0.01358	0.04297	0.04821
	0.75	0.25607	0.28714	0.34713	0.00810	0.03808	0.06347
	1.00	0.27823	0.23396	0.37489	0.00538	0.03351	0.07403
	4.00	0.34575	0.07268	0.45790	0.00052	0.01272	0.11044
	10.00	0.36345	0.03056	0.47930	0.00009	0.00560	0.12100
1100	0.01	0.01004	0.93759	0.01852	0.03232	0.00150	0.00003
	0.05	0.04489	0.83994	0.08267	0.02594	0.00600	0.00056
	0.10	0.07934	0.74340	0.14583	0.02032	0.00936	0.00174
	0.30	0.16262	0.50984	0.29762	0.00956	0.01311	0.00726
	0.50	0.20595	0.38820	0.37611	0.00554	0.01261	0.01159
	0.75	0.23766	0.29911	0.43336	0.00329	0.01120	0.01539
	1.00	0.25752	0.24330	0.46912	0.00218	0.00986	0.01803
	4.00	0.31728	0.07516	0.57639	0.00021	0.00374	0.02722
	10.00	0.33277	0.03156	0.60409	0.00004	0.00165	0.02990
1200	0.01	0.00986	0.95575	0.01924	0.01469	0.00046	0.00001
	0.05	0.04408	0.85611	0.08605	0.01179	0.00184	0.00013
	0.10	0.07789	0.75752	0.15208	0.00923	0.00288	0.00041
	0.30	0.15949	0.51891	0.31152	0.00433	0.00405	0.00170
	0.50	0.20183	0.39474	0.39430	0.00251	0.00390	0.00273
	0.75	0.23275	0.30390	0.45478	0.00149	0.00346	0.00363
	1.00	0.25207	0.24706	0.49258	0.00098	0.00305	0.00426
	4.00	0.31006	0.07617	0.60607	0.00009	0.00116	0.00645
	10.00	0.32504	0.03196	0.63539	0.00002	0.00051	0.00709
1300	0.01	0.00978	0.96330	0.01940	0.00736	0.00016	0.00000
	0.05	0.04377	0.86284	0.08680	0.00591	0.00066	0.00004
	0.10	0.07737	0.76339	0.15348	0.00462	0.00103	0.00011
	0.30	0.15854	0.52269	0.31469	0.00217	0.00144	0.00048
	0.50	0.20068	0.39747	0.39845	0.00125	0.00139	0.00076
	0.75	0.23146	0.30589	0.45966	0.00074	0.00123	0.00101
	1.00	0.25069	0.24863	0.49792	0.00049	0.00109	0.00119
	4.00	0.30839	0.07659	0.61276	0.00005	0.00041	0.00180
	10.00	0.32328	0.03213	0.64242	0.00001	0.00018	0.00198
1400	0.01	0.00975	0.96671	0.01943	0.00404	0.00007	0.00000
	0.05	0.04363	0.86587	0.08697	0.00324	0.00027	0.00001
	0.10	0.07715	0.76604	0.15381	0.00254	0.00042	0.00004
	0.30	0.15820	0.52437	0.31549	0.00119	0.00059	0.00016
	0.50	0.20030	0.39866	0.39953	0.00069	0.00057	0.00025
	0.75	0.23106	0.30676	0.46093	0.00041	0.00051	0.00034
	1.00	0.25028	0.24929	0.49932	0.00027	0.00045	0.00040
	4.00	0.30794	0.07676	0.61450	0.00003	0.00017	0.00060
	10.00	0.32282	0.03220	0.64424	0.00000	0.00007	0.00066
1500	0.01	0.00973	0.96841	0.01943	0.00240	0.00003	0.00000
	0.05	0.04357	0.86738	0.08700	0.00192	0.00012	0.00000
	0.10	0.07705	0.76734	0.15389	0.00151	0.00019	0.00001
	0.30	0.15806	0.52518	0.31572	0.00071	0.00027	0.00006
	0.50	0.20015	0.39923	0.39985	0.00041	0.00026	0.00010
	0.75	0.23091	0.30716	0.46132	0.00024	0.00023	0.00013
	1.00	0.25013	0.24961	0.49975	0.00016	0.00021	0.00015
	4.00	0.30779	0.07684	0.61504	0.00002	0.00008	0.00023
	10.00	0.32268	0.03223	0.64480	0.00000	0.00003	0.00026

TABLE- 3 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM, N/O= 2.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.03739	0.01841	0.00000	0.90693	0.03714	0.00012
	0.05	0.15262	0.01596	0.00000	0.68142	0.14739	0.00261
	0.10	0.24829	0.01365	0.00000	0.49852	0.23078	0.00875
	0.30	0.42678	0.00834	0.00001	0.18619	0.33058	0.04810
	0.50	0.49856	0.00576	0.00001	0.08880	0.31519	0.09168
	0.75	0.54434	0.00405	0.00002	0.04398	0.27088	0.13672
	1.00	0.57054	0.00310	0.00002	0.02569	0.23078	0.16987
	4.00	0.63974	0.00079	0.00002	0.00167	0.07583	0.28194
	10.00	0.65563	0.00032	0.00002	0.00027	0.03193	0.31184
600	0.01	0.03601	0.09143	0.00002	0.83675	0.03558	0.00021
	0.05	0.14774	0.07930	0.00009	0.62943	0.13923	0.00421
	0.10	0.24148	0.06798	0.00016	0.46261	0.21420	0.01356
	0.30	0.41935	0.04268	0.00034	0.18235	0.29154	0.06373
	0.50	0.49223	0.03064	0.00045	0.09394	0.27371	0.10904
	0.75	0.53919	0.02244	0.00053	0.05042	0.23617	0.15124
	1.00	0.56622	0.01764	0.00058	0.03115	0.20318	0.18123
	4.00	0.63821	0.00487	0.00073	0.00237	0.07016	0.28366
	10.00	0.65484	0.00198	0.00076	0.00039	0.02997	0.31205
700	0.01	0.03260	0.27188	0.00028	0.66321	0.03173	0.00030
	0.05	0.13561	0.23579	0.00125	0.49885	0.12263	0.00587
	0.10	0.22444	0.20228	0.00221	0.36712	0.18568	0.01827
	0.30	0.40006	0.12852	0.00453	0.14819	0.24188	0.07682
	0.50	0.47511	0.09381	0.00573	0.07895	0.22340	0.12299
	0.75	0.52457	0.06998	0.00660	0.04393	0.19187	0.16305
	1.00	0.55346	0.05574	0.00714	0.02788	0.16523	0.19055
	4.00	0.63206	0.01613	0.00869	0.00233	0.05821	0.28258
	10.00	0.65058	0.00665	0.00908	0.00040	0.02508	0.30821
800	0.01	0.02756	0.53737	0.00203	0.40789	0.02478	0.00038
	0.05	0.11732	0.46593	0.00887	0.30665	0.09399	0.00723
	0.10	0.19812	0.39972	0.01535	0.22569	0.13950	0.02163
	0.30	0.36749	0.25514	0.02990	0.09195	0.17344	0.08208
	0.50	0.44391	0.18745	0.03689	0.04963	0.15720	0.12492
	0.75	0.49567	0.14078	0.04176	0.02800	0.13367	0.16012
	1.00	0.52644	0.11273	0.04472	0.01795	0.11460	0.18357
	4.00	0.61235	0.03324	0.05317	0.00156	0.04018	0.25950
	10.00	0.63310	0.01379	0.05525	0.00027	0.01732	0.28026
900	0.01	0.02317	0.76420	0.00804	0.18981	0.01446	0.00034
	0.05	0.10021	0.66289	0.03435	0.14282	0.05360	0.00613
	0.10	0.17157	0.56919	0.05826	0.10530	0.07806	0.01762
	0.30	0.32700	0.36473	0.10925	0.04324	0.09380	0.06198
	0.50	0.39963	0.26873	0.13273	0.02347	0.08396	0.09147
	0.75	0.44969	0.20232	0.14882	0.01330	0.07087	0.11500
	1.00	0.47979	0.16226	0.15847	0.00856	0.06052	0.13040
	4.00	0.56516	0.04811	0.18576	0.00075	0.02103	0.17918
	10.00	0.58609	0.01999	0.19244	0.00013	0.00905	0.19230
1000	0.01	0.02080	0.88205	0.01537	0.07647	0.00518	0.00012
	0.05	0.08993	0.76494	0.06603	0.05751	0.01930	0.00230
	0.10	0.15389	0.65652	0.11239	0.04236	0.02819	0.00665
	0.30	0.29318	0.41996	0.21189	0.01733	0.03400	0.02365

TABLE- 3 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.35828	0.30906	0.25782	0.00939	0.03044	0.03501
	0.75	0.40316	0.23246	0.28930	0.00531	0.02569	0.04408
	1.00	0.43015	0.18631	0.30817	0.00341	0.02194	0.05002
	4.00	0.50669	0.05513	0.36145	0.00030	0.00761	0.06881
	10.00	0.52546	0.02289	0.37446	0.00005	0.00328	0.07386
1100	0.01	0.01987	0.92858	0.01834	0.03171	0.00147	0.00003
	0.05	0.08582	0.80504	0.07928	0.02383	0.00551	0.00051
	0.10	0.14673	0.69051	0.13563	0.01753	0.00809	0.00151
	0.30	0.27884	0.44063	0.25810	0.00714	0.00982	0.00546
	0.50	0.34027	0.32375	0.31518	0.00385	0.00881	0.00814
	0.75	0.38247	0.24318	0.35444	0.00217	0.00744	0.01029
	1.00	0.40778	0.19474	0.37801	0.00139	0.00636	0.01171
	4.00	0.47931	0.05746	0.44470	0.00012	0.00221	0.01620
	10.00	0.49677	0.02385	0.46100	0.00002	0.00095	0.01741
1200	0.01	0.01952	0.94656	0.01905	0.01441	0.00045	0.00001
	0.05	0.08439	0.82052	0.08245	0.01083	0.00169	0.00012
	0.10	0.14440	0.70359	0.14121	0.00796	0.00249	0.00035
	0.30	0.27478	0.44848	0.26921	0.00324	0.00302	0.00127
	0.50	0.33545	0.32925	0.32894	0.00174	0.00271	0.00190
	0.75	0.37713	0.24716	0.37003	0.00098	0.00229	0.00240
	1.00	0.40213	0.19785	0.39470	0.00063	0.00195	0.00273
	4.00	0.47272	0.05830	0.46446	0.00005	0.00068	0.00379
	10.00	0.48994	0.02419	0.48151	0.00001	0.00029	0.00407
1300	0.01	0.01937	0.95404	0.01921	0.00722	0.00016	0.00000
	0.05	0.08384	0.82693	0.08317	0.00542	0.00060	0.00003
	0.10	0.14357	0.70898	0.14249	0.00399	0.00089	0.00010
	0.30	0.27356	0.45162	0.27177	0.00162	0.00108	0.00035
	0.50	0.33412	0.33141	0.33210	0.00087	0.00097	0.00053
	0.75	0.37574	0.24870	0.37359	0.00049	0.00081	0.00067
	1.00	0.40071	0.19903	0.39849	0.00031	0.00070	0.00076
	4.00	0.47121	0.05861	0.46886	0.00003	0.00024	0.00106
	10.00	0.48841	0.02431	0.48604	0.00000	0.00010	0.00113
1400	0.01	0.01931	0.95742	0.01924	0.00397	0.00007	0.00000
	0.05	0.08360	0.82982	0.08333	0.00298	0.00025	0.00001
	0.10	0.14323	0.71139	0.14280	0.00219	0.00036	0.00003
	0.30	0.27312	0.45299	0.27244	0.00089	0.00044	0.00012
	0.50	0.33368	0.33233	0.33293	0.00048	0.00040	0.00018
	0.75	0.37531	0.24933	0.37453	0.00027	0.00033	0.00022
	1.00	0.40028	0.19951	0.39949	0.00017	0.00029	0.00025
	4.00	0.47081	0.05872	0.47001	0.00001	0.00010	0.00035
	10.00	0.48801	0.02435	0.48721	0.00000	0.00004	0.00038
1500	0.01	0.01928	0.95910	0.01925	0.00235	0.00003	0.00000
	0.05	0.08349	0.83126	0.08337	0.00177	0.00011	0.00000
	0.10	0.14307	0.71258	0.14288	0.00130	0.00017	0.00001
	0.30	0.27294	0.45364	0.27264	0.00053	0.00020	0.00005
	0.50	0.33351	0.33276	0.33319	0.00028	0.00018	0.00007
	0.75	0.37515	0.24963	0.37482	0.00016	0.00015	0.00009
	1.00	0.40013	0.19973	0.39980	0.00010	0.00013	0.00010
	4.00	0.47068	0.05877	0.47036	0.00001	0.00005	0.00014
	10.00	0.48789	0.02437	0.48757	0.00000	0.00002	0.00015

TABLE- 4 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O= 3.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.05505	0.01824	0.00000	0.89013	0.03645	0.00012
	0.05	0.21264	0.01538	0.00000	0.63265	0.13690	0.00243
	0.10	0.33119	0.01287	0.00000	0.44294	0.20521	0.00779
	0.30	0.52741	0.00757	0.00001	0.15310	0.27225	0.03967
	0.50	0.59845	0.00515	0.00001	0.07088	0.25206	0.07345
	0.75	0.64170	0.00359	0.00001	0.03446	0.21268	0.10755
	1.00	0.66575	0.00273	0.00002	0.01993	0.17933	0.13224
	4.00	0.72702	0.00069	0.00002	0.00126	0.05737	0.21364
	10.00	0.74063	0.00027	0.00002	0.00020	0.02401	0.23486
600	0.01	0.05304	0.09058	0.00002	0.82123	0.03493	0.00020
	0.05	0.20609	0.07639	0.00009	0.58405	0.12946	0.00392
	0.10	0.32264	0.06403	0.00015	0.41036	0.19071	0.01212
	0.30	0.51911	0.03859	0.00031	0.14907	0.24005	0.05285
	0.50	0.59170	0.02726	0.00040	0.07436	0.21850	0.08778
	0.75	0.63635	0.01977	0.00047	0.03911	0.18484	0.11946
	1.00	0.66135	0.01545	0.00051	0.02388	0.15724	0.14157
	4.00	0.72551	0.00420	0.00063	0.00177	0.05273	0.21516
	10.00	0.73986	0.00171	0.00066	0.00029	0.02237	0.23510
700	0.01	0.04807	0.26933	0.00028	0.65085	0.03118	0.00029
	0.05	0.18984	0.22696	0.00121	0.46215	0.11434	0.00550
	0.10	0.30130	0.19010	0.00210	0.32423	0.16578	0.01649
	0.30	0.49777	0.11537	0.00415	0.11943	0.19885	0.06442
	0.50	0.57367	0.08261	0.00517	0.06123	0.17736	0.09996
	0.75	0.62140	0.06086	0.00589	0.03323	0.14886	0.12976
	1.00	0.64851	0.04813	0.00633	0.02078	0.12648	0.14977
	4.00	0.71955	0.01366	0.00757	0.00167	0.04296	0.21458
	10.00	0.73575	0.00561	0.00788	0.00028	0.01835	0.23213
800	0.01	0.04071	0.53229	0.00201	0.40022	0.02438	0.00037
	0.05	0.16537	0.44788	0.00864	0.28335	0.08792	0.00685
	0.10	0.26850	0.37433	0.01467	0.19792	0.12483	0.01975
	0.30	0.46214	0.22665	0.02750	0.07256	0.14171	0.06944
	0.50	0.54119	0.16269	0.03334	0.03739	0.12332	0.10206
	0.75	0.59220	0.12030	0.03730	0.02044	0.10202	0.12774
	1.00	0.62163	0.09544	0.03966	0.01287	0.08604	0.14436
	4.00	0.70049	0.02743	0.04621	0.00106	0.02882	0.19599
	10.00	0.71885	0.01131	0.04778	0.00018	0.01229	0.20958
900	0.01	0.03431	0.75694	0.00798	0.18622	0.01423	0.00033
	0.05	0.14250	0.63658	0.03339	0.13171	0.05003	0.00579
	0.10	0.23547	0.53168	0.05551	0.09187	0.06947	0.01600
	0.30	0.41788	0.32158	0.09975	0.03361	0.07551	0.05167
	0.50	0.49509	0.23085	0.11884	0.01732	0.06457	0.07333
	0.75	0.54572	0.17075	0.13147	0.00948	0.05284	0.08975
	1.00	0.57521	0.13550	0.13888	0.00597	0.04430	0.10015
	4.00	0.65522	0.03900	0.15915	0.00049	0.01461	0.13152
	10.00	0.67405	0.01609	0.16397	0.00008	0.00621	0.13960
1000	0.01	0.03086	0.87366	0.01524	0.07502	0.00509	0.00012
	0.05	0.12876	0.73450	0.06370	0.05303	0.01787	0.00214
	0.10	0.21352	0.61308	0.10578	0.03694	0.02478	0.00589
	0.30	0.38130	0.36997	0.18956	0.01345	0.02679	0.01893

TABLE- 4 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.45280	0.26520	0.22547	0.00691	0.02284	0.02678
	0.75	0.49979	0.19593	0.24915	0.00377	0.01865	0.03270
	1.00	0.52721	0.15538	0.26300	0.00237	0.01561	0.03643
	4.00	0.60169	0.04462	0.30073	0.00020	0.00513	0.04764
	10.00	0.61924	0.01840	0.30965	0.00003	0.00218	0.05050
1100	0.01	0.02950	0.91975	0.01817	0.03111	0.00144	0.00003
	0.05	0.12330	0.77300	0.07617	0.02197	0.00509	0.00048
	0.10	0.20473	0.64481	0.12679	0.01529	0.00706	0.00132
	0.30	0.36628	0.38825	0.22802	0.00554	0.00765	0.00426
	0.50	0.43517	0.27792	0.27152	0.00284	0.00652	0.00604
	0.75	0.48043	0.20511	0.30020	0.00155	0.00532	0.00738
	1.00	0.50683	0.16255	0.31697	0.00097	0.00445	0.00823
	4.00	0.57846	0.04659	0.36264	0.00008	0.00146	0.01077
	10.00	0.59533	0.01920	0.37342	0.00001	0.00062	0.01142
1200	0.01	0.02899	0.93755	0.01887	0.01414	0.00044	0.00001
	0.05	0.12140	0.78780	0.07915	0.00998	0.00156	0.00011
	0.10	0.20188	0.65689	0.13181	0.00694	0.00217	0.00030
	0.30	0.36210	0.39497	0.23708	0.00251	0.00234	0.00099
	0.50	0.43058	0.28249	0.28226	0.00128	0.00200	0.00140
	0.75	0.47560	0.20835	0.31202	0.00070	0.00163	0.00171
	1.00	0.50185	0.16505	0.32940	0.00044	0.00136	0.00190
	4.00	0.57313	0.04724	0.37666	0.00004	0.00045	0.00249
	10.00	0.58990	0.01946	0.38780	0.00001	0.00019	0.00264
1300	0.01	0.02878	0.94495	0.01902	0.00708	0.00016	0.00000
	0.05	0.12067	0.79391	0.07983	0.00500	0.00056	0.00003
	0.10	0.20087	0.66183	0.13297	0.00347	0.00077	0.00008
	0.30	0.36085	0.39760	0.23918	0.00125	0.00083	0.00027
	0.50	0.42932	0.28422	0.28472	0.00064	0.00071	0.00039
	0.75	0.47435	0.20955	0.31470	0.00035	0.00058	0.00048
	1.00	0.50062	0.16595	0.33220	0.00022	0.00048	0.00053
	4.00	0.57192	0.04747	0.37974	0.00002	0.00016	0.00069
	10.00	0.58871	0.01955	0.39094	0.00000	0.00007	0.00073
1400	0.01	0.02868	0.94830	0.01906	0.00389	0.00006	0.00000
	0.05	0.12036	0.79667	0.07999	0.00275	0.00023	0.00001
	0.10	0.20045	0.66404	0.13326	0.00191	0.00032	0.00003
	0.30	0.36040	0.39873	0.23974	0.00069	0.00034	0.00009
	0.50	0.42890	0.28494	0.28538	0.00035	0.00029	0.00013
	0.75	0.47396	0.21003	0.31542	0.00019	0.00024	0.00016
	1.00	0.50025	0.16631	0.33295	0.00012	0.00020	0.00018
	4.00	0.57160	0.04755	0.38054	0.00001	0.00006	0.00023
	10.00	0.58840	0.01958	0.39175	0.00000	0.00003	0.00024
1500	0.01	0.02864	0.94996	0.01906	0.00231	0.00003	0.00000
	0.05	0.12021	0.79803	0.08003	0.00163	0.00011	0.00000
	0.10	0.20026	0.66512	0.13334	0.00113	0.00015	0.00001
	0.30	0.36022	0.39927	0.23992	0.00041	0.00016	0.00004
	0.50	0.42874	0.28528	0.28559	0.00021	0.00013	0.00005
	0.75	0.47382	0.21025	0.31565	0.00011	0.00011	0.00006
	1.00	0.50012	0.16647	0.33318	0.00007	0.00009	0.00007
	4.00	0.57150	0.04758	0.38079	0.00001	0.00003	0.00009
	10.00	0.58830	0.01960	0.39200	0.00000	0.00001	0.00009

TABLE- 5 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O= 3.76

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.06808	0.01811	0.00000	0.87774	0.03595	0.00012
	0.05	0.25293	0.01498	0.00000	0.59992	0.12986	0.00230
	0.10	0.38299	0.01235	0.00000	0.40823	0.18923	0.00719
	0.30	0.58311	0.00710	0.00001	0.13480	0.23997	0.03501
	0.50	0.65133	0.00479	0.00001	0.06141	0.21866	0.06380
	0.75	0.69183	0.00332	0.00001	0.02957	0.18273	0.09253
	1.00	0.71403	0.00252	0.00001	0.01701	0.15326	0.11316
	4.00	0.76955	0.00063	0.00002	0.00106	0.04838	0.18036
	10.00	0.78169	0.00025	0.00002	0.00017	0.02019	0.19768
600	0.01	0.06561	0.08995	0.00002	0.80977	0.03446	0.00020
	0.05	0.24536	0.07437	0.00008	0.55357	0.12290	0.00373
	0.10	0.37351	0.06143	0.00014	0.37771	0.17600	0.01121
	0.30	0.57453	0.03614	0.00030	0.13070	0.21153	0.04681
	0.50	0.64452	0.02529	0.00038	0.06404	0.18928	0.07649
	0.75	0.68651	0.01824	0.00044	0.03331	0.15845	0.10304
	1.00	0.70969	0.01421	0.00048	0.02022	0.13399	0.12141
	4.00	0.76810	0.00384	0.00058	0.00147	0.04426	0.18175
	10.00	0.78095	0.00156	0.00061	0.00024	0.01872	0.19793
700	0.01	0.05950	0.26744	0.00028	0.64172	0.03078	0.00029
	0.05	0.22656	0.22081	0.00119	0.43745	0.10874	0.00526
	0.10	0.34990	0.18206	0.00203	0.29739	0.15326	0.01537
	0.30	0.55260	0.10747	0.00392	0.10362	0.17493	0.05746
	0.50	0.62647	0.07611	0.00484	0.05198	0.15298	0.08761
	0.75	0.67180	0.05568	0.00548	0.02782	0.12678	0.11244
	1.00	0.69716	0.04386	0.00587	0.01726	0.10694	0.12891
	4.00	0.76238	0.01232	0.00696	0.00136	0.03562	0.18136
	10.00	0.77700	0.00505	0.00723	0.00023	0.01515	0.19535
800	0.01	0.05047	0.52851	0.00201	0.39455	0.02409	0.00037
	0.05	0.19830	0.43525	0.00847	0.26760	0.08379	0.00658
	0.10	0.31375	0.35748	0.01421	0.18051	0.11550	0.01854
	0.30	0.51628	0.20949	0.02604	0.06199	0.12399	0.06222
	0.50	0.59427	0.14836	0.03125	0.03109	0.10539	0.08964
	0.75	0.64328	0.10874	0.03473	0.01670	0.08585	0.11071
	1.00	0.67111	0.08583	0.03677	0.01041	0.07175	0.12413
	4.00	0.74412	0.02433	0.04238	0.00084	0.02344	0.16489
	10.00	0.76080	0.01000	0.04371	0.00014	0.00994	0.17541
900	0.01	0.04261	0.75151	0.00794	0.18356	0.01405	0.00033
	0.05	0.17192	0.61808	0.03271	0.12416	0.04758	0.00555
	0.10	0.27742	0.50662	0.05364	0.08342	0.06397	0.01494
	0.30	0.47127	0.29553	0.09383	0.02838	0.06527	0.04572
	0.50	0.54862	0.20894	0.11050	0.01419	0.05435	0.06341
	0.75	0.59793	0.15301	0.12132	0.00761	0.04370	0.07643
	1.00	0.62618	0.12072	0.12759	0.00474	0.03625	0.08453
	4.00	0.70104	0.03420	0.14443	0.00038	0.01163	0.10832
	10.00	0.71830	0.01406	0.14837	0.00006	0.00491	0.11430
1000	0.01	0.03838	0.86738	0.01515	0.07395	0.00502	0.00012
	0.05	0.15609	0.71299	0.06203	0.04997	0.01690	0.00203
	0.10	0.25335	0.58385	0.10129	0.03350	0.02259	0.00540
	0.30	0.43445	0.33950	0.17567	0.01133	0.02279	0.01626

TABLE- 5 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.50739	0.23959	0.20612	0.00564	0.01887	0.02238
	0.75	0.55405	0.17522	0.22575	0.00302	0.01511	0.02684
	1.00	0.58082	0.13813	0.23707	0.00188	0.01251	0.02960
	4.00	0.65189	0.03903	0.26731	0.00015	0.00399	0.03764
	10.00	0.66829	0.01603	0.27433	0.00003	0.00168	0.03964
1100	0.01	0.03671	0.91314	0.01804	0.03066	0.00142	0.00003
	0.05	0.14982	0.75028	0.07396	0.02070	0.00479	0.00045
	0.10	0.24380	0.61393	0.12081	0.01386	0.00641	0.00120
	0.30	0.41970	0.35611	0.20949	0.00466	0.00644	0.00360
	0.50	0.49077	0.25095	0.24569	0.00232	0.00533	0.00495
	0.75	0.53626	0.18333	0.26898	0.00124	0.00426	0.00593
	1.00	0.56237	0.14443	0.28238	0.00077	0.00352	0.00653
	4.00	0.63168	0.04074	0.31812	0.00006	0.00112	0.00829
	10.00	0.64767	0.01672	0.32640	0.00001	0.00047	0.00873
1200	0.01	0.03608	0.93081	0.01873	0.01394	0.00044	0.00001
	0.05	0.14763	0.76458	0.07681	0.00940	0.00147	0.00010
	0.10	0.24071	0.62531	0.12545	0.00629	0.00196	0.00028
	0.30	0.41565	0.36210	0.21734	0.00211	0.00197	0.00083
	0.50	0.48652	0.25493	0.25474	0.00105	0.00163	0.00114
	0.75	0.53191	0.18611	0.27876	0.00056	0.00130	0.00136
	1.00	0.55797	0.14655	0.29256	0.00035	0.00107	0.00150
	4.00	0.62717	0.04128	0.32928	0.00003	0.00034	0.00190
	10.00	0.64314	0.01694	0.33777	0.00000	0.00014	0.00200
1300	0.01	0.03582	0.93815	0.01889	0.00698	0.00016	0.00000
	0.05	0.14680	0.77048	0.07746	0.00471	0.00052	0.00003
	0.10	0.23961	0.62993	0.12653	0.00315	0.00070	0.00008
	0.30	0.41444	0.36441	0.21917	0.00105	0.00070	0.00023
	0.50	0.48535	0.25641	0.25682	0.00052	0.00058	0.00032
	0.75	0.53080	0.18711	0.28097	0.00028	0.00046	0.00038
	1.00	0.55688	0.14730	0.29484	0.00017	0.00038	0.00042
	4.00	0.62616	0.04146	0.33171	0.00001	0.00012	0.00053
	10.00	0.64215	0.01701	0.34023	0.00000	0.00005	0.00056
1400	0.01	0.03571	0.94147	0.01892	0.00384	0.00006	0.00000
	0.05	0.14644	0.77313	0.07762	0.00259	0.00021	0.00001
	0.10	0.23916	0.63199	0.12681	0.00173	0.00029	0.00003
	0.30	0.41401	0.36539	0.21966	0.00058	0.00029	0.00008
	0.50	0.48497	0.25702	0.25738	0.00029	0.00024	0.00011
	0.75	0.53046	0.18751	0.28157	0.00015	0.00019	0.00013
	1.00	0.55656	0.14760	0.29545	0.00009	0.00016	0.00014
	4.00	0.62589	0.04153	0.33234	0.00001	0.00005	0.00018
	10.00	0.64189	0.01704	0.34086	0.00000	0.00002	0.00018
1500	0.01	0.03565	0.94312	0.01892	0.00227	0.00003	0.00000
	0.05	0.14627	0.77444	0.07765	0.00153	0.00010	0.00000
	0.10	0.23895	0.63300	0.12688	0.00102	0.00013	0.00001
	0.30	0.41383	0.36586	0.21981	0.00034	0.00013	0.00003
	0.50	0.48482	0.25730	0.25756	0.00017	0.00011	0.00004
	0.75	0.53033	0.18769	0.28175	0.00009	0.00009	0.00005
	1.00	0.55645	0.14773	0.29564	0.00006	0.00007	0.00005
	4.00	0.62581	0.04156	0.33254	0.00000	0.00002	0.00007
	10.00	0.64181	0.01705	0.34106	0.00000	0.00001	0.00007

TABLE- 6 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O= 5.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.08849	0.01791	0.00000	0.85832	0.03516	0.00012
	0.05	0.31025	0.01438	0.00000	0.55339	0.11985	0.00213
	0.10	0.45190	0.01163	0.00000	0.36209	0.16798	0.00639
	0.30	0.65005	0.00649	0.00001	0.11283	0.20121	0.02940
	0.50	0.71273	0.00434	0.00001	0.05043	0.17990	0.05259
	0.75	0.74887	0.00300	0.00001	0.02401	0.14868	0.07543
	1.00	0.76835	0.00227	0.00001	0.01373	0.12395	0.09169
	4.00	0.81609	0.00056	0.00002	0.00085	0.03855	0.14394
	10.00	0.82635	0.00022	0.00002	0.00013	0.01604	0.15724
600	0.01	0.08531	0.08894	0.00002	0.79181	0.03371	0.00020
	0.05	0.30133	0.07140	0.00008	0.51020	0.11354	0.00345
	0.10	0.44138	0.05779	0.00014	0.33428	0.15640	0.01001
	0.30	0.64134	0.03295	0.00027	0.10869	0.17723	0.03952
	0.50	0.70601	0.02282	0.00034	0.05211	0.15537	0.06334
	0.75	0.74372	0.01635	0.00040	0.02676	0.12846	0.08432
	1.00	0.76418	0.01269	0.00043	0.01613	0.10789	0.09868
	4.00	0.81473	0.00340	0.00052	0.00116	0.03503	0.14517
	10.00	0.82565	0.00137	0.00054	0.00019	0.01476	0.15748
700	0.01	0.07747	0.26444	0.00027	0.62739	0.03015	0.00028
	0.05	0.27924	0.21174	0.00115	0.40224	0.10073	0.00491
	0.10	0.41530	0.17077	0.00192	0.26166	0.13649	0.01385
	0.30	0.61930	0.09720	0.00362	0.08478	0.14611	0.04900
	0.50	0.68845	0.06791	0.00442	0.04138	0.12471	0.07313
	0.75	0.72966	0.04926	0.00497	0.02177	0.10177	0.09256
	1.00	0.75234	0.03862	0.00530	0.01338	0.08509	0.10527
	4.00	0.80941	0.01071	0.00622	0.00103	0.02770	0.14492
	10.00	0.82197	0.00438	0.00644	0.00017	0.01172	0.15531
800	0.01	0.06587	0.52251	0.00199	0.38564	0.02363	0.00036
	0.05	0.24613	0.41654	0.00822	0.24508	0.07783	0.00620
	0.10	0.37562	0.33372	0.01356	0.15731	0.10290	0.01689
	0.30	0.58326	0.18723	0.02410	0.04952	0.10258	0.05331
	0.50	0.65753	0.13036	0.02856	0.02400	0.08465	0.07490
	0.75	0.70275	0.09452	0.03148	0.01262	0.06765	0.09099
	1.00	0.72795	0.07414	0.03318	0.00776	0.05592	0.10104
	4.00	0.79248	0.02068	0.03774	0.00060	0.01774	0.13076
	10.00	0.80691	0.00847	0.03881	0.00010	0.00747	0.13824
900	0.01	0.05577	0.74288	0.00788	0.17936	0.01378	0.00032
	0.05	0.21529	0.59048	0.03167	0.11332	0.04402	0.00521
	0.10	0.33591	0.47108	0.05094	0.07213	0.05648	0.01347
	0.30	0.53881	0.26174	0.08592	0.02227	0.05294	0.03833
	0.50	0.61385	0.18152	0.09970	0.01071	0.04260	0.05162
	0.75	0.66010	0.13131	0.10843	0.00560	0.03351	0.06105
	1.00	0.68605	0.10287	0.11340	0.00344	0.02746	0.06678
	4.00	0.75302	0.02860	0.12650	0.00027	0.00852	0.08309
	10.00	0.76810	0.01170	0.12950	0.00004	0.00357	0.08708
1000	0.01	0.05034	0.85739	0.01499	0.07225	0.00491	0.00012
	0.05	0.19683	0.68075	0.05952	0.04555	0.01548	0.00187
	0.10	0.30978	0.54215	0.09481	0.02889	0.01964	0.00473
	0.30	0.50316	0.29977	0.15722	0.00883	0.01801	0.01302

TABLE- 6 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.57549	0.20738	0.18124	0.00423	0.01436	0.01730
	0.75	0.62024	0.14976	0.19628	0.00220	0.01123	0.02029
	1.00	0.64538	0.11721	0.20480	0.00135	0.00917	0.02209
	4.00	0.71040	0.03249	0.22704	0.00010	0.00282	0.02715
	10.00	0.72505	0.01329	0.23209	0.00002	0.00118	0.02837
1100	0.01	0.04819	0.90260	0.01784	0.02996	0.00139	0.00003
	0.05	0.18956	0.71616	0.07064	0.01886	0.00437	0.00041
	0.10	0.29956	0.56972	0.11224	0.01193	0.00552	0.00103
	0.30	0.48941	0.31400	0.18513	0.00363	0.00502	0.00281
	0.50	0.56079	0.21687	0.21290	0.00173	0.00399	0.00371
	0.75	0.60501	0.15643	0.23021	0.00090	0.00311	0.00434
	1.00	0.62988	0.12234	0.23998	0.00055	0.00254	0.00472
	4.00	0.69420	0.03385	0.26537	0.00004	0.00078	0.00577
	10.00	0.70870	0.01384	0.27111	0.00001	0.00032	0.00602
1200	0.01	0.04739	0.92005	0.01852	0.01362	0.00043	0.00001
	0.05	0.18704	0.72968	0.07329	0.00856	0.00134	0.00009
	0.10	0.29628	0.58004	0.11635	0.00541	0.00169	0.00024
	0.30	0.48571	0.31901	0.19147	0.00164	0.00153	0.00064
	0.50	0.55713	0.22008	0.21994	0.00078	0.00121	0.00085
	0.75	0.60140	0.15862	0.23764	0.00040	0.00094	0.00099
	1.00	0.62631	0.12400	0.24760	0.00025	0.00077	0.00108
	4.00	0.69074	0.03426	0.27343	0.00002	0.00023	0.00131
	10.00	0.70526	0.01400	0.27927	0.00000	0.00010	0.00137
1300	0.01	0.04705	0.92730	0.01867	0.00682	0.00015	0.00000
	0.05	0.18607	0.73524	0.07390	0.00429	0.00048	0.00003
	0.10	0.29511	0.58420	0.11731	0.00271	0.00060	0.00007
	0.30	0.48462	0.32090	0.19295	0.00082	0.00054	0.00018
	0.50	0.55614	0.22125	0.22156	0.00039	0.00043	0.00024
	0.75	0.60049	0.15939	0.23931	0.00020	0.00033	0.00027
	1.00	0.62543	0.12457	0.24930	0.00012	0.00027	0.00030
	4.00	0.68997	0.03440	0.27518	0.00001	0.00008	0.00036
	10.00	0.70452	0.01405	0.28101	0.00000	0.00003	0.00038
1400	0.01	0.04691	0.93058	0.01870	0.00375	0.00006	0.00000
	0.05	0.18566	0.73773	0.07405	0.00236	0.00020	0.00001
	0.10	0.29463	0.58605	0.11756	0.00149	0.00025	0.00002
	0.30	0.48422	0.32170	0.19335	0.00045	0.00022	0.00006
	0.50	0.55582	0.22172	0.22199	0.00021	0.00018	0.00008
	0.75	0.60020	0.15970	0.23976	0.00011	0.00014	0.00009
	1.00	0.62517	0.12479	0.24976	0.00007	0.00011	0.00010
	4.00	0.68977	0.03444	0.27563	0.00001	0.00003	0.00012
	10.00	0.70432	0.01407	0.28146	0.00000	0.00001	0.00013
1500	0.01	0.04683	0.93221	0.01870	0.00222	0.00003	0.00000
	0.05	0.18546	0.73896	0.07409	0.00140	0.00009	0.00000
	0.10	0.29441	0.58695	0.11763	0.00088	0.00011	0.00001
	0.30	0.48406	0.32207	0.19348	0.00027	0.00010	0.00002
	0.50	0.55569	0.22194	0.22213	0.00013	0.00008	0.00003
	0.75	0.60010	0.15983	0.23991	0.00007	0.00006	0.00004
	1.00	0.62508	0.12489	0.24990	0.00004	0.00005	0.00004
	4.00	0.68970	0.03446	0.27577	0.00000	0.00002	0.00005
	10.00	0.70426	0.01408	0.28160	0.00000	0.00001	0.00005

TABLE- 7 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O=10.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.16253	0.01716	0.00000	0.78791	0.03229	0.00011
	0.05	0.47320	0.01255	0.00000	0.42123	0.09139	0.00162
	0.10	0.62199	0.00964	0.00000	0.24839	0.11558	0.00441
	0.30	0.78748	0.00504	0.00001	0.06787	0.12172	0.01789
	0.50	0.83195	0.00330	0.00001	0.02917	0.10474	0.03082
	0.75	0.85617	0.00225	0.00001	0.01359	0.08471	0.04326
	1.00	0.86882	0.00170	0.00001	0.00769	0.06982	0.05197
	4.00	0.89868	0.00042	0.00001	0.00046	0.02113	0.07930
	10.00	0.90490	0.00016	0.00001	0.00007	0.00874	0.08611
600	0.01	0.15695	0.08520	0.00002	0.72664	0.03101	0.00018
	0.05	0.46137	0.06217	0.00007	0.38685	0.08687	0.00267
	0.10	0.61007	0.04765	0.00011	0.22726	0.10789	0.00700
	0.30	0.77942	0.02526	0.00021	0.06387	0.10682	0.02443
	0.50	0.82610	0.01709	0.00027	0.02922	0.08969	0.03763
	0.75	0.85184	0.01208	0.00030	0.01461	0.07228	0.04889
	1.00	0.86538	0.00931	0.00032	0.00868	0.05986	0.05644
	4.00	0.89760	0.00245	0.00039	0.00060	0.01878	0.08017
	10.00	0.90435	0.00099	0.00040	0.00010	0.00786	0.08630
700	0.01	0.14316	0.25321	0.00026	0.57526	0.02784	0.00026
	0.05	0.43228	0.18339	0.00102	0.30176	0.07766	0.00389
	0.10	0.58101	0.13913	0.00164	0.17367	0.09454	0.01001
	0.30	0.75975	0.07241	0.00289	0.04704	0.08677	0.03115
	0.50	0.81147	0.04903	0.00344	0.02157	0.07013	0.04436
	0.75	0.84055	0.03490	0.00382	0.01093	0.05532	0.05449
	1.00	0.85604	0.02708	0.00403	0.00658	0.04537	0.06090
	4.00	0.89351	0.00732	0.00462	0.00048	0.01406	0.08001
	10.00	0.90148	0.00297	0.00476	0.00008	0.00588	0.08483
800	0.01	0.12280	0.49994	0.00193	0.35305	0.02194	0.00034
	0.05	0.38932	0.35742	0.00742	0.18045	0.06032	0.00506
	0.10	0.53806	0.26653	0.01169	0.10035	0.07083	0.01254
	0.30	0.72904	0.13385	0.01925	0.02530	0.05856	0.03400
	0.50	0.78678	0.08958	0.02215	0.01133	0.04511	0.04505
	0.75	0.81970	0.06340	0.02396	0.00568	0.03454	0.05272
	1.00	0.83737	0.04907	0.02499	0.00340	0.02787	0.05731
	4.00	0.88052	0.01322	0.02763	0.00025	0.00830	0.07009
	10.00	0.88977	0.00537	0.02823	0.00004	0.00345	0.07314
900	0.01	0.10509	0.71024	0.00764	0.16395	0.01277	0.00030
	0.05	0.34986	0.50231	0.02826	0.08200	0.03342	0.00415
	0.10	0.49604	0.36983	0.04285	0.04445	0.03730	0.00953
	0.30	0.69200	0.18129	0.06564	0.01068	0.02801	0.02237
	0.50	0.75257	0.12029	0.07354	0.00470	0.02082	0.02808
	0.75	0.78730	0.08471	0.07826	0.00233	0.01560	0.03180
	1.00	0.80598	0.06538	0.08086	0.00139	0.01244	0.03395
	4.00	0.85173	0.01749	0.08741	0.00010	0.00360	0.03967
	10.00	0.86156	0.00710	0.08885	0.00002	0.00148	0.04099
1000	0.01	0.09559	0.81941	0.01439	0.06599	0.00451	0.00011
	0.05	0.32668	0.57668	0.05127	0.03269	0.01130	0.00138
	0.10	0.46943	0.42219	0.07565	0.01752	0.01220	0.00301
	0.30	0.66478	0.20466	0.11123	0.00412	0.00870	0.00652

TABLE- 7 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.72579	0.13521	0.12290	0.00180	0.00635	0.00796
	0.75	0.76084	0.09497	0.12973	0.00089	0.00471	0.00886
	1.00	0.77972	0.07319	0.13345	0.00053	0.00373	0.00938
	4.00	0.82598	0.01951	0.14269	0.00004	0.00106	0.01072
	10.00	0.83593	0.00791	0.14469	0.00001	0.00044	0.01103
1100	0.01	0.09184	0.86246	0.01705	0.02735	0.00127	0.00002
	0.05	0.31778	0.60547	0.05984	0.01348	0.00313	0.00029
	0.10	0.45961	0.44191	0.08734	0.00718	0.00333	0.00062
	0.30	0.65562	0.21289	0.12620	0.00167	0.00232	0.00130
	0.50	0.71713	0.14030	0.13860	0.00072	0.00168	0.00157
	0.75	0.75250	0.09838	0.14578	0.00036	0.00124	0.00174
	1.00	0.77156	0.07575	0.14966	0.00021	0.00098	0.00184
	4.00	0.81826	0.02015	0.15922	0.00001	0.00028	0.00208
	10.00	0.82830	0.00816	0.16128	0.00000	0.00011	0.00213
1200	0.01	0.09043	0.87906	0.01769	0.01243	0.00039	0.00001
	0.05	0.31473	0.61628	0.06186	0.00611	0.00095	0.00007
	0.10	0.45654	0.44905	0.09001	0.00324	0.00101	0.00014
	0.30	0.65331	0.21558	0.12938	0.00075	0.00070	0.00029
	0.50	0.71513	0.14187	0.14182	0.00032	0.00050	0.00035
	0.75	0.75069	0.09940	0.14899	0.00016	0.00037	0.00039
	1.00	0.76984	0.07650	0.15286	0.00009	0.00029	0.00041
	4.00	0.81678	0.02032	0.16235	0.00001	0.00008	0.00046
	10.00	0.82687	0.00823	0.16439	0.00000	0.00003	0.00047
1300	0.01	0.08985	0.88595	0.01783	0.00623	0.00014	0.00000
	0.05	0.31357	0.62068	0.06234	0.00306	0.00034	0.00002
	0.10	0.45546	0.45186	0.09065	0.00162	0.00036	0.00004
	0.30	0.65263	0.21655	0.13012	0.00037	0.00025	0.00008
	0.50	0.71460	0.14242	0.14255	0.00016	0.00018	0.00010
	0.75	0.75024	0.09974	0.14970	0.00008	0.00013	0.00011
	1.00	0.76943	0.07675	0.15356	0.00005	0.00010	0.00011
	4.00	0.81646	0.02038	0.16301	0.00000	0.00003	0.00013
	10.00	0.82656	0.00825	0.16504	0.00000	0.00001	0.00013
1400	0.01	0.08960	0.88906	0.01786	0.00342	0.00006	0.00000
	0.05	0.31307	0.62265	0.06246	0.00168	0.00014	0.00001
	0.10	0.45502	0.45310	0.09083	0.00089	0.00015	0.00001
	0.30	0.65239	0.21695	0.13032	0.00020	0.00010	0.00003
	0.50	0.71442	0.14264	0.14275	0.00009	0.00007	0.00003
	0.75	0.75010	0.09987	0.14989	0.00004	0.00005	0.00004
	1.00	0.76931	0.07684	0.15374	0.00003	0.00004	0.00004
	4.00	0.81637	0.02039	0.16318	0.00000	0.00001	0.00004
	10.00	0.82649	0.00826	0.16521	0.00000	0.00000	0.00004
1500	0.01	0.08947	0.89061	0.01787	0.00203	0.00003	0.00000
	0.05	0.31283	0.62361	0.06250	0.00099	0.00006	0.00000
	0.10	0.45482	0.45370	0.09089	0.00053	0.00007	0.00001
	0.30	0.65229	0.21714	0.13039	0.00012	0.00005	0.00001
	0.50	0.71436	0.14273	0.14281	0.00005	0.00003	0.00001
	0.75	0.75005	0.09993	0.14996	0.00003	0.00002	0.00001
	1.00	0.76927	0.07688	0.15381	0.00002	0.00002	0.00001
	4.00	0.81635	0.02040	0.16323	0.00000	0.00001	0.00002
	10.00	0.82646	0.00826	0.16526	0.00000	0.00000	0.00002

TABLE- 8 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 1 ATM,N/O=20.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.27945	0.01591	0.00000	0.67679	0.02776	0.00009
	0.05	0.64183	0.01032	0.00000	0.28477	0.06197	0.00111
	0.10	0.76633	0.00754	0.00000	0.15222	0.07118	0.00273
	0.30	0.88070	0.00375	0.00000	0.03755	0.06793	0.01007
	0.50	0.90799	0.00242	0.00001	0.01571	0.05695	0.01692
	0.75	0.92232	0.00164	0.00001	0.00722	0.04541	0.02341
	1.00	0.92966	0.00123	0.00001	0.00405	0.03715	0.02791
	4.00	0.94660	0.00030	0.00001	0.00024	0.01105	0.04180
	10.00	0.95006	0.00012	0.00001	0.00004	0.00456	0.04522
600	0.01	0.27057	0.07893	0.00002	0.62360	0.02673	0.00016
	0.05	0.62872	0.05090	0.00006	0.25935	0.05913	0.00184
	0.10	0.75497	0.03699	0.00009	0.13697	0.06656	0.00442
	0.30	0.87414	0.01844	0.00016	0.03405	0.05915	0.01405
	0.50	0.90343	0.01225	0.00020	0.01501	0.04807	0.02104
	0.75	0.91902	0.00857	0.00022	0.00735	0.03799	0.02684
	1.00	0.92706	0.00657	0.00024	0.00432	0.03114	0.03067
	4.00	0.94580	0.00171	0.00028	0.00029	0.00953	0.04239
	10.00	0.94965	0.00069	0.00029	0.00005	0.00397	0.04535
700	0.01	0.24866	0.23427	0.00025	0.49243	0.02416	0.00023
	0.05	0.59700	0.14843	0.00086	0.19766	0.05325	0.00279
	0.10	0.72810	0.10561	0.00133	0.10008	0.05828	0.00660
	0.30	0.85906	0.05058	0.00222	0.02295	0.04670	0.01849
	0.50	0.89276	0.03333	0.00260	0.00997	0.03602	0.02533
	0.75	0.91099	0.02335	0.00285	0.00489	0.02761	0.03032
	1.00	0.92049	0.01796	0.00299	0.00289	0.02228	0.03339
	4.00	0.94291	0.00475	0.00336	0.00020	0.00663	0.04215
	10.00	0.94757	0.00192	0.00344	0.00003	0.00275	0.04428
800	0.01	0.21644	0.46145	0.00183	0.30078	0.01920	0.00031
	0.05	0.55166	0.28345	0.00640	0.11349	0.04124	0.00376
	0.10	0.69049	0.19513	0.00959	0.05378	0.04256	0.00845
	0.30	0.83699	0.08813	0.01469	0.01097	0.02942	0.01980
	0.50	0.87568	0.05703	0.01646	0.00459	0.02135	0.02488
	0.75	0.89672	0.03958	0.01752	0.00221	0.01577	0.02819
	1.00	0.90771	0.03031	0.01811	0.00130	0.01248	0.03009
	4.00	0.93372	0.00795	0.01956	0.00009	0.00354	0.03514
	10.00	0.93915	0.00321	0.01988	0.00001	0.00145	0.03629
900	0.01	0.18858	0.65387	0.00721	0.13896	0.01110	0.00027
	0.05	0.51153	0.39062	0.02363	0.04959	0.02173	0.00290
	0.10	0.65548	0.26238	0.03337	0.02237	0.02061	0.00578
	0.30	0.81148	0.11429	0.04636	0.00425	0.01247	0.01116
	0.50	0.85296	0.07315	0.05033	0.00174	0.00867	0.01315
	0.75	0.87551	0.05047	0.05259	0.00083	0.00625	0.01436
	1.00	0.88729	0.03852	0.05380	0.00048	0.00488	0.01503
	4.00	0.91514	0.01003	0.05674	0.00003	0.00134	0.01672
	10.00	0.92094	0.00405	0.05737	0.00001	0.00055	0.01709
1000	0.01	0.17372	0.75324	0.01334	0.05576	0.00384	0.00009
	0.05	0.48906	0.44355	0.04035	0.01934	0.00684	0.00086
	0.10	0.63511	0.29441	0.05430	0.00852	0.00611	0.00155
	0.30	0.79549	0.12605	0.07085	0.00156	0.00341	0.00264

TABLE- 8 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.83829	0.08025	0.07551	0.00063	0.00231	0.00300
	0.75	0.86156	0.05519	0.07809	0.00030	0.00165	0.00321
	1.00	0.87372	0.04206	0.07945	0.00017	0.00128	0.00332
	4.00	0.90243	0.01091	0.08269	0.00001	0.00034	0.00360
	10.00	0.90842	0.00440	0.08338	0.00000	0.00014	0.00366
1100	0.01	0.16790	0.79225	0.01568	0.02308	0.00107	0.00002
	0.05	0.48091	0.46328	0.04591	0.00789	0.00184	0.00017
	0.10	0.62834	0.30569	0.06063	0.00344	0.00160	0.00030
	0.30	0.79103	0.12974	0.07726	0.00062	0.00087	0.00049
	0.50	0.83448	0.08237	0.08177	0.00025	0.00058	0.00055
	0.75	0.85809	0.05656	0.08424	0.00012	0.00041	0.00058
	1.00	0.87042	0.04307	0.08553	0.00007	0.00032	0.00060
	4.00	0.89954	0.01115	0.08858	0.00000	0.00009	0.00064
	10.00	0.90560	0.00449	0.08922	0.00000	0.00003	0.00065
1200	0.01	0.16571	0.80725	0.01623	0.01048	0.00033	0.00000
	0.05	0.47817	0.47049	0.04718	0.00356	0.00056	0.00004
	0.10	0.62631	0.30959	0.06201	0.00154	0.00048	0.00007
	0.30	0.78998	0.13086	0.07852	0.00028	0.00026	0.00011
	0.50	0.83367	0.08297	0.08295	0.00011	0.00017	0.00012
	0.75	0.85740	0.05693	0.08536	0.00005	0.00012	0.00013
	1.00	0.86979	0.04334	0.08662	0.00003	0.00009	0.00013
	4.00	0.89903	0.01121	0.08960	0.00000	0.00003	0.00014
	10.00	0.90512	0.00451	0.09022	0.00000	0.00001	0.00014
1300	0.01	0.16481	0.81346	0.01636	0.00525	0.00012	0.00000
	0.05	0.47714	0.47338	0.04749	0.00178	0.00020	0.00001
	0.10	0.62560	0.31109	0.06235	0.00077	0.00017	0.00002
	0.30	0.78968	0.13125	0.07882	0.00014	0.00009	0.00003
	0.50	0.83346	0.08318	0.08322	0.00005	0.00006	0.00003
	0.75	0.85723	0.05705	0.08561	0.00003	0.00004	0.00004
	1.00	0.86964	0.04342	0.08686	0.00001	0.00003	0.00004
	4.00	0.89892	0.01123	0.08981	0.00000	0.00001	0.00004
	10.00	0.90502	0.00452	0.09042	0.00000	0.00000	0.00004
1400	0.01	0.16441	0.81626	0.01639	0.00288	0.00005	0.00000
	0.05	0.47669	0.47466	0.04758	0.00097	0.00008	0.00000
	0.10	0.62531	0.31174	0.06245	0.00042	0.00007	0.00001
	0.30	0.78957	0.13141	0.07890	0.00007	0.00004	0.00001
	0.50	0.83339	0.08325	0.08329	0.00003	0.00002	0.00001
	0.75	0.85718	0.05710	0.08568	0.00001	0.00002	0.00001
	1.00	0.86959	0.04345	0.08692	0.00001	0.00001	0.00001
	4.00	0.89889	0.01123	0.08986	0.00000	0.00000	0.00001
	10.00	0.90499	0.00452	0.09047	0.00000	0.00000	0.00001
1500	0.01	0.16422	0.81765	0.01640	0.00171	0.00002	0.00000
	0.05	0.47648	0.47529	0.04761	0.00058	0.00004	0.00000
	0.10	0.62518	0.31206	0.06248	0.00025	0.00003	0.00000
	0.30	0.78953	0.13148	0.07893	0.00004	0.00002	0.00000
	0.50	0.83336	0.08329	0.08332	0.00002	0.00001	0.00000
	0.75	0.85716	0.05712	0.08570	0.00001	0.00001	0.00000
	1.00	0.86958	0.04346	0.08694	0.00000	0.00001	0.00000
	4.00	0.89888	0.01123	0.08988	0.00000	0.00000	0.00000
	10.00	0.90498	0.00452	0.09049	0.00000	0.00000	0.00001

TABLE- 9 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O= 0.0

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.0	0.00844	0.00000	0.95264	0.03879	0.00013
	0.05	0.0	0.00780	0.00000	0.81417	0.17495	0.00308
	0.10	0.0	0.00709	0.00000	0.67239	0.30889	0.01163
	0.30	0.0	0.00497	0.00001	0.33054	0.58084	0.08364
	0.50	0.0	0.00367	0.00001	0.18046	0.63358	0.18229
	0.75	0.0	0.00271	0.00001	0.09835	0.59949	0.29943
	1.00	0.0	0.00213	0.00001	0.06094	0.54194	0.39497
	4.00	0.0	0.00059	0.00002	0.00471	0.21214	0.78254
	10.00	0.0	0.00024	0.00002	0.00079	0.09340	0.90555
600	0.01	0.0	0.04285	0.00001	0.91899	0.03794	0.00021
	0.05	0.0	0.03966	0.00004	0.78706	0.16832	0.00492
	0.10	0.0	0.03616	0.00008	0.65432	0.29166	0.01778
	0.30	0.0	0.02616	0.00020	0.34257	0.52222	0.10885
	0.50	0.0	0.02015	0.00028	0.20329	0.56305	0.21323
	0.75	0.0	0.01553	0.00035	0.12064	0.53685	0.32664
	1.00	0.0	0.01258	0.00039	0.07924	0.49129	0.41650
	4.00	0.0	0.00380	0.00054	0.00721	0.20351	0.78493
	10.00	0.0	0.00158	0.00058	0.00125	0.09105	0.90554
700	0.01	0.0	0.13585	0.00013	0.82790	0.03582	0.00030
	0.05	0.0	0.12585	0.00060	0.71052	0.15634	0.00669
	0.10	0.0	0.11509	0.00111	0.59418	0.26638	0.02324
	0.30	0.0	0.08509	0.00261	0.32481	0.46047	0.12702
	0.50	0.0	0.06714	0.00354	0.20220	0.49312	0.23400
	0.75	0.0	0.05298	0.00429	0.12594	0.47223	0.34456
	1.00	0.0	0.04371	0.00480	0.08570	0.43539	0.43040
	4.00	0.0	0.01402	0.00647	0.00882	0.18829	0.78240
	10.00	0.0	0.00594	0.00694	0.00158	0.08553	0.90002
800	0.01	0.0	0.30597	0.00091	0.66121	0.03154	0.00038
	0.05	0.0	0.28376	0.00419	0.56868	0.13529	0.00808
	0.10	0.0	0.26019	0.00767	0.47815	0.22696	0.02703
	0.30	0.0	0.19547	0.01719	0.26986	0.38188	0.13559
	0.50	0.0	0.15662	0.02287	0.17324	0.40717	0.24011
	0.75	0.0	0.12547	0.02741	0.11119	0.39098	0.34494
	1.00	0.0	0.10467	0.03044	0.07738	0.36218	0.42532
	4.00	0.0	0.03504	0.04054	0.00867	0.16145	0.75431
	10.00	0.0	0.01504	0.04343	0.00160	0.07422	0.86571
900	0.01	0.0	0.52450	0.00391	0.44705	0.02415	0.00040
	0.05	0.0	0.48694	0.01776	0.38532	0.10179	0.00819
	0.10	0.0	0.44758	0.03197	0.32554	0.16839	0.02653
	0.30	0.0	0.34023	0.06932	0.18811	0.27758	0.12476
	0.50	0.0	0.27533	0.09107	0.12319	0.29510	0.21532
	0.75	0.0	0.22265	0.10832	0.08056	0.28385	0.30463
	1.00	0.0	0.18702	0.11981	0.05684	0.26370	0.37264
	4.00	0.0	0.06428	0.15834	0.00671	0.11978	0.65089
	10.00	0.0	0.02782	0.16950	0.00126	0.05550	0.74591
1000	0.01	0.0	0.72037	0.01024	0.25502	0.01409	0.00028
	0.05	0.0	0.66894	0.04631	0.21991	0.05918	0.00565
	0.10	0.0	0.61520	0.08304	0.18600	0.09759	0.01816
	0.30	0.0	0.46894	0.17874	0.10807	0.16011	0.08414

TABLE- 9 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.0	0.38042	0.23407	0.07112	0.17010	0.14429
	0.75	0.0	0.30836	0.27787	0.04673	0.16368	0.20335
	1.00	0.0	0.25948	0.30701	0.03309	0.15218	0.24824
	4.00	0.0	0.08983	0.40492	0.00397	0.06949	0.43180
	10.00	0.0	0.03898	0.43337	0.00075	0.03227	0.49463
1100	0.01	0.0	0.84616	0.01618	0.13164	0.00591	0.00011
	0.05	0.0	0.78520	0.07408	0.11335	0.02512	0.00225
	0.10	0.0	0.72101	0.13423	0.09558	0.04180	0.00738
	0.30	0.0	0.54585	0.29445	0.05478	0.06941	0.03551
	0.50	0.0	0.44045	0.38827	0.03567	0.07385	0.06175
	0.75	0.0	0.35534	0.46273	0.02321	0.07101	0.08771
	1.00	0.0	0.29800	0.51226	0.01633	0.06592	0.10749
	4.00	0.0	0.10191	0.67803	0.00191	0.02984	0.18832
	10.00	0.0	0.04405	0.72592	0.00036	0.01381	0.21586
1200	0.01	0.0	0.91216	0.01876	0.06691	0.00214	0.00003
	0.05	0.0	0.84606	0.08655	0.05757	0.00917	0.00066
	0.10	0.0	0.77609	0.15794	0.04844	0.01534	0.00219
	0.30	0.0	0.58437	0.35159	0.02746	0.02572	0.01085
	0.50	0.0	0.46928	0.46650	0.01771	0.02740	0.01910
	0.75	0.0	0.37686	0.55806	0.01142	0.02633	0.02733
	1.00	0.0	0.31498	0.61901	0.00798	0.02441	0.03363
	4.00	0.0	0.10627	0.82250	0.00091	0.01094	0.05938
	10.00	0.0	0.04573	0.88094	0.00017	0.00504	0.06812
1300	0.01	0.0	0.94432	0.01949	0.03537	0.00081	0.00001
	0.05	0.0	0.87577	0.09015	0.03042	0.00346	0.00020
	0.10	0.0	0.80307	0.16489	0.02558	0.00581	0.00065
	0.30	0.0	0.60352	0.36900	0.01445	0.00976	0.00327
	0.50	0.0	0.48376	0.49077	0.00928	0.01041	0.00578
	0.75	0.0	0.38778	0.58796	0.00596	0.01000	0.00830
	1.00	0.0	0.32364	0.65272	0.00415	0.00926	0.01022
	4.00	0.0	0.10856	0.86872	0.00047	0.00414	0.01811
	10.00	0.0	0.04663	0.93060	0.00009	0.00190	0.02078
1400	0.01	0.0	0.96006	0.01966	0.01994	0.00034	0.00000
	0.05	0.0	0.89031	0.09102	0.01715	0.00145	0.00007
	0.10	0.0	0.81629	0.16664	0.01442	0.00243	0.00022
	0.30	0.0	0.61298	0.37368	0.00813	0.00410	0.00111
	0.50	0.0	0.49098	0.49747	0.00522	0.00437	0.00197
	0.75	0.0	0.39326	0.59637	0.00335	0.00419	0.00283
	1.00	0.0	0.32803	0.66227	0.00233	0.00389	0.00349
	4.00	0.0	0.10977	0.88205	0.00026	0.00173	0.00619
	10.00	0.0	0.04711	0.94495	0.00005	0.00080	0.00710
1500	0.01	0.0	0.96817	0.01969	0.01198	0.00016	0.00000
	0.05	0.0	0.89781	0.09118	0.01030	0.00067	0.00003
	0.10	0.0	0.82311	0.16701	0.00866	0.00113	0.00009
	0.30	0.0	0.61785	0.37494	0.00488	0.00190	0.00043
	0.50	0.0	0.49468	0.49940	0.00313	0.00203	0.00077
	0.75	0.0	0.39606	0.59888	0.00201	0.00195	0.00111
	1.00	0.0	0.33026	0.66518	0.00139	0.00181	0.00136
	4.00	0.0	0.11037	0.88625	0.00016	0.00080	0.00242
	10.00	0.0	0.04734	0.94948	0.00003	0.00037	0.00278

TABLE-10 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O= 1.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.01915	0.00836	0.00000	0.93432	0.03805	0.00013
	0.05	0.08302	0.00747	0.00000	0.74629	0.16039	0.00282
	0.10	0.14239	0.00656	0.00000	0.57625	0.26483	0.00997
	0.30	0.27215	0.00424	0.00000	0.24021	0.42250	0.06090
	0.50	0.33283	0.00300	0.00001	0.12016	0.42235	0.12165
	0.75	0.37460	0.00214	0.00001	0.06138	0.37456	0.18731
	1.00	0.39967	0.00165	0.00001	0.03650	0.32501	0.23716
	4.00	0.47048	0.00043	0.00001	0.00249	0.11221	0.41437
	10.00	0.48776	0.00017	0.00001	0.00040	0.04780	0.46386
600	0.01	0.01882	0.04244	0.00001	0.90130	0.03722	0.00021
	0.05	0.08175	0.03796	0.00004	0.72131	0.15442	0.00452
	0.10	0.14046	0.03346	0.00008	0.56043	0.25028	0.01528
	0.30	0.26967	0.02227	0.00017	0.24828	0.38006	0.07955
	0.50	0.33056	0.01641	0.00023	0.13475	0.37520	0.14284
	0.75	0.37266	0.01223	0.00028	0.07483	0.33498	0.20503
	1.00	0.39800	0.00970	0.00031	0.04713	0.29404	0.25083
	4.00	0.46985	0.00275	0.00039	0.00377	0.10717	0.41607
	10.00	0.48743	0.00112	0.00042	0.00063	0.04635	0.46404
700	0.01	0.01794	0.13453	0.00013	0.81195	0.03515	0.00030
	0.05	0.07829	0.12045	0.00057	0.65085	0.14367	0.00617
	0.10	0.13518	0.10643	0.00104	0.50813	0.22912	0.02010
	0.30	0.26258	0.07219	0.00224	0.23378	0.33552	0.09370
	0.50	0.32379	0.05435	0.00291	0.13250	0.32824	0.15822
	0.75	0.36660	0.04140	0.00341	0.07690	0.29359	0.21809
	1.00	0.39257	0.03339	0.00374	0.05003	0.25912	0.26115
	4.00	0.46713	0.00999	0.00471	0.00448	0.09783	0.41585
	10.00	0.48558	0.00415	0.00497	0.00077	0.04286	0.46167
800	0.01	0.01631	0.30301	0.00090	0.64844	0.03098	0.00037
	0.05	0.07185	0.27146	0.00404	0.52047	0.12468	0.00749
	0.10	0.12518	0.24029	0.00717	0.40779	0.19594	0.02362
	0.30	0.24822	0.16486	0.01487	0.19196	0.27862	0.10147
	0.50	0.30925	0.12555	0.01894	0.11133	0.27029	0.16464
	0.75	0.35274	0.09675	0.02195	0.06611	0.24136	0.22109
	1.00	0.37949	0.07870	0.02384	0.04375	0.21329	0.26092
	4.00	0.45790	0.02431	0.02960	0.00418	0.08181	0.40220
	10.00	0.47773	0.01021	0.03111	0.00074	0.03609	0.44413
900	0.01	0.01420	0.51940	0.00388	0.43840	0.02373	0.00039
	0.05	0.06322	0.46564	0.01715	0.35235	0.09400	0.00764
	0.10	0.11123	0.41278	0.03000	0.27689	0.14574	0.02336
	0.30	0.22561	0.28525	0.06027	0.13223	0.20234	0.09431
	0.50	0.28429	0.21853	0.07575	0.07760	0.19484	0.14899
	0.75	0.32693	0.16931	0.08704	0.04658	0.17344	0.19669
	1.00	0.35353	0.13826	0.09410	0.03107	0.15313	0.22991
	4.00	0.43323	0.04333	0.11545	0.00305	0.05888	0.34606
	10.00	0.45383	0.01827	0.12103	0.00054	0.02603	0.38030
1000	0.01	0.01227	0.71336	0.01016	0.25009	0.01384	0.00027
	0.05	0.05482	0.63969	0.04462	0.20110	0.05453	0.00524
	0.10	0.09679	0.56734	0.07765	0.15818	0.08416	0.01588
	0.30	0.19810	0.39277	0.15451	0.07581	0.11593	0.06288

TABLE-10 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.25089	0.30126	0.19342	0.04460	0.11131	0.09852
	0.75	0.28964	0.23363	0.22163	0.02682	0.09891	0.12937
	1.00	0.31397	0.19091	0.23924	0.01791	0.08724	0.15073
	4.00	0.38773	0.05994	0.29222	0.00177	0.03346	0.22489
	10.00	0.40700	0.02529	0.30600	0.00031	0.01478	0.24661
1100	0.01	0.01102	0.83795	0.01603	0.12909	0.00580	0.00011
	0.05	0.04908	0.75111	0.07100	0.10372	0.02303	0.00206
	0.10	0.08643	0.66561	0.12441	0.08145	0.03576	0.00634
	0.30	0.17593	0.45919	0.25067	0.03877	0.04971	0.02574
	0.50	0.22224	0.35129	0.31525	0.02269	0.04782	0.04071
	0.75	0.25612	0.27181	0.36223	0.01358	0.04252	0.05375
	1.00	0.27734	0.22176	0.39156	0.00904	0.03750	0.06281
	4.00	0.34140	0.06924	0.47983	0.00088	0.01435	0.09431
	10.00	0.35807	0.02916	0.50274	0.00016	0.00633	0.10353
1200	0.01	0.01037	0.90331	0.01857	0.06562	0.00210	0.00003
	0.05	0.04616	0.80943	0.08274	0.05269	0.00838	0.00060
	0.10	0.08125	0.71679	0.14570	0.04132	0.01307	0.00186
	0.30	0.16509	0.49292	0.29645	0.01954	0.01829	0.00771
	0.50	0.20826	0.37614	0.37430	0.01138	0.01762	0.01230
	0.75	0.23972	0.29039	0.43113	0.00678	0.01567	0.01631
	1.00	0.25936	0.23654	0.46667	0.00450	0.01382	0.01911
	4.00	0.31833	0.07344	0.57363	0.00043	0.00527	0.02888
	10.00	0.33359	0.03088	0.60138	0.00008	0.00232	0.03174
1300	0.01	0.01005	0.93516	0.01930	0.03469	0.00079	0.00001
	0.05	0.04483	0.83783	0.08615	0.02784	0.00316	0.00018
	0.10	0.07902	0.74167	0.15200	0.02182	0.00494	0.00055
	0.30	0.16098	0.50910	0.31040	0.01028	0.00693	0.00231
	0.50	0.20327	0.38792	0.39247	0.00597	0.00668	0.00370
	0.75	0.23409	0.29909	0.45242	0.00355	0.00593	0.00491
	1.00	0.25333	0.24341	0.48992	0.00235	0.00523	0.00576
	4.00	0.31106	0.07532	0.60269	0.00023	0.00199	0.00872
	10.00	0.32597	0.03164	0.63189	0.00004	0.00088	0.00958
1400	0.01	0.00990	0.95074	0.01947	0.01956	0.00033	0.00000
	0.05	0.04422	0.85170	0.08700	0.01569	0.00133	0.00006
	0.10	0.07804	0.75377	0.15364	0.01229	0.00207	0.00019
	0.30	0.15939	0.51684	0.31430	0.00578	0.00291	0.00079
	0.50	0.20148	0.39346	0.39765	0.00335	0.00280	0.00126
	0.75	0.23219	0.30312	0.45854	0.00199	0.00249	0.00167
	1.00	0.25137	0.24655	0.49662	0.00132	0.00219	0.00196
	4.00	0.30890	0.07614	0.61103	0.00013	0.00083	0.00297
	10.00	0.32376	0.03197	0.64062	0.00002	0.00037	0.00326
1500	0.01	0.00982	0.95878	0.01949	0.01175	0.00015	0.00000
	0.05	0.04392	0.85885	0.08717	0.00943	0.00062	0.00002
	0.10	0.07757	0.75998	0.15403	0.00738	0.00096	0.00007
	0.30	0.15870	0.52073	0.31544	0.00347	0.00135	0.00031
	0.50	0.20076	0.39621	0.39924	0.00201	0.00130	0.00049
	0.75	0.23146	0.30508	0.46046	0.00119	0.00116	0.00065
	1.00	0.25064	0.24805	0.49873	0.00079	0.00102	0.00077
	4.00	0.30819	0.07651	0.61368	0.00007	0.00039	0.00116
	10.00	0.32305	0.03211	0.64338	0.00001	0.00017	0.00128

TABLE-11 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O= 2.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.03758	0.00828	0.00000	0.91669	0.03733	0.00012
	0.05	0.15329	0.00718	0.00000	0.68884	0.14808	0.00261
	0.10	0.24923	0.00614	0.00000	0.50413	0.23177	0.00873
	0.30	0.42777	0.00376	0.00000	0.18860	0.33199	0.04789
	0.50	0.49935	0.00259	0.00001	0.09002	0.31672	0.09131
	0.75	0.54495	0.00183	0.00001	0.04458	0.27232	0.13632
	1.00	0.57103	0.00140	0.00001	0.02603	0.23205	0.16949
	4.00	0.63988	0.00036	0.00001	0.00169	0.07625	0.28181
	10.00	0.65569	0.00014	0.00001	0.00027	0.03210	0.31179
600	0.01	0.03694	0.04204	0.00001	0.88429	0.03652	0.00021
	0.05	0.15104	0.03647	0.00004	0.66563	0.14264	0.00418
	0.10	0.24608	0.03129	0.00007	0.48996	0.21919	0.01341
	0.30	0.42432	0.01971	0.00015	0.19440	0.29868	0.06274
	0.50	0.49641	0.01417	0.00020	0.10053	0.28117	0.10752
	0.75	0.54256	0.01039	0.00024	0.05406	0.24318	0.14957
	1.00	0.56902	0.00817	0.00026	0.03341	0.20951	0.17962
	4.00	0.63917	0.00225	0.00033	0.00254	0.07256	0.28315
	10.00	0.65532	0.00092	0.00034	0.00042	0.03101	0.31199
700	0.01	0.03522	0.13326	0.00012	0.79660	0.03451	0.00029
	0.05	0.14491	0.11567	0.00055	0.60024	0.13290	0.00573
	0.10	0.23745	0.09942	0.00097	0.44341	0.20101	0.01773
	0.30	0.41450	0.06365	0.00199	0.18176	0.26366	0.07442
	0.50	0.48770	0.04669	0.00253	0.09779	0.24543	0.11986
	0.75	0.53513	0.03495	0.00292	0.05478	0.21224	0.15998
	1.00	0.56255	0.02789	0.00317	0.03490	0.18358	0.18790
	4.00	0.63616	0.00811	0.00389	0.00295	0.06552	0.28337
	10.00	0.65330	0.00335	0.00407	0.00050	0.02831	0.31046
800	0.01	0.03206	0.30012	0.00089	0.63614	0.03043	0.00037
	0.05	0.13350	0.26055	0.00390	0.47944	0.11561	0.00699
	0.10	0.22114	0.22408	0.00677	0.35464	0.17235	0.02101
	0.30	0.39476	0.14447	0.01332	0.14740	0.21867	0.08139
	0.50	0.46915	0.10685	0.01655	0.08063	0.20104	0.12578
	0.75	0.51831	0.08067	0.01886	0.04596	0.17294	0.16326
	1.00	0.54712	0.06482	0.02028	0.02967	0.14939	0.18872
	4.00	0.62600	0.01932	0.02443	0.00264	0.05366	0.27396
	10.00	0.64475	0.00804	0.02548	0.00046	0.02328	0.29799
900	0.01	0.02796	0.51443	0.00385	0.43005	0.02333	0.00039
	0.05	0.11821	0.44660	0.01661	0.32413	0.08729	0.00716
	0.10	0.19843	0.38418	0.02837	0.23985	0.12827	0.02089
	0.30	0.36380	0.24819	0.05407	0.10010	0.15794	0.07590
	0.50	0.43744	0.18399	0.06623	0.05501	0.14343	0.11389
	0.75	0.48710	0.13925	0.07472	0.03151	0.12246	0.14496
	1.00	0.51658	0.11208	0.07988	0.02042	0.10538	0.16566
	4.00	0.59890	0.03365	0.09479	0.00184	0.03754	0.23329
	10.00	0.61883	0.01403	0.09853	0.00032	0.01627	0.25202
1000	0.01	0.02422	0.70652	0.01008	0.24531	0.01360	0.00027
	0.05	0.10335	0.61332	0.04309	0.18486	0.05048	0.00489
	0.10	0.17493	0.52749	0.07311	0.13674	0.07367	0.01408
	0.30	0.32618	0.34040	0.13740	0.05695	0.08935	0.04972

TABLE-11 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.39516	0.25212	0.16726	0.03124	0.08055	0.07367
	0.75	0.44222	0.19066	0.18788	0.01786	0.06843	0.09296
	1.00	0.47037	0.15337	0.20032	0.01156	0.05869	0.10568
	4.00	0.54980	0.04594	0.23592	0.00104	0.02071	0.14659
	10.00	0.56921	0.01915	0.24475	0.00018	0.00895	0.15776
1100	0.01	0.02178	0.82992	0.01588	0.12663	0.00569	0.00010
	0.05	0.09320	0.72015	0.06819	0.09535	0.02121	0.00190
	0.10	0.15814	0.61884	0.11608	0.07041	0.03102	0.00552
	0.30	0.29631	0.39795	0.21925	0.02912	0.03768	0.01969
	0.50	0.35969	0.29398	0.26725	0.01589	0.03393	0.02926
	0.75	0.40304	0.22183	0.30036	0.00905	0.02877	0.03695
	1.00	0.42900	0.17818	0.32031	0.00584	0.02465	0.04203
	4.00	0.50232	0.05310	0.37714	0.00052	0.00865	0.05826
	10.00	0.52024	0.02210	0.39116	0.00009	0.00373	0.06268
1200	0.01	0.02051	0.89464	0.01839	0.06437	0.00206	0.00003
	0.05	0.08806	0.77601	0.07926	0.04843	0.00770	0.00055
	0.10	0.14980	0.66630	0.13530	0.03570	0.01128	0.00161
	0.30	0.28205	0.42703	0.25675	0.01466	0.01372	0.00579
	0.50	0.34298	0.31470	0.31339	0.00796	0.01235	0.00862
	0.75	0.38470	0.23698	0.35244	0.00452	0.01045	0.01090
	1.00	0.40970	0.19009	0.37595	0.00291	0.00895	0.01241
	4.00	0.48028	0.05640	0.44274	0.00026	0.00313	0.01720
	10.00	0.49751	0.02344	0.45915	0.00004	0.00135	0.01850
1300	0.01	0.01990	0.92619	0.01911	0.03402	0.00078	0.00001
	0.05	0.08572	0.80314	0.08249	0.02558	0.00290	0.00016
	0.10	0.14623	0.68919	0.14101	0.01884	0.00426	0.00048
	0.30	0.27671	0.44061	0.26808	0.00770	0.00518	0.00172
	0.50	0.33713	0.32414	0.32734	0.00417	0.00465	0.00257
	0.75	0.37858	0.24374	0.36814	0.00236	0.00393	0.00325
	1.00	0.40343	0.19533	0.39267	0.00151	0.00336	0.00370
	4.00	0.47361	0.05777	0.46219	0.00013	0.00117	0.00513
	10.00	0.49075	0.02399	0.47922	0.00002	0.00050	0.00551
1400	0.01	0.01961	0.94161	0.01928	0.01918	0.00032	0.00000
	0.05	0.08464	0.81635	0.08331	0.01442	0.00122	0.00006
	0.10	0.14465	0.70025	0.14254	0.01061	0.00179	0.00016
	0.30	0.27466	0.44695	0.27132	0.00432	0.00217	0.00059
	0.50	0.33505	0.32844	0.33136	0.00233	0.00195	0.00087
	0.75	0.37653	0.24674	0.37267	0.00132	0.00164	0.00110
	1.00	0.40140	0.19761	0.39748	0.00084	0.00140	0.00126
	4.00	0.47167	0.05832	0.46770	0.00007	0.00049	0.00174
	10.00	0.48883	0.02421	0.48488	0.00001	0.00021	0.00187
1500	0.01	0.01946	0.94956	0.01930	0.01153	0.00015	0.00000
	0.05	0.08410	0.82315	0.08350	0.00866	0.00057	0.00002
	0.10	0.14389	0.70590	0.14294	0.00637	0.00083	0.00006
	0.30	0.27377	0.45010	0.27231	0.00259	0.00101	0.00023
	0.50	0.33421	0.33052	0.33263	0.00140	0.00090	0.00034
	0.75	0.37574	0.24816	0.37412	0.00079	0.00076	0.00043
	1.00	0.40066	0.19867	0.39903	0.00050	0.00065	0.00049
	4.00	0.47103	0.05857	0.46945	0.00004	0.00023	0.00068
	10.00	0.48821	0.02430	0.48666	0.00001	0.00010	0.00073

TABLE-12 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O= 3.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.05533	0.00820	0.00000	0.89971	0.03664	0.00012
	0.05	0.21354	0.00692	0.00000	0.63960	0.13752	0.00242
	0.10	0.33237	0.00579	0.00000	0.44803	0.20605	0.00777
	0.30	0.52851	0.00341	0.00000	0.15521	0.27340	0.03947
	0.50	0.59930	0.00232	0.00001	0.07194	0.25333	0.07310
	0.75	0.64234	0.00162	0.00001	0.03499	0.21389	0.10716
	1.00	0.66625	0.00123	0.00001	0.02022	0.18041	0.13188
	4.00	0.72716	0.00031	0.00001	0.00128	0.05773	0.21352
	10.00	0.74069	0.00012	0.00001	0.00020	0.02416	0.23481
600	0.01	0.05440	0.04164	0.00001	0.86789	0.03585	0.00020
	0.05	0.21052	0.03514	0.00004	0.61789	0.13253	0.00389
	0.10	0.32841	0.02949	0.00007	0.43511	0.19498	0.01195
	0.30	0.52465	0.01786	0.00014	0.15957	0.24595	0.05184
	0.50	0.59615	0.01265	0.00018	0.08004	0.22472	0.08627
	0.75	0.63984	0.00919	0.00021	0.04222	0.19074	0.11781
	1.00	0.66420	0.00718	0.00023	0.02582	0.16258	0.13999
	4.00	0.72646	0.00195	0.00028	0.00191	0.05476	0.21463
	10.00	0.74034	0.00079	0.00030	0.00031	0.02326	0.23500
700	0.01	0.05189	0.13201	0.00012	0.78180	0.03389	0.00029
	0.05	0.20229	0.11141	0.00053	0.55678	0.12364	0.00534
	0.10	0.31758	0.09359	0.00092	0.39298	0.17905	0.01587
	0.30	0.51372	0.05747	0.00182	0.14817	0.21699	0.06183
	0.50	0.58688	0.04145	0.00227	0.07707	0.19567	0.09666
	0.75	0.63216	0.03069	0.00260	0.04225	0.16576	0.12654
	1.00	0.65762	0.02434	0.00280	0.02658	0.14170	0.14696
	4.00	0.72351	0.00696	0.00339	0.00217	0.04899	0.21498
	10.00	0.73837	0.00286	0.00354	0.00037	0.02102	0.23385
800	0.01	0.04727	0.29730	0.00089	0.62427	0.02991	0.00036
	0.05	0.18701	0.25076	0.00378	0.44411	0.10777	0.00656
	0.10	0.29717	0.21056	0.00643	0.31311	0.15379	0.01895
	0.30	0.49187	0.12964	0.01218	0.11869	0.17950	0.06811
	0.50	0.56732	0.09402	0.01491	0.06244	0.15932	0.10200
	0.75	0.61493	0.07008	0.01681	0.03468	0.13386	0.12964
	1.00	0.64206	0.05587	0.01796	0.02205	0.11405	0.14802
	4.00	0.71361	0.01630	0.02126	0.00188	0.03941	0.20753
	10.00	0.73006	0.00675	0.02208	0.00032	0.01694	0.22384
900	0.01	0.04129	0.50958	0.00383	0.42198	0.02294	0.00038
	0.05	0.16655	0.42945	0.01611	0.29971	0.08144	0.00674
	0.10	0.26881	0.36013	0.02699	0.21076	0.11440	0.01891
	0.30	0.45780	0.22109	0.04946	0.07943	0.12870	0.06352
	0.50	0.53406	0.16025	0.05955	0.04173	0.11232	0.09208
	0.75	0.58312	0.11944	0.06641	0.02318	0.09335	0.11449
	1.00	0.61141	0.09526	0.07050	0.01475	0.07904	0.12903
	4.00	0.68732	0.02786	0.08202	0.00126	0.02689	0.17465
	10.00	0.70505	0.01154	0.08483	0.00022	0.01153	0.18684
1000	0.01	0.03584	0.69984	0.01000	0.24069	0.01337	0.00026
	0.05	0.14667	0.58940	0.04169	0.17072	0.04694	0.00458
	0.10	0.23953	0.49365	0.06920	0.11976	0.06526	0.01261
	0.30	0.41661	0.30171	0.12445	0.04473	0.07172	0.04079

TABLE-12 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.49002	0.21806	0.14856	0.02337	0.06188	0.05812
	0.75	0.53780	0.16216	0.16468	0.01292	0.05101	0.07142
	1.00	0.56555	0.12915	0.17421	0.00820	0.04298	0.07992
	4.00	0.64064	0.03759	0.20064	0.00069	0.01441	0.10602
	10.00	0.65831	0.01555	0.20701	0.00012	0.00615	0.11286
1100	0.01	0.03228	0.82205	0.01573	0.12424	0.00559	0.00010
	0.05	0.13313	0.69188	0.06562	0.08801	0.01961	0.00176
	0.10	0.21873	0.57873	0.10889	0.06158	0.02721	0.00486
	0.30	0.38452	0.35199	0.19538	0.02278	0.02970	0.01564
	0.50	0.45408	0.25358	0.23282	0.01182	0.02550	0.02220
	0.75	0.49957	0.18809	0.25770	0.00650	0.02093	0.02720
	1.00	0.52604	0.14954	0.27234	0.00411	0.01759	0.03038
	4.00	0.59784	0.04329	0.31264	0.00034	0.00584	0.04004
	10.00	0.61476	0.01789	0.32227	0.00006	0.00249	0.04254
1200	0.01	0.03043	0.88615	0.01821	0.06315	0.00202	0.00003
	0.05	0.12627	0.74537	0.07607	0.04468	0.00710	0.00051
	0.10	0.20849	0.62273	0.12634	0.03119	0.00985	0.00140
	0.30	0.36959	0.37709	0.22668	0.01144	0.01070	0.00451
	0.50	0.43776	0.27089	0.26990	0.00590	0.00915	0.00639
	0.75	0.48247	0.20048	0.29851	0.00323	0.00749	0.00782
	1.00	0.50852	0.15915	0.31528	0.00204	0.00628	0.00872
	4.00	0.57925	0.04586	0.36119	0.00017	0.00207	0.01145
	10.00	0.59592	0.01892	0.37209	0.00003	0.00088	0.01215
1300	0.01	0.02955	0.91738	0.01892	0.03338	0.00076	0.00001
	0.05	0.12317	0.77127	0.07914	0.02359	0.00268	0.00015
	0.10	0.20411	0.64379	0.13153	0.01644	0.00371	0.00042
	0.30	0.36408	0.38854	0.23603	0.00599	0.00402	0.00134
	0.50	0.43217	0.27853	0.28090	0.00308	0.00343	0.00189
	0.75	0.47690	0.20580	0.31051	0.00168	0.00280	0.00231
	1.00	0.50299	0.16320	0.32782	0.00106	0.00235	0.00258
	4.00	0.57385	0.04688	0.37504	0.00009	0.00077	0.00338
	10.00	0.59054	0.01933	0.38621	0.00001	0.00033	0.00358
1400	0.01	0.02912	0.93265	0.01909	0.01882	0.00032	0.00000
	0.05	0.12174	0.78386	0.07993	0.01329	0.00112	0.00005
	0.10	0.20219	0.65391	0.13296	0.00925	0.00156	0.00014
	0.30	0.36198	0.39380	0.23873	0.00336	0.00168	0.00045
	0.50	0.43020	0.28193	0.28408	0.00172	0.00143	0.00064
	0.75	0.47505	0.20809	0.31397	0.00094	0.00117	0.00078
	1.00	0.50122	0.16492	0.33142	0.00059	0.00098	0.00087
	4.00	0.57229	0.04727	0.37892	0.00005	0.00032	0.00114
	10.00	0.58903	0.01948	0.39013	0.00001	0.00014	0.00121
1500	0.01	0.02890	0.94053	0.01912	0.01131	0.00015	0.00000
	0.05	0.12102	0.79033	0.08012	0.00799	0.00052	0.00002
	0.10	0.20127	0.65906	0.13335	0.00555	0.00072	0.00005
	0.30	0.36107	0.39639	0.23958	0.00201	0.00078	0.00018
	0.50	0.42940	0.28355	0.28510	0.00103	0.00066	0.00025
	0.75	0.47435	0.20916	0.31508	0.00056	0.00054	0.00031
	1.00	0.50057	0.16570	0.33258	0.00035	0.00045	0.00034
	4.00	0.57178	0.04744	0.38015	0.00003	0.00015	0.00045
	10.00	0.58855	0.01955	0.39136	0.00000	0.00006	0.00047

TABLE-13 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM, N/O= 3.76

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.06842	0.00814	0.00000	0.88719	0.03613	0.00012
	0.05	0.25399	0.00673	0.00000	0.60655	0.13043	0.00230
	0.10	0.38430	0.00556	0.00000	0.41300	0.18998	0.00716
	0.30	0.58425	0.00320	0.00000	0.13674	0.24100	0.03480
	0.50	0.65219	0.00216	0.00000	0.06238	0.21980	0.06346
	0.75	0.69247	0.00150	0.00001	0.03005	0.18383	0.09215
	1.00	0.71453	0.00114	0.00001	0.01728	0.15424	0.11281
	4.00	0.76969	0.00028	0.00001	0.00108	0.04871	0.18024
	10.00	0.78175	0.00011	0.00001	0.00017	0.02032	0.19763
600	0.01	0.06728	0.04135	0.00001	0.85580	0.03536	0.00020
	0.05	0.25048	0.03421	0.00004	0.58583	0.12574	0.00369
	0.10	0.37991	0.02830	0.00006	0.40085	0.17984	0.01103
	0.30	0.58025	0.01674	0.00013	0.14031	0.21677	0.04579
	0.50	0.64900	0.01176	0.00017	0.06921	0.19485	0.07501
	0.75	0.68998	0.00850	0.00019	0.03615	0.16375	0.10143
	1.00	0.71249	0.00663	0.00021	0.02198	0.13881	0.11988
	4.00	0.76901	0.00179	0.00026	0.00160	0.04611	0.18123
	10.00	0.78141	0.00073	0.00027	0.00026	0.01952	0.19781
700	0.01	0.06419	0.13109	0.00012	0.77088	0.03344	0.00028
	0.05	0.24096	0.10844	0.00052	0.52758	0.11741	0.00508
	0.10	0.36791	0.08976	0.00089	0.36145	0.16529	0.01471
	0.30	0.56896	0.05375	0.00171	0.12963	0.19112	0.05483
	0.50	0.63967	0.03841	0.00212	0.06617	0.16932	0.08431
	0.75	0.68236	0.02827	0.00242	0.03585	0.14187	0.10924
	1.00	0.70602	0.02235	0.00260	0.02241	0.12051	0.12612
	4.00	0.76616	0.00633	0.00312	0.00180	0.04098	0.18161
	10.00	0.77951	0.00260	0.00324	0.00030	0.01751	0.19683
800	0.01	0.05853	0.29521	0.00088	0.61550	0.02952	0.00036
	0.05	0.22329	0.24395	0.00370	0.42032	0.10247	0.00627
	0.10	0.34533	0.20162	0.00620	0.28711	0.14210	0.01765
	0.30	0.54651	0.12071	0.01150	0.10290	0.15773	0.06066
	0.50	0.62008	0.08657	0.01394	0.05293	0.13722	0.08925
	0.75	0.66538	0.06406	0.01563	0.02898	0.11381	0.11215
	1.00	0.69081	0.05086	0.01665	0.01827	0.09623	0.12719
	4.00	0.75663	0.01467	0.01953	0.00152	0.03257	0.17508
	10.00	0.77152	0.00606	0.02024	0.00026	0.01393	0.18800
900	0.01	0.05119	0.50596	0.00380	0.41601	0.02266	0.00038
	0.05	0.19964	0.41747	0.01577	0.28321	0.07746	0.00645
	0.10	0.31403	0.34417	0.02607	0.19249	0.10559	0.01764
	0.30	0.51164	0.20473	0.04664	0.06811	0.11239	0.05649
	0.50	0.58693	0.14646	0.05561	0.03486	0.09586	0.08028
	0.75	0.63414	0.10822	0.06160	0.01903	0.07847	0.09853
	1.00	0.66095	0.08588	0.06515	0.01198	0.06585	0.11019
	4.00	0.73140	0.02476	0.07499	0.00100	0.02185	0.14600
	10.00	0.74756	0.01022	0.07736	0.00017	0.00931	0.15538
1000	0.01	0.04449	0.69485	0.00994	0.23727	0.01319	0.00026
	0.05	0.17670	0.57260	0.04070	0.16113	0.04452	0.00436
	0.10	0.28178	0.47104	0.06657	0.10904	0.05990	0.01167
	0.30	0.46972	0.27823	0.11643	0.03804	0.06188	0.03570

TABLE-13 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.54334	0.19822	0.13740	0.01931	0.05202	0.04972
	0.75	0.59002	0.14600	0.15116	0.01048	0.04216	0.06018
	1.00	0.61670	0.11562	0.15920	0.00657	0.03516	0.06675
	4.00	0.68733	0.03313	0.18113	0.00054	0.01146	0.08640
	10.00	0.70362	0.01366	0.18633	0.00009	0.00486	0.09144
1100	0.01	0.04013	0.81617	0.01563	0.12247	0.00551	0.00010
	0.05	0.16110	0.67192	0.06380	0.08301	0.01851	0.00167
	0.10	0.25901	0.55176	0.10404	0.05597	0.02479	0.00443
	0.30	0.43757	0.32388	0.18063	0.01929	0.02526	0.01337
	0.50	0.50854	0.22985	0.21234	0.00971	0.02108	0.01847
	0.75	0.55378	0.16881	0.23296	0.00524	0.01698	0.02223
	1.00	0.57969	0.13343	0.24492	0.00327	0.01411	0.02457
	4.00	0.64846	0.03801	0.27723	0.00027	0.00455	0.03148
	10.00	0.66435	0.01565	0.28481	0.00005	0.00192	0.03323
1200	0.01	0.03786	0.87980	0.01808	0.06225	0.00199	0.00003
	0.05	0.15323	0.72368	0.07382	0.04212	0.00669	0.00048
	0.10	0.24787	0.59332	0.12030	0.02831	0.00893	0.00127
	0.30	0.42292	0.34640	0.20820	0.00965	0.00903	0.00380
	0.50	0.49318	0.24504	0.24423	0.00483	0.00749	0.00524
	0.75	0.53810	0.17952	0.26750	0.00259	0.00601	0.00628
	1.00	0.56387	0.14167	0.28093	0.00161	0.00498	0.00693
	4.00	0.63234	0.04017	0.31695	0.00013	0.00159	0.00882
	10.00	0.64817	0.01651	0.32533	0.00002	0.00067	0.00929
1300	0.01	0.03677	0.91079	0.01878	0.03290	0.00075	0.00001
	0.05	0.14966	0.74868	0.07676	0.02223	0.00252	0.00014
	0.10	0.24313	0.61309	0.12514	0.01491	0.00336	0.00038
	0.30	0.41757	0.35652	0.21636	0.00504	0.00338	0.00112
	0.50	0.48799	0.25161	0.25355	0.00251	0.00280	0.00154
	0.75	0.53309	0.18401	0.27747	0.00134	0.00224	0.00185
	1.00	0.55897	0.14506	0.29124	0.00083	0.00185	0.00204
	4.00	0.62777	0.04100	0.32799	0.00007	0.00059	0.00258
	10.00	0.64367	0.01684	0.33651	0.00001	0.00025	0.00272
1400	0.01	0.03624	0.92594	0.01895	0.01855	0.00031	0.00000
	0.05	0.14802	0.76081	0.07754	0.01252	0.00106	0.00005
	0.10	0.24104	0.62255	0.12648	0.00839	0.00141	0.00013
	0.30	0.41553	0.36112	0.21873	0.00282	0.00141	0.00038
	0.50	0.48617	0.25449	0.25625	0.00140	0.00117	0.00052
	0.75	0.53143	0.18592	0.28034	0.00075	0.00093	0.00063
	1.00	0.55741	0.14647	0.29419	0.00046	0.00077	0.00069
	4.00	0.62647	0.04131	0.33106	0.00004	0.00024	0.00087
	10.00	0.64242	0.01696	0.33959	0.00001	0.00010	0.00092
1500	0.01	0.03597	0.93376	0.01898	0.01115	0.00015	0.00000
	0.05	0.14720	0.76704	0.07773	0.00752	0.00049	0.00002
	0.10	0.24004	0.62736	0.12686	0.00503	0.00065	0.00005
	0.30	0.41465	0.36337	0.21949	0.00169	0.00066	0.00015
	0.50	0.48544	0.25586	0.25712	0.00084	0.00054	0.00020
	0.75	0.53080	0.18680	0.28127	0.00045	0.00043	0.00024
	1.00	0.55685	0.14711	0.29514	0.00028	0.00036	0.00027
	4.00	0.62605	0.04145	0.33203	0.00002	0.00011	0.00034
	10.00	0.64202	0.01701	0.34056	0.00000	0.00005	0.00036

TABLE-14 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O= 5.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.08893	0.00805	0.00000	0.86757	0.03533	0.00012
	0.05	0.31149	0.00647	0.00000	0.55957	0.12035	0.00212
	0.10	0.45336	0.00523	0.00000	0.36643	0.16862	0.00636
	0.30	0.65122	0.00293	0.00000	0.11457	0.20207	0.02921
	0.50	0.71358	0.00196	0.00000	0.05129	0.18089	0.05227
	0.75	0.74949	0.00135	0.00001	0.02444	0.14963	0.07508
	1.00	0.76884	0.00102	0.00001	0.01397	0.12480	0.09136
	4.00	0.81622	0.00025	0.00001	0.00086	0.03884	0.14382
	10.00	0.82640	0.00010	0.00001	0.00014	0.01616	0.15720
600	0.01	0.08746	0.04089	0.00001	0.83686	0.03458	0.00020
	0.05	0.30736	0.03286	0.00004	0.54025	0.11609	0.00341
	0.10	0.44848	0.02664	0.00006	0.35530	0.15970	0.00981
	0.30	0.64714	0.01530	0.00012	0.11721	0.18171	0.03852
	0.50	0.71043	0.01064	0.00015	0.05667	0.16019	0.06191
	0.75	0.74707	0.00764	0.00018	0.02925	0.13308	0.08279
	1.00	0.76687	0.00594	0.00019	0.01767	0.11209	0.09723
	4.00	0.81558	0.00159	0.00023	0.00127	0.03665	0.14468
	10.00	0.82608	0.00064	0.00024	0.00021	0.01546	0.15736
700	0.01	0.08349	0.12962	0.00012	0.75376	0.03272	0.00028
	0.05	0.29616	0.10408	0.00050	0.48601	0.10853	0.00472
	0.10	0.43517	0.08439	0.00084	0.31951	0.14694	0.01315
	0.30	0.63570	0.04894	0.00157	0.10744	0.15999	0.04636
	0.50	0.70125	0.03456	0.00193	0.05359	0.13876	0.06991
	0.75	0.73971	0.02526	0.00219	0.02863	0.11474	0.08948
	1.00	0.76068	0.01989	0.00234	0.01775	0.09674	0.10259
	4.00	0.81291	0.00558	0.00278	0.00140	0.03227	0.14505
	10.00	0.82431	0.00229	0.00289	0.00023	0.01373	0.15655
800	0.01	0.07622	0.29189	0.00087	0.60175	0.02892	0.00035
	0.05	0.27540	0.23390	0.00357	0.38639	0.09489	0.00585
	0.10	0.41024	0.18907	0.00588	0.25248	0.12644	0.01589
	0.30	0.61314	0.10911	0.01060	0.08408	0.13148	0.05159
	0.50	0.68218	0.07717	0.01272	0.04206	0.11159	0.07428
	0.75	0.72347	0.05659	0.01416	0.02262	0.09110	0.09206
	1.00	0.74626	0.04470	0.01502	0.01411	0.07633	0.10358
	4.00	0.80402	0.01272	0.01743	0.00114	0.02520	0.13949
	10.00	0.81684	0.00523	0.01802	0.00019	0.01072	0.14900
900	0.01	0.06679	0.50023	0.00377	0.40664	0.02220	0.00037
	0.05	0.24766	0.39969	0.01525	0.25961	0.07174	0.00604
	0.10	0.37582	0.32165	0.02476	0.16813	0.09373	0.01592
	0.30	0.57835	0.18347	0.04293	0.05470	0.09270	0.04785
	0.50	0.65013	0.12909	0.05055	0.02708	0.07680	0.06635
	0.75	0.69378	0.09437	0.05555	0.01447	0.06170	0.08013
	1.00	0.71812	0.07441	0.05848	0.00900	0.05121	0.08878
	4.00	0.78060	0.02109	0.06645	0.00072	0.01649	0.11465
	10.00	0.79462	0.00867	0.06834	0.00012	0.00698	0.12126
1000	0.01	0.05818	0.68692	0.00984	0.23189	0.01292	0.00026
	0.05	0.22082	0.54756	0.03921	0.14734	0.04102	0.00405
	0.10	0.34051	0.43897	0.06279	0.09470	0.05265	0.01038
	0.30	0.53693	0.24764	0.10579	0.03014	0.05004	0.02947

TABLE-14 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.60849	0.17321	0.12300	0.01474	0.04070	0.03985
	0.75	0.65245	0.12608	0.13405	0.00781	0.03228	0.04732
	1.00	0.67709	0.09916	0.14041	0.00483	0.02660	0.05192
	4.00	0.74070	0.02789	0.15740	0.00038	0.00838	0.06525
	10.00	0.75504	0.01144	0.16136	0.00006	0.00353	0.06857
1100	0.01	0.05258	0.80681	0.01545	0.11968	0.00538	0.00010
	0.05	0.20264	0.64205	0.06107	0.07579	0.01693	0.00153
	0.10	0.31583	0.51327	0.09709	0.04843	0.02152	0.00386
	0.30	0.50602	0.28706	0.16115	0.01515	0.01998	0.01064
	0.50	0.57644	0.19983	0.18613	0.00734	0.01606	0.01419
	0.75	0.61992	0.14495	0.20193	0.00386	0.01264	0.01670
	1.00	0.64435	0.11375	0.21093	0.00238	0.01036	0.01822
	4.00	0.70756	0.03179	0.23468	0.00019	0.00322	0.02256
	10.00	0.72183	0.01302	0.24014	0.00003	0.00135	0.02362
1200	0.01	0.04966	0.86967	0.01786	0.06083	0.00194	0.00003
	0.05	0.19351	0.69111	0.07044	0.03841	0.00609	0.00044
	0.10	0.30389	0.55121	0.11166	0.02443	0.00770	0.00109
	0.30	0.49237	0.30612	0.18396	0.00754	0.00705	0.00297
	0.50	0.56288	0.21228	0.21166	0.00362	0.00562	0.00393
	0.75	0.60654	0.15355	0.22901	0.00190	0.00440	0.00460
	1.00	0.63110	0.12030	0.23883	0.00116	0.00360	0.00501
	4.00	0.69472	0.03345	0.26450	0.00009	0.00111	0.00614
	10.00	0.70908	0.01369	0.27034	0.00002	0.00046	0.00641
1300	0.01	0.04827	0.90029	0.01856	0.03215	0.00073	0.00001
	0.05	0.18939	0.71473	0.07320	0.02026	0.00229	0.00013
	0.10	0.29884	0.56910	0.11600	0.01285	0.00289	0.00032
	0.30	0.48746	0.31450	0.19061	0.00392	0.00263	0.00087
	0.50	0.55840	0.21752	0.21897	0.00188	0.00209	0.00115
	0.75	0.60237	0.15705	0.23663	0.00098	0.00163	0.00134
	1.00	0.62712	0.12290	0.24660	0.00060	0.00133	0.00146
	4.00	0.69120	0.03406	0.27251	0.00005	0.00041	0.00178
	10.00	0.70566	0.01393	0.27837	0.00001	0.00017	0.00186
1400	0.01	0.04759	0.91525	0.01872	0.01812	0.00031	0.00000
	0.05	0.18748	0.72616	0.07395	0.01141	0.00096	0.00004
	0.10	0.29663	0.57761	0.11722	0.00722	0.00121	0.00011
	0.30	0.48560	0.31826	0.19256	0.00219	0.00110	0.00029
	0.50	0.55683	0.21977	0.22109	0.00105	0.00087	0.00039
	0.75	0.60100	0.15850	0.23882	0.00054	0.00068	0.00045
	1.00	0.62586	0.12396	0.24881	0.00033	0.00055	0.00049
	4.00	0.69020	0.03429	0.27471	0.00003	0.00017	0.00060
	10.00	0.70472	0.01402	0.28056	0.00000	0.00007	0.00063
1500	0.01	0.04724	0.92297	0.01875	0.01089	0.00014	0.00000
	0.05	0.18654	0.73201	0.07414	0.00685	0.00045	0.00002
	0.10	0.29557	0.58192	0.11758	0.00433	0.00056	0.00004
	0.30	0.48481	0.32008	0.19318	0.00131	0.00051	0.00012
	0.50	0.55621	0.22083	0.22178	0.00062	0.00040	0.00015
	0.75	0.60049	0.15917	0.23953	0.00032	0.00031	0.00018
	1.00	0.62540	0.12443	0.24952	0.00020	0.00026	0.00019
	4.00	0.68988	0.03439	0.27541	0.00002	0.00008	0.00023
	10.00	0.70442	0.01405	0.28125	0.00000	0.00003	0.00024

TABLE-15 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O=10.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.16330	0.00772	0.00000	0.79643	0.03244	0.00011
	0.05	0.47485	0.00564	0.00000	0.42616	0.09173	0.00162
	0.10	0.62364	0.00434	0.00000	0.25167	0.11597	0.00438
	0.30	0.78858	0.00227	0.00000	0.06915	0.12228	0.01772
	0.50	0.83271	0.00149	0.00000	0.02981	0.10543	0.03056
	0.75	0.85670	0.00102	0.00000	0.01391	0.08539	0.04297
	1.00	0.86923	0.00077	0.00000	0.00786	0.07043	0.05170
	4.00	0.89879	0.00019	0.00001	0.00047	0.02134	0.07921
	10.00	0.90494	0.00007	0.00001	0.00007	0.00883	0.08608
600	0.01	0.16072	0.03918	0.00001	0.76814	0.03178	0.00018
	0.05	0.46936	0.02865	0.00003	0.41073	0.08861	0.00261
	0.10	0.61810	0.02204	0.00005	0.24305	0.10996	0.00680
	0.30	0.78477	0.01183	0.00009	0.06999	0.10978	0.02354
	0.50	0.82993	0.00805	0.00012	0.03246	0.09301	0.03643
	0.75	0.85464	0.00572	0.00013	0.01636	0.07551	0.04764
	1.00	0.86758	0.00442	0.00014	0.00976	0.06282	0.05528
	4.00	0.89827	0.00117	0.00017	0.00068	0.01993	0.07978
	10.00	0.90468	0.00047	0.00018	0.00011	0.00836	0.08620
700	0.01	0.15375	0.12416	0.00012	0.69160	0.03012	0.00026
	0.05	0.45453	0.09053	0.00044	0.36769	0.08315	0.00366
	0.10	0.60309	0.06941	0.00070	0.21614	0.10140	0.00926
	0.30	0.77427	0.03729	0.00124	0.06237	0.09605	0.02878
	0.50	0.82201	0.02568	0.00149	0.02957	0.07958	0.04167
	0.75	0.84851	0.01848	0.00167	0.01532	0.06400	0.05202
	1.00	0.86252	0.01443	0.00177	0.00934	0.05313	0.05880
	4.00	0.89617	0.00396	0.00207	0.00070	0.01703	0.08007
	10.00	0.90328	0.00162	0.00214	0.00012	0.00718	0.08567
800	0.01	0.14096	0.27949	0.00084	0.55169	0.02670	0.00032
	0.05	0.42723	0.20246	0.00317	0.28949	0.07303	0.00462
	0.10	0.57537	0.15384	0.00499	0.16715	0.08724	0.01142
	0.30	0.75415	0.08107	0.00841	0.04641	0.07749	0.03246
	0.50	0.80610	0.05551	0.00986	0.02176	0.06219	0.04459
	0.75	0.83541	0.03989	0.01081	0.01124	0.04902	0.05363
	1.00	0.85108	0.03115	0.01137	0.00685	0.04025	0.05930
	4.00	0.88922	0.00860	0.01288	0.00052	0.01259	0.07619
	10.00	0.89740	0.00351	0.01324	0.00009	0.00529	0.08048
900	0.01	0.12440	0.47869	0.00365	0.37238	0.02054	0.00035
	0.05	0.39114	0.34359	0.01360	0.19184	0.05501	0.00481
	0.10	0.53784	0.25792	0.02099	0.10811	0.06371	0.01144
	0.30	0.72401	0.13219	0.03365	0.02840	0.05235	0.02940
	0.50	0.78002	0.08946	0.03850	0.01300	0.04054	0.03848
	0.75	0.81198	0.06382	0.04155	0.00662	0.03121	0.04482
	1.00	0.82917	0.04963	0.04328	0.00400	0.02528	0.04864
	4.00	0.87129	0.01355	0.04783	0.00030	0.00763	0.05940
	10.00	0.88036	0.00553	0.04887	0.00005	0.00318	0.06201
1000	0.01	0.10931	0.65696	0.00948	0.21211	0.01190	0.00024
	0.05	0.35666	0.46765	0.03439	0.10748	0.03072	0.00311
	0.10	0.50029	0.34738	0.05169	0.05930	0.03430	0.00704
	0.30	0.68967	0.17393	0.07891	0.01487	0.02622	0.01640

TABLE-15 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.74788	0.11652	0.08856	0.00667	0.01971	0.02065
	0.75	0.78129	0.08258	0.09441	0.00335	0.01489	0.02348
	1.00	0.79929	0.06397	0.09767	0.00201	0.01194	0.02512
	4.00	0.84346	0.01729	0.10600	0.00015	0.00350	0.02959
	10.00	0.85299	0.00703	0.10787	0.00002	0.00145	0.03064
1100	0.01	0.09950	0.77131	0.01479	0.10938	0.00493	0.00009
	0.05	0.33381	0.54578	0.05222	0.05477	0.01231	0.00112
	0.10	0.47524	0.40236	0.07686	0.02976	0.01335	0.00242
	0.30	0.66661	0.19809	0.11315	0.00721	0.00968	0.00524
	0.50	0.72625	0.13174	0.12527	0.00319	0.00713	0.00643
	0.75	0.76056	0.09292	0.13243	0.00159	0.00531	0.00718
	1.00	0.77907	0.07179	0.13635	0.00095	0.00423	0.00762
	4.00	0.82452	0.01926	0.14618	0.00007	0.00122	0.00875
	10.00	0.83432	0.00782	0.14834	0.00001	0.00050	0.00901
1200	0.01	0.09441	0.83118	0.01706	0.05556	0.00177	0.00003
	0.05	0.32258	0.58563	0.05953	0.02758	0.00436	0.00031
	0.10	0.46371	0.42939	0.08676	0.01483	0.00466	0.00066
	0.30	0.65750	0.20887	0.12546	0.00351	0.00328	0.00138
	0.50	0.71828	0.13820	0.13793	0.00154	0.00239	0.00167
	0.75	0.75328	0.09715	0.14519	0.00076	0.00177	0.00185
	1.00	0.77216	0.07491	0.14913	0.00045	0.00140	0.00195
	4.00	0.81849	0.02000	0.15887	0.00003	0.00040	0.00222
	10.00	0.82847	0.00811	0.16098	0.00001	0.00016	0.00227
1300	0.01	0.09197	0.86029	0.01771	0.02935	0.00067	0.00001
	0.05	0.31757	0.60451	0.06170	0.01449	0.00164	0.00009
	0.10	0.45894	0.44173	0.08967	0.00774	0.00174	0.00019
	0.30	0.65440	0.21332	0.12888	0.00180	0.00121	0.00040
	0.50	0.71581	0.14072	0.14133	0.00079	0.00087	0.00048
	0.75	0.75117	0.09874	0.14853	0.00039	0.00064	0.00053
	1.00	0.77023	0.07606	0.15242	0.00023	0.00051	0.00056
	4.00	0.81697	0.02025	0.16199	0.00002	0.00014	0.00063
	10.00	0.82703	0.00821	0.16406	0.00000	0.00006	0.00065
1400	0.01	0.09079	0.87451	0.01787	0.01655	0.00028	0.00000
	0.05	0.31527	0.61356	0.06231	0.00814	0.00068	0.00003
	0.10	0.45687	0.44748	0.09052	0.00433	0.00072	0.00007
	0.30	0.65324	0.21524	0.12988	0.00100	0.00050	0.00013
	0.50	0.71497	0.14176	0.14231	0.00043	0.00036	0.00016
	0.75	0.75049	0.09937	0.14948	0.00021	0.00027	0.00018
	1.00	0.76963	0.07650	0.15334	0.00013	0.00021	0.00019
	4.00	0.81655	0.02034	0.16283	0.00001	0.00006	0.00021
	10.00	0.82665	0.00824	0.16487	0.00000	0.00002	0.00022
1500	0.01	0.09019	0.88184	0.01791	0.00994	0.00013	0.00000
	0.05	0.31413	0.61817	0.06248	0.00489	0.00032	0.00001
	0.10	0.45589	0.45037	0.09079	0.00259	0.00034	0.00003
	0.30	0.65275	0.21616	0.13021	0.00060	0.00023	0.00005
	0.50	0.71463	0.14224	0.14263	0.00026	0.00017	0.00006
	0.75	0.75024	0.09966	0.14979	0.00013	0.00012	0.00007
	1.00	0.76942	0.07669	0.15364	0.00008	0.00010	0.00007
	4.00	0.81642	0.02037	0.16309	0.00001	0.00003	0.00008
	10.00	0.82653	0.00825	0.16513	0.00000	0.00001	0.00008

TABLE-16 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P= 5 ATM,N/O=20.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.28068	0.00715	0.00000	0.68419	0.02788	0.00009
	0.05	0.64366	0.00464	0.00000	0.28842	0.06217	0.00110
	0.10	0.76792	0.00340	0.00000	0.15459	0.07139	0.00270
	0.30	0.88160	0.00170	0.00000	0.03847	0.06829	0.00993
	0.50	0.90859	0.00110	0.00000	0.01617	0.05743	0.01672
	0.75	0.92273	0.00075	0.00000	0.00744	0.04589	0.02319
	1.00	0.92997	0.00056	0.00000	0.00418	0.03758	0.02771
	4.00	0.94668	0.00014	0.00000	0.00025	0.01120	0.04173
	10.00	0.95009	0.00005	0.00000	0.00004	0.00462	0.04519
600	0.01	0.27658	0.03630	0.00001	0.65962	0.02734	0.00015
	0.05	0.63756	0.02352	0.00003	0.27694	0.06016	0.00179
	0.10	0.76260	0.01721	0.00004	0.14817	0.06775	0.00424
	0.30	0.87846	0.00875	0.00007	0.03828	0.06110	0.01334
	0.50	0.90639	0.00587	0.00009	0.01722	0.05033	0.02011
	0.75	0.92113	0.00413	0.00010	0.00853	0.04021	0.02590
	1.00	0.92871	0.00318	0.00011	0.00505	0.03317	0.02980
	4.00	0.94629	0.00083	0.00013	0.00035	0.01031	0.04210
	10.00	0.94990	0.00033	0.00013	0.00006	0.00430	0.04528
700	0.01	0.26548	0.11499	0.00011	0.59320	0.02600	0.00022
	0.05	0.62119	0.07394	0.00037	0.24529	0.05666	0.00255
	0.10	0.74839	0.05363	0.00056	0.12903	0.06250	0.00589
	0.30	0.87004	0.02697	0.00094	0.03262	0.05280	0.01663
	0.50	0.90032	0.01818	0.00112	0.01483	0.04219	0.02336
	0.75	0.91654	0.01292	0.00124	0.00749	0.03319	0.02861
	1.00	0.92496	0.01002	0.00131	0.00451	0.02722	0.03199
	4.00	0.94475	0.00271	0.00150	0.00033	0.00845	0.04226
	10.00	0.94886	0.00110	0.00155	0.00005	0.00354	0.04490
800	0.01	0.24517	0.25853	0.00079	0.47207	0.02316	0.00029
	0.05	0.59152	0.16360	0.00268	0.18903	0.04987	0.00330
	0.10	0.72288	0.11647	0.00403	0.09581	0.05335	0.00745
	0.30	0.85465	0.05638	0.00642	0.02245	0.04116	0.01894
	0.50	0.88868	0.03751	0.00738	0.00994	0.03147	0.02501
	0.75	0.90716	0.02649	0.00799	0.00496	0.02407	0.02933
	1.00	0.91682	0.02049	0.00834	0.00296	0.01943	0.03196
	4.00	0.93975	0.00551	0.00927	0.00021	0.00581	0.03945
	10.00	0.94455	0.00224	0.00948	0.00004	0.00241	0.04128
900	0.01	0.21895	0.44199	0.00343	0.31747	0.01785	0.00031
	0.05	0.55327	0.27338	0.01149	0.12145	0.03698	0.00343
	0.10	0.68970	0.18999	0.01679	0.05866	0.03754	0.00732
	0.30	0.83257	0.08784	0.02499	0.01254	0.02584	0.01621
	0.50	0.87031	0.05746	0.02787	0.00536	0.01884	0.02016
	0.75	0.89088	0.04016	0.02960	0.00262	0.01399	0.02275
	1.00	0.90166	0.03088	0.03056	0.00155	0.01111	0.02425
	4.00	0.92725	0.00819	0.03300	0.00011	0.00318	0.02827
	10.00	0.93261	0.00332	0.03354	0.00002	0.00131	0.02921
1000	0.01	0.19518	0.60540	0.00886	0.18012	0.01025	0.00021
	0.05	0.51793	0.36638	0.02803	0.06597	0.01962	0.00207
	0.10	0.65827	0.24937	0.03913	0.03056	0.01864	0.00403
	0.30	0.80942	0.11125	0.05406	0.00608	0.01149	0.00770

TABLE-16 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.84974	0.07184	0.05874	0.00254	0.00806	0.00909
	0.75	0.87172	0.04983	0.06144	0.00122	0.00585	0.00994
	1.00	0.88323	0.03815	0.06290	0.00072	0.00458	0.01042
	4.00	0.91053	0.01001	0.06649	0.00005	0.00127	0.01164
	10.00	0.91624	0.00405	0.06727	0.00001	0.00052	0.01192
1100	0.01	0.17981	0.70968	0.01365	0.09260	0.00418	0.00008
	0.05	0.49569	0.42259	0.04077	0.03283	0.00744	0.00068
	0.10	0.63918	0.28336	0.05476	0.01476	0.00670	0.00123
	0.30	0.79635	0.12332	0.07162	0.00280	0.00381	0.00210
	0.50	0.83846	0.07895	0.07645	0.00115	0.00261	0.00239
	0.75	0.86141	0.05447	0.07915	0.00055	0.00186	0.00257
	1.00	0.87341	0.04159	0.08058	0.00032	0.00145	0.00266
	4.00	0.90185	0.01084	0.08401	0.00002	0.00039	0.00289
	10.00	0.90779	0.00437	0.08474	0.00000	0.00016	0.00294
1200	0.01	0.17188	0.76401	0.01565	0.04694	0.00150	0.00002
	0.05	0.48526	0.45010	0.04559	0.01629	0.00257	0.00018
	0.10	0.63110	0.29892	0.06022	0.00719	0.00225	0.00032
	0.30	0.79190	0.12811	0.07692	0.00132	0.00123	0.00052
	0.50	0.83496	0.08159	0.08150	0.00054	0.00083	0.00058
	0.75	0.85840	0.05613	0.08401	0.00025	0.00059	0.00062
	1.00	0.87065	0.04278	0.08533	0.00015	0.00046	0.00064
	4.00	0.89961	0.01110	0.08846	0.00001	0.00012	0.00069
	10.00	0.90565	0.00448	0.08912	0.00000	0.00005	0.00070
1300	0.01	0.16809	0.79033	0.01623	0.02477	0.00056	0.00001
	0.05	0.48071	0.46277	0.04701	0.00849	0.00095	0.00005
	0.10	0.62789	0.30570	0.06178	0.00371	0.00083	0.00009
	0.30	0.79047	0.12996	0.07831	0.00067	0.00045	0.00015
	0.50	0.83395	0.08255	0.08277	0.00027	0.00030	0.00016
	0.75	0.85758	0.05671	0.08520	0.00013	0.00021	0.00017
	1.00	0.86993	0.04318	0.08647	0.00007	0.00016	0.00018
	4.00	0.89909	0.01118	0.08948	0.00000	0.00004	0.00019
	10.00	0.90517	0.00451	0.09011	0.00000	0.00002	0.00019
1400	0.01	0.16626	0.80316	0.01639	0.01396	0.00024	0.00000
	0.05	0.47865	0.46875	0.04743	0.00475	0.00040	0.00002
	0.10	0.62652	0.30879	0.06225	0.00206	0.00034	0.00003
	0.30	0.78995	0.13073	0.07871	0.00037	0.00018	0.00005
	0.50	0.83361	0.08294	0.08313	0.00015	0.00012	0.00005
	0.75	0.85733	0.05693	0.08553	0.00007	0.00009	0.00006
	1.00	0.86971	0.04334	0.08678	0.00004	0.00007	0.00006
	4.00	0.89895	0.01121	0.08975	0.00000	0.00002	0.00006
	10.00	0.90504	0.00452	0.09037	0.00000	0.00001	0.00006
1500	0.01	0.16533	0.80976	0.01642	0.00838	0.00011	0.00000
	0.05	0.47764	0.47176	0.04757	0.00285	0.00018	0.00001
	0.10	0.62588	0.31032	0.06240	0.00123	0.00016	0.00001
	0.30	0.78973	0.13110	0.07885	0.00022	0.00008	0.00002
	0.50	0.83347	0.08311	0.08325	0.00009	0.00006	0.00002
	0.75	0.85723	0.05703	0.08564	0.00004	0.00004	0.00002
	1.00	0.86963	0.04340	0.08689	0.00002	0.00003	0.00002
	4.00	0.89891	0.01122	0.08983	0.00000	0.00001	0.00002
	10.00	0.90500	0.00452	0.09045	0.00000	0.00000	0.00003

TABLE-17 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O= 0.0

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.0	0.00598	0.00000	0.95506	0.03884	0.00013
	0.05	0.0	0.00552	0.00000	0.81624	0.17516	0.00308
	0.10	0.0	0.00502	0.00000	0.67411	0.30924	0.01163
	0.30	0.0	0.00352	0.00000	0.33140	0.58147	0.08360
	0.50	0.0	0.00260	0.00001	0.18092	0.63426	0.18222
	0.75	0.0	0.00192	0.00001	0.09859	0.60013	0.29935
	1.00	0.0	0.00151	0.00001	0.06107	0.54250	0.39490
	4.00	0.0	0.00042	0.00001	0.00472	0.21231	0.78253
	10.00	0.0	0.00017	0.00001	0.00079	0.09348	0.90555
600	0.01	0.0	0.03050	0.00001	0.93110	0.03818	0.00021
	0.05	0.0	0.02823	0.00003	0.79744	0.16938	0.00492
	0.10	0.0	0.02574	0.00006	0.66299	0.29346	0.01776
	0.30	0.0	0.01862	0.00014	0.34713	0.52538	0.10872
	0.50	0.0	0.01434	0.00020	0.20596	0.56647	0.21303
	0.75	0.0	0.01105	0.00025	0.12217	0.54009	0.32644
	1.00	0.0	0.00895	0.00028	0.08021	0.49421	0.41634
	4.00	0.0	0.00270	0.00038	0.00729	0.20460	0.78503
	10.00	0.0	0.00112	0.00041	0.00126	0.09151	0.90569
700	0.01	0.0	0.09818	0.00009	0.86483	0.03660	0.00030
	0.05	0.0	0.09095	0.00042	0.74222	0.15971	0.00669
	0.10	0.0	0.08317	0.00079	0.62070	0.27212	0.02321
	0.30	0.0	0.06149	0.00184	0.33923	0.47048	0.12697
	0.50	0.0	0.04850	0.00250	0.21106	0.50387	0.23406
	0.75	0.0	0.03826	0.00304	0.13136	0.48250	0.34484
	1.00	0.0	0.03155	0.00339	0.08933	0.44479	0.43092
	4.00	0.0	0.01011	0.00458	0.00916	0.19216	0.78400
	10.00	0.0	0.00428	0.00491	0.00164	0.08724	0.90193
800	0.01	0.0	0.22845	0.00064	0.73720	0.03333	0.00038
	0.05	0.0	0.21185	0.00297	0.63396	0.14311	0.00811
	0.10	0.0	0.19423	0.00544	0.53289	0.24026	0.02718
	0.30	0.0	0.14581	0.01221	0.30033	0.40477	0.13688
	0.50	0.0	0.11675	0.01626	0.19255	0.43165	0.24279
	0.75	0.0	0.09348	0.01950	0.12344	0.41445	0.34913
	1.00	0.0	0.07795	0.02166	0.08583	0.38385	0.43071
	4.00	0.0	0.02605	0.02886	0.00958	0.17090	0.76460
	10.00	0.0	0.01117	0.03092	0.00176	0.07853	0.87761
900	0.01	0.0	0.41354	0.00282	0.55582	0.02741	0.00041
	0.05	0.0	0.38387	0.01282	0.47892	0.11586	0.00854
	0.10	0.0	0.35272	0.02313	0.40436	0.19202	0.02777
	0.30	0.0	0.26778	0.05033	0.23306	0.31727	0.13155
	0.50	0.0	0.21652	0.06620	0.15237	0.33738	0.22753
	0.75	0.0	0.17498	0.07878	0.09952	0.32448	0.32224
	1.00	0.0	0.14692	0.08715	0.07016	0.30140	0.39437
	4.00	0.0	0.05045	0.11521	0.00827	0.13682	0.68924
	10.00	0.0	0.02183	0.12334	0.00155	0.06339	0.78989
1000	0.01	0.0	0.60885	0.00795	0.36436	0.01850	0.00033
	0.05	0.0	0.56542	0.03593	0.31423	0.07762	0.00680
	0.10	0.0	0.52006	0.06437	0.26584	0.12790	0.02183
	0.30	0.0	0.39669	0.13830	0.15467	0.20960	0.10074

TABLE-17 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.0	0.32203	0.18095	0.10193	0.22263	0.17247
	0.75	0.0	0.26123	0.21468	0.06707	0.21426	0.24276
	1.00	0.0	0.21995	0.23711	0.04755	0.19925	0.29613
	4.00	0.0	0.07638	0.31246	0.00573	0.09117	0.51425
	10.00	0.0	0.03318	0.33435	0.00108	0.04239	0.58896
1100	0.01	0.0	0.76243	0.01426	0.21375	0.00939	0.00017
	0.05	0.0	0.70771	0.06496	0.18417	0.03971	0.00346
	0.10	0.0	0.65031	0.11714	0.15551	0.06580	0.01124
	0.30	0.0	0.49404	0.25453	0.08975	0.10861	0.05308
	0.50	0.0	0.39986	0.33432	0.05879	0.11546	0.09157
	0.75	0.0	0.32354	0.39747	0.03849	0.11107	0.12943
	1.00	0.0	0.27194	0.43945	0.02719	0.10322	0.15821
	4.00	0.0	0.09384	0.58016	0.00324	0.04702	0.27575
	10.00	0.0	0.04069	0.62097	0.00061	0.02182	0.31591
1200	0.01	0.0	0.85928	0.01802	0.11876	0.00388	0.00006
	0.05	0.0	0.79718	0.08287	0.10221	0.01654	0.00121
	0.10	0.0	0.73161	0.15070	0.08609	0.02760	0.00399
	0.30	0.0	0.55241	0.33299	0.04908	0.04605	0.01946
	0.50	0.0	0.44478	0.44034	0.03182	0.04903	0.03404
	0.75	0.0	0.35812	0.52563	0.02063	0.04712	0.04850
	1.00	0.0	0.29992	0.58236	0.01447	0.04372	0.05953
	4.00	0.0	0.10204	0.77196	0.00167	0.01972	0.10461
	10.00	0.0	0.04404	0.82659	0.00031	0.00911	0.11994
1300	0.01	0.0	0.91297	0.01935	0.06612	0.00155	0.00002
	0.05	0.0	0.84679	0.08932	0.05688	0.00663	0.00038
	0.10	0.0	0.77672	0.16305	0.04785	0.01111	0.00128
	0.30	0.0	0.58469	0.36324	0.02712	0.01862	0.00633
	0.50	0.0	0.46943	0.48209	0.01748	0.01985	0.01115
	0.75	0.0	0.37692	0.57678	0.01127	0.01906	0.01597
	1.00	0.0	0.31498	0.63982	0.00787	0.01767	0.01965
	4.00	0.0	0.10623	0.85025	0.00090	0.00792	0.03470
	10.00	0.0	0.04571	0.91067	0.00017	0.00365	0.03980
1400	0.01	0.0	0.94129	0.01970	0.03834	0.00066	0.00001
	0.05	0.0	0.87298	0.09107	0.03298	0.00284	0.00013
	0.10	0.0	0.80055	0.16651	0.02773	0.00477	0.00044
	0.30	0.0	0.60182	0.37228	0.01567	0.00802	0.00221
	0.50	0.0	0.48256	0.49492	0.01008	0.00854	0.00390
	0.75	0.0	0.38695	0.59278	0.00648	0.00821	0.00559
	1.00	0.0	0.32303	0.65796	0.00452	0.00760	0.00689
	4.00	0.0	0.10848	0.87542	0.00051	0.00340	0.01219
	10.00	0.0	0.04661	0.93774	0.00009	0.00156	0.01399
1500	0.01	0.0	0.95654	0.01976	0.02339	0.00031	0.00000
	0.05	0.0	0.88707	0.09143	0.02012	0.00133	0.00005
	0.10	0.0	0.81337	0.16730	0.01692	0.00224	0.00017
	0.30	0.0	0.61100	0.37482	0.00955	0.00377	0.00087
	0.50	0.0	0.48957	0.49876	0.00613	0.00402	0.00153
	0.75	0.0	0.39227	0.59774	0.00393	0.00386	0.00220
	1.00	0.0	0.32729	0.66368	0.00274	0.00357	0.00271
	4.00	0.0	0.10965	0.88364	0.00031	0.00159	0.00481
	10.00	0.0	0.04707	0.94661	0.00006	0.00073	0.00552

TABLE-18 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O= 1.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.01917	0.00592	0.00000	0.93669	0.03809	0.00013
	0.05	0.08311	0.00529	0.00000	0.74820	0.16058	0.00282
	0.10	0.14253	0.00465	0.00000	0.57775	0.26511	0.00997
	0.30	0.27232	0.00300	0.00000	0.24089	0.42293	0.06085
	0.50	0.33298	0.00212	0.00000	0.12051	0.42282	0.12157
	0.75	0.37471	0.00152	0.00001	0.06155	0.37500	0.18721
	1.00	0.39976	0.00117	0.00001	0.03660	0.32539	0.23706
	4.00	0.47051	0.00031	0.00001	0.00250	0.11233	0.41434
	10.00	0.48777	0.00012	0.00001	0.00040	0.04785	0.46385
600	0.01	0.01894	0.03021	0.00001	0.91318	0.03745	0.00021
	0.05	0.08221	0.02702	0.00003	0.73087	0.15535	0.00452
	0.10	0.14115	0.02382	0.00005	0.56798	0.25174	0.01526
	0.30	0.27055	0.01586	0.00012	0.25184	0.38229	0.07934
	0.50	0.33136	0.01169	0.00016	0.13675	0.37753	0.14251
	0.75	0.37333	0.00871	0.00020	0.07595	0.33716	0.20465
	1.00	0.39857	0.00691	0.00022	0.04783	0.29600	0.25047
	4.00	0.47006	0.00196	0.00028	0.00383	0.10791	0.41597
	10.00	0.48754	0.00080	0.00029	0.00064	0.04667	0.46406
700	0.01	0.01830	0.09723	0.00009	0.84818	0.03591	0.00030
	0.05	0.07969	0.08706	0.00041	0.68003	0.14666	0.00615
	0.10	0.13731	0.07694	0.00073	0.53116	0.23383	0.02003
	0.30	0.26539	0.05224	0.00158	0.24488	0.34263	0.09328
	0.50	0.32643	0.03936	0.00205	0.13898	0.33554	0.15763
	0.75	0.36892	0.03000	0.00241	0.08074	0.30042	0.21751
	1.00	0.39463	0.02420	0.00264	0.05255	0.26532	0.26065
	4.00	0.46810	0.00724	0.00334	0.00471	0.10036	0.41625
	10.00	0.48621	0.00301	0.00352	0.00081	0.04398	0.46246
800	0.01	0.01705	0.22624	0.00064	0.72299	0.03272	0.00037
	0.05	0.07477	0.20272	0.00286	0.58047	0.13169	0.00750
	0.10	0.12967	0.17950	0.00507	0.45511	0.20702	0.02363
	0.30	0.25447	0.12335	0.01052	0.21490	0.29509	0.10167
	0.50	0.31542	0.09405	0.01342	0.12495	0.28689	0.16527
	0.75	0.35848	0.07255	0.01556	0.07436	0.25670	0.22235
	1.00	0.38480	0.05907	0.01692	0.04928	0.22718	0.26276
	4.00	0.46133	0.01830	0.02106	0.00473	0.08758	0.40701
	10.00	0.48053	0.00769	0.02214	0.00083	0.03870	0.45011
900	0.01	0.01527	0.40953	0.00279	0.54508	0.02693	0.00041
	0.05	0.06752	0.36718	0.01236	0.43819	0.10682	0.00793
	0.10	0.11805	0.32560	0.02164	0.34455	0.16584	0.02431
	0.30	0.23605	0.22539	0.04359	0.16510	0.23123	0.09864
	0.50	0.29536	0.17295	0.05486	0.09722	0.22334	0.15627
	0.75	0.33800	0.13422	0.06310	0.05855	0.19936	0.20677
	1.00	0.36440	0.10974	0.06828	0.03914	0.17637	0.24207
	4.00	0.44269	0.03456	0.08401	0.00388	0.06835	0.36651
	10.00	0.46274	0.01460	0.08816	0.00069	0.03029	0.40352
1000	0.01	0.01336	0.60294	0.00789	0.35731	0.01817	0.00033
	0.05	0.05936	0.54079	0.03461	0.28744	0.07150	0.00631
	0.10	0.10428	0.47987	0.06016	0.22634	0.11029	0.01906
	0.30	0.21101	0.33312	0.11950	0.10907	0.15209	0.07521

TABLE-18 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.26572	0.25614	0.14954	0.06448	0.14633	0.11778
	0.75	0.30554	0.19910	0.17137	0.03896	0.13035	0.15468
	1.00	0.33040	0.16298	0.18501	0.02611	0.11520	0.18029
	4.00	0.40521	0.05153	0.22632	0.00261	0.04455	0.26978
	10.00	0.42465	0.02179	0.23714	0.00047	0.01974	0.29621
1100	0.01	0.01183	0.75504	0.01413	0.20962	0.00921	0.00016
	0.05	0.05253	0.67704	0.06228	0.16855	0.03642	0.00318
	0.10	0.09220	0.60048	0.10868	0.13259	0.05637	0.00968
	0.30	0.18637	0.41595	0.21731	0.06362	0.07807	0.03869
	0.50	0.23470	0.31928	0.27254	0.03748	0.07516	0.06085
	0.75	0.26991	0.24780	0.31269	0.02258	0.06692	0.08010
	1.00	0.29192	0.20262	0.33778	0.01510	0.05911	0.09347
	4.00	0.35827	0.06379	0.41355	0.00150	0.02279	0.14011
	10.00	0.37554	0.02694	0.43333	0.00027	0.01008	0.15384
1200	0.01	0.01088	0.85096	0.01784	0.11647	0.00380	0.00006
	0.05	0.04825	0.76276	0.07918	0.09358	0.01512	0.00110
	0.10	0.08465	0.67596	0.13899	0.07349	0.02352	0.00339
	0.30	0.17079	0.46649	0.28104	0.03500	0.03282	0.01386
	0.50	0.21483	0.35701	0.35402	0.02050	0.03164	0.02200
	0.75	0.24682	0.27636	0.40725	0.01228	0.02818	0.02911
	1.00	0.26678	0.22554	0.44055	0.00818	0.02487	0.03407
	4.00	0.32669	0.07052	0.54105	0.00080	0.00955	0.05139
	10.00	0.34221	0.02972	0.56723	0.00014	0.00422	0.05648
1300	0.01	0.01035	0.90412	0.01915	0.06484	0.00152	0.00002
	0.05	0.04602	0.81021	0.08528	0.05207	0.00606	0.00035
	0.10	0.08088	0.71761	0.15014	0.04085	0.00945	0.00108
	0.30	0.16374	0.49389	0.30532	0.01935	0.01322	0.00447
	0.50	0.20623	0.37715	0.38545	0.01128	0.01275	0.00713
	0.75	0.23712	0.29135	0.44398	0.00673	0.01134	0.00946
	1.00	0.25639	0.23744	0.48060	0.00447	0.01001	0.01109
	4.00	0.31416	0.07385	0.59097	0.00043	0.00383	0.01676
	10.00	0.32909	0.03107	0.61964	0.00008	0.00169	0.01843
1400	0.01	0.01008	0.93217	0.01950	0.03760	0.00065	0.00001
	0.05	0.04491	0.83521	0.08698	0.03018	0.00260	0.00012
	0.10	0.07908	0.73946	0.15336	0.02366	0.00406	0.00037
	0.30	0.16080	0.50799	0.31280	0.01117	0.00568	0.00156
	0.50	0.20289	0.38732	0.39533	0.00649	0.00548	0.00249
	0.75	0.23355	0.29880	0.45562	0.00386	0.00487	0.00330
	1.00	0.25268	0.24327	0.49333	0.00256	0.00429	0.00387
	4.00	0.31007	0.07539	0.60680	0.00025	0.00164	0.00586
	10.00	0.32490	0.03168	0.63621	0.00004	0.00072	0.00644
1500	0.01	0.00993	0.94726	0.01956	0.02294	0.00030	0.00000
	0.05	0.04433	0.84863	0.08735	0.01841	0.00122	0.00005
	0.10	0.07819	0.75115	0.15418	0.01443	0.00190	0.00015
	0.30	0.15949	0.51537	0.31508	0.00679	0.00267	0.00061
	0.50	0.20150	0.39254	0.39847	0.00394	0.00257	0.00098
	0.75	0.23214	0.30255	0.45939	0.00234	0.00229	0.00130
	1.00	0.25127	0.24616	0.49748	0.00155	0.00201	0.00153
	4.00	0.30868	0.07611	0.61198	0.00015	0.00077	0.00231
	10.00	0.32352	0.03196	0.64162	0.00003	0.00034	0.00254

TABLE-19 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O= 2.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.03763	0.00586	0.00000	0.91901	0.03738	0.00012
	0.05	0.15346	0.00508	0.00000	0.69062	0.14824	0.00261
	0.10	0.24946	0.00435	0.00000	0.50547	0.23200	0.00873
	0.30	0.42800	0.00266	0.00000	0.18918	0.33232	0.04784
	0.50	0.49954	0.00184	0.00000	0.09031	0.31708	0.09123
	0.75	0.54510	0.00129	0.00000	0.04472	0.27266	0.13622
	1.00	0.57114	0.00099	0.00001	0.02612	0.23235	0.16939
	4.00	0.63992	0.00025	0.00001	0.00170	0.07635	0.28178
	10.00	0.65570	0.00010	0.00001	0.00027	0.03214	0.31178
600	0.01	0.03717	0.02992	0.00001	0.89595	0.03675	0.00021
	0.05	0.15185	0.02596	0.00003	0.67452	0.14347	0.00417
	0.10	0.24721	0.02228	0.00005	0.49668	0.22041	0.01337
	0.30	0.42554	0.01404	0.00011	0.19739	0.30041	0.06251
	0.50	0.49744	0.01010	0.00014	0.10218	0.28298	0.10716
	0.75	0.54339	0.00741	0.00017	0.05498	0.24490	0.14916
	1.00	0.56971	0.00583	0.00018	0.03398	0.21106	0.17923
	4.00	0.63941	0.00161	0.00023	0.00259	0.07315	0.28302
	10.00	0.65544	0.00065	0.00024	0.00043	0.03126	0.31197
700	0.01	0.03592	0.09631	0.00009	0.83215	0.03525	0.00029
	0.05	0.14738	0.08362	0.00039	0.62732	0.13559	0.00570
	0.10	0.24093	0.07190	0.00069	0.46387	0.20499	0.01763
	0.30	0.41838	0.04613	0.00141	0.19096	0.26925	0.07387
	0.50	0.49108	0.03389	0.00178	0.10304	0.25112	0.11909
	0.75	0.53797	0.02539	0.00206	0.05785	0.21755	0.15918
	1.00	0.56500	0.02028	0.00224	0.03690	0.18841	0.18717
	4.00	0.63723	0.00590	0.00275	0.00313	0.06750	0.28349
	10.00	0.65399	0.00244	0.00288	0.00053	0.02919	0.31096
800	0.01	0.03350	0.22408	0.00063	0.70929	0.03213	0.00037
	0.05	0.13866	0.19462	0.00276	0.53503	0.12196	0.00698
	0.10	0.22846	0.16753	0.00477	0.39647	0.18184	0.02093
	0.30	0.40332	0.10842	0.00940	0.16605	0.23169	0.08112
	0.50	0.47697	0.08041	0.01170	0.09133	0.21390	0.12569
	0.75	0.52522	0.06085	0.01335	0.05231	0.18468	0.16360
	1.00	0.55333	0.04897	0.01437	0.03387	0.15995	0.18951
	4.00	0.62974	0.01467	0.01738	0.00304	0.05796	0.27720
	10.00	0.64778	0.00611	0.01814	0.00053	0.02522	0.30221
900	0.01	0.03003	0.40562	0.00277	0.53472	0.02646	0.00040
	0.05	0.12583	0.35232	0.01195	0.40344	0.09906	0.00741
	0.10	0.20952	0.30341	0.02042	0.29919	0.14581	0.02165
	0.30	0.37801	0.19696	0.03902	0.12608	0.18089	0.07905
	0.50	0.45139	0.14655	0.04790	0.06980	0.16523	0.11913
	0.75	0.50034	0.11127	0.05414	0.04024	0.14180	0.15220
	1.00	0.52922	0.08977	0.05796	0.02619	0.12246	0.17440
	4.00	0.60919	0.02717	0.06910	0.00240	0.04419	0.24795
	10.00	0.62843	0.01136	0.07193	0.00042	0.01923	0.26864
1000	0.01	0.02632	0.59717	0.00782	0.35051	0.01785	0.00032
	0.05	0.11138	0.51869	0.03341	0.26443	0.06621	0.00588
	0.10	0.18709	0.44664	0.05664	0.19608	0.09665	0.01690
	0.30	0.34366	0.28981	0.10644	0.08255	0.11786	0.05968

TABLE-19 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.41369	0.21555	0.12969	0.04567	0.10680	0.08860
	0.75	0.46106	0.16360	0.14584	0.02631	0.09116	0.11203
	1.00	0.48926	0.13195	0.15564	0.01711	0.07846	0.12758
	4.00	0.56838	0.03989	0.18394	0.00156	0.02803	0.17820
	10.00	0.58764	0.01667	0.19103	0.00027	0.01217	0.19222
1100	0.01	0.02336	0.74781	0.01400	0.20563	0.00904	0.00016
	0.05	0.09929	0.64932	0.05986	0.15503	0.03357	0.00294
	0.10	0.16746	0.55873	0.10156	0.11479	0.04901	0.00845
	0.30	0.31022	0.36139	0.19091	0.04802	0.05959	0.02986
	0.50	0.37485	0.26814	0.23247	0.02644	0.05384	0.04427
	0.75	0.41883	0.20308	0.26121	0.01516	0.04582	0.05590
	1.00	0.44511	0.16354	0.27859	0.00983	0.03935	0.06358
	4.00	0.51916	0.04917	0.32845	0.00089	0.01395	0.08838
	10.00	0.53726	0.02051	0.34085	0.00015	0.00604	0.09518
1200	0.01	0.02150	0.84280	0.01766	0.11425	0.00373	0.00005
	0.05	0.09175	0.73146	0.07584	0.08606	0.01389	0.00101
	0.10	0.15526	0.62880	0.12909	0.06360	0.02032	0.00293
	0.30	0.28952	0.40503	0.24390	0.02639	0.02473	0.01044
	0.50	0.35076	0.29958	0.29740	0.01444	0.02230	0.01553
	0.75	0.39255	0.22629	0.33436	0.00824	0.01894	0.01962
	1.00	0.41756	0.18189	0.35666	0.00532	0.01624	0.02233
	4.00	0.48810	0.05434	0.42035	0.00048	0.00572	0.03102
	10.00	0.50534	0.02263	0.43610	0.00008	0.00247	0.03338
1300	0.01	0.02048	0.89545	0.01896	0.06360	0.00149	0.00002
	0.05	0.08781	0.77683	0.08161	0.04787	0.00556	0.00032
	0.10	0.14920	0.66722	0.13919	0.03531	0.00814	0.00093
	0.30	0.28030	0.42819	0.26373	0.01454	0.00990	0.00334
	0.50	0.34060	0.31586	0.32175	0.00791	0.00891	0.00497
	0.75	0.38187	0.23804	0.36176	0.00449	0.00755	0.00628
	1.00	0.40660	0.19105	0.38585	0.00290	0.00646	0.00715
	4.00	0.47644	0.05678	0.45436	0.00026	0.00226	0.00991
	10.00	0.49350	0.02361	0.47121	0.00004	0.00098	0.01066
1400	0.01	0.01995	0.92322	0.01930	0.03688	0.00064	0.00001
	0.05	0.08585	0.80066	0.08325	0.02774	0.00238	0.00011
	0.10	0.14632	0.68724	0.14218	0.02044	0.00350	0.00032
	0.30	0.27648	0.43982	0.26992	0.00837	0.00425	0.00116
	0.50	0.33669	0.32380	0.32942	0.00454	0.00382	0.00173
	0.75	0.37799	0.24363	0.37040	0.00257	0.00323	0.00218
	1.00	0.40276	0.19532	0.39503	0.00165	0.00276	0.00248
	4.00	0.47273	0.05784	0.46489	0.00014	0.00096	0.00344
	10.00	0.48982	0.02403	0.48202	0.00002	0.00041	0.00370
1500	0.01	0.01967	0.93816	0.01937	0.02250	0.00030	0.00000
	0.05	0.08484	0.81344	0.08363	0.01692	0.00112	0.00004
	0.10	0.14489	0.69790	0.14300	0.01245	0.00164	0.00013
	0.30	0.27478	0.44581	0.27188	0.00508	0.00199	0.00046
	0.50	0.33507	0.32779	0.33192	0.00275	0.00179	0.00068
	0.75	0.37647	0.24636	0.37324	0.00155	0.00151	0.00086
	1.00	0.40131	0.19737	0.39806	0.00100	0.00129	0.00098
	4.00	0.47148	0.05831	0.46832	0.00009	0.00045	0.00135
	10.00	0.48862	0.02421	0.48552	0.00001	0.00019	0.00145

TABLE-20 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O= 3.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.05539	0.00581	0.00000	0.90199	0.03668	0.00012
	0.05	0.21376	0.00490	0.00000	0.64126	0.13766	0.00242
	0.10	0.33265	0.00410	0.00000	0.44924	0.20625	0.00776
	0.30	0.52877	0.00241	0.00000	0.15572	0.27368	0.03942
	0.50	0.59951	0.00164	0.00000	0.07220	0.25363	0.07302
	0.75	0.64249	0.00115	0.00000	0.03511	0.21418	0.10707
	1.00	0.66637	0.00087	0.00000	0.02029	0.18066	0.13179
	4.00	0.72719	0.00022	0.00001	0.00128	0.05781	0.21349
	10.00	0.74071	0.00009	0.00001	0.00020	0.02419	0.23480
600	0.01	0.05473	0.02964	0.00001	0.87934	0.03608	0.00020
	0.05	0.21160	0.02501	0.00003	0.62619	0.13328	0.00388
	0.10	0.32983	0.02100	0.00005	0.44120	0.19602	0.01191
	0.30	0.52602	0.01273	0.00010	0.16217	0.24739	0.05160
	0.50	0.59726	0.00902	0.00013	0.08146	0.22623	0.08591
	0.75	0.64070	0.00656	0.00015	0.04301	0.19218	0.11740
	1.00	0.66490	0.00513	0.00016	0.02631	0.16389	0.13961
	4.00	0.72669	0.00139	0.00020	0.00195	0.05527	0.21450
	10.00	0.74045	0.00057	0.00021	0.00032	0.02347	0.23498
700	0.01	0.05290	0.09541	0.00009	0.81671	0.03461	0.00029
	0.05	0.20562	0.08055	0.00038	0.58208	0.12607	0.00531
	0.10	0.32194	0.06772	0.00065	0.41146	0.18248	0.01575
	0.30	0.51803	0.04171	0.00128	0.15612	0.22163	0.06122
	0.50	0.59048	0.03015	0.00160	0.08155	0.20040	0.09582
	0.75	0.63508	0.02236	0.00183	0.04485	0.17020	0.12568
	1.00	0.66009	0.01775	0.00198	0.02827	0.14574	0.14617
	4.00	0.72455	0.00509	0.00240	0.00232	0.05065	0.21499
	10.00	0.73904	0.00209	0.00250	0.00039	0.02175	0.23422
800	0.01	0.04937	0.22199	0.00063	0.69608	0.03157	0.00036
	0.05	0.19392	0.18738	0.00267	0.49594	0.11357	0.00652
	0.10	0.30632	0.15757	0.00453	0.35070	0.16209	0.01880
	0.30	0.50131	0.09759	0.00858	0.13452	0.19039	0.06761
	0.50	0.57553	0.07106	0.01052	0.07133	0.16996	0.10160
	0.75	0.62196	0.05313	0.01188	0.03988	0.14353	0.12961
	1.00	0.64828	0.04246	0.01271	0.02546	0.12271	0.14838
	4.00	0.71724	0.01247	0.01513	0.00220	0.04290	0.21007
	10.00	0.73300	0.00517	0.01573	0.00038	0.01850	0.22721
900	0.01	0.04432	0.40181	0.00275	0.52472	0.02601	0.00039
	0.05	0.17673	0.33897	0.01157	0.37344	0.09234	0.00695
	0.10	0.28263	0.28482	0.01939	0.26365	0.12999	0.01952
	0.30	0.47333	0.17621	0.03565	0.10091	0.14788	0.06601
	0.50	0.54856	0.12840	0.04306	0.05359	0.13013	0.09626
	0.75	0.59649	0.09613	0.04813	0.03003	0.10891	0.12031
	1.00	0.62397	0.07690	0.05119	0.01922	0.09266	0.13607
	4.00	0.69722	0.02271	0.05992	0.00168	0.03204	0.18643
	10.00	0.71425	0.00944	0.06209	0.00029	0.01379	0.20015
1000	0.01	0.03891	0.59154	0.00776	0.34393	0.01754	0.00032
	0.05	0.15739	0.49872	0.03233	0.24447	0.06159	0.00550
	0.10	0.25463	0.41857	0.05365	0.17220	0.08579	0.01516
	0.30	0.43555	0.25792	0.09667	0.06538	0.09526	0.04922

TABLE-20 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.50907	0.18746	0.11565	0.03454	0.08283	0.07045
	0.75	0.55655	0.14006	0.12846	0.01928	0.06874	0.08692
	1.00	0.58401	0.11189	0.13608	0.01230	0.05817	0.09754
	4.00	0.65803	0.03291	0.15752	0.00106	0.01980	0.13068
	10.00	0.67541	0.01366	0.16275	0.00018	0.00849	0.13951
1100	0.01	0.03459	0.74074	0.01387	0.20176	0.00888	0.00016
	0.05	0.14124	0.62410	0.05764	0.14322	0.03107	0.00272
	0.10	0.23024	0.52311	0.09544	0.10062	0.04312	0.00746
	0.30	0.39928	0.32067	0.17095	0.03781	0.04735	0.02394
	0.50	0.46918	0.23224	0.20383	0.01983	0.04089	0.03404
	0.75	0.51467	0.17299	0.22582	0.01100	0.03374	0.04178
	1.00	0.54109	0.13792	0.23882	0.00699	0.02845	0.04673
	4.00	0.61263	0.04029	0.27497	0.00060	0.00957	0.06194
	10.00	0.62949	0.01669	0.28370	0.00010	0.00409	0.06594
1200	0.01	0.03188	0.83482	0.01749	0.11210	0.00366	0.00005
	0.05	0.13118	0.70284	0.07279	0.07945	0.01281	0.00093
	0.10	0.21519	0.58824	0.12060	0.05566	0.01776	0.00255
	0.30	0.37736	0.35856	0.21584	0.02068	0.01938	0.00818
	0.50	0.44529	0.25869	0.25702	0.01076	0.01664	0.01160
	0.75	0.48970	0.19210	0.28439	0.00594	0.01368	0.01420
	1.00	0.51555	0.15284	0.30050	0.00376	0.01150	0.01585
	4.00	0.58573	0.04435	0.34489	0.00032	0.00383	0.02088
	10.00	0.60228	0.01834	0.35551	0.00005	0.00163	0.02219
1300	0.01	0.03040	0.88695	0.01877	0.06240	0.00146	0.00002
	0.05	0.12595	0.74621	0.07826	0.04417	0.00512	0.00029
	0.10	0.20775	0.62370	0.12979	0.03086	0.00710	0.00081
	0.30	0.36779	0.37825	0.23231	0.01135	0.00771	0.00259
	0.50	0.43548	0.27199	0.27640	0.00587	0.00659	0.00367
	0.75	0.47989	0.20145	0.30557	0.00322	0.00540	0.00448
	1.00	0.50578	0.16000	0.32266	0.00203	0.00453	0.00500
	4.00	0.57612	0.04618	0.36948	0.00017	0.00150	0.00655
	10.00	0.59272	0.01906	0.38060	0.00003	0.00064	0.00695
1400	0.01	0.02962	0.91445	0.01911	0.03618	0.00063	0.00001
	0.05	0.12335	0.76894	0.07983	0.02558	0.00220	0.00010
	0.10	0.20423	0.64205	0.13255	0.01784	0.00304	0.00028
	0.30	0.36385	0.38796	0.23748	0.00651	0.00330	0.00090
	0.50	0.43176	0.27832	0.28249	0.00335	0.00281	0.00127
	0.75	0.47637	0.20576	0.31218	0.00183	0.00230	0.00155
	1.00	0.50240	0.16324	0.32955	0.00115	0.00192	0.00173
	4.00	0.57314	0.04694	0.37694	0.00010	0.00063	0.00226
	10.00	0.58981	0.01936	0.38815	0.00002	0.00027	0.00240
1500	0.01	0.02921	0.92924	0.01918	0.02208	0.00029	0.00000
	0.05	0.12200	0.78111	0.08022	0.01560	0.00103	0.00004
	0.10	0.20248	0.65178	0.13334	0.01086	0.00143	0.00011
	0.30	0.36210	0.39290	0.23915	0.00395	0.00155	0.00035
	0.50	0.43022	0.28144	0.28450	0.00203	0.00132	0.00050
	0.75	0.47500	0.20783	0.31438	0.00110	0.00107	0.00061
	1.00	0.50114	0.16476	0.33183	0.00069	0.00090	0.00068
	4.00	0.57214	0.04727	0.37936	0.00006	0.00029	0.00089
	10.00	0.58887	0.01948	0.39057	0.00001	0.00013	0.00094

TABLE-21 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O= 3.76

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.06850	0.00577	0.00000	0.88944	0.03618	0.00012
	0.05	0.25424	0.00477	0.00000	0.60813	0.13057	0.00230
	0.10	0.38461	0.00393	0.00000	0.41413	0.19016	0.00716
	0.30	0.58453	0.00226	0.00000	0.13721	0.24124	0.03476
	0.50	0.65240	0.00153	0.00000	0.06262	0.22007	0.06338
	0.75	0.69262	0.00106	0.00000	0.03016	0.18409	0.09206
	1.00	0.71465	0.00081	0.00000	0.01735	0.15447	0.11273
	4.00	0.76972	0.00020	0.00001	0.00108	0.04879	0.18021
	10.00	0.78176	0.00008	0.00001	0.00017	0.02036	0.19762
600	0.01	0.06769	0.02943	0.00001	0.86710	0.03558	0.00020
	0.05	0.25174	0.02436	0.00003	0.59376	0.12644	0.00368
	0.10	0.38148	0.02015	0.00005	0.40655	0.18078	0.01099
	0.30	0.58167	0.01194	0.00009	0.14271	0.21804	0.04555
	0.50	0.65012	0.00839	0.00012	0.07051	0.19621	0.07465
	0.75	0.69084	0.00607	0.00014	0.03686	0.16505	0.10104
	1.00	0.71319	0.00473	0.00015	0.02242	0.14000	0.11950
	4.00	0.76923	0.00128	0.00018	0.00164	0.04657	0.18110
	10.00	0.78152	0.00052	0.00019	0.00027	0.01972	0.19778
700	0.01	0.06544	0.09474	0.00009	0.80531	0.03414	0.00028
	0.05	0.24480	0.07841	0.00037	0.55169	0.11968	0.00505
	0.10	0.37273	0.06497	0.00062	0.37871	0.16839	0.01457
	0.30	0.57341	0.03906	0.00120	0.13688	0.19525	0.05419
	0.50	0.64328	0.02798	0.00149	0.07022	0.17356	0.08347
	0.75	0.68525	0.02063	0.00170	0.03819	0.14585	0.10837
	1.00	0.70845	0.01633	0.00183	0.02392	0.12414	0.12533
	4.00	0.76716	0.00464	0.00220	0.00193	0.04247	0.18159
	10.00	0.78015	0.00191	0.00230	0.00033	0.01818	0.19714
800	0.01	0.06110	0.22043	0.00062	0.68634	0.03115	0.00035
	0.05	0.23128	0.18234	0.00260	0.46965	0.10791	0.00622
	0.10	0.35544	0.15100	0.00436	0.32206	0.14969	0.01746
	0.30	0.55618	0.09107	0.00809	0.11714	0.16746	0.06007
	0.50	0.62826	0.06563	0.00983	0.06084	0.14669	0.08874
	0.75	0.67227	0.04875	0.01104	0.03356	0.12239	0.11198
	1.00	0.69686	0.03880	0.01178	0.02126	0.10391	0.12739
	4.00	0.76011	0.01128	0.01390	0.00180	0.03564	0.17728
	10.00	0.77433	0.00467	0.01442	0.00031	0.01530	0.19097
900	0.01	0.05490	0.39897	0.00273	0.51734	0.02568	0.00039
	0.05	0.21140	0.32966	0.01131	0.35321	0.08778	0.00665
	0.10	0.32926	0.27251	0.01871	0.24136	0.12000	0.01817
	0.30	0.52746	0.16369	0.03361	0.08709	0.12950	0.05865
	0.50	0.60130	0.11785	0.04021	0.04514	0.11154	0.08396
	0.75	0.64718	0.08752	0.04468	0.02490	0.09205	0.10366
	1.00	0.67310	0.06969	0.04735	0.01578	0.07767	0.11641
	4.00	0.74086	0.02031	0.05488	0.00134	0.02624	0.15637
	10.00	0.75633	0.00841	0.05672	0.00023	0.01123	0.16707
1000	0.01	0.04826	0.58734	0.00772	0.33906	0.01731	0.00031
	0.05	0.18906	0.48474	0.03156	0.23095	0.05845	0.00525
	0.10	0.29837	0.39988	0.05164	0.15717	0.07889	0.01405
	0.30	0.48885	0.23860	0.09066	0.05595	0.08264	0.04329

TABLE-21 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.56201	0.17109	0.10732	0.02877	0.07015	0.06066
	0.75	0.60808	0.12668	0.11837	0.01577	0.05729	0.07381
	1.00	0.63431	0.10066	0.12489	0.00996	0.04803	0.08215
	4.00	0.70356	0.02916	0.14292	0.00084	0.01592	0.10759
	10.00	0.71952	0.01206	0.14727	0.00014	0.00678	0.11423
1100	0.01	0.04296	0.73546	0.01378	0.19889	0.00875	0.00016
	0.05	0.17044	0.60634	0.05608	0.13519	0.02937	0.00258
	0.10	0.27158	0.49923	0.09133	0.09164	0.03938	0.00683
	0.30	0.45222	0.29581	0.15864	0.03218	0.04053	0.02062
	0.50	0.52298	0.21117	0.18679	0.01640	0.03407	0.02859
	0.75	0.56788	0.15580	0.20526	0.00893	0.02762	0.03452
	1.00	0.59356	0.12351	0.21604	0.00561	0.02305	0.03824
	4.00	0.66164	0.03551	0.24548	0.00046	0.00753	0.04937
	10.00	0.67738	0.01465	0.25247	0.00008	0.00320	0.05222
1200	0.01	0.03963	0.82885	0.01736	0.11050	0.00360	0.00005
	0.05	0.15886	0.68261	0.07063	0.07495	0.01207	0.00088
	0.10	0.25516	0.56091	0.11488	0.05060	0.01613	0.00232
	0.30	0.43052	0.33002	0.19862	0.01752	0.01641	0.00692
	0.50	0.50022	0.23455	0.23316	0.00885	0.01369	0.00954
	0.75	0.54467	0.17244	0.25560	0.00478	0.01103	0.01147
	1.00	0.57016	0.13640	0.26861	0.00299	0.00917	0.01267
	4.00	0.63789	0.03894	0.30377	0.00024	0.00296	0.01620
	10.00	0.65356	0.01604	0.31202	0.00004	0.00125	0.01709
1300	0.01	0.03781	0.88059	0.01863	0.06151	0.00144	0.00002
	0.05	0.15285	0.72452	0.07589	0.04164	0.00482	0.00028
	0.10	0.24707	0.59429	0.12345	0.02802	0.00643	0.00073
	0.30	0.42117	0.34752	0.21306	0.00958	0.00649	0.00218
	0.50	0.49106	0.24607	0.24969	0.00480	0.00539	0.00299
	0.75	0.53577	0.18040	0.27334	0.00258	0.00432	0.00359
	1.00	0.56143	0.14243	0.28699	0.00161	0.00358	0.00395
	4.00	0.62969	0.04044	0.32357	0.00013	0.00115	0.00503
	10.00	0.64548	0.01663	0.33209	0.00002	0.00048	0.00529
1400	0.01	0.03686	0.90788	0.01897	0.03567	0.00062	0.00001
	0.05	0.14987	0.74645	0.07742	0.02411	0.00207	0.00010
	0.10	0.24326	0.61149	0.12606	0.01618	0.00276	0.00025
	0.30	0.41735	0.35605	0.21760	0.00549	0.00277	0.00075
	0.50	0.48761	0.25146	0.25487	0.00274	0.00229	0.00103
	0.75	0.53261	0.18400	0.27884	0.00147	0.00184	0.00124
	1.00	0.55845	0.14510	0.29265	0.00091	0.00152	0.00136
	4.00	0.62718	0.04105	0.32949	0.00007	0.00048	0.00173
	10.00	0.64307	0.01687	0.33803	0.00001	0.00020	0.00182
1500	0.01	0.03635	0.92256	0.01903	0.02176	0.00029	0.00000
	0.05	0.14832	0.75817	0.07781	0.01470	0.00097	0.00004
	0.10	0.24136	0.62058	0.12682	0.00985	0.00129	0.00010
	0.30	0.41565	0.36035	0.21908	0.00332	0.00130	0.00030
	0.50	0.48619	0.25410	0.25659	0.00165	0.00107	0.00041
	0.75	0.53139	0.18571	0.28067	0.00088	0.00086	0.00049
	1.00	0.55734	0.14635	0.29452	0.00055	0.00071	0.00053
	4.00	0.62634	0.04131	0.33140	0.00004	0.00023	0.00068
	10.00	0.64228	0.01696	0.33994	0.00001	0.00009	0.00071

TABLE-22 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O= 5.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.08903	0.00570	0.00000	0.86977	0.03538	0.00012
	0.05	0.31178	0.00458	0.00000	0.56104	0.12047	0.00212
	0.10	0.45370	0.00371	0.00000	0.36746	0.16878	0.00635
	0.30	0.65150	0.00207	0.00000	0.11499	0.20228	0.02916
	0.50	0.71379	0.00139	0.00000	0.05150	0.18112	0.05220
	0.75	0.74964	0.00096	0.00000	0.02454	0.14986	0.07499
	1.00	0.76895	0.00072	0.00000	0.01403	0.12501	0.09128
	4.00	0.81625	0.00018	0.00001	0.00086	0.03891	0.14379
	10.00	0.82641	0.00007	0.00001	0.00014	0.01618	0.15719
600	0.01	0.08799	0.02911	0.00001	0.84791	0.03480	0.00020
	0.05	0.30884	0.02339	0.00003	0.54763	0.11671	0.00340
	0.10	0.45022	0.01898	0.00004	0.36048	0.16050	0.00977
	0.30	0.64859	0.01092	0.00008	0.11934	0.18279	0.03828
	0.50	0.71153	0.00760	0.00011	0.05782	0.16136	0.06157
	0.75	0.74790	0.00546	0.00012	0.02988	0.13421	0.08241
	1.00	0.76755	0.00425	0.00013	0.01806	0.11313	0.09688
	4.00	0.81579	0.00114	0.00016	0.00130	0.03705	0.14455
	10.00	0.82619	0.00046	0.00017	0.00021	0.01564	0.15733
700	0.01	0.08510	0.09368	0.00009	0.78745	0.03340	0.00028
	0.05	0.30068	0.07528	0.00035	0.50844	0.11056	0.00468
	0.10	0.44052	0.06112	0.00059	0.33515	0.14962	0.01300
	0.30	0.64020	0.03562	0.00111	0.11382	0.16354	0.04572
	0.50	0.70479	0.02523	0.00136	0.05713	0.14241	0.06907
	0.75	0.74249	0.01849	0.00154	0.03066	0.11818	0.08864
	1.00	0.76299	0.01458	0.00165	0.01907	0.09989	0.10183
	4.00	0.81385	0.00410	0.00197	0.00151	0.03356	0.14500
	10.00	0.82491	0.00168	0.00205	0.00025	0.01431	0.15680
800	0.01	0.07953	0.21796	0.00062	0.67105	0.03050	0.00035
	0.05	0.28478	0.17492	0.00251	0.43218	0.09983	0.00579
	0.10	0.42138	0.14178	0.00413	0.28394	0.13311	0.01566
	0.30	0.62281	0.08260	0.00745	0.09638	0.13985	0.05091
	0.50	0.69010	0.05877	0.00896	0.04879	0.11970	0.07369
	0.75	0.73001	0.04329	0.01000	0.02648	0.09842	0.09179
	1.00	0.75195	0.03430	0.01063	0.01662	0.08285	0.10365
	4.00	0.80724	0.00985	0.01241	0.00137	0.02778	0.14136
	10.00	0.81946	0.00406	0.01285	0.00023	0.01186	0.15154
900	0.01	0.07155	0.39447	0.00271	0.50574	0.02515	0.00038
	0.05	0.26144	0.31588	0.01093	0.32431	0.08125	0.00620
	0.10	0.39252	0.25518	0.01774	0.21164	0.10657	0.01635
	0.30	0.59402	0.14742	0.03093	0.07063	0.10733	0.04967
	0.50	0.66389	0.10453	0.03658	0.03551	0.09001	0.06948
	0.75	0.70604	0.07687	0.04035	0.01920	0.07300	0.08453
	1.00	0.72945	0.06085	0.04257	0.01203	0.06098	0.09412
	4.00	0.78930	0.01745	0.04876	0.00099	0.02003	0.12346
	10.00	0.80270	0.00720	0.05026	0.00017	0.00852	0.13115
1000	0.01	0.06302	0.58067	0.00764	0.33141	0.01695	0.00031
	0.05	0.23525	0.46395	0.03042	0.21157	0.05393	0.00488
	0.10	0.35859	0.37344	0.04878	0.13707	0.06959	0.01253
	0.30	0.55561	0.21342	0.08272	0.04477	0.06745	0.03604

TABLE-22 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.62606	0.15043	0.09660	0.02224	0.05552	0.04915
	0.75	0.66909	0.11013	0.10564	0.01192	0.04445	0.05878
	1.00	0.69314	0.08694	0.11089	0.00743	0.03683	0.06477
	4.00	0.75514	0.02473	0.12517	0.00060	0.01183	0.08253
	10.00	0.76912	0.01018	0.12855	0.00010	0.00500	0.08705
1100	0.01	0.05622	0.72707	0.01363	0.19438	0.00856	0.00015
	0.05	0.21350	0.57984	0.05375	0.12363	0.02692	0.00237
	0.10	0.32939	0.46525	0.08545	0.07959	0.03434	0.00598
	0.30	0.51990	0.26326	0.14237	0.02548	0.03237	0.01661
	0.50	0.58949	0.18449	0.16494	0.01251	0.02628	0.02229
	0.75	0.63231	0.13448	0.17937	0.00665	0.02083	0.02636
	1.00	0.65633	0.10586	0.18767	0.00412	0.01716	0.02885
	4.00	0.71849	0.02986	0.20984	0.00033	0.00541	0.03607
	10.00	0.73254	0.01226	0.21500	0.00006	0.00228	0.03787
1200	0.01	0.05194	0.81935	0.01715	0.10798	0.00352	0.00005
	0.05	0.20005	0.65230	0.06741	0.06844	0.01101	0.00080
	0.10	0.31169	0.52184	0.10673	0.04380	0.01394	0.00200
	0.30	0.49940	0.29252	0.17600	0.01376	0.01289	0.00544
	0.50	0.56903	0.20389	0.20282	0.00669	0.01035	0.00722
	0.75	0.61209	0.14803	0.21974	0.00352	0.00814	0.00848
	1.00	0.63630	0.11624	0.22937	0.00217	0.00667	0.00924
	4.00	0.69906	0.03254	0.25476	0.00017	0.00208	0.01139
	10.00	0.71325	0.01334	0.26059	0.00003	0.00087	0.01192
1300	0.01	0.04960	0.87047	0.01840	0.06010	0.00140	0.00002
	0.05	0.19308	0.69196	0.07234	0.03798	0.00439	0.00025
	0.10	0.30305	0.55218	0.11442	0.02419	0.00554	0.00063
	0.30	0.49076	0.30715	0.18786	0.00748	0.00506	0.00169
	0.50	0.56104	0.21317	0.21591	0.00360	0.00404	0.00224
	0.75	0.60460	0.15429	0.23345	0.00189	0.00316	0.00262
	1.00	0.62911	0.12092	0.24338	0.00116	0.00258	0.00284
	4.00	0.69267	0.03366	0.26931	0.00009	0.00079	0.00348
	10.00	0.70703	0.01378	0.27521	0.00002	0.00033	0.00364
1400	0.01	0.04839	0.89742	0.01874	0.03485	0.00060	0.00001
	0.05	0.18962	0.71264	0.07379	0.02198	0.00188	0.00009
	0.10	0.29898	0.56770	0.11679	0.01395	0.00237	0.00022
	0.30	0.48726	0.31415	0.19158	0.00427	0.00215	0.00058
	0.50	0.55807	0.21743	0.21998	0.00205	0.00171	0.00077
	0.75	0.60198	0.15706	0.23766	0.00107	0.00134	0.00090
	1.00	0.62670	0.12294	0.24764	0.00065	0.00109	0.00098
	4.00	0.69074	0.03410	0.27358	0.00005	0.00033	0.00119
	10.00	0.70520	0.01395	0.27946	0.00001	0.00014	0.00124
1500	0.01	0.04774	0.91191	0.01881	0.02126	0.00028	0.00000
	0.05	0.18783	0.72368	0.07418	0.01339	0.00088	0.00003
	0.10	0.29696	0.57586	0.11750	0.00848	0.00111	0.00009
	0.30	0.48572	0.31764	0.19282	0.00258	0.00101	0.00023
	0.50	0.55685	0.21948	0.22134	0.00123	0.00080	0.00030
	0.75	0.60097	0.15835	0.23906	0.00064	0.00062	0.00035
	1.00	0.62580	0.12387	0.24905	0.00039	0.00051	0.00038
	4.00	0.69010	0.03429	0.27495	0.00003	0.00016	0.00047
	10.00	0.70462	0.01402	0.28081	0.00001	0.00006	0.00049

TABLE-23 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM,N/O=10.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.16349	0.00546	0.00000	0.79846	0.03248	0.00011
	0.05	0.47524	0.00400	0.00000	0.42733	0.09181	0.00162
	0.10	0.62404	0.00307	0.00000	0.25245	0.11606	0.00437
	0.30	0.78884	0.00161	0.00000	0.06946	0.12241	0.01768
	0.50	0.83289	0.00106	0.00000	0.02996	0.10559	0.03049
	0.75	0.85683	0.00072	0.00000	0.01398	0.08556	0.04290
	1.00	0.86933	0.00054	0.00000	0.00790	0.07058	0.05164
	4.00	0.89881	0.00013	0.00000	0.00047	0.02139	0.07918
	10.00	0.90495	0.00005	0.00000	0.00007	0.00885	0.08607
600	0.01	0.16165	0.02789	0.00001	0.77832	0.03196	0.00018
	0.05	0.47133	0.02040	0.00002	0.41661	0.08904	0.00260
	0.10	0.62008	0.01571	0.00004	0.24695	0.11047	0.00676
	0.30	0.78611	0.00845	0.00007	0.07154	0.11049	0.02333
	0.50	0.83090	0.00577	0.00008	0.03330	0.09382	0.03614
	0.75	0.85535	0.00410	0.00009	0.01682	0.07631	0.04733
	1.00	0.86814	0.00317	0.00010	0.01004	0.06356	0.05499
	4.00	0.89845	0.00084	0.00012	0.00070	0.02022	0.07967
	10.00	0.90477	0.00034	0.00013	0.00011	0.00848	0.08617
700	0.01	0.15657	0.08974	0.00008	0.72262	0.03072	0.00025
	0.05	0.46051	0.06554	0.00031	0.38545	0.08457	0.00361
	0.10	0.60910	0.05039	0.00049	0.22778	0.10315	0.00909
	0.30	0.77836	0.02730	0.00087	0.06686	0.09842	0.02819
	0.50	0.82503	0.01889	0.00105	0.03202	0.08208	0.04094
	0.75	0.85079	0.01365	0.00117	0.01671	0.06638	0.05131
	1.00	0.86438	0.01068	0.00125	0.01023	0.05530	0.05816
	4.00	0.89689	0.00295	0.00146	0.00078	0.01791	0.08000
	10.00	0.90375	0.00120	0.00151	0.00013	0.00757	0.08583
800	0.01	0.14678	0.20874	0.00059	0.61545	0.02812	0.00032
	0.05	0.43953	0.15176	0.00222	0.32533	0.07663	0.00453
	0.10	0.58767	0.11597	0.00348	0.18996	0.09179	0.01113
	0.30	0.76263	0.06212	0.00588	0.05450	0.08309	0.03178
	0.50	0.81257	0.04292	0.00692	0.02602	0.06756	0.04401
	0.75	0.84057	0.03105	0.00762	0.01361	0.05380	0.05334
	1.00	0.85549	0.02434	0.00804	0.00837	0.04447	0.05929
	4.00	0.89169	0.00680	0.00919	0.00065	0.01419	0.07748
	10.00	0.89944	0.00278	0.00946	0.00011	0.00599	0.08222
900	0.01	0.13277	0.37761	0.00261	0.46343	0.02323	0.00035
	0.05	0.40897	0.27260	0.00971	0.24152	0.06230	0.00489
	0.10	0.55584	0.20632	0.01500	0.13835	0.07282	0.01168
	0.30	0.73723	0.10805	0.02430	0.03794	0.06181	0.03067
	0.50	0.79086	0.07392	0.02800	0.01776	0.04873	0.04072
	0.75	0.82134	0.05314	0.03038	0.00918	0.03801	0.04794
	1.00	0.83770	0.04152	0.03176	0.00560	0.03104	0.05237
	4.00	0.87778	0.01149	0.03545	0.00043	0.00959	0.06526
	10.00	0.88642	0.00470	0.03631	0.00007	0.00402	0.06848
1000	0.01	0.11779	0.55557	0.00736	0.30337	0.01563	0.00029
	0.05	0.37505	0.39801	0.02677	0.15570	0.04070	0.00377
	0.10	0.51916	0.29822	0.04047	0.08741	0.04611	0.00863
	0.30	0.70449	0.15252	0.06279	0.02286	0.03658	0.02076

TABLE-23 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.76074	0.10321	0.07102	0.01047	0.02800	0.02656
	0.75	0.79296	0.07365	0.07612	0.00533	0.02142	0.03052
	1.00	0.81031	0.05729	0.07901	0.00323	0.01729	0.03288
	4.00	0.85295	0.01566	0.08653	0.00024	0.00518	0.03944
	10.00	0.86216	0.00639	0.08824	0.00004	0.00215	0.04102
1100	0.01	0.10587	0.69532	0.01305	0.17777	0.00784	0.00014
	0.05	0.34736	0.49487	0.04622	0.09005	0.01975	0.00175
	0.10	0.48875	0.36764	0.06838	0.04970	0.02171	0.00383
	0.30	0.67647	0.18428	0.10201	0.01249	0.01624	0.00852
	0.50	0.73451	0.12355	0.11362	0.00561	0.01213	0.01058
	0.75	0.76790	0.08761	0.12062	0.00282	0.00913	0.01192
	1.00	0.78592	0.06790	0.12449	0.00170	0.00730	0.01270
	4.00	0.83024	0.01838	0.13434	0.00012	0.00213	0.01479
	10.00	0.83981	0.00748	0.13654	0.00002	0.00088	0.01527
1200	0.01	0.09839	0.78330	0.01637	0.09869	0.00321	0.00005
	0.05	0.33060	0.55441	0.05706	0.04944	0.00792	0.00057
	0.10	0.47120	0.40889	0.08328	0.02689	0.00852	0.00122
	0.30	0.66210	0.20152	0.12115	0.00653	0.00611	0.00258
	0.50	0.72179	0.13409	0.13361	0.00289	0.00449	0.00313
	0.75	0.75620	0.09461	0.14093	0.00144	0.00334	0.00349
	1.00	0.77477	0.07311	0.14493	0.00086	0.00265	0.00369
	4.00	0.82044	0.01963	0.15490	0.00006	0.00076	0.00421
	10.00	0.83029	0.00797	0.15708	0.00001	0.00031	0.00433
1300	0.01	0.09430	0.83195	0.01755	0.05490	0.00128	0.00001
	0.05	0.32206	0.58643	0.06092	0.02728	0.00313	0.00018
	0.10	0.46291	0.43021	0.08849	0.01468	0.00334	0.00038
	0.30	0.65648	0.20952	0.12740	0.00348	0.00234	0.00078
	0.50	0.71726	0.13870	0.13987	0.00153	0.00170	0.00094
	0.75	0.75229	0.09754	0.14712	0.00075	0.00126	0.00104
	1.00	0.77118	0.07522	0.15105	0.00045	0.00100	0.00110
	4.00	0.81760	0.02009	0.16076	0.00003	0.00028	0.00124
	10.00	0.82760	0.00815	0.16286	0.00001	0.00012	0.00127
1400	0.01	0.09218	0.85757	0.01788	0.03182	0.00055	0.00001
	0.05	0.31785	0.60291	0.06211	0.01573	0.00134	0.00006
	0.10	0.45907	0.44083	0.09013	0.00841	0.00142	0.00013
	0.30	0.65427	0.21317	0.12934	0.00197	0.00099	0.00027
	0.50	0.71564	0.14070	0.14177	0.00086	0.00071	0.00032
	0.75	0.75098	0.09876	0.14896	0.00042	0.00053	0.00035
	1.00	0.77003	0.07609	0.15285	0.00025	0.00042	0.00037
	4.00	0.81678	0.02027	0.16240	0.00002	0.00012	0.00042
	10.00	0.82684	0.00821	0.16446	0.00000	0.00005	0.00043
1500	0.01	0.09104	0.87134	0.01795	0.01941	0.00026	0.00000
	0.05	0.31569	0.61163	0.06246	0.00956	0.00063	0.00002
	0.10	0.45719	0.44633	0.09067	0.00509	0.00067	0.00005
	0.30	0.65331	0.21495	0.12999	0.00118	0.00046	0.00010
	0.50	0.71498	0.14164	0.14241	0.00051	0.00033	0.00013
	0.75	0.75048	0.09931	0.14958	0.00025	0.00024	0.00014
	1.00	0.76961	0.07647	0.15344	0.00015	0.00019	0.00015
	4.00	0.81651	0.02034	0.16292	0.00001	0.00005	0.00016
	10.00	0.82660	0.00824	0.16496	0.00000	0.00002	0.00017

TABLE-24 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=10 ATM, N/O=20.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.28098	0.00506	0.00000	0.68595	0.02791	0.00009
	0.05	0.64410	0.00329	0.00000	0.28930	0.06222	0.00110
	0.10	0.76830	0.00241	0.00000	0.15515	0.07144	0.00270
	0.30	0.88182	0.00120	0.00000	0.03869	0.06838	0.00990
	0.50	0.90874	0.00078	0.00000	0.01628	0.05754	0.01667
	0.75	0.92283	0.00053	0.00000	0.00749	0.04600	0.02314
	1.00	0.93005	0.00040	0.00000	0.00421	0.03769	0.02766
	4.00	0.94670	0.00010	0.00000	0.00025	0.01124	0.04171
	10.00	0.95010	0.00004	0.00000	0.00004	0.00463	0.04519
600	0.01	0.27805	0.02584	0.00001	0.66846	0.02749	0.00015
	0.05	0.63975	0.01676	0.00002	0.28129	0.06041	0.00177
	0.10	0.76450	0.01228	0.00003	0.15097	0.06804	0.00419
	0.30	0.87956	0.00627	0.00005	0.03937	0.06157	0.01317
	0.50	0.90715	0.00422	0.00006	0.01781	0.05089	0.01988
	0.75	0.92167	0.00297	0.00007	0.00885	0.04077	0.02567
	1.00	0.92913	0.00229	0.00007	0.00524	0.03368	0.02958
	4.00	0.94642	0.00060	0.00009	0.00036	0.01051	0.04202
	10.00	0.94996	0.00024	0.00009	0.00006	0.00439	0.04526
700	0.01	0.26997	0.08314	0.00008	0.62012	0.02648	0.00022
	0.05	0.62777	0.05365	0.00026	0.25829	0.05753	0.00249
	0.10	0.75404	0.03910	0.00039	0.13718	0.06355	0.00573
	0.30	0.87327	0.01993	0.00066	0.03562	0.05437	0.01615
	0.50	0.90259	0.01353	0.00078	0.01643	0.04387	0.02280
	0.75	0.91822	0.00967	0.00087	0.00838	0.03478	0.02809
	1.00	0.92631	0.00752	0.00092	0.00507	0.02866	0.03153
	4.00	0.94527	0.00204	0.00106	0.00038	0.00902	0.04222
	10.00	0.94920	0.00083	0.00110	0.00006	0.00379	0.04502
800	0.01	0.25440	0.19320	0.00055	0.52724	0.02432	0.00028
	0.05	0.60480	0.12327	0.00186	0.21464	0.05224	0.00319
	0.10	0.73406	0.08866	0.00279	0.11104	0.05629	0.00716
	0.30	0.86096	0.04400	0.00448	0.02735	0.04480	0.01841
	0.50	0.89327	0.02963	0.00518	0.01240	0.03489	0.02463
	0.75	0.91074	0.02110	0.00564	0.00629	0.02705	0.02919
	1.00	0.91986	0.01639	0.00591	0.00380	0.02201	0.03203
	4.00	0.94149	0.00447	0.00663	0.00028	0.00674	0.04039
	10.00	0.94602	0.00182	0.00680	0.00005	0.00282	0.04249
900	0.01	0.23219	0.34901	0.00245	0.39589	0.02014	0.00031
	0.05	0.57195	0.21877	0.00817	0.15555	0.04209	0.00347
	0.10	0.70527	0.15430	0.01200	0.07738	0.04358	0.00748
	0.30	0.84186	0.07358	0.01821	0.01760	0.03154	0.01722
	0.50	0.87760	0.04876	0.02051	0.00773	0.02354	0.02185
	0.75	0.89708	0.03437	0.02194	0.00384	0.01775	0.02500
	1.00	0.90730	0.02656	0.02275	0.00229	0.01422	0.02688
	4.00	0.93160	0.00714	0.02485	0.00017	0.00418	0.03207
	10.00	0.93671	0.00290	0.02533	0.00003	0.00173	0.03331
1000	0.01	0.20852	0.51261	0.00688	0.25827	0.01347	0.00025
	0.05	0.53646	0.31495	0.02203	0.09750	0.02651	0.00256
	0.10	0.67352	0.21768	0.03118	0.04657	0.02593	0.00512
	0.30	0.81873	0.09992	0.04429	0.00981	0.01691	0.01033

TABLE-24 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.85732	0.06524	0.04866	0.00418	0.01213	0.01247
	0.75	0.87840	0.04556	0.05125	0.00204	0.00892	0.01383
	1.00	0.88945	0.03502	0.05267	0.00121	0.00705	0.01461
	4.00	0.91573	0.00928	0.05625	0.00008	0.00199	0.01666
	10.00	0.92124	0.00376	0.05704	0.00001	0.00082	0.01713
1100	0.01	0.18978	0.64051	0.01206	0.15085	0.00667	0.00012
	0.05	0.50868	0.38659	0.03650	0.05495	0.01219	0.00109
	0.10	0.64914	0.26260	0.04962	0.02536	0.01126	0.00202
	0.30	0.80156	0.11686	0.06627	0.00502	0.00669	0.00360
	0.50	0.84241	0.07542	0.07127	0.00209	0.00464	0.00416
	0.75	0.86473	0.05229	0.07412	0.00101	0.00335	0.00450
	1.00	0.87643	0.04003	0.07565	0.00059	0.00262	0.00469
	4.00	0.90420	0.01050	0.07938	0.00004	0.00072	0.00516
	10.00	0.91002	0.00424	0.08018	0.00001	0.00029	0.00527
1200	0.01	0.17808	0.72063	0.01502	0.08353	0.00271	0.00004
	0.05	0.49268	0.42882	0.04388	0.02958	0.00471	0.00034
	0.10	0.63629	0.28739	0.05825	0.01328	0.00419	0.00060
	0.30	0.79409	0.12498	0.07508	0.00251	0.00235	0.00099
	0.50	0.83645	0.07999	0.07981	0.00103	0.00160	0.00112
	0.75	0.85956	0.05519	0.08243	0.00049	0.00114	0.00119
	1.00	0.87165	0.04213	0.08382	0.00029	0.00088	0.00123
	4.00	0.90031	0.01098	0.08713	0.00002	0.00024	0.00133
	10.00	0.90629	0.00443	0.08782	0.00000	0.00010	0.00135
1300	0.01	0.17172	0.76473	0.01607	0.04639	0.00108	0.00001
	0.05	0.48479	0.45072	0.04644	0.01611	0.00184	0.00010
	0.10	0.63056	0.29945	0.06109	0.00711	0.00160	0.00018
	0.30	0.79143	0.12841	0.07769	0.00131	0.00087	0.00029
	0.50	0.83454	0.08180	0.08222	0.00053	0.00059	0.00032
	0.75	0.85801	0.05628	0.08469	0.00025	0.00042	0.00034
	1.00	0.87028	0.04290	0.08599	0.00015	0.00032	0.00035
	4.00	0.89931	0.01113	0.08908	0.00001	0.00009	0.00038
	10.00	0.90536	0.00449	0.08973	0.00000	0.00004	0.00039
1400	0.01	0.16841	0.78789	0.01637	0.02686	0.00046	0.00000
	0.05	0.48097	0.46174	0.04725	0.00923	0.00078	0.00004
	0.10	0.62798	0.30525	0.06200	0.00403	0.00068	0.00006
	0.30	0.79042	0.12991	0.07848	0.00073	0.00036	0.00010
	0.50	0.83387	0.08255	0.08292	0.00029	0.00024	0.00011
	0.75	0.85751	0.05672	0.08535	0.00014	0.00017	0.00012
	1.00	0.86986	0.04320	0.08661	0.00008	0.00013	0.00012
	4.00	0.89903	0.01119	0.08961	0.00001	0.00004	0.00013
	10.00	0.90511	0.00451	0.09024	0.00000	0.00001	0.00013
1500	0.01	0.16665	0.80031	0.01645	0.01638	0.00022	0.00000
	0.05	0.47903	0.46749	0.04751	0.00559	0.00037	0.00001
	0.10	0.62673	0.30819	0.06231	0.00243	0.00032	0.00002
	0.30	0.78998	0.13062	0.07875	0.00044	0.00017	0.00004
	0.50	0.83361	0.08290	0.08316	0.00018	0.00011	0.00004
	0.75	0.85732	0.05691	0.08556	0.00008	0.00008	0.00005
	1.00	0.86970	0.04333	0.08682	0.00005	0.00006	0.00005
	4.00	0.89894	0.01121	0.08978	0.00000	0.00002	0.00005
	10.00	0.90503	0.00452	0.09040	0.00000	0.00001	0.00005

TABLE-25 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O= 0.0

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.0	0.00488	0.00000	0.95613	0.03886	0.00013
	0.05	0.0	0.00451	0.00000	0.81716	0.17525	0.00308
	0.10	0.0	0.00410	0.00000	0.67487	0.30940	0.01162
	0.30	0.0	0.00288	0.00000	0.33179	0.58175	0.08359
	0.50	0.0	0.00212	0.00000	0.18112	0.63456	0.18218
	0.75	0.0	0.00157	0.00001	0.09869	0.60041	0.29932
	1.00	0.0	0.00123	0.00001	0.06113	0.54275	0.39487
	4.00	0.0	0.00034	0.00001	0.00472	0.21239	0.78253
	10.00	0.0	0.00014	0.00001	0.00079	0.09351	0.90555
600	0.01	0.0	0.02498	0.00001	0.93651	0.03829	0.00021
	0.05	0.0	0.02311	0.00002	0.80209	0.16985	0.00492
	0.10	0.0	0.02108	0.00005	0.66687	0.29426	0.01775
	0.30	0.0	0.01525	0.00012	0.34918	0.52679	0.10867
	0.50	0.0	0.01175	0.00016	0.20715	0.56800	0.21294
	0.75	0.0	0.00905	0.00020	0.12286	0.54153	0.32636
	1.00	0.0	0.00733	0.00023	0.08065	0.49552	0.41627
	4.00	0.0	0.00221	0.00031	0.00733	0.20508	0.78507
	10.00	0.0	0.00092	0.00034	0.00127	0.09172	0.90576
700	0.01	0.0	0.08094	0.00007	0.88173	0.03695	0.00030
	0.05	0.0	0.07499	0.00035	0.75673	0.16125	0.00669
	0.10	0.0	0.06857	0.00064	0.63284	0.27474	0.02321
	0.30	0.0	0.05069	0.00150	0.34584	0.47502	0.12695
	0.50	0.0	0.03998	0.00204	0.21513	0.50875	0.23410
	0.75	0.0	0.03154	0.00248	0.13385	0.48715	0.34498
	1.00	0.0	0.02600	0.00277	0.09101	0.44906	0.43116
	4.00	0.0	0.00832	0.00374	0.00932	0.19391	0.78470
	10.00	0.0	0.00352	0.00401	0.00167	0.08802	0.90278
800	0.01	0.0	0.19111	0.00052	0.77382	0.03418	0.00038
	0.05	0.0	0.17722	0.00243	0.66542	0.14680	0.00813
	0.10	0.0	0.16247	0.00445	0.55928	0.24653	0.02727
	0.30	0.0	0.12194	0.00999	0.31504	0.41552	0.13751
	0.50	0.0	0.09761	0.01331	0.20189	0.44314	0.24404
	0.75	0.0	0.07814	0.01597	0.12938	0.42546	0.35105
	1.00	0.0	0.06515	0.01774	0.08993	0.39403	0.43316
	4.00	0.0	0.02176	0.02364	0.01003	0.17536	0.76922
	10.00	0.0	0.00933	0.02532	0.00184	0.08057	0.88293
900	0.01	0.0	0.35473	0.00232	0.61347	0.02906	0.00042
	0.05	0.0	0.32926	0.01057	0.52853	0.12293	0.00871
	0.10	0.0	0.30251	0.01909	0.44614	0.20389	0.02838
	0.30	0.0	0.22956	0.04160	0.25690	0.33716	0.13478
	0.50	0.0	0.18556	0.05473	0.16787	0.35856	0.23328
	0.75	0.0	0.14993	0.06514	0.10960	0.34484	0.33049
	1.00	0.0	0.12588	0.07207	0.07725	0.32030	0.40450
	4.00	0.0	0.04322	0.09527	0.00911	0.14540	0.70700
	10.00	0.0	0.01871	0.10199	0.00171	0.06737	0.81022
1000	0.01	0.0	0.54076	0.00677	0.43112	0.02098	0.00036
	0.05	0.0	0.50219	0.03058	0.37182	0.08802	0.00739
	0.10	0.0	0.46192	0.05478	0.31457	0.14501	0.02371
	0.30	0.0	0.35243	0.11761	0.18312	0.23754	0.10929

TABLE-25 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.0	0.28619	0.15382	0.12076	0.25228	0.18694
	0.75	0.0	0.23225	0.18244	0.07953	0.24282	0.26296
	1.00	0.0	0.19562	0.20146	0.05642	0.22585	0.32065
	4.00	0.0	0.06805	0.26535	0.00683	0.10348	0.55630
	10.00	0.0	0.02958	0.28395	0.00129	0.04814	0.63703
1100	0.01	0.0	0.70268	0.01297	0.27234	0.01180	0.00021
	0.05	0.0	0.65237	0.05888	0.23473	0.04976	0.00426
	0.10	0.0	0.59969	0.10590	0.19836	0.08228	0.01378
	0.30	0.0	0.45646	0.22888	0.11492	0.13536	0.06438
	0.50	0.0	0.37007	0.29998	0.07554	0.14383	0.11058
	0.75	0.0	0.29993	0.35617	0.04962	0.13840	0.15589
	1.00	0.0	0.25241	0.39350	0.03514	0.12868	0.19028
	4.00	0.0	0.08756	0.51872	0.00423	0.05884	0.33065
	10.00	0.0	0.03804	0.55512	0.00080	0.02736	0.37869
1200	0.01	0.0	0.81641	0.01738	0.16081	0.00533	0.00008
	0.05	0.0	0.75752	0.07969	0.13845	0.02267	0.00167
	0.10	0.0	0.69548	0.14456	0.11670	0.03776	0.00550
	0.30	0.0	0.52621	0.31765	0.06681	0.06277	0.02657
	0.50	0.0	0.42450	0.41900	0.04348	0.06679	0.04623
	0.75	0.0	0.34246	0.49936	0.02830	0.06422	0.06566
	1.00	0.0	0.28723	0.55278	0.01990	0.05962	0.08046
	4.00	0.0	0.09835	0.73144	0.00233	0.02701	0.14087
	10.00	0.0	0.04254	0.78306	0.00044	0.01251	0.16146
1300	0.01	0.0	0.88529	0.01919	0.09325	0.00223	0.00003
	0.05	0.0	0.82120	0.08844	0.08024	0.00955	0.00056
	0.10	0.0	0.75343	0.16118	0.06754	0.01597	0.00187
	0.30	0.0	0.56796	0.35772	0.03838	0.02672	0.00921
	0.50	0.0	0.45664	0.47392	0.02481	0.02847	0.01617
	0.75	0.0	0.36716	0.56635	0.01604	0.02735	0.02309
	1.00	0.0	0.30717	0.62785	0.01123	0.02537	0.02838
	4.00	0.0	0.10409	0.83323	0.00129	0.01141	0.04998
	10.00	0.0	0.04487	0.89231	0.00024	0.00527	0.05732
1400	0.01	0.0	0.92389	0.01972	0.05540	0.00098	0.00001
	0.05	0.0	0.85690	0.09106	0.04766	0.00419	0.00020
	0.10	0.0	0.78594	0.16629	0.04009	0.00701	0.00066
	0.30	0.0	0.59142	0.37083	0.02270	0.01177	0.00328
	0.50	0.0	0.47468	0.49236	0.01463	0.01254	0.00579
	0.75	0.0	0.38101	0.58923	0.00942	0.01205	0.00829
	1.00	0.0	0.31833	0.65373	0.00658	0.01117	0.01020
	4.00	0.0	0.10726	0.86897	0.00075	0.00500	0.01802
	10.00	0.0	0.04614	0.93074	0.00014	0.00230	0.02067
1500	0.01	0.0	0.94543	0.01982	0.03428	0.00046	0.00000
	0.05	0.0	0.87682	0.09164	0.02949	0.00198	0.00008
	0.10	0.0	0.80407	0.16755	0.02480	0.00332	0.00026
	0.30	0.0	0.60445	0.37465	0.01401	0.00559	0.00130
	0.50	0.0	0.48466	0.49809	0.00901	0.00595	0.00229
	0.75	0.0	0.38862	0.59658	0.00579	0.00572	0.00329
	1.00	0.0	0.32442	0.66219	0.00404	0.00530	0.00405
	4.00	0.0	0.10894	0.88106	0.00046	0.00237	0.00718
	10.00	0.0	0.04681	0.94378	0.00008	0.00109	0.00824

TABLE-26 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O= 1.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.01918	0.00483	0.00000	0.93774	0.03811	0.00013
	0.05	0.08315	0.00432	0.00000	0.74904	0.16066	0.00282
	0.10	0.14259	0.00380	0.00000	0.57841	0.26524	0.00997
	0.30	0.27239	0.00245	0.00000	0.24120	0.42313	0.06083
	0.50	0.33304	0.00173	0.00000	0.12066	0.42302	0.12153
	0.75	0.37477	0.00124	0.00000	0.06163	0.37519	0.18717
	1.00	0.39981	0.00096	0.00001	0.03664	0.32556	0.23702
	4.00	0.47053	0.00025	0.00001	0.00250	0.11239	0.41433
	10.00	0.48778	0.00010	0.00001	0.00040	0.04787	0.46384
600	0.01	0.01899	0.02473	0.00001	0.91850	0.03756	0.00021
	0.05	0.08241	0.02213	0.00002	0.73515	0.15577	0.00451
	0.10	0.14146	0.01951	0.00004	0.57135	0.25239	0.01524
	0.30	0.27094	0.01299	0.00010	0.25344	0.38328	0.07925
	0.50	0.33172	0.00957	0.00013	0.13764	0.37857	0.14236
	0.75	0.37363	0.00714	0.00016	0.07645	0.33814	0.20448
	1.00	0.39883	0.00566	0.00018	0.04815	0.29688	0.25030
	4.00	0.47016	0.00160	0.00023	0.00385	0.10824	0.41593
	10.00	0.48759	0.00066	0.00024	0.00065	0.04681	0.46406
700	0.01	0.01846	0.08016	0.00007	0.86476	0.03625	0.00030
	0.05	0.08033	0.07178	0.00033	0.69338	0.14803	0.00615
	0.10	0.13828	0.06344	0.00060	0.54171	0.23597	0.02000
	0.30	0.26667	0.04310	0.00129	0.24998	0.34585	0.09310
	0.50	0.32764	0.03248	0.00167	0.14197	0.33886	0.15737
	0.75	0.36999	0.02476	0.00197	0.08252	0.30352	0.21724
	1.00	0.39557	0.01998	0.00215	0.05372	0.26815	0.26042
	4.00	0.46854	0.00598	0.00272	0.00482	0.10152	0.41642
	10.00	0.48650	0.00249	0.00287	0.00083	0.04450	0.46281
800	0.01	0.01741	0.18925	0.00052	0.75890	0.03355	0.00037
	0.05	0.07617	0.16959	0.00233	0.60940	0.13500	0.00750
	0.10	0.13183	0.15019	0.00414	0.47795	0.21223	0.02365
	0.30	0.25747	0.10329	0.00860	0.22607	0.30281	0.10177
	0.50	0.31837	0.07882	0.01096	0.13162	0.29469	0.16554
	0.75	0.36121	0.06084	0.01272	0.07842	0.26393	0.22288
	1.00	0.38732	0.04955	0.01383	0.05202	0.23374	0.26354
	4.00	0.46292	0.01537	0.01724	0.00501	0.09035	0.40912
	10.00	0.48181	0.00646	0.01813	0.00088	0.03995	0.45276
900	0.01	0.01583	0.35129	0.00230	0.60163	0.02854	0.00041
	0.05	0.06978	0.31500	0.01018	0.48373	0.11324	0.00807
	0.10	0.12163	0.27937	0.01783	0.38051	0.17589	0.02477
	0.30	0.24143	0.19360	0.03594	0.18273	0.24569	0.10061
	0.50	0.30100	0.14872	0.04526	0.10782	0.23765	0.15955
	0.75	0.34357	0.11552	0.05209	0.06506	0.21245	0.21130
	1.00	0.36982	0.09453	0.05638	0.04356	0.18816	0.24755
	4.00	0.44722	0.02986	0.06947	0.00435	0.07325	0.37586
	10.00	0.46694	0.01263	0.07293	0.00078	0.03251	0.41422
1000	0.01	0.01402	0.53551	0.00671	0.42279	0.02061	0.00036
	0.05	0.06209	0.48037	0.02944	0.34021	0.08105	0.00685
	0.10	0.10875	0.42639	0.05115	0.26804	0.12499	0.02067
	0.30	0.21845	0.29648	0.10153	0.12960	0.17250	0.08144

TABLE-26 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.27411	0.22831	0.12703	0.07685	0.16621	0.12749
	0.75	0.31438	0.17774	0.14558	0.04657	0.14828	0.16745
	1.00	0.33943	0.14566	0.15719	0.03128	0.13121	0.19523
	4.00	0.41442	0.04626	0.19247	0.00316	0.05103	0.29267
	10.00	0.43382	0.01959	0.20176	0.00057	0.02266	0.32161
1100	0.01	0.01242	0.69587	0.01285	0.26708	0.01158	0.00020
	0.05	0.05498	0.62414	0.05646	0.21486	0.04565	0.00392
	0.10	0.09628	0.55385	0.09829	0.16919	0.07052	0.01187
	0.30	0.19360	0.38464	0.19564	0.08160	0.09749	0.04703
	0.50	0.24319	0.29589	0.24497	0.04829	0.09391	0.07375
	0.75	0.27920	0.23012	0.28083	0.02921	0.08373	0.09692
	1.00	0.30166	0.18845	0.30326	0.01959	0.07404	0.11301
	4.00	0.36922	0.05968	0.37116	0.00196	0.02870	0.16929
	10.00	0.38678	0.02525	0.38897	0.00035	0.01272	0.18593
1200	0.01	0.01129	0.80850	0.01720	0.15771	0.00522	0.00008
	0.05	0.04996	0.72488	0.07614	0.12677	0.02073	0.00153
	0.10	0.08742	0.64274	0.13331	0.09967	0.03218	0.00468
	0.30	0.17550	0.44474	0.26828	0.04772	0.04481	0.01895
	0.50	0.22025	0.34113	0.33735	0.02808	0.04322	0.02997
	0.75	0.25269	0.26461	0.38770	0.01689	0.03852	0.03958
	1.00	0.27290	0.21628	0.41921	0.01129	0.03405	0.04627
	4.00	0.33353	0.06801	0.51451	0.00112	0.01314	0.06970
	10.00	0.34924	0.02871	0.53942	0.00020	0.00582	0.07662
1300	0.01	0.01062	0.87672	0.01899	0.09146	0.00219	0.00003
	0.05	0.04707	0.78582	0.08440	0.07347	0.00872	0.00051
	0.10	0.08253	0.69631	0.14830	0.05769	0.01358	0.00158
	0.30	0.16625	0.48030	0.30052	0.02745	0.01899	0.00650
	0.50	0.20894	0.36744	0.37890	0.01606	0.01831	0.01034
	0.75	0.23991	0.28433	0.43613	0.00962	0.01631	0.01369
	1.00	0.25921	0.23200	0.47195	0.00640	0.01440	0.01604
	4.00	0.31704	0.07248	0.58010	0.00063	0.00553	0.02423
	10.00	0.33200	0.03053	0.60828	0.00011	0.00244	0.02664
1400	0.01	0.01025	0.91494	0.01952	0.05433	0.00096	0.00001
	0.05	0.04555	0.81990	0.08691	0.04363	0.00382	0.00018
	0.10	0.08006	0.72616	0.15303	0.03423	0.00596	0.00056
	0.30	0.16214	0.49970	0.31130	0.01621	0.00835	0.00231
	0.50	0.20424	0.38153	0.39305	0.00945	0.00805	0.00369
	0.75	0.23485	0.29470	0.45276	0.00564	0.00716	0.00489
	1.00	0.25395	0.24015	0.49011	0.00374	0.00632	0.00573
	4.00	0.31121	0.07467	0.60268	0.00036	0.00241	0.00867
	10.00	0.32602	0.03141	0.63191	0.00006	0.00107	0.00953
1500	0.01	0.01004	0.93627	0.01962	0.03362	0.00045	0.00000
	0.05	0.04473	0.83888	0.08751	0.02699	0.00181	0.00007
	0.10	0.07878	0.74271	0.15430	0.02116	0.00283	0.00022
	0.30	0.16024	0.51021	0.31469	0.00998	0.00396	0.00092
	0.50	0.20222	0.38901	0.39769	0.00580	0.00382	0.00146
	0.75	0.23280	0.30010	0.45832	0.00345	0.00339	0.00194
	1.00	0.25189	0.24432	0.49623	0.00229	0.00299	0.00228
	4.00	0.30917	0.07571	0.61031	0.00022	0.00114	0.00344
	10.00	0.32398	0.03182	0.63988	0.00004	0.00050	0.00379

TABLE-27 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O= 2.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.03765	0.00479	0.00000	0.92004	0.03740	0.00012
	0.05	0.15353	0.00415	0.00000	0.69140	0.14831	0.00261
	0.10	0.24956	0.00355	0.00000	0.50606	0.23211	0.00872
	0.30	0.42811	0.00217	0.00000	0.18943	0.33247	0.04782
	0.50	0.49962	0.00150	0.00000	0.09044	0.31724	0.09119
	0.75	0.54517	0.00106	0.00000	0.04479	0.27281	0.13617
	1.00	0.57120	0.00081	0.00000	0.02615	0.23248	0.16935
	4.00	0.63993	0.00021	0.00001	0.00170	0.07639	0.28177
	10.00	0.65571	0.00008	0.00001	0.00027	0.03216	0.31177
600	0.01	0.03727	0.02450	0.00001	0.90116	0.03686	0.00021
	0.05	0.15221	0.02126	0.00002	0.67849	0.14385	0.00417
	0.10	0.24771	0.01824	0.00004	0.49969	0.22096	0.01336
	0.30	0.42609	0.01150	0.00009	0.19873	0.30118	0.06241
	0.50	0.49790	0.00828	0.00012	0.10292	0.28379	0.10700
	0.75	0.54376	0.00607	0.00014	0.05539	0.24566	0.14898
	1.00	0.57002	0.00478	0.00015	0.03424	0.21176	0.17906
	4.00	0.63952	0.00132	0.00019	0.00260	0.07341	0.28296
	10.00	0.65550	0.00054	0.00020	0.00043	0.03138	0.31196
700	0.01	0.03624	0.07940	0.00007	0.84842	0.03558	0.00029
	0.05	0.14852	0.06894	0.00032	0.63971	0.13681	0.00569
	0.10	0.24252	0.05930	0.00056	0.47325	0.20679	0.01758
	0.30	0.42016	0.03808	0.00115	0.19521	0.27177	0.07362
	0.50	0.49264	0.02799	0.00145	0.10547	0.25370	0.11874
	0.75	0.53927	0.02099	0.00168	0.05928	0.21996	0.15881
	1.00	0.56612	0.01677	0.00182	0.03784	0.19061	0.18684
	4.00	0.63772	0.00488	0.00225	0.00321	0.06841	0.28353
	10.00	0.65430	0.00202	0.00235	0.00055	0.02960	0.31117
800	0.01	0.03419	0.18745	0.00052	0.74453	0.03294	0.00037
	0.05	0.14115	0.16284	0.00225	0.56184	0.12495	0.00697
	0.10	0.23198	0.14024	0.00390	0.41669	0.18629	0.02090
	0.30	0.40744	0.09093	0.00767	0.17518	0.23779	0.08099
	0.50	0.48073	0.06753	0.00955	0.09663	0.21995	0.12562
	0.75	0.52853	0.05117	0.01090	0.05547	0.19024	0.16369
	1.00	0.55630	0.04121	0.01174	0.03598	0.16498	0.18979
	4.00	0.63149	0.01238	0.01422	0.00325	0.06006	0.27860
	10.00	0.64917	0.00516	0.01486	0.00056	0.02617	0.30407
900	0.01	0.03113	0.34794	0.00228	0.59021	0.02803	0.00041
	0.05	0.12984	0.30231	0.00983	0.44555	0.10495	0.00753
	0.10	0.21534	0.26050	0.01680	0.33082	0.15455	0.02199
	0.30	0.38535	0.16956	0.03213	0.14016	0.19237	0.08042
	0.50	0.45852	0.12643	0.03948	0.07793	0.17624	0.12140
	0.75	0.50704	0.09618	0.04466	0.04510	0.15166	0.15536
	1.00	0.53556	0.07769	0.04784	0.02943	0.13123	0.17825
	4.00	0.61414	0.02363	0.05718	0.00272	0.04770	0.25463
	10.00	0.63297	0.00989	0.05956	0.00048	0.02080	0.27630
1000	0.01	0.02760	0.53039	0.00666	0.41475	0.02024	0.00035
	0.05	0.11621	0.46084	0.02841	0.31311	0.07504	0.00638
	0.10	0.19434	0.39712	0.04815	0.23251	0.10957	0.01831
	0.30	0.35379	0.25853	0.09046	0.09854	0.13402	0.06465

TABLE-27 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.42423	0.19280	0.11027	0.05480	0.12183	0.09607
	0.75	0.47161	0.14668	0.12407	0.03172	0.10429	0.12162
	1.00	0.49972	0.11850	0.13247	0.02070	0.08996	0.13865
	4.00	0.57826	0.03604	0.15689	0.00192	0.03241	0.19448
	10.00	0.59733	0.01509	0.16306	0.00034	0.01410	0.21008
1100	0.01	0.02449	0.68922	0.01273	0.26200	0.01137	0.00020
	0.05	0.10362	0.59869	0.05428	0.19769	0.04210	0.00362
	0.10	0.17406	0.51562	0.09190	0.14664	0.06139	0.01038
	0.30	0.31991	0.33481	0.17226	0.06183	0.07472	0.03647
	0.50	0.38530	0.24916	0.20963	0.03424	0.06767	0.05400
	0.75	0.42962	0.18919	0.23554	0.01974	0.05773	0.06818
	1.00	0.45604	0.15264	0.25123	0.01285	0.04968	0.07756
	4.00	0.53034	0.04619	0.29651	0.00118	0.01775	0.10804
	10.00	0.54847	0.01931	0.30785	0.00021	0.00770	0.11646
1200	0.01	0.02231	0.80076	0.01703	0.15470	0.00512	0.00008
	0.05	0.09476	0.69526	0.07292	0.11662	0.01904	0.00140
	0.10	0.15974	0.59821	0.12384	0.08634	0.02782	0.00404
	0.30	0.29571	0.38679	0.23320	0.03610	0.03387	0.01432
	0.50	0.35724	0.28691	0.28412	0.01986	0.03061	0.02126
	0.75	0.39911	0.21725	0.31935	0.01139	0.02605	0.02685
	1.00	0.42412	0.17492	0.34064	0.00738	0.02238	0.03055
	4.00	0.49463	0.05257	0.40172	0.00067	0.00793	0.04249
	10.00	0.51186	0.02193	0.41690	0.00012	0.00343	0.04576
1300	0.01	0.02100	0.86832	0.01880	0.08971	0.00215	0.00003
	0.05	0.08967	0.75356	0.08073	0.06757	0.00800	0.00047
	0.10	0.15186	0.64773	0.13743	0.04992	0.01171	0.00136
	0.30	0.28358	0.41701	0.25963	0.02069	0.01424	0.00485
	0.50	0.34379	0.30833	0.31652	0.01131	0.01284	0.00721
	0.75	0.38492	0.23282	0.35580	0.00645	0.01090	0.00911
	1.00	0.40955	0.18710	0.37947	0.00417	0.00934	0.01037
	4.00	0.47908	0.05586	0.44702	0.00037	0.00328	0.01439
	10.00	0.49608	0.02326	0.46370	0.00006	0.00142	0.01548
1400	0.01	0.02027	0.90616	0.01932	0.05330	0.00094	0.00001
	0.05	0.08698	0.78609	0.08314	0.04011	0.00351	0.00016
	0.10	0.14789	0.67512	0.14179	0.02958	0.00514	0.00048
	0.30	0.27822	0.43311	0.26854	0.01218	0.00624	0.00172
	0.50	0.33827	0.31941	0.32753	0.00662	0.00561	0.00256
	0.75	0.37941	0.24066	0.36818	0.00376	0.00475	0.00324
	1.00	0.40407	0.19312	0.39264	0.00242	0.00407	0.00368
	4.00	0.47376	0.05737	0.46214	0.00021	0.00142	0.00510
	10.00	0.49080	0.02385	0.47922	0.00004	0.00061	0.00548
1500	0.01	0.01987	0.92728	0.01942	0.03298	0.00044	0.00000
	0.05	0.08554	0.80417	0.08375	0.02480	0.00166	0.00006
	0.10	0.14584	0.69023	0.14303	0.01827	0.00244	0.00019
	0.30	0.27576	0.44168	0.27144	0.00748	0.00296	0.00068
	0.50	0.33591	0.32514	0.33122	0.00405	0.00266	0.00101
	0.75	0.37718	0.24462	0.37237	0.00229	0.00225	0.00128
	1.00	0.40194	0.19610	0.39710	0.00147	0.00192	0.00146
	4.00	0.47191	0.05806	0.46721	0.00013	0.00067	0.00202
	10.00	0.48901	0.02412	0.48439	0.00002	0.00029	0.00217

TABLE-28 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O= 3.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.05542	0.00474	0.00000	0.90301	0.03670	0.00012
	0.05	0.21386	0.00400	0.00000	0.64199	0.13773	0.00242
	0.10	0.33278	0.00335	0.00000	0.44978	0.20634	0.00776
	0.30	0.52889	0.00197	0.00000	0.15594	0.27380	0.03939
	0.50	0.59960	0.00134	0.00000	0.07231	0.25377	0.07298
	0.75	0.64256	0.00094	0.00000	0.03517	0.21431	0.10703
	1.00	0.66643	0.00071	0.00000	0.02033	0.18078	0.13175
	4.00	0.72721	0.00018	0.00001	0.00128	0.05785	0.21347
	10.00	0.74071	0.00007	0.00001	0.00020	0.02421	0.23480
600	0.01	0.05488	0.02427	0.00001	0.88446	0.03618	0.00020
	0.05	0.21209	0.02048	0.00002	0.62991	0.13362	0.00388
	0.10	0.33046	0.01720	0.00004	0.44393	0.19649	0.01189
	0.30	0.52663	0.01043	0.00008	0.16335	0.24802	0.05149
	0.50	0.59775	0.00739	0.00010	0.08210	0.22691	0.08575
	0.75	0.64109	0.00537	0.00012	0.04337	0.19282	0.11723
	1.00	0.66522	0.00420	0.00013	0.02653	0.16448	0.13943
	4.00	0.72680	0.00114	0.00016	0.00196	0.05550	0.21444
	10.00	0.74051	0.00046	0.00017	0.00032	0.02357	0.23496
700	0.01	0.05337	0.07866	0.00007	0.83268	0.03494	0.00029
	0.05	0.20714	0.06642	0.00031	0.59366	0.12718	0.00530
	0.10	0.32394	0.05586	0.00053	0.41994	0.18404	0.01569
	0.30	0.52001	0.03446	0.00104	0.15980	0.22373	0.06095
	0.50	0.59213	0.02493	0.00130	0.08364	0.20255	0.09545
	0.75	0.63643	0.01850	0.00149	0.04607	0.17222	0.12528
	1.00	0.66123	0.01470	0.00161	0.02907	0.14758	0.14581
	4.00	0.72503	0.00422	0.00196	0.00239	0.05142	0.21499
	10.00	0.73934	0.00174	0.00204	0.00041	0.02210	0.23438
800	0.01	0.05038	0.18570	0.00051	0.73068	0.03236	0.00036
	0.05	0.19725	0.15680	0.00218	0.52096	0.11630	0.00651
	0.10	0.31073	0.13195	0.00369	0.36891	0.16599	0.01874
	0.30	0.50587	0.08196	0.00700	0.14231	0.19549	0.06738
	0.50	0.57949	0.05980	0.00858	0.07577	0.17498	0.10138
	0.75	0.62534	0.04479	0.00970	0.04250	0.14813	0.12953
	1.00	0.65126	0.03583	0.01038	0.02720	0.12686	0.14846
	4.00	0.71893	0.01057	0.01238	0.00237	0.04461	0.21114
	10.00	0.73434	0.00439	0.01289	0.00041	0.01928	0.22870
900	0.01	0.04592	0.34468	0.00226	0.57919	0.02755	0.00040
	0.05	0.18209	0.29093	0.00952	0.41263	0.09777	0.00706
	0.10	0.28989	0.24471	0.01594	0.29193	0.13773	0.01979
	0.30	0.48140	0.15203	0.02934	0.11268	0.15750	0.06705
	0.50	0.55602	0.11112	0.03547	0.06019	0.13918	0.09802
	0.75	0.60329	0.08340	0.03970	0.03391	0.11691	0.12279
	1.00	0.63030	0.06683	0.04226	0.02177	0.09972	0.13911
	4.00	0.70201	0.01986	0.04962	0.00192	0.03480	0.19179
	10.00	0.71862	0.00827	0.05147	0.00033	0.01502	0.20630
1000	0.01	0.04078	0.52540	0.00661	0.40698	0.01989	0.00034
	0.05	0.16385	0.44324	0.02748	0.28964	0.06981	0.00597
	0.10	0.26366	0.37247	0.04560	0.20453	0.09732	0.01643
	0.30	0.44659	0.23066	0.08222	0.07844	0.10868	0.05341

TABLE-28 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.51998	0.16824	0.09848	0.04173	0.09495	0.07662
	0.75	0.56714	0.12608	0.10950	0.02343	0.07912	0.09474
	1.00	0.59433	0.10093	0.11610	0.01502	0.06715	0.10649
	4.00	0.66739	0.02989	0.13478	0.00132	0.02309	0.14353
	10.00	0.68451	0.01243	0.13939	0.00023	0.00993	0.15351
1100	0.01	0.03624	0.68271	0.01261	0.25708	0.01116	0.00020
	0.05	0.14701	0.57560	0.05229	0.18274	0.03900	0.00336
	0.10	0.23841	0.48311	0.08645	0.12873	0.05411	0.00919
	0.30	0.40966	0.29773	0.15466	0.04889	0.05966	0.02939
	0.50	0.47973	0.21643	0.18447	0.02584	0.05172	0.04182
	0.75	0.52515	0.16171	0.20449	0.01442	0.04284	0.05139
	1.00	0.55148	0.12920	0.21637	0.00921	0.03622	0.05753
	4.00	0.62267	0.03800	0.24965	0.00080	0.01229	0.07659
	10.00	0.63944	0.01577	0.25775	0.00014	0.00527	0.08164
1200	0.01	0.03305	0.79319	0.01686	0.15179	0.00502	0.00007
	0.05	0.13519	0.66824	0.06999	0.10773	0.01756	0.00129
	0.10	0.22071	0.56002	0.11574	0.07567	0.02434	0.00353
	0.30	0.38387	0.34308	0.20676	0.02840	0.02664	0.01126
	0.50	0.45163	0.24836	0.24620	0.01488	0.02296	0.01596
	0.75	0.49582	0.18494	0.27251	0.00825	0.01893	0.01955
	1.00	0.52152	0.14741	0.28804	0.00524	0.01594	0.02185
	4.00	0.59123	0.04303	0.33108	0.00045	0.00535	0.02886
	10.00	0.60768	0.01782	0.34144	0.00008	0.00228	0.03070
1300	0.01	0.03115	0.86009	0.01861	0.08802	0.00211	0.00002
	0.05	0.12842	0.72402	0.07738	0.06237	0.00737	0.00043
	0.10	0.21101	0.60582	0.12810	0.04367	0.01021	0.00118
	0.30	0.37118	0.36893	0.22881	0.01620	0.01110	0.00377
	0.50	0.43855	0.26600	0.27217	0.00842	0.00952	0.00533
	0.75	0.48267	0.19743	0.30093	0.00464	0.00781	0.00652
	1.00	0.50839	0.15703	0.31782	0.00293	0.00656	0.00727
	4.00	0.57827	0.04552	0.36423	0.00025	0.00218	0.00955
	10.00	0.59477	0.01881	0.37530	0.00004	0.00093	0.01014
1400	0.01	0.03009	0.89756	0.01912	0.05229	0.00092	0.00001
	0.05	0.12485	0.75507	0.07970	0.03701	0.00323	0.00015
	0.10	0.20615	0.63100	0.13212	0.02584	0.00447	0.00042
	0.30	0.36564	0.38243	0.23625	0.00949	0.00485	0.00133
	0.50	0.43326	0.27488	0.28093	0.00490	0.00414	0.00188
	0.75	0.47765	0.20352	0.31045	0.00269	0.00339	0.00230
	1.00	0.50355	0.16162	0.32773	0.00170	0.00284	0.00256
	4.00	0.57396	0.04661	0.37499	0.00014	0.00094	0.00336
	10.00	0.59058	0.01924	0.38620	0.00002	0.00040	0.00356
1500	0.01	0.02951	0.91847	0.01923	0.03235	0.00044	0.00000
	0.05	0.12294	0.77229	0.08031	0.02287	0.00153	0.00006
	0.10	0.20365	0.64481	0.13331	0.01595	0.00212	0.00016
	0.30	0.36311	0.38952	0.23873	0.00582	0.00229	0.00053
	0.50	0.43101	0.27940	0.28389	0.00299	0.00196	0.00075
	0.75	0.47565	0.20653	0.31368	0.00164	0.00160	0.00091
	1.00	0.50169	0.16383	0.33110	0.00103	0.00134	0.00101
	4.00	0.57249	0.04710	0.37857	0.00009	0.00044	0.00132
	10.00	0.58918	0.01942	0.38979	0.00001	0.00019	0.00140

TABLE-29 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O= 3.76

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.06854	0.00471	0.00000	0.89044	0.03619	0.00012
	0.05	0.25435	0.00390	0.00000	0.60884	0.13063	0.00230
	0.10	0.38475	0.00321	0.00000	0.41464	0.19024	0.00715
	0.30	0.58465	0.00185	0.00000	0.13742	0.24135	0.03474
	0.50	0.65249	0.00125	0.00000	0.06272	0.22019	0.06335
	0.75	0.69269	0.00087	0.00000	0.03022	0.18420	0.09202
	1.00	0.71470	0.00066	0.00000	0.01737	0.15457	0.11269
	4.00	0.76973	0.00016	0.00000	0.00108	0.04882	0.18020
	10.00	0.78177	0.00007	0.00000	0.00017	0.02037	0.19762
600	0.01	0.06787	0.02410	0.00000	0.87215	0.03568	0.00020
	0.05	0.25230	0.01995	0.00002	0.59730	0.12675	0.00368
	0.10	0.38218	0.01651	0.00004	0.40910	0.18120	0.01097
	0.30	0.58231	0.00979	0.00008	0.14378	0.21861	0.04545
	0.50	0.65062	0.00688	0.00010	0.07110	0.19681	0.07449
	0.75	0.69122	0.00498	0.00011	0.03719	0.16563	0.10087
	1.00	0.71351	0.00388	0.00012	0.02263	0.14053	0.11934
	4.00	0.76934	0.00105	0.00015	0.00165	0.04677	0.18104
	10.00	0.78157	0.00043	0.00016	0.00027	0.01981	0.19777
700	0.01	0.06601	0.07811	0.00007	0.82107	0.03446	0.00028
	0.05	0.24657	0.06466	0.00030	0.56273	0.12071	0.00504
	0.10	0.37495	0.05360	0.00051	0.38663	0.16980	0.01451
	0.30	0.57546	0.03228	0.00098	0.14024	0.19712	0.05391
	0.50	0.64494	0.02315	0.00122	0.07212	0.17548	0.08309
	0.75	0.68659	0.01709	0.00139	0.03929	0.14767	0.10798
	1.00	0.70957	0.01353	0.00149	0.02464	0.12580	0.12497
	4.00	0.76762	0.00385	0.00180	0.00200	0.04317	0.18156
	10.00	0.78044	0.00158	0.00187	0.00034	0.01849	0.19727
800	0.01	0.06235	0.18440	0.00051	0.72046	0.03193	0.00035
	0.05	0.23513	0.15261	0.00212	0.49347	0.11047	0.00620
	0.10	0.36031	0.12649	0.00355	0.33902	0.15324	0.01738
	0.30	0.56086	0.07656	0.00659	0.12419	0.17202	0.05978
	0.50	0.63223	0.05531	0.00802	0.06482	0.15117	0.08846
	0.75	0.67560	0.04116	0.00901	0.03590	0.12649	0.11183
	1.00	0.69977	0.03281	0.00962	0.02280	0.10760	0.12740
	4.00	0.76173	0.00958	0.01138	0.00194	0.03716	0.17821
	10.00	0.77563	0.00397	0.01182	0.00033	0.01598	0.19227
900	0.01	0.05686	0.34225	0.00225	0.57105	0.02719	0.00039
	0.05	0.21760	0.28300	0.00930	0.39045	0.09291	0.00673
	0.10	0.33727	0.23427	0.01537	0.26756	0.12713	0.01840
	0.30	0.53571	0.14146	0.02765	0.09756	0.13809	0.05953
	0.50	0.60872	0.10221	0.03313	0.05093	0.11955	0.08547
	0.75	0.65384	0.07613	0.03686	0.02826	0.09909	0.10583
	1.00	0.67925	0.06074	0.03910	0.01798	0.08385	0.11908
	4.00	0.74543	0.01782	0.04548	0.00155	0.02862	0.16110
	10.00	0.76051	0.00740	0.04706	0.00027	0.01229	0.17248
1000	0.01	0.05055	0.52168	0.00657	0.40123	0.01963	0.00034
	0.05	0.19652	0.43092	0.02683	0.27377	0.06626	0.00569
	0.10	0.30830	0.35608	0.04389	0.18693	0.08957	0.01522
	0.30	0.50006	0.21378	0.07718	0.06738	0.09455	0.04706

TABLE-29 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.57278	0.15393	0.09150	0.03493	0.08071	0.06615
	0.75	0.61834	0.11436	0.10107	0.01928	0.06624	0.08071
	1.00	0.64422	0.09108	0.10674	0.01223	0.05571	0.09002
	4.00	0.71238	0.02658	0.12259	0.00104	0.01867	0.11873
	10.00	0.72806	0.01101	0.12644	0.00018	0.00798	0.12632
1100	0.01	0.04498	0.67786	0.01253	0.25344	0.01100	0.00019
	0.05	0.17708	0.55938	0.05089	0.17258	0.03688	0.00318
	0.10	0.28052	0.46137	0.08280	0.11740	0.04949	0.00842
	0.30	0.46261	0.27513	0.14383	0.04175	0.05127	0.02542
	0.50	0.53318	0.19723	0.16951	0.02146	0.04331	0.03531
	0.75	0.57779	0.14600	0.18646	0.01176	0.03527	0.04272
	1.00	0.60327	0.11600	0.19640	0.00742	0.02952	0.04740
	4.00	0.67074	0.03359	0.22377	0.00062	0.00974	0.06154
	10.00	0.68633	0.01389	0.23034	0.00011	0.00414	0.06520
1200	0.01	0.04107	0.78753	0.01674	0.14963	0.00495	0.00007
	0.05	0.16347	0.64916	0.06792	0.10167	0.01656	0.00121
	0.10	0.26116	0.53432	0.11030	0.06888	0.02213	0.00320
	0.30	0.43691	0.31624	0.19053	0.02413	0.02263	0.00956
	0.50	0.50620	0.22560	0.22378	0.01228	0.01896	0.01319
	0.75	0.55029	0.16635	0.24548	0.00668	0.01533	0.01587
	1.00	0.57555	0.13183	0.25812	0.00419	0.01278	0.01754
	4.00	0.64266	0.03786	0.29246	0.00035	0.00416	0.02252
	10.00	0.65820	0.01562	0.30058	0.00006	0.00176	0.02379
1300	0.01	0.03873	0.85394	0.01847	0.08676	0.00207	0.00002
	0.05	0.15569	0.70312	0.07502	0.05882	0.00694	0.00041
	0.10	0.25061	0.57754	0.12184	0.03969	0.00926	0.00107
	0.30	0.42447	0.33933	0.20995	0.01370	0.00937	0.00317
	0.50	0.49391	0.24096	0.24606	0.00691	0.00780	0.00436
	0.75	0.53828	0.17705	0.26944	0.00373	0.00627	0.00523
	1.00	0.56375	0.13998	0.28297	0.00233	0.00521	0.00576
	4.00	0.63151	0.03991	0.31937	0.00019	0.00168	0.00734
	10.00	0.64720	0.01643	0.32789	0.00003	0.00071	0.00774
1400	0.01	0.03744	0.89113	0.01898	0.05154	0.00091	0.00001
	0.05	0.15159	0.73308	0.07726	0.03488	0.00304	0.00014
	0.10	0.24533	0.60116	0.12562	0.02346	0.00405	0.00038
	0.30	0.41908	0.35123	0.21648	0.00801	0.00408	0.00112
	0.50	0.48899	0.24856	0.25352	0.00401	0.00338	0.00153
	0.75	0.53376	0.18216	0.27738	0.00215	0.00271	0.00184
	1.00	0.55947	0.14378	0.29114	0.00134	0.00225	0.00202
	4.00	0.62787	0.04079	0.32795	0.00011	0.00072	0.00257
	10.00	0.64370	0.01677	0.33650	0.00002	0.00030	0.00270
1500	0.01	0.03672	0.91187	0.01909	0.03189	0.00043	0.00000
	0.05	0.14940	0.74968	0.07787	0.02155	0.00144	0.00006
	0.10	0.24262	0.61408	0.12677	0.01446	0.00192	0.00015
	0.30	0.41663	0.35743	0.21868	0.00490	0.00193	0.00044
	0.50	0.48692	0.25238	0.25606	0.00244	0.00159	0.00061
	0.75	0.53196	0.18465	0.28008	0.00131	0.00128	0.00073
	1.00	0.55783	0.14560	0.29391	0.00081	0.00106	0.00080
	4.00	0.62663	0.04118	0.33078	0.00007	0.00034	0.00101
	10.00	0.64254	0.01692	0.33933	0.00001	0.00014	0.00106

TABLE-30 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O= 5.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.08908	0.00466	0.00000	0.87075	0.03540	0.00012
	0.05	0.31192	0.00374	0.00000	0.56170	0.12053	0.00212
	0.10	0.45386	0.00303	0.00000	0.36792	0.16884	0.00635
	0.30	0.65162	0.00169	0.00000	0.11517	0.20237	0.02914
	0.50	0.71388	0.00113	0.00000	0.05160	0.18123	0.05216
	0.75	0.74971	0.00078	0.00000	0.02459	0.14997	0.07496
	1.00	0.76900	0.00059	0.00000	0.01405	0.12510	0.09125
	4.00	0.81626	0.00015	0.00000	0.00086	0.03894	0.14378
	10.00	0.82642	0.00006	0.00000	0.00014	0.01620	0.15718
600	0.01	0.08822	0.02383	0.00000	0.85285	0.03489	0.00020
	0.05	0.30950	0.01916	0.00002	0.55094	0.11699	0.00340
	0.10	0.45100	0.01554	0.00003	0.36280	0.16086	0.00975
	0.30	0.64923	0.00895	0.00007	0.12030	0.18327	0.03818
	0.50	0.71203	0.00623	0.00009	0.05834	0.16189	0.06142
	0.75	0.74828	0.00448	0.00010	0.03017	0.13472	0.08225
	1.00	0.76785	0.00349	0.00011	0.01824	0.11360	0.09672
	4.00	0.81589	0.00093	0.00013	0.00131	0.03724	0.14449
	10.00	0.82623	0.00038	0.00014	0.00021	0.01572	0.15732
700	0.01	0.08583	0.07724	0.00007	0.80287	0.03371	0.00028
	0.05	0.30275	0.06208	0.00029	0.51872	0.11149	0.00466
	0.10	0.44297	0.05043	0.00048	0.34233	0.15084	0.01293
	0.30	0.64227	0.02946	0.00090	0.11679	0.16514	0.04544
	0.50	0.70643	0.02090	0.00111	0.05880	0.14407	0.06869
	0.75	0.74378	0.01533	0.00125	0.03163	0.11976	0.08825
	1.00	0.76406	0.01210	0.00134	0.01969	0.10133	0.10147
	4.00	0.81428	0.00341	0.00161	0.00157	0.03417	0.14497
	10.00	0.82518	0.00140	0.00167	0.00026	0.01458	0.15691
800	0.01	0.08112	0.18234	0.00050	0.70444	0.03125	0.00035
	0.05	0.28930	0.14643	0.00205	0.45431	0.10215	0.00576
	0.10	0.42677	0.11884	0.00336	0.29924	0.13623	0.01556
	0.30	0.62752	0.06956	0.00606	0.10251	0.14377	0.05059
	0.50	0.69395	0.04964	0.00730	0.05220	0.12355	0.07337
	0.75	0.73320	0.03665	0.00816	0.02846	0.10194	0.09159
	1.00	0.75471	0.02908	0.00867	0.01792	0.08602	0.10360
	4.00	0.80876	0.00839	0.01016	0.00149	0.02907	0.14214
	10.00	0.82066	0.00346	0.01053	0.00025	0.01244	0.15265
900	0.01	0.07408	0.33840	0.00223	0.55828	0.02663	0.00039
	0.05	0.26871	0.27129	0.00897	0.35879	0.08596	0.00627
	0.10	0.40133	0.21959	0.01456	0.23507	0.11292	0.01652
	0.30	0.60223	0.12773	0.02543	0.07953	0.11470	0.05038
	0.50	0.67104	0.09096	0.03014	0.04033	0.09679	0.07074
	0.75	0.71234	0.06712	0.03330	0.02196	0.07891	0.08636
	1.00	0.73522	0.05325	0.03518	0.01382	0.06614	0.09638
	4.00	0.79353	0.01539	0.04046	0.00115	0.02198	0.12749
	10.00	0.80657	0.00636	0.04175	0.00020	0.00938	0.13575
1000	0.01	0.06597	0.51577	0.00650	0.39220	0.01922	0.00033
	0.05	0.24398	0.41266	0.02586	0.25105	0.06116	0.00528
	0.10	0.36945	0.33293	0.04147	0.16342	0.07913	0.01359
	0.30	0.56664	0.19178	0.07053	0.05423	0.07752	0.03930

TABLE-30 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.63629	0.13584	0.08256	0.02720	0.06427	0.05385
	0.75	0.67864	0.09984	0.09045	0.01469	0.05175	0.06463
	1.00	0.70228	0.07901	0.09506	0.00920	0.04304	0.07140
	4.00	0.76310	0.02265	0.10776	0.00076	0.01399	0.09175
	10.00	0.77680	0.00934	0.11080	0.00013	0.00593	0.09699
1100	0.01	0.05882	0.67015	0.01239	0.24770	0.01076	0.00019
	0.05	0.22125	0.53519	0.04881	0.15798	0.03384	0.00293
	0.10	0.33908	0.43048	0.07758	0.10221	0.04326	0.00740
	0.30	0.52987	0.24554	0.12952	0.03325	0.04120	0.02061
	0.50	0.59885	0.17289	0.15033	0.01649	0.03367	0.02777
	0.75	0.64116	0.12649	0.16374	0.00883	0.02683	0.03295
	1.00	0.66488	0.09981	0.17149	0.00549	0.02218	0.03614
	4.00	0.72621	0.02836	0.19242	0.00044	0.00707	0.04550
	10.00	0.74008	0.01167	0.19734	0.00008	0.00298	0.04786
1200	0.01	0.05379	0.77853	0.01654	0.14623	0.00483	0.00007
	0.05	0.20540	0.62062	0.06484	0.09293	0.01511	0.00111
	0.10	0.31814	0.49763	0.10255	0.05974	0.01916	0.00277
	0.30	0.50537	0.28097	0.16922	0.01905	0.01785	0.00754
	0.50	0.57432	0.19665	0.19524	0.00933	0.01442	0.01004
	0.75	0.61689	0.14322	0.21175	0.00495	0.01139	0.01181
	1.00	0.64082	0.11268	0.22120	0.00306	0.00936	0.01288
	4.00	0.70286	0.03172	0.24627	0.00024	0.00293	0.01597
	10.00	0.71690	0.01302	0.25207	0.00004	0.00123	0.01673
1300	0.01	0.05079	0.84414	0.01824	0.08478	0.00203	0.00002
	0.05	0.19637	0.67176	0.07149	0.05369	0.00632	0.00037
	0.10	0.30683	0.53704	0.11292	0.03432	0.00798	0.00092
	0.30	0.49380	0.30041	0.18526	0.01074	0.00732	0.00247
	0.50	0.56352	0.20914	0.21301	0.00520	0.00586	0.00327
	0.75	0.60670	0.15171	0.23043	0.00274	0.00460	0.00382
	1.00	0.63101	0.11906	0.24032	0.00169	0.00376	0.00416
	4.00	0.69407	0.03327	0.26625	0.00013	0.00117	0.00510
	10.00	0.70834	0.01363	0.27218	0.00002	0.00049	0.00533
1400	0.01	0.04912	0.88087	0.01875	0.05036	0.00089	0.00001
	0.05	0.19161	0.70006	0.07362	0.03181	0.00277	0.00013
	0.10	0.30119	0.55842	0.11634	0.02024	0.00349	0.00032
	0.30	0.48885	0.31023	0.19063	0.00625	0.00317	0.00087
	0.50	0.55926	0.21517	0.21889	0.00301	0.00253	0.00114
	0.75	0.60293	0.15566	0.23653	0.00157	0.00198	0.00134
	1.00	0.62752	0.12196	0.24649	0.00097	0.00161	0.00145
	4.00	0.69127	0.03392	0.27247	0.00007	0.00050	0.00177
	10.00	0.70568	0.01388	0.27837	0.00001	0.00021	0.00185
1500	0.01	0.04820	0.90136	0.01886	0.03116	0.00042	0.00000
	0.05	0.18908	0.71570	0.07422	0.01965	0.00131	0.00005
	0.10	0.29831	0.57004	0.11742	0.01246	0.00165	0.00013
	0.30	0.48661	0.31528	0.19246	0.00381	0.00150	0.00034
	0.50	0.55748	0.21815	0.22090	0.00183	0.00119	0.00045
	0.75	0.60144	0.15755	0.23860	0.00095	0.00093	0.00053
	1.00	0.62619	0.12332	0.24858	0.00058	0.00076	0.00057
	4.00	0.69033	0.03420	0.27451	0.00004	0.00023	0.00070
	10.00	0.70481	0.01398	0.28037	0.00001	0.00010	0.00073

TABLE-31 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O=10.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.16357	0.00446	0.00000	0.79936	0.03250	0.00011
	0.05	0.47541	0.00327	0.00000	0.42785	0.09185	0.00162
	0.10	0.62422	0.00251	0.00000	0.25280	0.11610	0.00437
	0.30	0.78895	0.00132	0.00000	0.06960	0.12247	0.01766
	0.50	0.83297	0.00087	0.00000	0.03003	0.10566	0.03046
	0.75	0.85689	0.00059	0.00000	0.01402	0.08563	0.04287
	1.00	0.86937	0.00044	0.00000	0.00792	0.07065	0.05161
	4.00	0.89883	0.00011	0.00000	0.00047	0.02141	0.07917
	10.00	0.90496	0.00004	0.00000	0.00007	0.00886	0.08607
600	0.01	0.16206	0.02283	0.00000	0.78287	0.03205	0.00018
	0.05	0.47221	0.01671	0.00002	0.41924	0.08923	0.00260
	0.10	0.62097	0.01287	0.00003	0.24870	0.11069	0.00674
	0.30	0.78671	0.00694	0.00005	0.07225	0.11081	0.02324
	0.50	0.83133	0.00474	0.00007	0.03368	0.09418	0.03601
	0.75	0.85567	0.00337	0.00008	0.01703	0.07667	0.04720
	1.00	0.86840	0.00260	0.00008	0.01017	0.06389	0.05485
	4.00	0.89852	0.00069	0.00010	0.00071	0.02035	0.07963
	10.00	0.90480	0.00028	0.00010	0.00012	0.00854	0.08616
700	0.01	0.15786	0.07399	0.00007	0.73682	0.03100	0.00025
	0.05	0.46325	0.05408	0.00025	0.39361	0.08522	0.00359
	0.10	0.61187	0.04162	0.00040	0.23315	0.10394	0.00902
	0.30	0.78026	0.02264	0.00071	0.06898	0.09950	0.02793
	0.50	0.82644	0.01570	0.00085	0.03318	0.08322	0.04061
	0.75	0.85186	0.01136	0.00095	0.01738	0.06747	0.05098
	1.00	0.86525	0.00890	0.00102	0.01066	0.05630	0.05787
	4.00	0.89723	0.00246	0.00119	0.00082	0.01833	0.07996
	10.00	0.90396	0.00101	0.00124	0.00014	0.00776	0.08590
800	0.01	0.14958	0.17464	0.00048	0.64619	0.02879	0.00032
	0.05	0.44548	0.12718	0.00181	0.34273	0.07831	0.00449
	0.10	0.59367	0.09744	0.00283	0.20116	0.09391	0.01100
	0.30	0.76682	0.05261	0.00478	0.05864	0.08572	0.03144
	0.50	0.81577	0.03651	0.00563	0.02825	0.07014	0.04369
	0.75	0.84312	0.02650	0.00621	0.01488	0.05614	0.05313
	1.00	0.85766	0.02082	0.00656	0.00919	0.04656	0.05921
	4.00	0.89286	0.00585	0.00753	0.00073	0.01502	0.07801
	10.00	0.90038	0.00240	0.00776	0.00012	0.00636	0.08298
900	0.01	0.13720	0.32399	0.00215	0.51173	0.02457	0.00036
	0.05	0.41845	0.23456	0.00795	0.26823	0.06588	0.00493
	0.10	0.56545	0.17827	0.01228	0.15494	0.07731	0.01175
	0.30	0.74430	0.09446	0.01999	0.04350	0.06665	0.03111
	0.50	0.79661	0.06503	0.02311	0.02062	0.05305	0.04158
	0.75	0.82624	0.04697	0.02514	0.01076	0.04169	0.04921
	1.00	0.84212	0.03680	0.02632	0.00660	0.03420	0.05395
	4.00	0.88098	0.01028	0.02954	0.00051	0.01072	0.06797
	10.00	0.88936	0.00421	0.03030	0.00009	0.00451	0.07153
1000	0.01	0.12296	0.49358	0.00626	0.35917	0.01771	0.00031
	0.05	0.38627	0.35489	0.02277	0.18568	0.04630	0.00409
	0.10	0.53070	0.26726	0.03450	0.10530	0.05284	0.00940
	0.30	0.71352	0.13849	0.05393	0.02827	0.04280	0.02298

TABLE-31 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.76850	0.09434	0.06127	0.01312	0.03312	0.02966
	0.75	0.79992	0.06763	0.06588	0.00674	0.02553	0.03429
	1.00	0.81684	0.05276	0.06850	0.00410	0.02071	0.03708
	4.00	0.85843	0.01455	0.07545	0.00031	0.00629	0.04497
	10.00	0.86742	0.00594	0.07705	0.00005	0.00263	0.04690
1100	0.01	0.11042	0.64103	0.01187	0.22664	0.00986	0.00017
	0.05	0.35713	0.45795	0.04210	0.11567	0.02498	0.00218
	0.10	0.49862	0.34196	0.06246	0.06450	0.02767	0.00479
	0.30	0.68387	0.17359	0.09395	0.01662	0.02113	0.01085
	0.50	0.74076	0.11709	0.10508	0.00756	0.01594	0.01357
	0.75	0.77347	0.08338	0.11186	0.00383	0.01208	0.01538
	1.00	0.79112	0.06478	0.11565	0.00231	0.00971	0.01644
	4.00	0.83458	0.01765	0.12540	0.00017	0.00287	0.01932
	10.00	0.84399	0.00719	0.12759	0.00003	0.00119	0.02001
1200	0.01	0.10162	0.74442	0.01578	0.13370	0.00441	0.00007
	0.05	0.33723	0.52868	0.05495	0.06743	0.01091	0.00079
	0.10	0.47751	0.39167	0.08030	0.03701	0.01181	0.00170
	0.30	0.66614	0.19508	0.11737	0.00918	0.00860	0.00363
	0.50	0.72492	0.13042	0.12976	0.00410	0.00636	0.00443
	0.75	0.75882	0.09231	0.13711	0.00206	0.00475	0.00495
	1.00	0.77713	0.07146	0.14115	0.00123	0.00379	0.00525
	4.00	0.82221	0.01928	0.15129	0.00009	0.00110	0.00603
	10.00	0.83196	0.00784	0.15353	0.00001	0.00045	0.00621
1300	0.01	0.09637	0.80691	0.01739	0.07747	0.00185	0.00002
	0.05	0.32608	0.57027	0.06018	0.03869	0.00451	0.00026
	0.10	0.46652	0.41976	0.08738	0.02097	0.00482	0.00055
	0.30	0.65844	0.20597	0.12599	0.00505	0.00341	0.00114
	0.50	0.71864	0.13678	0.13848	0.00223	0.00249	0.00138
	0.75	0.75336	0.09639	0.14576	0.00111	0.00185	0.00153
	1.00	0.77211	0.07443	0.14973	0.00066	0.00147	0.00161
	4.00	0.81820	0.01994	0.15956	0.00005	0.00042	0.00183
	10.00	0.82815	0.00809	0.16169	0.00001	0.00017	0.00188
1400	0.01	0.09347	0.84185	0.01787	0.04600	0.00081	0.00001
	0.05	0.32028	0.59294	0.06190	0.02282	0.00197	0.00009
	0.10	0.46116	0.43455	0.08975	0.01226	0.00209	0.00019
	0.30	0.65527	0.21118	0.12880	0.00289	0.00146	0.00040
	0.50	0.71629	0.13967	0.14125	0.00127	0.00106	0.00048
	0.75	0.75145	0.09816	0.14846	0.00063	0.00078	0.00053
	1.00	0.77042	0.07568	0.15236	0.00037	0.00062	0.00055
	4.00	0.81700	0.02020	0.16197	0.00003	0.00018	0.00063
	10.00	0.82704	0.00819	0.16405	0.00000	0.00007	0.00064
1500	0.01	0.09186	0.86132	0.01798	0.02845	0.00038	0.00000
	0.05	0.31719	0.60535	0.06243	0.01405	0.00093	0.00004
	0.10	0.45844	0.44244	0.09055	0.00751	0.00099	0.00008
	0.30	0.65386	0.21377	0.12978	0.00175	0.00068	0.00016
	0.50	0.71532	0.14104	0.14219	0.00076	0.00049	0.00019
	0.75	0.75071	0.09898	0.14936	0.00038	0.00036	0.00021
	1.00	0.76979	0.07624	0.15324	0.00022	0.00029	0.00022
	4.00	0.81661	0.02030	0.16275	0.00002	0.00008	0.00024
	10.00	0.82668	0.00823	0.16480	0.00000	0.00003	0.00025

TABLE-32 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=15 ATM,N/O=20.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.28111	0.00414	0.00000	0.68674	0.02792	0.00009
	0.05	0.64429	0.00269	0.00000	0.28968	0.06224	0.00110
	0.10	0.76847	0.00197	0.00000	0.15540	0.07146	0.00269
	0.30	0.88192	0.00098	0.00000	0.03879	0.06842	0.00989
	0.50	0.90880	0.00064	0.00000	0.01633	0.05759	0.01665
	0.75	0.92288	0.00043	0.00000	0.00752	0.04605	0.02312
	1.00	0.93008	0.00032	0.00000	0.00422	0.03774	0.02764
	4.00	0.94671	0.00008	0.00000	0.00025	0.01126	0.04171
	10.00	0.95010	0.00003	0.00000	0.00004	0.00464	0.04518
600	0.01	0.27871	0.02116	0.00000	0.67241	0.02756	0.00015
	0.05	0.64073	0.01373	0.00001	0.28323	0.06052	0.00177
	0.10	0.76535	0.01007	0.00002	0.15222	0.06816	0.00417
	0.30	0.88006	0.00515	0.00004	0.03987	0.06178	0.01309
	0.50	0.90749	0.00347	0.00005	0.01807	0.05113	0.01978
	0.75	0.92192	0.00245	0.00006	0.00900	0.04102	0.02556
	1.00	0.92933	0.00188	0.00006	0.00533	0.03391	0.02948
	4.00	0.94648	0.00049	0.00007	0.00037	0.01060	0.04199
	10.00	0.94999	0.00020	0.00008	0.00006	0.00443	0.04525
700	0.01	0.27203	0.06855	0.00006	0.63244	0.02670	0.00022
	0.05	0.63080	0.04431	0.00021	0.26428	0.05793	0.00247
	0.10	0.75666	0.03236	0.00032	0.14097	0.06403	0.00566
	0.30	0.87480	0.01659	0.00053	0.03706	0.05508	0.01593
	0.50	0.90366	0.01131	0.00063	0.01721	0.04465	0.02254
	0.75	0.91901	0.00810	0.00070	0.00882	0.03553	0.02784
	1.00	0.92695	0.00631	0.00075	0.00535	0.02934	0.03130
	4.00	0.94552	0.00172	0.00087	0.00040	0.00930	0.04219
	10.00	0.94936	0.00070	0.00090	0.00007	0.00391	0.04506
800	0.01	0.25885	0.16168	0.00045	0.55386	0.02487	0.00028
	0.05	0.61127	0.10355	0.00151	0.22719	0.05333	0.00314
	0.10	0.73958	0.07483	0.00226	0.11866	0.05765	0.00703
	0.30	0.86416	0.03760	0.00363	0.02995	0.04652	0.01813
	0.50	0.89560	0.02548	0.00421	0.01376	0.03657	0.02439
	0.75	0.91255	0.01822	0.00459	0.00704	0.02854	0.02906
	1.00	0.92139	0.01420	0.00482	0.00427	0.02333	0.03199
	4.00	0.94232	0.00390	0.00544	0.00032	0.00724	0.04078
	10.00	0.94671	0.00159	0.00559	0.00005	0.00303	0.04302
900	0.01	0.23921	0.29960	0.00201	0.43759	0.02128	0.00032
	0.05	0.58203	0.18903	0.00668	0.17421	0.04458	0.00347
	0.10	0.71378	0.13435	0.00981	0.08799	0.04656	0.00750
	0.30	0.84697	0.06518	0.01502	0.02071	0.03456	0.01756
	0.50	0.88157	0.04354	0.01700	0.00924	0.02613	0.02251
	0.75	0.90041	0.03086	0.01825	0.00464	0.01989	0.02595
	1.00	0.91029	0.02392	0.01897	0.00279	0.01602	0.02802
	4.00	0.93380	0.00649	0.02085	0.00021	0.00478	0.03387
	10.00	0.93875	0.00264	0.02129	0.00003	0.00198	0.03530
1000	0.01	0.21668	0.45573	0.00585	0.30620	0.01528	0.00027
	0.05	0.54800	0.28241	0.01880	0.11758	0.03042	0.00279
	0.10	0.68318	0.19697	0.02677	0.05720	0.03022	0.00566
	0.30	0.82470	0.09209	0.03858	0.01250	0.02036	0.01176

TABLE-32 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.86216	0.06058	0.04266	0.00541	0.01481	0.01438
	0.75	0.88263	0.04252	0.04511	0.00267	0.01099	0.01608
	1.00	0.89337	0.03277	0.04648	0.00158	0.00873	0.01707
	4.00	0.91895	0.00875	0.04996	0.00011	0.00251	0.01972
	10.00	0.92433	0.00355	0.05073	0.00002	0.00103	0.02033
1100	0.01	0.19691	0.59094	0.01098	0.19261	0.00841	0.00015
	0.05	0.51829	0.35984	0.03347	0.07142	0.01560	0.00138
	0.10	0.65674	0.24662	0.04585	0.03355	0.01465	0.00258
	0.30	0.80573	0.11158	0.06211	0.00687	0.00898	0.00474
	0.50	0.84562	0.07246	0.06717	0.00290	0.00631	0.00554
	0.75	0.86745	0.05044	0.07009	0.00140	0.00458	0.00604
	1.00	0.87890	0.03870	0.07167	0.00083	0.00359	0.00631
	4.00	0.90614	0.01021	0.07558	0.00006	0.00100	0.00702
	10.00	0.91185	0.00413	0.07642	0.00001	0.00041	0.00718
1200	0.01	0.18313	0.68531	0.01448	0.11331	0.00373	0.00006
	0.05	0.49893	0.41091	0.04240	0.04074	0.00654	0.00047
	0.10	0.64081	0.27739	0.05651	0.01856	0.00589	0.00084
	0.30	0.79609	0.12212	0.07341	0.00360	0.00337	0.00142
	0.50	0.83784	0.07850	0.07825	0.00149	0.00231	0.00161
	0.75	0.86065	0.05430	0.08096	0.00071	0.00165	0.00173
	1.00	0.87260	0.04151	0.08240	0.00042	0.00128	0.00179
	4.00	0.90096	0.01086	0.08586	0.00003	0.00035	0.00194
	10.00	0.90690	0.00438	0.08660	0.00000	0.00014	0.00197
1300	0.01	0.17493	0.74207	0.01590	0.06552	0.00155	0.00002
	0.05	0.48849	0.43980	0.04589	0.02301	0.00265	0.00015
	0.10	0.63304	0.29366	0.06044	0.01026	0.00233	0.00026
	0.30	0.79234	0.12694	0.07709	0.00192	0.00129	0.00043
	0.50	0.83511	0.08108	0.08168	0.00078	0.00087	0.00048
	0.75	0.85843	0.05587	0.08420	0.00037	0.00062	0.00051
	1.00	0.87063	0.04262	0.08553	0.00022	0.00048	0.00053
	4.00	0.89951	0.01109	0.08869	0.00001	0.00013	0.00057
	10.00	0.90555	0.00447	0.08935	0.00000	0.00005	0.00057
1400	0.01	0.17042	0.77370	0.01635	0.03885	0.00068	0.00001
	0.05	0.48317	0.45513	0.04706	0.01344	0.00115	0.00005
	0.10	0.62938	0.30186	0.06176	0.00591	0.00100	0.00009
	0.30	0.79087	0.12911	0.07825	0.00108	0.00054	0.00015
	0.50	0.83414	0.08217	0.08272	0.00044	0.00036	0.00016
	0.75	0.85769	0.05651	0.08516	0.00021	0.00026	0.00017
	1.00	0.87000	0.04306	0.08644	0.00012	0.00020	0.00018
	4.00	0.89910	0.01117	0.08947	0.00001	0.00005	0.00019
	10.00	0.90517	0.00450	0.09011	0.00000	0.00002	0.00019
1500	0.01	0.16792	0.79127	0.01647	0.02401	0.00032	0.00000
	0.05	0.48038	0.46337	0.04745	0.00823	0.00054	0.00002
	0.10	0.62756	0.30612	0.06221	0.00359	0.00047	0.00004
	0.30	0.79023	0.13015	0.07866	0.00065	0.00025	0.00006
	0.50	0.83375	0.08268	0.08308	0.00026	0.00017	0.00006
	0.75	0.85741	0.05679	0.08549	0.00012	0.00012	0.00007
	1.00	0.86977	0.04325	0.08675	0.00007	0.00009	0.00007
	4.00	0.89897	0.01120	0.08972	0.00000	0.00002	0.00007
	10.00	0.90506	0.00451	0.09034	0.00000	0.00001	0.00008

TABLE-33 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O= 0.0

T, K	O/H	N2	H2	CC	CH4	H2O	CO2
500	0.01	0.0	0.00378	0.00000	0.95720	0.03888	0.00013
	0.05	0.0	0.00350	0.00000	0.81808	0.17534	0.00308
	0.10	0.0	0.00318	0.00000	0.67564	0.30956	0.01162
	0.30	0.0	0.00223	0.00000	0.33218	0.58202	0.08357
	0.50	0.0	0.00165	0.00000	0.18133	0.63487	0.18215
	0.75	0.0	0.00122	0.00000	0.09880	0.60070	0.29928
	1.00	0.0	0.00096	0.00001	0.06119	0.54300	0.39484
	4.00	0.0	0.00027	0.00001	0.00473	0.21247	0.78253
	10.00	0.0	0.00011	0.00001	0.00079	0.09354	0.90555
600	0.01	0.0	0.01940	0.00000	0.94198	0.03840	0.00021
	0.05	0.0	0.01796	0.00002	0.80678	0.17033	0.00492
	0.10	0.0	0.01637	0.00004	0.67078	0.29507	0.01775
	0.30	0.0	0.01185	0.00009	0.35124	0.52821	0.10861
	0.50	0.0	0.00913	0.00013	0.20836	0.56953	0.21286
	0.75	0.0	0.00703	0.00016	0.12356	0.54299	0.32627
	1.00	0.0	0.00569	0.00018	0.08109	0.49683	0.41620
	4.00	0.0	0.00171	0.00024	0.00736	0.20557	0.78511
	10.00	0.0	0.00071	0.00026	0.00128	0.09193	0.90582
700	0.01	0.0	0.06331	0.00006	0.89902	0.03731	0.00030
	0.05	0.0	0.05865	0.00027	0.77157	0.16282	0.00669
	0.10	0.0	0.05363	0.00050	0.64526	0.27740	0.02321
	0.30	0.0	0.03965	0.00117	0.35261	0.47963	0.12695
	0.50	0.0	0.03127	0.00158	0.21930	0.51370	0.23414
	0.75	0.0	0.02466	0.00192	0.13641	0.49188	0.34512
	1.00	0.0	0.02033	0.00215	0.09272	0.45340	0.43140
	4.00	0.0	0.00650	0.00290	0.00949	0.19570	0.78541
	10.00	0.0	0.00275	0.00311	0.00170	0.08881	0.90363
800	0.01	0.0	0.15168	0.00041	0.81246	0.03507	0.00038
	0.05	0.0	0.14066	0.00188	0.69864	0.15067	0.00815
	0.10	0.0	0.12895	0.00345	0.58716	0.25308	0.02737
	0.30	0.0	0.09676	0.00776	0.33061	0.42670	0.13818
	0.50	0.0	0.07744	0.01034	0.21179	0.45508	0.24534
	0.75	0.0	0.06198	0.01240	0.13567	0.43691	0.35303
	1.00	0.0	0.05167	0.01378	0.09428	0.40461	0.43566
	4.00	0.0	0.01725	0.01836	0.01051	0.18001	0.77388
	10.00	0.0	0.00740	0.01967	0.00193	0.08269	0.88831
900	0.01	0.0	0.28887	0.00181	0.67804	0.03085	0.00043
	0.05	0.0	0.26811	0.00828	0.58409	0.13062	0.00890
	0.10	0.0	0.24631	0.01496	0.49294	0.21677	0.02903
	0.30	0.0	0.18684	0.03263	0.28364	0.35872	0.13818
	0.50	0.0	0.15100	0.04293	0.18526	0.38151	0.23929
	0.75	0.0	0.12200	0.05111	0.12093	0.36690	0.33906
	1.00	0.0	0.10242	0.05654	0.08523	0.34079	0.41501
	4.00	0.0	0.03518	0.07475	0.01005	0.15473	0.72530
	10.00	0.0	0.01523	0.08002	0.00188	0.07171	0.83116
1000	0.01	0.0	0.45702	0.00547	0.51323	0.02389	0.00039
	0.05	0.0	0.42442	0.02471	0.44263	0.10019	0.00804
	0.10	0.0	0.39040	0.04426	0.37451	0.16504	0.02580
	0.30	0.0	0.29795	0.09496	0.21813	0.27023	0.11874

TABLE-33 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.0	0.24204	0.12413	0.14395	0.28697	0.20291
	0.75	0.0	0.19651	0.14717	0.09489	0.27623	0.28520
	1.00	0.0	0.16559	0.16247	0.06738	0.25697	0.34759
	4.00	0.0	0.05773	0.21386	0.00819	0.11793	0.60228
	10.00	0.0	0.02513	0.22884	0.00155	0.05492	0.68957
1100	0.01	0.0	0.62003	0.01125	0.35340	0.01507	0.00026
	0.05	0.0	0.57574	0.05092	0.30472	0.06331	0.00531
	0.10	0.0	0.52949	0.09131	0.25772	0.10440	0.01708
	0.30	0.0	0.40390	0.19619	0.14997	0.17111	0.07883
	0.50	0.0	0.32809	0.25650	0.09895	0.18171	0.13475
	0.75	0.0	0.26641	0.30407	0.06524	0.17492	0.18937
	1.00	0.0	0.22453	0.33565	0.04634	0.16273	0.23075
	4.00	0.0	0.07839	0.44167	0.00565	0.07476	0.39954
	10.00	0.0	0.03414	0.47257	0.00107	0.03483	0.45739
1200	0.01	0.0	0.74984	0.01631	0.22609	0.00765	0.00012
	0.05	0.0	0.69591	0.07448	0.19474	0.03244	0.00243
	0.10	0.0	0.63927	0.13460	0.16433	0.05385	0.00795
	0.30	0.0	0.48510	0.29341	0.09462	0.08908	0.03778
	0.50	0.0	0.39240	0.38568	0.06192	0.09472	0.06528
	0.75	0.0	0.31743	0.45863	0.04052	0.09111	0.09231
	1.00	0.0	0.26680	0.50707	0.02862	0.08467	0.11284
	4.00	0.0	0.09218	0.66924	0.00342	0.03861	0.19656
	10.00	0.0	0.04000	0.71627	0.00064	0.01793	0.22515
1300	0.01	0.0	0.83828	0.01886	0.13935	0.00347	0.00004
	0.05	0.0	0.77772	0.08666	0.11995	0.01478	0.00090
	0.10	0.0	0.71382	0.15751	0.10105	0.02465	0.00298
	0.30	0.0	0.53933	0.34742	0.05768	0.04108	0.01448
	0.50	0.0	0.43459	0.45895	0.03745	0.04373	0.02527
	0.75	0.0	0.35024	0.54744	0.02433	0.04203	0.03596
	1.00	0.0	0.29354	0.60625	0.01709	0.03901	0.04410
	4.00	0.0	0.10025	0.80278	0.00199	0.01764	0.07733
	10.00	0.0	0.04334	0.85949	0.00037	0.00817	0.08864
1400	0.01	0.0	0.89251	0.01972	0.08617	0.00157	0.00002
	0.05	0.0	0.82789	0.09090	0.07415	0.00673	0.00033
	0.10	0.0	0.75956	0.16569	0.06241	0.01126	0.00109
	0.30	0.0	0.57254	0.36779	0.03546	0.01883	0.00538
	0.50	0.0	0.46031	0.48727	0.02292	0.02006	0.00944
	0.75	0.0	0.37012	0.58230	0.01482	0.01927	0.01349
	1.00	0.0	0.30965	0.64552	0.01037	0.01788	0.01657
	4.00	0.0	0.10496	0.85663	0.00119	0.00804	0.02919
	10.00	0.0	0.04525	0.91735	0.00022	0.00371	0.03347
1500	0.01	0.0	0.92466	0.01992	0.05465	0.00076	0.00001
	0.05	0.0	0.85763	0.09199	0.04701	0.00324	0.00013
	0.10	0.0	0.78664	0.16794	0.03955	0.00543	0.00043
	0.30	0.0	0.59212	0.37420	0.02241	0.00911	0.00216
	0.50	0.0	0.47538	0.49667	0.01445	0.00971	0.00380
	0.75	0.0	0.38168	0.59424	0.00931	0.00933	0.00544
	1.00	0.0	0.31896	0.65919	0.00650	0.00864	0.00670
	4.00	0.0	0.10758	0.87598	0.00074	0.00387	0.01182
	10.00	0.0	0.04630	0.93822	0.00014	0.00179	0.01356

TABLE-34 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O= 1.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.01919	0.00375	0.00000	0.93880	0.03814	0.00013
	0.05	0.08319	0.00335	0.00000	0.74989	0.16074	0.00282
	0.10	0.14265	0.00294	0.00000	0.57908	0.26536	0.00996
	0.30	0.27247	0.00190	0.00000	0.24150	0.42332	0.06081
	0.50	0.33311	0.00134	0.00000	0.12082	0.42323	0.12149
	0.75	0.37482	0.00096	0.00000	0.06171	0.37538	0.18713
	1.00	0.39985	0.00074	0.00000	0.03669	0.32573	0.23698
	4.00	0.47054	0.00019	0.00001	0.00250	0.11244	0.41432
	10.00	0.48778	0.00008	0.00001	0.00041	0.04789	0.46384
600	0.01	0.01905	0.01921	0.00000	0.92386	0.03767	0.00021
	0.05	0.08262	0.01719	0.00002	0.73947	0.15619	0.00451
	0.10	0.14177	0.01516	0.00003	0.57476	0.25305	0.01523
	0.30	0.27134	0.01010	0.00008	0.25505	0.38428	0.07916
	0.50	0.33208	0.00744	0.00010	0.13855	0.37962	0.14222
	0.75	0.37394	0.00555	0.00012	0.07696	0.33912	0.20432
	1.00	0.39909	0.00440	0.00014	0.04846	0.29776	0.25014
	4.00	0.47025	0.00124	0.00018	0.00388	0.10857	0.41588
	10.00	0.48764	0.00051	0.00019	0.00065	0.04695	0.46406
700	0.01	0.01863	0.06270	0.00006	0.88172	0.03661	0.00030
	0.05	0.08098	0.05614	0.00026	0.70705	0.14942	0.00614
	0.10	0.13928	0.04963	0.00046	0.55251	0.23815	0.01997
	0.30	0.26799	0.03373	0.00100	0.25522	0.34913	0.09293
	0.50	0.32888	0.02543	0.00130	0.14505	0.34223	0.15712
	0.75	0.37108	0.01939	0.00152	0.08435	0.30668	0.21697
	1.00	0.39654	0.01565	0.00167	0.05493	0.27102	0.26019
	4.00	0.46899	0.00469	0.00211	0.00493	0.10271	0.41658
	10.00	0.48679	0.00195	0.00223	0.00085	0.04503	0.46316
800	0.01	0.01778	0.15021	0.00040	0.79681	0.03442	0.00037
	0.05	0.07765	0.13462	0.00181	0.63995	0.13846	0.00752
	0.10	0.13411	0.11924	0.00321	0.50210	0.21766	0.02367
	0.30	0.26063	0.08208	0.00666	0.23792	0.31082	0.10188
	0.50	0.32147	0.06268	0.00850	0.13873	0.30280	0.16582
	0.75	0.36407	0.04841	0.00987	0.08277	0.27147	0.22340
	1.00	0.38996	0.03945	0.01073	0.05496	0.24060	0.26430
	4.00	0.46455	0.01226	0.01339	0.00531	0.09326	0.41123
	10.00	0.48311	0.00516	0.01409	0.00094	0.04128	0.45543
900	0.01	0.01646	0.28607	0.00180	0.66496	0.03029	0.00042
	0.05	0.07231	0.25654	0.00796	0.53475	0.12020	0.00823
	0.10	0.12560	0.22758	0.01395	0.42085	0.18677	0.02525
	0.30	0.24736	0.15792	0.02812	0.20264	0.26132	0.10264
	0.50	0.30719	0.12146	0.03542	0.11987	0.25318	0.16288
	0.75	0.34964	0.09447	0.04078	0.07251	0.22671	0.21590
	1.00	0.37569	0.07737	0.04416	0.04864	0.20104	0.25310
	4.00	0.45199	0.02454	0.05449	0.00489	0.07868	0.38541
	10.00	0.47131	0.01039	0.05723	0.00088	0.03499	0.42520
1000	0.01	0.01483	0.45259	0.00543	0.50332	0.02345	0.00039
	0.05	0.06542	0.40604	0.02377	0.40512	0.09219	0.00744
	0.10	0.11416	0.36055	0.04128	0.31942	0.14215	0.02244
	0.30	0.22731	0.25121	0.08184	0.15506	0.19637	0.08820

TABLE-34 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.28397	0.19381	0.10238	0.09230	0.18952	0.13802
	0.75	0.32466	0.15117	0.11733	0.05615	0.16941	0.18129
	1.00	0.34985	0.12406	0.12671	0.03782	0.15014	0.21142
	4.00	0.42472	0.03964	0.15532	0.00386	0.05881	0.31765
	10.00	0.44397	0.01683	0.16290	0.00070	0.02618	0.34943
1100	0.01	0.01322	0.61402	0.01115	0.34658	0.01478	0.00025
	0.05	0.05835	0.55088	0.04883	0.27897	0.05809	0.00488
	0.10	0.10186	0.48917	0.08476	0.21996	0.08953	0.01472
	0.30	0.20337	0.34082	0.16783	0.10678	0.12351	0.05769
	0.50	0.25455	0.26292	0.20977	0.06355	0.11909	0.09012
	0.75	0.29151	0.20503	0.24024	0.03864	0.10636	0.11821
	1.00	0.31449	0.16824	0.25932	0.02602	0.09421	0.13773
	4.00	0.38329	0.05371	0.31732	0.00265	0.03680	0.20623
	10.00	0.40112	0.02279	0.33263	0.00048	0.01637	0.22662
1200	0.01	0.01194	0.74258	0.01614	0.22173	0.00750	0.00011
	0.05	0.05262	0.66601	0.07114	0.17836	0.02965	0.00222
	0.10	0.09178	0.59099	0.12412	0.14044	0.04591	0.00676
	0.30	0.18292	0.41049	0.24809	0.06776	0.06374	0.02701
	0.50	0.22883	0.31589	0.31116	0.04012	0.06152	0.04249
	0.75	0.26196	0.24578	0.35708	0.02429	0.05493	0.05596
	1.00	0.28256	0.20134	0.38584	0.01630	0.04862	0.06533
	4.00	0.34424	0.06387	0.47311	0.00164	0.01891	0.09823
	10.00	0.36022	0.02704	0.49606	0.00029	0.00839	0.10799
1300	0.01	0.01107	0.83017	0.01866	0.13667	0.00340	0.00004
	0.05	0.04888	0.74432	0.08263	0.10987	0.01348	0.00082
	0.10	0.08537	0.66001	0.14477	0.08639	0.02095	0.00251
	0.30	0.17065	0.45685	0.29168	0.04139	0.02921	0.01021
	0.50	0.21375	0.35055	0.36697	0.02437	0.02820	0.01616
	0.75	0.24489	0.27201	0.42190	0.01467	0.02516	0.02136
	1.00	0.26426	0.22240	0.45630	0.00981	0.02225	0.02498
	4.00	0.32224	0.07001	0.56048	0.00097	0.00860	0.03769
	10.00	0.33724	0.02957	0.58776	0.00017	0.00381	0.04145
1400	0.01	0.01054	0.88387	0.01952	0.08451	0.00154	0.00002
	0.05	0.04671	0.79227	0.08668	0.06790	0.00614	0.00030
	0.10	0.08183	0.70210	0.15226	0.05333	0.00956	0.00092
	0.30	0.16461	0.48455	0.30830	0.02540	0.01336	0.00378
	0.50	0.20675	0.37086	0.38861	0.01488	0.01289	0.00601
	0.75	0.23731	0.28710	0.44723	0.00892	0.01148	0.00796
	1.00	0.25635	0.23433	0.48393	0.00594	0.01014	0.00931
	4.00	0.31340	0.07329	0.59476	0.00058	0.00390	0.01407
	10.00	0.32816	0.03089	0.62366	0.00010	0.00172	0.01547
1500	0.01	0.01024	0.91570	0.01972	0.05360	0.00074	0.00001
	0.05	0.04548	0.82062	0.08777	0.04305	0.00296	0.00012
	0.10	0.07990	0.72688	0.15446	0.03377	0.00462	0.00037
	0.30	0.16168	0.50046	0.31387	0.01601	0.00646	0.00152
	0.50	0.20360	0.38229	0.39613	0.00934	0.00623	0.00242
	0.75	0.23408	0.29540	0.45620	0.00558	0.00554	0.00321
	1.00	0.25309	0.24079	0.49377	0.00371	0.00489	0.00376
	4.00	0.31013	0.07494	0.60702	0.00036	0.00187	0.00568
	10.00	0.32488	0.03154	0.63645	0.00006	0.00083	0.00624

TABLE-35 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O= 2.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.03767	0.00371	0.00000	0.92108	0.03742	0.00012
	0.05	0.15360	0.00322	0.00000	0.69219	0.14838	0.00261
	0.10	0.24966	0.00275	0.00000	0.50666	0.23221	0.00872
	0.30	0.42821	0.00168	0.00000	0.18969	0.33262	0.04779
	0.50	0.49971	0.00116	0.00000	0.09057	0.31740	0.09115
	0.75	0.54523	0.00082	0.00000	0.04485	0.27296	0.13613
	1.00	0.57125	0.00063	0.00000	0.02619	0.23262	0.16931
	4.00	0.63995	0.00016	0.00000	0.00170	0.07644	0.28175
	10.00	0.65572	0.00006	0.00000	0.00027	0.03218	0.31177
600	0.01	0.03738	0.01903	0.00000	0.90642	0.03696	0.00021
	0.05	0.15257	0.01652	0.00002	0.68250	0.14422	0.00417
	0.10	0.24822	0.01417	0.00003	0.50272	0.22150	0.01334
	0.30	0.42664	0.00894	0.00007	0.20008	0.30196	0.06231
	0.50	0.49837	0.00644	0.00009	0.10366	0.28461	0.10684
	0.75	0.54414	0.00472	0.00011	0.05580	0.24643	0.14880
	1.00	0.57033	0.00371	0.00012	0.03450	0.21245	0.17888
	4.00	0.63963	0.00102	0.00015	0.00262	0.07368	0.28290
	10.00	0.65555	0.00042	0.00015	0.00043	0.03149	0.31195
700	0.01	0.03656	0.06210	0.00006	0.86506	0.03593	0.00029
	0.05	0.14968	0.05393	0.00025	0.65240	0.13806	0.00569
	0.10	0.24415	0.04640	0.00043	0.48285	0.20863	0.01754
	0.30	0.42199	0.02983	0.00089	0.19957	0.27434	0.07338
	0.50	0.49423	0.02194	0.00113	0.10798	0.25632	0.11839
	0.75	0.54061	0.01646	0.00130	0.06076	0.22243	0.15844
	1.00	0.56727	0.01315	0.00141	0.03881	0.19286	0.18650
	4.00	0.63822	0.00384	0.00174	0.00330	0.06934	0.28357
	10.00	0.65462	0.00158	0.00182	0.00056	0.03002	0.31139
800	0.01	0.03492	0.14879	0.00040	0.78174	0.03379	0.00037
	0.05	0.14377	0.12928	0.00174	0.59016	0.12808	0.00697
	0.10	0.23570	0.11138	0.00302	0.43810	0.19093	0.02088
	0.30	0.41179	0.07236	0.00594	0.18492	0.24413	0.08087
	0.50	0.48469	0.05383	0.00740	0.10231	0.22624	0.12553
	0.75	0.53201	0.04084	0.00845	0.05889	0.19605	0.16376
	1.00	0.55942	0.03292	0.00910	0.03827	0.17025	0.19004
	4.00	0.63329	0.00992	0.01105	0.00348	0.06229	0.27998
	10.00	0.65059	0.00414	0.01155	0.00061	0.02718	0.30594
900	0.01	0.03236	0.28335	0.00178	0.65235	0.02975	0.00041
	0.05	0.13431	0.24626	0.00768	0.49277	0.11131	0.00766
	0.10	0.22182	0.21235	0.01312	0.36638	0.16398	0.02236
	0.30	0.39348	0.13864	0.02510	0.15618	0.20480	0.08179
	0.50	0.46638	0.10363	0.03086	0.08726	0.18822	0.12365
	0.75	0.51438	0.07901	0.03494	0.05072	0.16246	0.15849
	1.00	0.54246	0.06393	0.03745	0.03321	0.14089	0.18206
	4.00	0.61938	0.01956	0.04488	0.00311	0.05165	0.26143
	10.00	0.63771	0.00820	0.04679	0.00055	0.02259	0.28417
1000	0.01	0.02918	0.44827	0.00538	0.49376	0.02303	0.00038
	0.05	0.12211	0.38964	0.02293	0.37306	0.08533	0.00692
	0.10	0.20314	0.33606	0.03882	0.27751	0.12462	0.01985
	0.30	0.36588	0.21967	0.07291	0.11857	0.15297	0.07000

TABLE-35 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.43668	0.16436	0.08891	0.06638	0.13957	0.10410
	0.75	0.48395	0.12542	0.10011	0.03865	0.11992	0.13196
	1.00	0.51186	0.10154	0.10694	0.02534	0.10372	0.15060
	4.00	0.58940	0.03114	0.12698	0.00238	0.03777	0.21233
	10.00	0.60814	0.01307	0.13210	0.00042	0.01649	0.22978
1100	0.01	0.02605	0.60815	0.01105	0.33999	0.01451	0.00025
	0.05	0.10958	0.52855	0.04696	0.25681	0.05359	0.00452
	0.10	0.18312	0.45572	0.07931	0.19092	0.07804	0.01288
	0.30	0.33310	0.29742	0.14812	0.08131	0.09512	0.04493
	0.50	0.39942	0.22221	0.18011	0.04539	0.08642	0.06644
	0.75	0.44408	0.16934	0.20236	0.02636	0.07399	0.08387
	1.00	0.47062	0.13697	0.21587	0.01725	0.06385	0.09545
	4.00	0.54495	0.04184	0.25517	0.00161	0.02306	0.13336
	10.00	0.56306	0.01754	0.26511	0.00028	0.01004	0.14395
1200	0.01	0.02356	0.73548	0.01598	0.21751	0.00735	0.00011
	0.05	0.09945	0.63896	0.06813	0.16417	0.02725	0.00204
	0.10	0.16677	0.55045	0.11535	0.12184	0.03974	0.00584
	0.30	0.30557	0.35787	0.21615	0.05150	0.04841	0.02050
	0.50	0.36760	0.26657	0.26301	0.02857	0.04388	0.03036
	0.75	0.40961	0.20260	0.29550	0.01650	0.03747	0.03832
	1.00	0.43465	0.16355	0.31519	0.01076	0.03226	0.04360
	4.00	0.50507	0.04961	0.37204	0.00099	0.01155	0.06074
	10.00	0.52228	0.02075	0.38629	0.00017	0.00502	0.06549
1300	0.01	0.02187	0.82223	0.01846	0.13407	0.00333	0.00004
	0.05	0.09285	0.71396	0.07899	0.10109	0.01236	0.00075
	0.10	0.15644	0.61441	0.13407	0.07486	0.01806	0.00216
	0.30	0.28935	0.39758	0.25212	0.03135	0.02198	0.00763
	0.50	0.34948	0.29508	0.30700	0.01727	0.01986	0.01131
	0.75	0.39041	0.22355	0.34495	0.00991	0.01691	0.01428
	1.00	0.41488	0.18006	0.36788	0.00643	0.01452	0.01624
	4.00	0.48390	0.05417	0.43363	0.00058	0.00515	0.02256
	10.00	0.50079	0.02261	0.44997	0.00010	0.00223	0.02430
1400	0.01	0.02085	0.87541	0.01931	0.08290	0.00151	0.00001
	0.05	0.08903	0.75977	0.08285	0.06245	0.00563	0.00027
	0.10	0.15074	0.65316	0.14093	0.04615	0.00823	0.00079
	0.30	0.28145	0.42077	0.26582	0.01915	0.01000	0.00281
	0.50	0.34122	0.31125	0.32386	0.01048	0.00902	0.00417
	0.75	0.38209	0.23511	0.36390	0.00598	0.00765	0.00527
	1.00	0.40656	0.18900	0.38803	0.00386	0.00656	0.00599
	4.00	0.47574	0.05647	0.45683	0.00034	0.00231	0.00830
	10.00	0.49268	0.02352	0.47382	0.00006	0.00100	0.00893
1500	0.01	0.02026	0.90692	0.01952	0.05257	0.00073	0.00001
	0.05	0.08687	0.78681	0.08393	0.03957	0.00272	0.00011
	0.10	0.14764	0.67584	0.14304	0.02920	0.00397	0.00032
	0.30	0.27763	0.43383	0.27055	0.01203	0.00483	0.00113
	0.50	0.33752	0.32008	0.32983	0.00655	0.00434	0.00168
	0.75	0.37857	0.24126	0.37066	0.00372	0.00368	0.00212
	1.00	0.40318	0.19365	0.39522	0.00240	0.00315	0.00241
	4.00	0.47277	0.05757	0.46501	0.00021	0.00110	0.00333
	10.00	0.48980	0.02394	0.48216	0.00004	0.00047	0.00358

TABLE-36 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O= 3.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.05545	0.00368	0.00000	0.90402	0.03672	0.00012
	0.05	0.21395	0.00310	0.00000	0.64273	0.13779	0.00242
	0.10	0.33290	0.00260	0.00000	0.45032	0.20642	0.00775
	0.30	0.52901	0.00153	0.00000	0.15617	0.27392	0.03937
	0.50	0.59969	0.00104	0.00000	0.07242	0.25390	0.07294
	0.75	0.64262	0.00073	0.00000	0.03522	0.21444	0.10699
	1.00	0.66648	0.00055	0.00000	0.02036	0.18089	0.13171
	4.00	0.72722	0.00014	0.00000	0.00129	0.05789	0.21346
	10.00	0.74072	0.00006	0.00000	0.00020	0.02423	0.23479
600	0.01	0.05503	0.01886	0.00000	0.88963	0.03628	0.00020
	0.05	0.21258	0.01591	0.00002	0.63366	0.13396	0.00387
	0.10	0.33110	0.01336	0.00003	0.44668	0.19696	0.01187
	0.30	0.52725	0.00811	0.00006	0.16453	0.24867	0.05139
	0.50	0.59825	0.00575	0.00008	0.08275	0.22759	0.08558
	0.75	0.64148	0.00418	0.00009	0.04373	0.19347	0.11705
	1.00	0.66554	0.00327	0.00010	0.02675	0.16507	0.13926
	4.00	0.72690	0.00089	0.00013	0.00198	0.05572	0.21438
	10.00	0.74056	0.00036	0.00013	0.00033	0.02367	0.23495
700	0.01	0.05385	0.06152	0.00006	0.84902	0.03527	0.00029
	0.05	0.20869	0.05196	0.00024	0.60551	0.12831	0.00529
	0.10	0.32598	0.04371	0.00041	0.42863	0.18563	0.01564
	0.30	0.52205	0.02701	0.00081	0.16359	0.22587	0.06068
	0.50	0.59383	0.01956	0.00101	0.08579	0.20474	0.09507
	0.75	0.63782	0.01453	0.00116	0.04733	0.17429	0.12488
	1.00	0.66240	0.01154	0.00125	0.02989	0.14947	0.14544
	4.00	0.72552	0.00332	0.00152	0.00247	0.05221	0.21498
	10.00	0.73965	0.00137	0.00158	0.00042	0.02245	0.23453
800	0.01	0.05145	0.14740	0.00040	0.76721	0.03318	0.00036
	0.05	0.20077	0.12450	0.00168	0.54739	0.11915	0.00651
	0.10	0.31538	0.10485	0.00285	0.38820	0.17003	0.01869
	0.30	0.51069	0.06532	0.00541	0.15067	0.20078	0.06713
	0.50	0.58368	0.04777	0.00664	0.08057	0.18021	0.10113
	0.75	0.62892	0.03584	0.00751	0.04536	0.15296	0.12941
	1.00	0.65442	0.02871	0.00804	0.02910	0.13123	0.14850
	4.00	0.72069	0.00850	0.00962	0.00255	0.04645	0.21219
	10.00	0.73572	0.00353	0.01001	0.00044	0.02011	0.23018
900	0.01	0.04771	0.28070	0.00177	0.64019	0.02922	0.00041
	0.05	0.18809	0.23706	0.00743	0.45662	0.10364	0.00716
	0.10	0.29799	0.19963	0.01244	0.32380	0.14608	0.02007
	0.30	0.49037	0.12461	0.02290	0.12617	0.16790	0.06806
	0.50	0.56427	0.09139	0.02771	0.06787	0.14905	0.09971
	0.75	0.61076	0.06880	0.03106	0.03846	0.12573	0.12519
	1.00	0.63722	0.05525	0.03308	0.02480	0.10756	0.14209
	4.00	0.70708	0.01654	0.03898	0.00222	0.03794	0.19724
	10.00	0.72320	0.00690	0.04047	0.00039	0.01643	0.21261
1000	0.01	0.04307	0.44406	0.00534	0.48453	0.02263	0.00037
	0.05	0.17174	0.37489	0.02217	0.34534	0.07938	0.00647
	0.10	0.27463	0.31550	0.03675	0.24458	0.11075	0.01779
	0.30	0.45983	0.19656	0.06630	0.09494	0.12448	0.05789

TABLE-36 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.53295	0.14402	0.07950	0.05096	0.10935	0.08322
	0.75	0.57959	0.10834	0.08851	0.02884	0.09158	0.10315
	1.00	0.60637	0.08696	0.09392	0.01858	0.07801	0.11616
	4.00	0.67802	0.02600	0.10944	0.00166	0.02718	0.15770
	10.00	0.69476	0.01084	0.11331	0.00029	0.01174	0.16906
1100	0.01	0.03852	0.60243	0.01095	0.33362	0.01424	0.00025
	0.05	0.15497	0.50835	0.04525	0.23756	0.04967	0.00419
	0.10	0.24965	0.42741	0.07468	0.16793	0.06892	0.01142
	0.30	0.42390	0.26525	0.13336	0.06468	0.07638	0.03643
	0.50	0.49413	0.19379	0.15912	0.03452	0.06658	0.05186
	0.75	0.53938	0.14542	0.17652	0.01944	0.05543	0.06382
	1.00	0.56553	0.11652	0.18690	0.01248	0.04702	0.07155
	4.00	0.63604	0.03463	0.21627	0.00110	0.01617	0.09579
	10.00	0.65262	0.01442	0.22350	0.00019	0.00696	0.10231
1200	0.01	0.03488	0.72855	0.01582	0.21343	0.00721	0.00011
	0.05	0.14145	0.61435	0.06540	0.15177	0.02515	0.00188
	0.10	0.22938	0.51581	0.10788	0.10699	0.03483	0.00511
	0.30	0.39428	0.31832	0.19216	0.04074	0.03828	0.01621
	0.50	0.46188	0.23161	0.22880	0.02157	0.03317	0.02297
	0.75	0.50575	0.17319	0.25336	0.01206	0.02746	0.02817
	1.00	0.53121	0.13844	0.26792	0.00771	0.02321	0.03150
	4.00	0.60020	0.04080	0.30864	0.00067	0.00788	0.04181
	10.00	0.61649	0.01694	0.31855	0.00012	0.00338	0.04453
1300	0.01	0.03242	0.81445	0.01827	0.13154	0.00326	0.00004
	0.05	0.13265	0.68622	0.07568	0.09338	0.01138	0.00069
	0.10	0.21665	0.57519	0.12493	0.06561	0.01575	0.00187
	0.30	0.37720	0.35261	0.22241	0.02466	0.01719	0.00594
	0.50	0.44406	0.25537	0.26445	0.01293	0.01480	0.00839
	0.75	0.48772	0.19022	0.29243	0.00718	0.01219	0.01026
	1.00	0.51314	0.15165	0.30892	0.00456	0.01027	0.01145
	4.00	0.58224	0.04430	0.35455	0.00039	0.00344	0.01508
	10.00	0.59857	0.01835	0.36551	0.00007	0.00147	0.01603
1400	0.01	0.03094	0.86711	0.01911	0.08134	0.00148	0.00001
	0.05	0.12757	0.72999	0.07936	0.05765	0.00518	0.00025
	0.10	0.20965	0.61090	0.13122	0.04037	0.00717	0.00068
	0.30	0.36898	0.37222	0.23385	0.01499	0.00778	0.00218
	0.50	0.43609	0.26846	0.27791	0.00780	0.00667	0.00307
	0.75	0.48009	0.19931	0.30708	0.00430	0.00547	0.00375
	1.00	0.50575	0.15855	0.32421	0.00272	0.00460	0.00418
	4.00	0.57556	0.04598	0.37122	0.00023	0.00153	0.00548
	10.00	0.59206	0.01901	0.38242	0.00004	0.00065	0.00582
1500	0.01	0.03007	0.89831	0.01932	0.05158	0.00071	0.00001
	0.05	0.12469	0.75577	0.08043	0.03651	0.00250	0.00010
	0.10	0.20585	0.63169	0.13322	0.02551	0.00346	0.00027
	0.30	0.36504	0.38309	0.23787	0.00938	0.00375	0.00087
	0.50	0.43255	0.27546	0.28270	0.00485	0.00320	0.00123
	0.75	0.47690	0.20401	0.31231	0.00266	0.00262	0.00150
	1.00	0.50277	0.16204	0.32964	0.00168	0.00220	0.00167
	4.00	0.57317	0.04676	0.37701	0.00014	0.00072	0.00219
	10.00	0.58980	0.01930	0.38824	0.00002	0.00031	0.00232

TABLE-37 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O= 3.76

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.06857	0.00365	0.00000	0.89144	0.03621	0.00012
	0.05	0.25446	0.00302	0.00000	0.60954	0.13069	0.00230
	0.10	0.38489	0.00249	0.00000	0.41515	0.19032	0.00715
	0.30	0.58477	0.00143	0.00000	0.13762	0.24145	0.03471
	0.50	0.65258	0.00097	0.00000	0.06283	0.22031	0.06331
	0.75	0.69275	0.00067	0.00000	0.03027	0.18432	0.09198
	1.00	0.71475	0.00051	0.00000	0.01740	0.15468	0.11265
	4.00	0.76975	0.00013	0.00000	0.00109	0.04885	0.18018
	10.00	0.78177	0.00005	0.00000	0.00017	0.02039	0.19761
600	0.01	0.06805	0.01872	0.00000	0.87724	0.03578	0.00020
	0.05	0.25287	0.01550	0.00002	0.60088	0.12707	0.00367
	0.10	0.38289	0.01283	0.00003	0.41167	0.18162	0.01096
	0.30	0.58295	0.00761	0.00006	0.14487	0.21918	0.04534
	0.50	0.65113	0.00535	0.00007	0.07169	0.19742	0.07433
	0.75	0.69162	0.00387	0.00009	0.03752	0.16622	0.10069
	1.00	0.71382	0.00302	0.00009	0.02283	0.14106	0.11917
	4.00	0.76944	0.00082	0.00012	0.00167	0.04698	0.18098
	10.00	0.78162	0.00033	0.00012	0.00027	0.01990	0.19776
700	0.01	0.06660	0.06109	0.00005	0.83719	0.03479	0.00028
	0.05	0.24837	0.05059	0.00023	0.57403	0.12176	0.00503
	0.10	0.37721	0.04195	0.00039	0.39475	0.17124	0.01445
	0.30	0.57756	0.02531	0.00076	0.14371	0.19903	0.05363
	0.50	0.64666	0.01817	0.00094	0.07408	0.17744	0.08270
	0.75	0.68796	0.01343	0.00107	0.04044	0.14952	0.10757
	1.00	0.71072	0.01064	0.00115	0.02539	0.12750	0.12459
	4.00	0.76809	0.00303	0.00139	0.00206	0.04388	0.18153
	10.00	0.78074	0.00125	0.00145	0.00035	0.01881	0.19740
800	0.01	0.06366	0.14636	0.00039	0.75649	0.03274	0.00036
	0.05	0.23919	0.12119	0.00164	0.51865	0.11314	0.00619
	0.10	0.36547	0.10055	0.00275	0.35700	0.15693	0.01731
	0.30	0.56583	0.06108	0.00509	0.13176	0.17675	0.05949
	0.50	0.63643	0.04424	0.00620	0.06913	0.15584	0.08815
	0.75	0.67914	0.03300	0.00697	0.03845	0.13080	0.11164
	1.00	0.70286	0.02634	0.00745	0.02450	0.11150	0.12735
	4.00	0.76342	0.00773	0.00883	0.00211	0.03879	0.17912
	10.00	0.77695	0.00320	0.00918	0.00036	0.01672	0.19357
900	0.01	0.05906	0.27872	0.00176	0.63122	0.02884	0.00040
	0.05	0.22453	0.23065	0.00725	0.43228	0.09845	0.00683
	0.10	0.34622	0.19123	0.01198	0.29713	0.13482	0.01863
	0.30	0.54490	0.11616	0.02156	0.10963	0.14740	0.06036
	0.50	0.61694	0.08427	0.02587	0.05770	0.12831	0.08690
	0.75	0.66117	0.06299	0.02883	0.03224	0.10687	0.10790
	1.00	0.68599	0.05037	0.03061	0.02062	0.09075	0.12167
	4.00	0.75030	0.01490	0.03575	0.00180	0.03135	0.16589
	10.00	0.76490	0.00620	0.03704	0.00031	0.01351	0.17805
1000	0.01	0.05337	0.44092	0.00530	0.47771	0.02233	0.00037
	0.05	0.20563	0.36459	0.02164	0.32663	0.07535	0.00617
	0.10	0.32039	0.30186	0.03538	0.22390	0.10199	0.01648
	0.30	0.51355	0.18259	0.06228	0.08192	0.10860	0.05107

TABLE-37 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.58561	0.13216	0.07395	0.04291	0.09335	0.07202
	0.75	0.63047	0.09861	0.08182	0.02389	0.07706	0.08815
	1.00	0.65586	0.07877	0.08651	0.01524	0.06508	0.09854
	4.00	0.72245	0.02323	0.09977	0.00133	0.02213	0.13109
	10.00	0.73774	0.00965	0.10305	0.00023	0.00950	0.13983
1100	0.01	0.04778	0.59816	0.01087	0.32891	0.01404	0.00024
	0.05	0.18626	0.49419	0.04406	0.22451	0.04701	0.00398
	0.10	0.29286	0.40852	0.07157	0.15341	0.06314	0.01049
	0.30	0.47693	0.24568	0.12431	0.05548	0.06594	0.03165
	0.50	0.54719	0.17713	0.14668	0.02884	0.05610	0.04406
	0.75	0.59137	0.13174	0.16154	0.01595	0.04595	0.05345
	1.00	0.61652	0.10500	0.17032	0.01013	0.03861	0.05941
	4.00	0.68300	0.03073	0.19478	0.00087	0.01292	0.07770
	10.00	0.69835	0.01274	0.20072	0.00015	0.00552	0.08251
1200	0.01	0.04331	0.72337	0.01570	0.21041	0.00711	0.00011
	0.05	0.17068	0.59702	0.06348	0.14333	0.02372	0.00177
	0.10	0.27064	0.49257	0.10288	0.09756	0.03171	0.00464
	0.30	0.44723	0.29406	0.17746	0.03477	0.03266	0.01382
	0.50	0.51594	0.21096	0.20857	0.01790	0.02754	0.01909
	0.75	0.55949	0.15626	0.22901	0.00982	0.02240	0.02302
	1.00	0.58440	0.12420	0.24098	0.00620	0.01873	0.02549
	4.00	0.65053	0.03601	0.27385	0.00052	0.00617	0.03291
	10.00	0.66585	0.01489	0.28171	0.00009	0.00263	0.03483
1300	0.01	0.04030	0.80864	0.01813	0.12967	0.00321	0.00004
	0.05	0.16056	0.66661	0.07335	0.08812	0.01072	0.00065
	0.10	0.25674	0.54874	0.11881	0.05971	0.01429	0.00169
	0.30	0.43037	0.32491	0.20424	0.02093	0.01455	0.00501
	0.50	0.49906	0.23183	0.23940	0.01066	0.01217	0.00688
	0.75	0.54287	0.17098	0.26227	0.00580	0.00983	0.00825
	1.00	0.56799	0.13551	0.27556	0.00364	0.00819	0.00911
	4.00	0.63489	0.03893	0.31157	0.00030	0.00266	0.01165
	10.00	0.65041	0.01606	0.32007	0.00005	0.00113	0.01229
1400	0.01	0.03847	0.86091	0.01897	0.08018	0.00146	0.00001
	0.05	0.15471	0.70891	0.07690	0.05436	0.00488	0.00024
	0.10	0.24913	0.58236	0.12471	0.03669	0.00650	0.00062
	0.30	0.42233	0.34230	0.21431	0.01267	0.00656	0.00183
	0.50	0.49163	0.24312	0.25090	0.00639	0.00546	0.00250
	0.75	0.53595	0.17866	0.27455	0.00345	0.00439	0.00300
	1.00	0.56141	0.14127	0.28821	0.00216	0.00364	0.00330
	4.00	0.62922	0.04029	0.32494	0.00018	0.00117	0.00420
	10.00	0.64494	0.01659	0.33353	0.00003	0.00049	0.00442
1500	0.01	0.03740	0.89187	0.01917	0.05084	0.00070	0.00001
	0.05	0.15141	0.73377	0.07796	0.03442	0.00235	0.00009
	0.10	0.24501	0.60183	0.12663	0.02315	0.00313	0.00025
	0.30	0.41850	0.35183	0.21787	0.00791	0.00315	0.00073
	0.50	0.48834	0.24908	0.25500	0.00397	0.00261	0.00100
	0.75	0.53308	0.18258	0.27891	0.00213	0.00209	0.00120
	1.00	0.55878	0.14414	0.29269	0.00133	0.00173	0.00132
	4.00	0.62721	0.04091	0.32954	0.00011	0.00055	0.00167
	10.00	0.64305	0.01682	0.33811	0.00002	0.00023	0.00176

TABLE-38 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O= 5.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.08912	0.00361	0.00000	0.87173	0.03541	0.00012
	0.05	0.31205	0.00290	0.00000	0.56235	0.12058	0.00212
	0.10	0.45401	0.00235	0.00000	0.36838	0.16891	0.00635
	0.30	0.65175	0.00131	0.00000	0.11536	0.20246	0.02912
	0.50	0.71397	0.00088	0.00000	0.05169	0.18133	0.05213
	0.75	0.74977	0.00061	0.00000	0.02463	0.15007	0.07492
	1.00	0.76905	0.00046	0.00000	0.01408	0.12519	0.09121
	4.00	0.81628	0.00011	0.00000	0.00087	0.03897	0.14377
	10.00	0.82643	0.00005	0.00000	0.00014	0.01621	0.15718
600	0.01	0.08846	0.01852	0.00000	0.85784	0.03499	0.00020
	0.05	0.31017	0.01488	0.00002	0.55427	0.11727	0.00339
	0.10	0.45179	0.01208	0.00003	0.36514	0.16122	0.00973
	0.30	0.64989	0.00696	0.00005	0.12127	0.18376	0.03807
	0.50	0.71253	0.00485	0.00007	0.05887	0.16242	0.06126
	0.75	0.74866	0.00349	0.00008	0.03046	0.13523	0.08208
	1.00	0.76815	0.00271	0.00008	0.01843	0.11407	0.09655
	4.00	0.81599	0.00073	0.00010	0.00133	0.03742	0.14444
	10.00	0.82628	0.00029	0.00011	0.00022	0.01580	0.15730
700	0.01	0.08659	0.06041	0.00005	0.81864	0.03403	0.00028
	0.05	0.30488	0.04857	0.00022	0.52925	0.11243	0.00465
	0.10	0.44549	0.03948	0.00037	0.34970	0.15208	0.01287
	0.30	0.64441	0.02312	0.00069	0.11986	0.16677	0.04515
	0.50	0.70811	0.01643	0.00085	0.06053	0.14577	0.06831
	0.75	0.74511	0.01206	0.00097	0.03263	0.12138	0.08785
	1.00	0.76517	0.00952	0.00104	0.02035	0.10282	0.10110
	4.00	0.81472	0.00269	0.00124	0.00163	0.03479	0.14492
	10.00	0.82545	0.00110	0.00130	0.00027	0.01486	0.15701
800	0.01	0.08281	0.14473	0.00039	0.73969	0.03204	0.00035
	0.05	0.29408	0.11631	0.00158	0.47772	0.10456	0.00574
	0.10	0.43247	0.09452	0.00260	0.31549	0.13946	0.01547
	0.30	0.63252	0.05559	0.00468	0.10913	0.14783	0.05025
	0.50	0.69806	0.03980	0.00564	0.05593	0.12757	0.07301
	0.75	0.73659	0.02946	0.00631	0.03066	0.10564	0.09134
	1.00	0.75764	0.02342	0.00672	0.01937	0.08937	0.10348
	4.00	0.81033	0.00679	0.00789	0.00163	0.03046	0.14289
	10.00	0.82190	0.00281	0.00819	0.00028	0.01307	0.15375
900	0.01	0.07690	0.27559	0.00174	0.61713	0.02823	0.00039
	0.05	0.27684	0.22120	0.00699	0.39757	0.09104	0.00635
	0.10	0.41119	0.17943	0.01134	0.26160	0.11974	0.01669
	0.30	0.61141	0.10517	0.01983	0.08987	0.12270	0.05102
	0.50	0.67900	0.07527	0.02354	0.04604	0.10425	0.07191
	0.75	0.71932	0.05577	0.02605	0.02527	0.08550	0.08809
	1.00	0.74157	0.04437	0.02755	0.01600	0.07195	0.09856
	4.00	0.79805	0.01294	0.03184	0.00136	0.02424	0.13157
	10.00	0.81064	0.00536	0.03290	0.00023	0.01038	0.14049
1000	0.01	0.06959	0.43595	0.00525	0.46699	0.02186	0.00036
	0.05	0.25466	0.34934	0.02085	0.29987	0.06957	0.00572
	0.10	0.38271	0.28263	0.03343	0.19628	0.09023	0.01471
	0.30	0.57999	0.16438	0.05699	0.06640	0.08948	0.04277

TABLE-38 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.64856	0.11716	0.06686	0.03373	0.07482	0.05887
	0.75	0.69002	0.08653	0.07341	0.01840	0.06067	0.07096
	1.00	0.71308	0.06871	0.07727	0.01160	0.05071	0.07863
	4.00	0.77226	0.01992	0.08804	0.00097	0.01675	0.10206
	10.00	0.78558	0.00824	0.09066	0.00017	0.00714	0.10822
1100	0.01	0.06240	0.59138	0.01075	0.32149	0.01373	0.00024
	0.05	0.23197	0.47313	0.04228	0.20578	0.04319	0.00366
	0.10	0.35252	0.38175	0.06717	0.13396	0.05536	0.00924
	0.30	0.54377	0.22007	0.11238	0.04452	0.05340	0.02586
	0.50	0.61189	0.15599	0.13072	0.02237	0.04403	0.03500
	0.75	0.65348	0.11472	0.14267	0.01210	0.03534	0.04169
	1.00	0.67674	0.09083	0.14963	0.00758	0.02935	0.04586
	4.00	0.73683	0.02609	0.16868	0.00063	0.00950	0.05828
	10.00	0.75042	0.01077	0.17322	0.00011	0.00403	0.06146
1200	0.01	0.05667	0.71513	0.01551	0.20564	0.00694	0.00011
	0.05	0.21379	0.57114	0.06062	0.13117	0.02167	0.00161
	0.10	0.32836	0.45944	0.09576	0.08488	0.02754	0.00402
	0.30	0.51511	0.26218	0.15814	0.02764	0.02595	0.01098
	0.50	0.58305	0.18467	0.18278	0.01371	0.02112	0.01466
	0.75	0.62486	0.13515	0.19855	0.00734	0.01679	0.01730
	1.00	0.64835	0.10666	0.20764	0.00457	0.01386	0.01892
	4.00	0.70924	0.03032	0.23204	0.00037	0.00440	0.02363
	10.00	0.72305	0.01248	0.23775	0.00006	0.00186	0.02481
1300	0.01	0.05280	0.79939	0.01790	0.12673	0.00314	0.00004
	0.05	0.20201	0.63724	0.06987	0.08053	0.00976	0.00059
	0.10	0.31340	0.51093	0.11012	0.05177	0.01233	0.00145
	0.30	0.49927	0.28844	0.18048	0.01650	0.01141	0.00391
	0.50	0.56803	0.20186	0.20767	0.00808	0.00919	0.00517
	0.75	0.61056	0.14700	0.22484	0.00429	0.00725	0.00607
	1.00	0.63450	0.11565	0.23464	0.00265	0.00595	0.00661
	4.00	0.69670	0.03256	0.26053	0.00021	0.00186	0.00814
	10.00	0.71080	0.01336	0.26650	0.00004	0.00078	0.00852
1400	0.01	0.05046	0.85103	0.01873	0.07835	0.00143	0.00001
	0.05	0.19523	0.67726	0.07323	0.04962	0.00444	0.00021
	0.10	0.30525	0.54147	0.11545	0.03172	0.00559	0.00053
	0.30	0.49183	0.30292	0.18878	0.00993	0.00511	0.00142
	0.50	0.56154	0.21090	0.21679	0.00481	0.00409	0.00187
	0.75	0.60475	0.15300	0.23433	0.00253	0.00321	0.00218
	1.00	0.62910	0.12008	0.24427	0.00156	0.00262	0.00237
	4.00	0.69230	0.03356	0.27030	0.00012	0.00081	0.00291
	10.00	0.70662	0.01375	0.27624	0.00002	0.00034	0.00304
1500	0.01	0.04908	0.88161	0.01894	0.04968	0.00069	0.00001
	0.05	0.19141	0.70073	0.07425	0.03139	0.00214	0.00008
	0.10	0.30085	0.55905	0.11722	0.01998	0.00269	0.00021
	0.30	0.48832	0.31075	0.19174	0.00617	0.00245	0.00057
	0.50	0.55870	0.21559	0.22004	0.00297	0.00195	0.00075
	0.75	0.60237	0.15600	0.23768	0.00156	0.00152	0.00087
	1.00	0.62697	0.12224	0.24765	0.00096	0.00124	0.00095
	4.00	0.69077	0.03401	0.27362	0.00007	0.00038	0.00115
	10.00	0.70519	0.01392	0.27951	0.00001	0.00016	0.00120

TABLE-39 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O=10.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.16365	0.00346	0.00000	0.80027	0.03251	0.00011
	0.05	0.47559	0.00253	0.00000	0.42838	0.09189	0.00162
	0.10	0.62439	0.00195	0.00000	0.25315	0.11614	0.00437
	0.30	0.78907	0.00102	0.00000	0.06974	0.12253	0.01764
	0.50	0.83305	0.00067	0.00000	0.03010	0.10574	0.03044
	0.75	0.85695	0.00046	0.00000	0.01405	0.08570	0.04284
	1.00	0.86941	0.00034	0.00000	0.00794	0.07071	0.05159
	4.00	0.89884	0.00008	0.00000	0.00048	0.02144	0.07916
	10.00	0.90496	0.00003	0.00000	0.00007	0.00887	0.08606
600	0.01	0.16248	0.01774	0.00000	0.78746	0.03213	0.00018
	0.05	0.47310	0.01298	0.00001	0.42189	0.08942	0.00259
	0.10	0.62187	0.01000	0.00002	0.25047	0.11092	0.00672
	0.30	0.78733	0.00540	0.00004	0.07296	0.11113	0.02315
	0.50	0.83177	0.00369	0.00005	0.03406	0.09454	0.03588
	0.75	0.85599	0.00262	0.00006	0.01724	0.07703	0.04706
	1.00	0.86866	0.00203	0.00006	0.01031	0.06422	0.05472
	4.00	0.89860	0.00054	0.00008	0.00072	0.02049	0.07958
	10.00	0.90484	0.00022	0.00008	0.00012	0.00860	0.08615
700	0.01	0.15919	0.05788	0.00005	0.75135	0.03128	0.00025
	0.05	0.46606	0.04233	0.00020	0.40196	0.08588	0.00357
	0.10	0.61471	0.03262	0.00031	0.23867	0.10474	0.00894
	0.30	0.78223	0.01781	0.00054	0.07117	0.10058	0.02766
	0.50	0.82790	0.01238	0.00066	0.03441	0.08438	0.04027
	0.75	0.85298	0.00898	0.00074	0.01808	0.06859	0.05063
	1.00	0.86616	0.00704	0.00078	0.01112	0.05734	0.05755
	4.00	0.89758	0.00196	0.00092	0.00086	0.01877	0.07991
	10.00	0.90418	0.00080	0.00096	0.00014	0.00796	0.08596
800	0.01	0.15254	0.13863	0.00037	0.67864	0.02949	0.00032
	0.05	0.45178	0.10113	0.00139	0.36118	0.08006	0.00445
	0.10	0.60004	0.07769	0.00218	0.21313	0.09609	0.01087
	0.30	0.77132	0.04230	0.00368	0.06318	0.08845	0.03107
	0.50	0.81923	0.02951	0.00434	0.03074	0.07286	0.04332
	0.75	0.84587	0.02150	0.00480	0.01632	0.05864	0.05287
	1.00	0.86000	0.01693	0.00507	0.01013	0.04882	0.05905
	4.00	0.89409	0.00479	0.00585	0.00081	0.01594	0.07852
	10.00	0.90135	0.00197	0.00604	0.00014	0.00677	0.08373
900	0.01	0.14217	0.26390	0.00168	0.56587	0.02603	0.00036
	0.05	0.42909	0.19164	0.00618	0.29841	0.06971	0.00496
	0.10	0.57630	0.14631	0.00954	0.17394	0.08211	0.01181
	0.30	0.75232	0.07855	0.01557	0.05013	0.07196	0.03147
	0.50	0.80311	0.05448	0.01806	0.02412	0.05790	0.04233
	0.75	0.83174	0.03957	0.01970	0.01272	0.04588	0.05038
	1.00	0.84705	0.03112	0.02067	0.00787	0.03785	0.05545
	4.00	0.88444	0.00879	0.02334	0.00063	0.01207	0.07074
	10.00	0.89249	0.00361	0.02399	0.00011	0.00510	0.07470
1000	0.01	0.12932	0.41729	0.00505	0.42787	0.02014	0.00034
	0.05	0.40009	0.30128	0.01835	0.22304	0.05280	0.00443
	0.10	0.54497	0.22824	0.02785	0.12801	0.06072	0.01021
	0.30	0.72471	0.12020	0.04387	0.03550	0.05037	0.02535

TABLE-39 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.77806	0.08259	0.05007	0.01676	0.03950	0.03302
	0.75	0.80845	0.05959	0.05404	0.00872	0.03075	0.03845
	1.00	0.82479	0.04667	0.05632	0.00535	0.02510	0.04177
	4.00	0.86495	0.01302	0.06246	0.00042	0.00777	0.05138
	10.00	0.87364	0.00534	0.06391	0.00007	0.00326	0.05378
1100	0.01	0.11671	0.56584	0.01031	0.29433	0.01260	0.00022
	0.05	0.37077	0.40616	0.03659	0.15165	0.03209	0.00274
	0.10	0.51257	0.30530	0.05446	0.08568	0.03590	0.00607
	0.30	0.69458	0.15766	0.08272	0.02285	0.02816	0.01402
	0.50	0.74988	0.10728	0.09300	0.01058	0.02154	0.01772
	0.75	0.78161	0.07686	0.09938	0.00543	0.01649	0.02023
	1.00	0.79873	0.05994	0.10298	0.00330	0.01333	0.02172
	4.00	0.84093	0.01651	0.11241	0.00025	0.00401	0.02588
	10.00	0.85008	0.00675	0.11457	0.00004	0.00167	0.02689
1200	0.01	0.10666	0.68399	0.01480	0.18812	0.00634	0.00010
	0.05	0.34772	0.48810	0.05149	0.09580	0.01573	0.00116
	0.10	0.48770	0.36398	0.07538	0.05327	0.01717	0.00249
	0.30	0.67294	0.18422	0.11098	0.01365	0.01280	0.00541
	0.50	0.73030	0.12411	0.12318	0.00619	0.00957	0.00666
	0.75	0.76337	0.08830	0.13051	0.00314	0.00721	0.00748
	1.00	0.78124	0.06857	0.13458	0.00189	0.00578	0.00795
	4.00	0.82535	0.01866	0.14494	0.00014	0.00169	0.00922
	10.00	0.83491	0.00760	0.14725	0.00002	0.00070	0.00952
1300	0.01	0.09989	0.76432	0.01705	0.11585	0.00286	0.00003
	0.05	0.33305	0.54241	0.05879	0.05834	0.00699	0.00041
	0.10	0.47288	0.40145	0.08532	0.03196	0.00751	0.00087
	0.30	0.66203	0.19950	0.12336	0.00789	0.00540	0.00183
	0.50	0.72122	0.13323	0.13585	0.00352	0.00397	0.00221
	0.75	0.75539	0.09424	0.14320	0.00176	0.00296	0.00246
	1.00	0.77385	0.07292	0.14722	0.00105	0.00235	0.00260
	4.00	0.81936	0.01965	0.15726	0.00008	0.00068	0.00297
	10.00	0.82921	0.00799	0.15946	0.00001	0.00028	0.00305
1400	0.01	0.09579	0.81347	0.01784	0.07159	0.00130	0.00001
	0.05	0.32470	0.57477	0.06148	0.03574	0.00316	0.00015
	0.10	0.46502	0.42295	0.08901	0.01935	0.00337	0.00032
	0.30	0.65718	0.20738	0.12777	0.00465	0.00237	0.00065
	0.50	0.71754	0.13768	0.14022	0.00205	0.00173	0.00078
	0.75	0.75237	0.09700	0.14747	0.00102	0.00128	0.00086
	1.00	0.77118	0.07489	0.15140	0.00061	0.00101	0.00091
	4.00	0.81744	0.02006	0.16113	0.00004	0.00029	0.00103
	10.00	0.82743	0.00814	0.16325	0.00001	0.00012	0.00106
1500	0.01	0.09339	0.84256	0.01804	0.04538	0.00063	0.00001
	0.05	0.32003	0.59351	0.06236	0.02252	0.00152	0.00006
	0.10	0.46084	0.43503	0.09030	0.01210	0.00162	0.00013
	0.30	0.65494	0.21147	0.12935	0.00286	0.00112	0.00026
	0.50	0.71598	0.13988	0.14176	0.00125	0.00082	0.00031
	0.75	0.75117	0.09832	0.14895	0.00062	0.00060	0.00034
	1.00	0.77016	0.07580	0.15284	0.00037	0.00048	0.00036
	4.00	0.81679	0.02023	0.16241	0.00003	0.00014	0.00041
	10.00	0.82684	0.00820	0.16448	0.00000	0.00006	0.00042

TABLE-40 EQUILIBRIUM GAS-PHASE MOLE FRACTIONS
P=25 ATM,N/O=20.00

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
500	0.01	0.28124	0.00321	0.00000	0.68752	0.02794	0.00009
	0.05	0.64449	0.00208	0.00000	0.29007	0.06226	0.00110
	0.10	0.76864	0.00153	0.00000	0.15566	0.07148	0.00269
	0.30	0.88202	0.00076	0.00000	0.03889	0.06845	0.00987
	0.50	0.90887	0.00049	0.00000	0.01638	0.05764	0.01662
	0.75	0.92292	0.00034	0.00000	0.00754	0.04611	0.02309
	1.00	0.93011	0.00025	0.00000	0.00424	0.03778	0.02761
	4.00	0.94672	0.00006	0.00000	0.00025	0.01127	0.04170
	10.00	0.95011	0.00002	0.00000	0.00004	0.00465	0.04518
600	0.01	0.27937	0.01644	0.00000	0.67640	0.02763	0.00015
	0.05	0.64171	0.01068	0.00001	0.28520	0.06063	0.00176
	0.10	0.76621	0.00783	0.00002	0.15349	0.06829	0.00415
	0.30	0.88057	0.00402	0.00003	0.04037	0.06199	0.01302
	0.50	0.90784	0.00271	0.00004	0.01835	0.05139	0.01968
	0.75	0.92217	0.00191	0.00004	0.00915	0.04127	0.02545
	1.00	0.92953	0.00147	0.00005	0.00543	0.03415	0.02938
	4.00	0.94654	0.00039	0.00006	0.00037	0.01070	0.04195
	10.00	0.95002	0.00016	0.00006	0.00006	0.00447	0.04523
700	0.01	0.27413	0.05363	0.00005	0.64505	0.02693	0.00022
	0.05	0.63391	0.03472	0.00016	0.27043	0.05833	0.00245
	0.10	0.75936	0.02541	0.00024	0.14488	0.06451	0.00559
	0.30	0.87639	0.01311	0.00041	0.03857	0.05581	0.01571
	0.50	0.90479	0.00897	0.00049	0.01804	0.04544	0.02228
	0.75	0.91986	0.00644	0.00054	0.00930	0.03629	0.02757
	1.00	0.92763	0.00502	0.00058	0.00566	0.03005	0.03107
	4.00	0.94578	0.00138	0.00067	0.00043	0.00960	0.04216
	10.00	0.94952	0.00056	0.00069	0.00007	0.00405	0.04511
800	0.01	0.26356	0.12838	0.00035	0.58199	0.02545	0.00028
	0.05	0.61816	0.08254	0.00116	0.24058	0.05447	0.00309
	0.10	0.74551	0.05994	0.00173	0.12689	0.05904	0.00689
	0.30	0.86766	0.03051	0.00279	0.03288	0.04833	0.01782
	0.50	0.89815	0.02083	0.00324	0.01532	0.03836	0.02411
	0.75	0.91453	0.01497	0.00355	0.00791	0.03017	0.02887
	1.00	0.92306	0.01170	0.00373	0.00483	0.02479	0.03190
	4.00	0.94321	0.00324	0.00423	0.00037	0.00780	0.04114
	10.00	0.94742	0.00133	0.00436	0.00006	0.00329	0.04355
900	0.01	0.24708	0.24416	0.00157	0.48437	0.02250	0.00032
	0.05	0.59345	0.15513	0.00517	0.19555	0.04722	0.00347
	0.10	0.72355	0.11117	0.00760	0.10043	0.04974	0.00750
	0.30	0.85291	0.05502	0.01172	0.02460	0.03794	0.01782
	0.50	0.88616	0.03711	0.01333	0.01119	0.02912	0.02308
	0.75	0.90422	0.02648	0.01437	0.00570	0.02240	0.02682
	1.00	0.91368	0.02061	0.01498	0.00345	0.01817	0.02911
	4.00	0.93621	0.00566	0.01660	0.00026	0.00552	0.03575
	10.00	0.94096	0.00231	0.01698	0.00004	0.00231	0.03741
1000	0.01	0.22672	0.38558	0.00472	0.36532	0.01737	0.00029
	0.05	0.56243	0.24130	0.01518	0.14307	0.03499	0.00304
	0.10	0.69543	0.17013	0.02175	0.07112	0.03534	0.00623
	0.30	0.83240	0.08141	0.03182	0.01629	0.02475	0.01334

TABLE-40 CONTINUED

T, K	O/H	N2	H2	CO	CH4	H2O	CO2
	0.50	0.86838	0.05412	0.03544	0.00720	0.01832	0.01654
	0.75	0.88804	0.03825	0.03767	0.00360	0.01376	0.01869
	1.00	0.89836	0.02960	0.03893	0.00215	0.01101	0.01995
	4.00	0.92299	0.00800	0.04219	0.00016	0.00322	0.02344
	10.00	0.92818	0.00325	0.04293	0.00003	0.00133	0.02427
1100	0.01	0.20681	0.52211	0.00955	0.25059	0.01076	0.00019
	0.05	0.53198	0.32154	0.02932	0.09504	0.02036	0.00176
	0.10	0.66787	0.22299	0.04054	0.04571	0.01952	0.00337
	0.30	0.81212	0.10327	0.05593	0.00980	0.01247	0.00641
	0.50	0.85061	0.06772	0.06094	0.00422	0.00891	0.00761
	0.75	0.87169	0.04743	0.06390	0.00207	0.00654	0.00836
	1.00	0.88277	0.03652	0.06552	0.00123	0.00517	0.00879
	4.00	0.90919	0.00973	0.06961	0.00009	0.00146	0.00992
	10.00	0.91475	0.00394	0.07051	0.00001	0.00060	0.01018
1200	0.01	0.19101	0.63025	0.01358	0.15972	0.00536	0.00008
	0.05	0.50903	0.38207	0.03995	0.05870	0.00955	0.00070
	0.10	0.64834	0.26075	0.05357	0.02734	0.00874	0.00126
	0.30	0.79962	0.11708	0.07044	0.00551	0.00516	0.00218
	0.50	0.84033	0.07583	0.07545	0.00231	0.00358	0.00250
	0.75	0.86262	0.05269	0.07830	0.00112	0.00258	0.00269
	1.00	0.87432	0.04039	0.07982	0.00066	0.00202	0.00280
	4.00	0.90217	0.01063	0.08354	0.00005	0.00056	0.00306
	10.00	0.90801	0.00430	0.08433	0.00001	0.00023	0.00312
1300	0.01	0.18042	0.70344	0.01558	0.09813	0.00240	0.00003
	0.05	0.49499	0.42066	0.04488	0.03509	0.00414	0.00024
	0.10	0.63751	0.28325	0.05923	0.01591	0.00368	0.00042
	0.30	0.79407	0.12416	0.07595	0.00306	0.00207	0.00069
	0.50	0.83621	0.07969	0.08065	0.00126	0.00141	0.00078
	0.75	0.85923	0.05507	0.08325	0.00060	0.00101	0.00083
	1.00	0.87130	0.04208	0.08463	0.00035	0.00078	0.00086
	4.00	0.89992	0.01099	0.08793	0.00002	0.00021	0.00093
	10.00	0.90591	0.00444	0.08862	0.00000	0.00009	0.00094
1400	0.01	0.17404	0.74804	0.01629	0.06053	0.00109	0.00001
	0.05	0.48722	0.44292	0.04670	0.02122	0.00185	0.00009
	0.10	0.63201	0.29549	0.06128	0.00945	0.00162	0.00015
	0.30	0.79175	0.12755	0.07781	0.00176	0.00089	0.00024
	0.50	0.83466	0.08143	0.08233	0.00072	0.00060	0.00027
	0.75	0.85804	0.05610	0.08481	0.00034	0.00043	0.00029
	1.00	0.87028	0.04279	0.08611	0.00020	0.00033	0.00029
	4.00	0.89925	0.01113	0.08920	0.00001	0.00009	0.00032
	10.00	0.90530	0.00449	0.08985	0.00000	0.00004	0.00032
1500	0.01	0.17030	0.77434	0.01650	0.03833	0.00053	0.00000
	0.05	0.48295	0.45553	0.04734	0.01326	0.00089	0.00003
	0.10	0.62917	0.30214	0.06203	0.00584	0.00077	0.00006
	0.30	0.79072	0.12923	0.07847	0.00107	0.00042	0.00009
	0.50	0.83402	0.08226	0.08291	0.00043	0.00028	0.00011
	0.75	0.85758	0.05656	0.08534	0.00020	0.00020	0.00011
	1.00	0.86990	0.04310	0.08661	0.00012	0.00015	0.00012
	4.00	0.89903	0.01118	0.08961	0.00001	0.00004	0.00012
	10.00	0.90511	0.00451	0.09024	0.00000	0.00002	0.00013

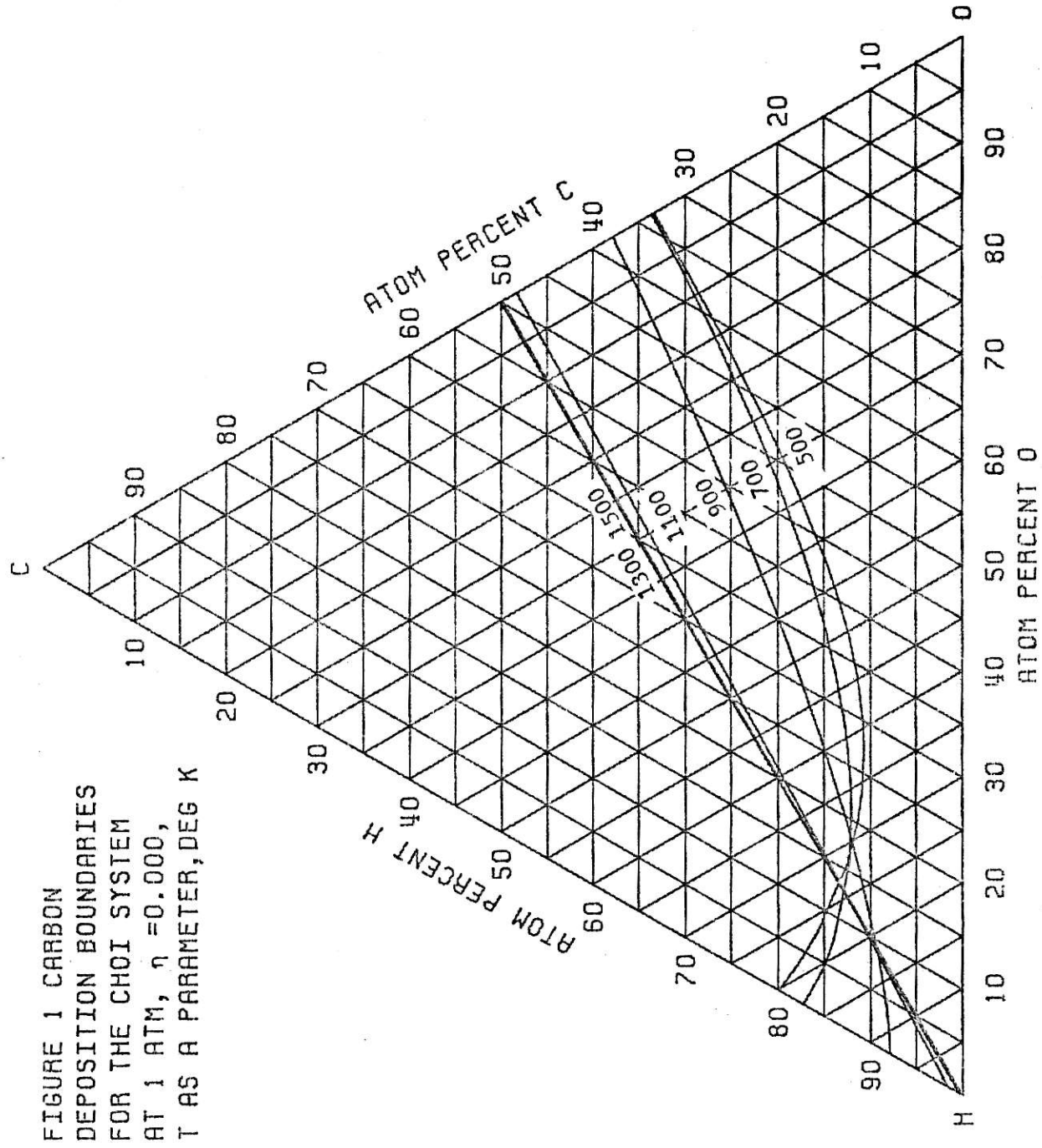
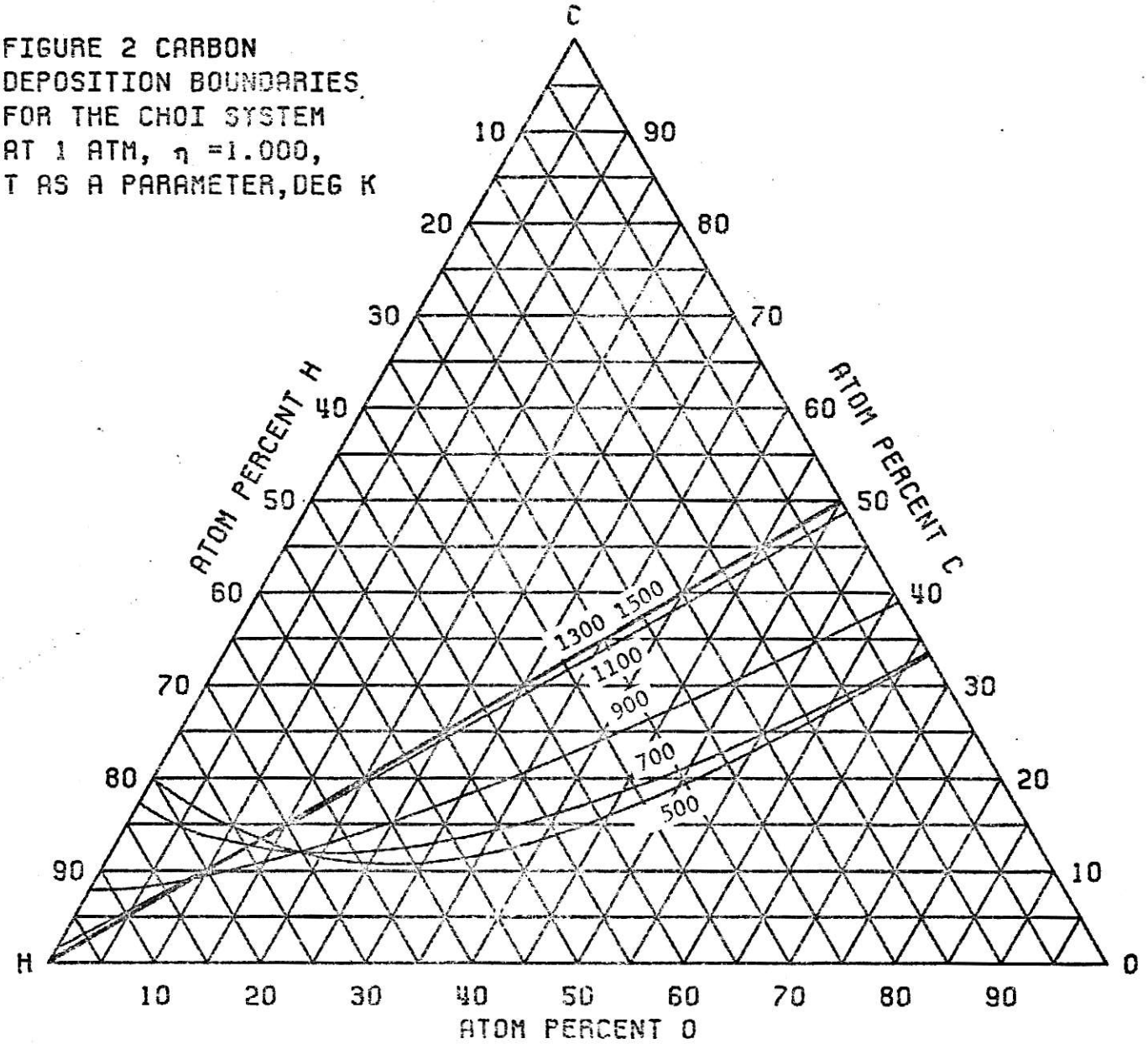


FIGURE 1 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =0.000,
T AS A PARAMETER, DEG K

FIGURE 2 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =1.000,
T AS A PARAMETER, DEG K



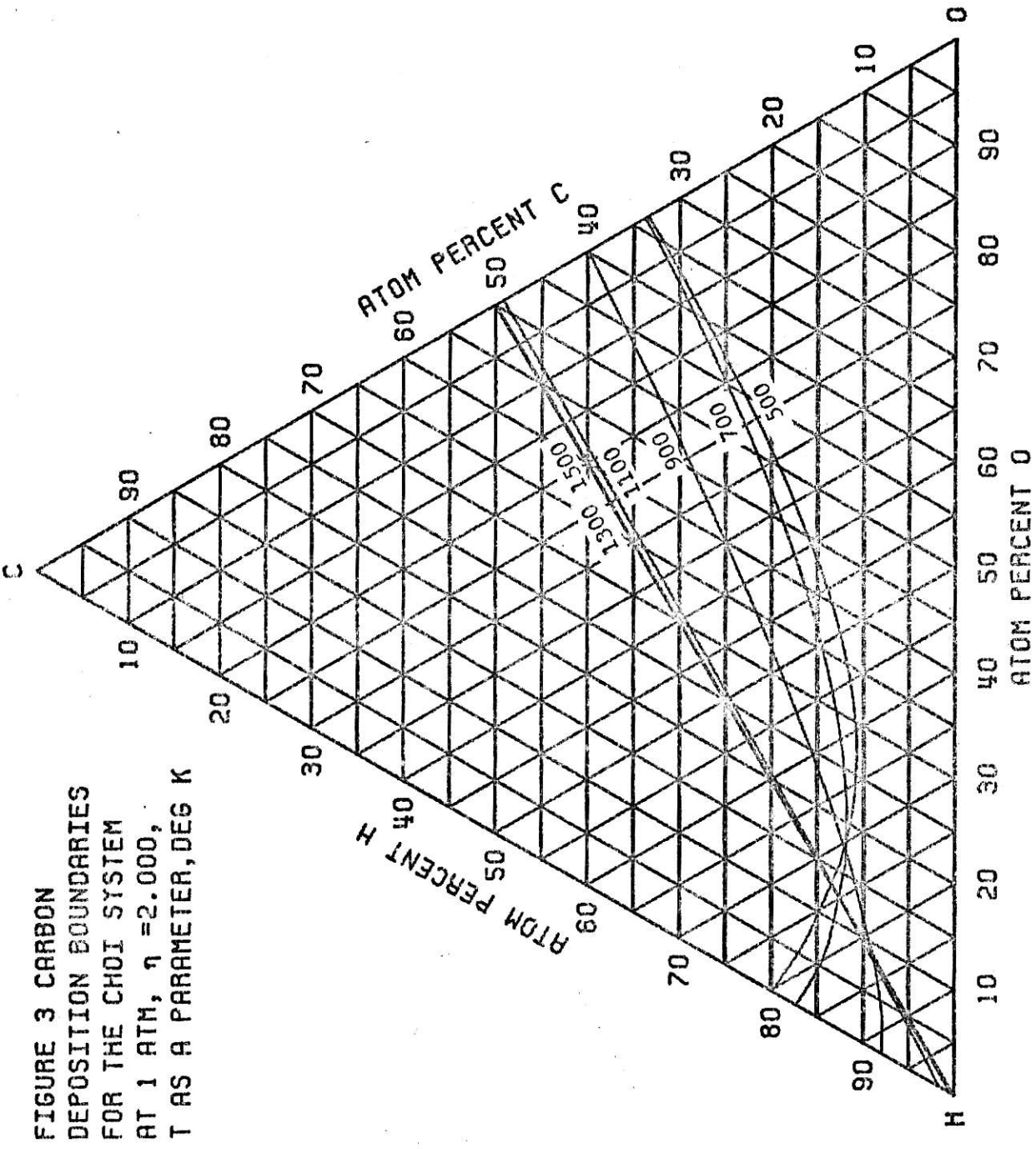


FIGURE 3 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =2.000,
T AS A PARAMETER, DEG K

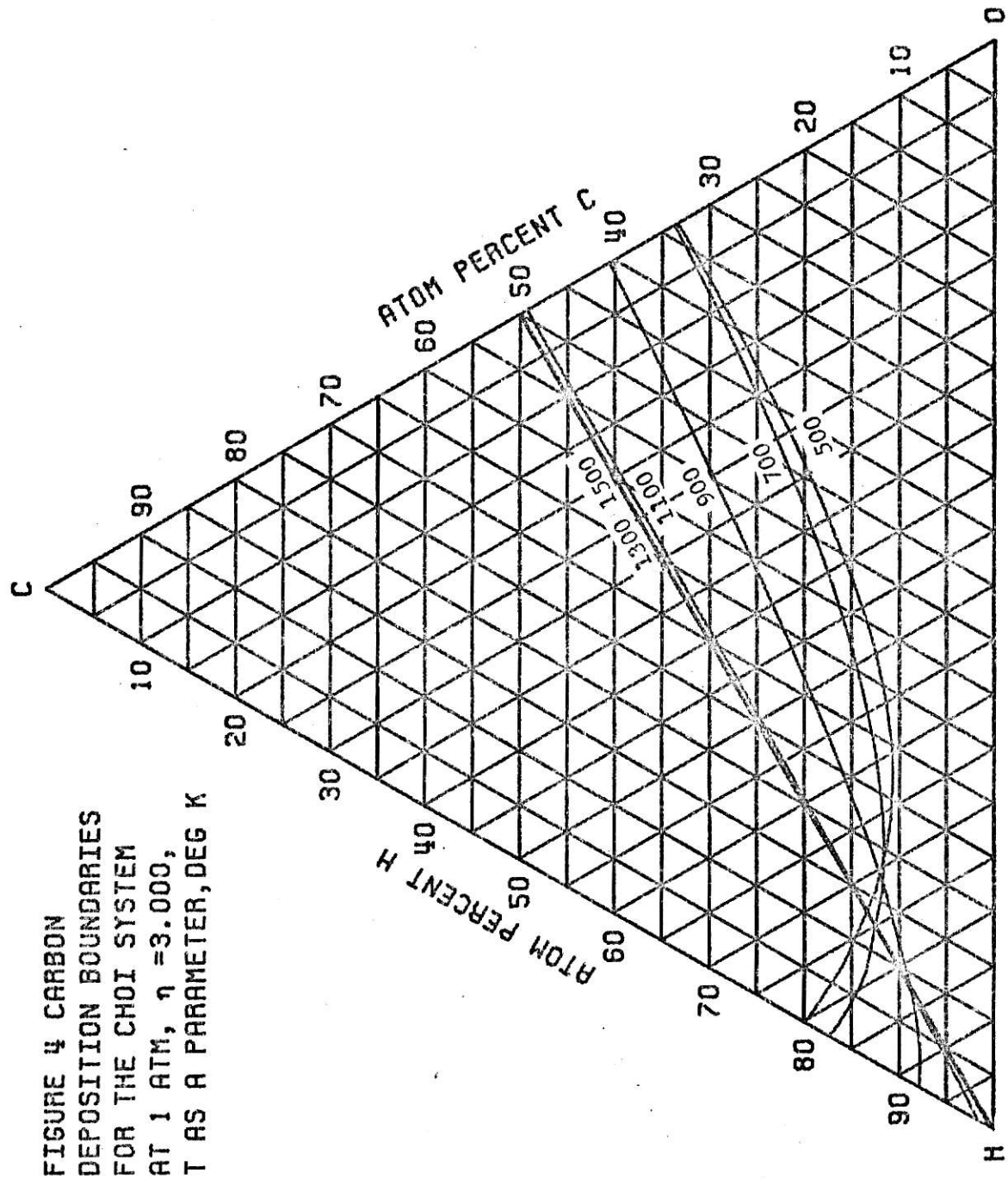


FIGURE 4 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =3.000,
T AS A PARAMETER, DEG K

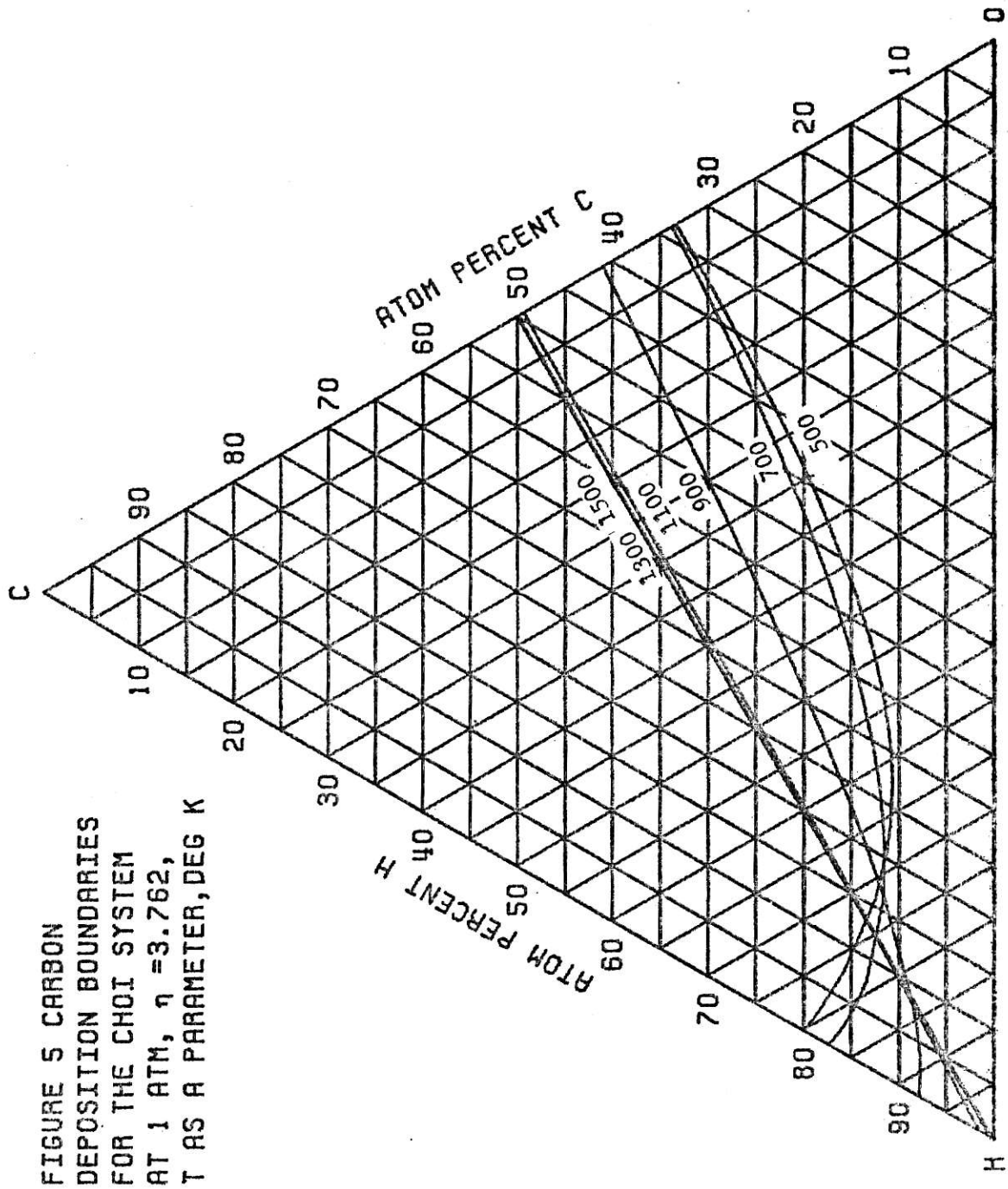


FIGURE 5 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =3.762,
T AS A PARAMETER, DEG K

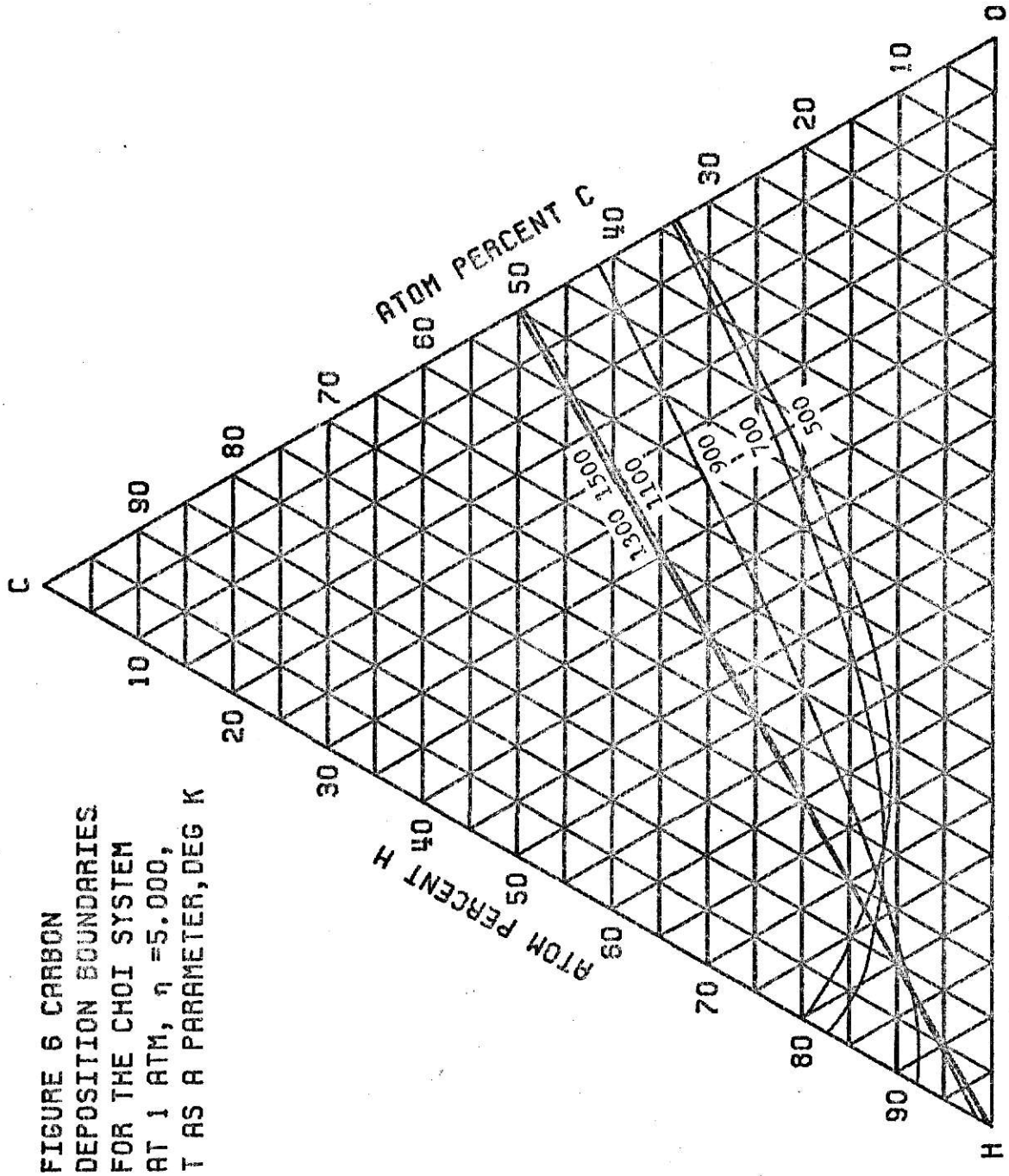


FIGURE 6 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =5.000,
T AS A PARAMETER, DEG K

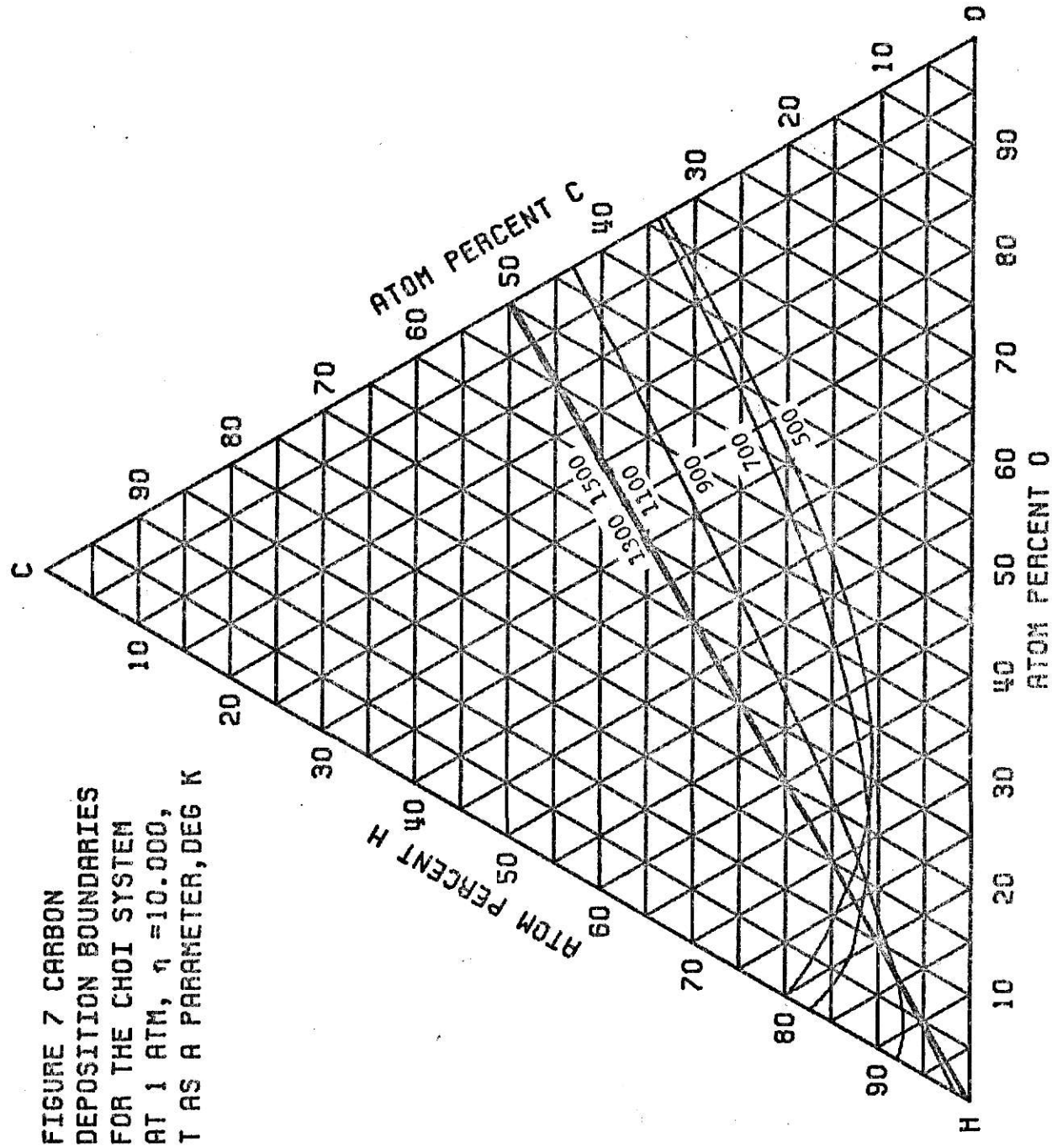


FIGURE 7 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =10.000,
T AS A PARAMETER, DEG K

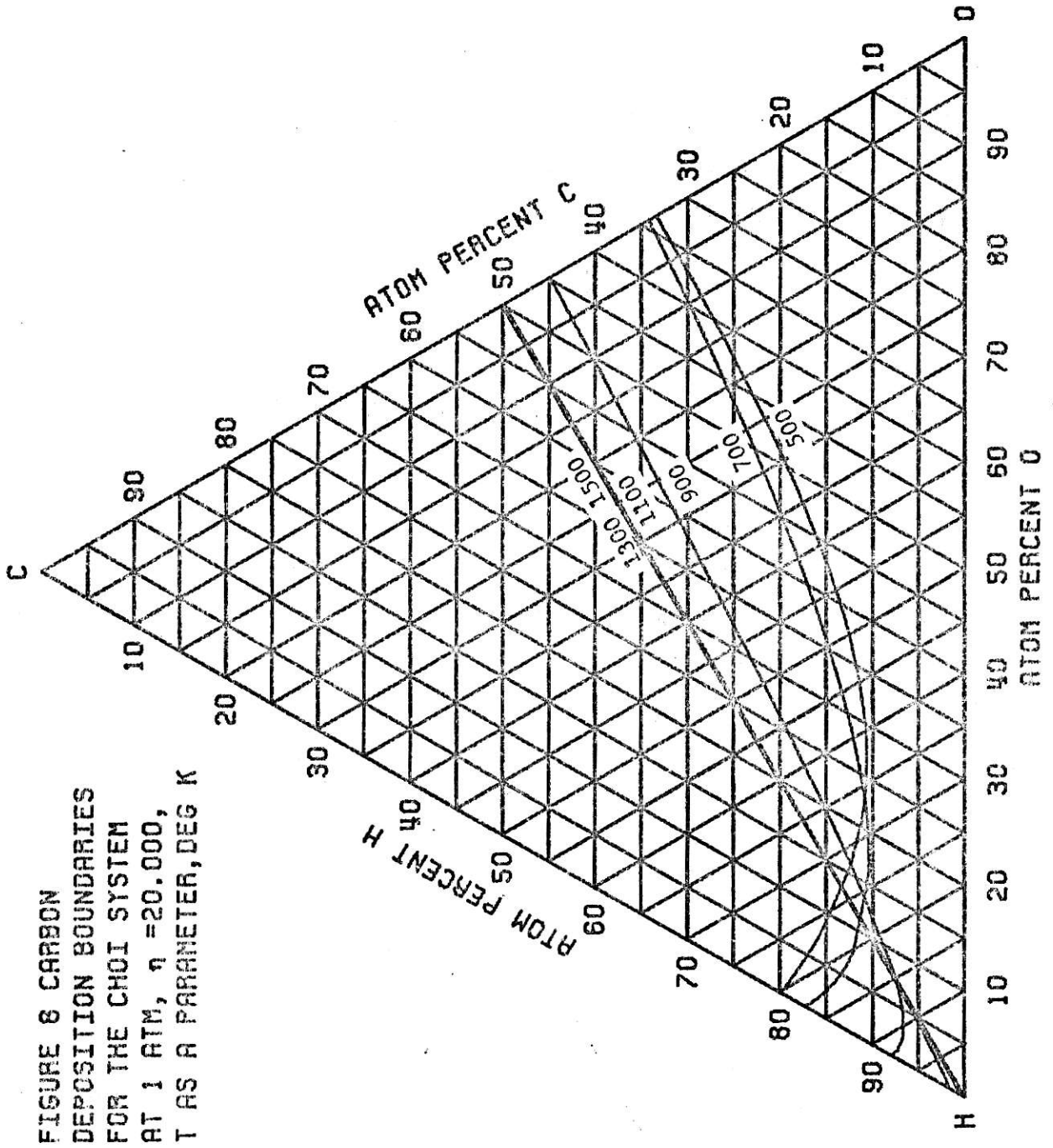


FIGURE 8 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 1 ATM, η =20.000,
T AS A PARAMETER, DEG K

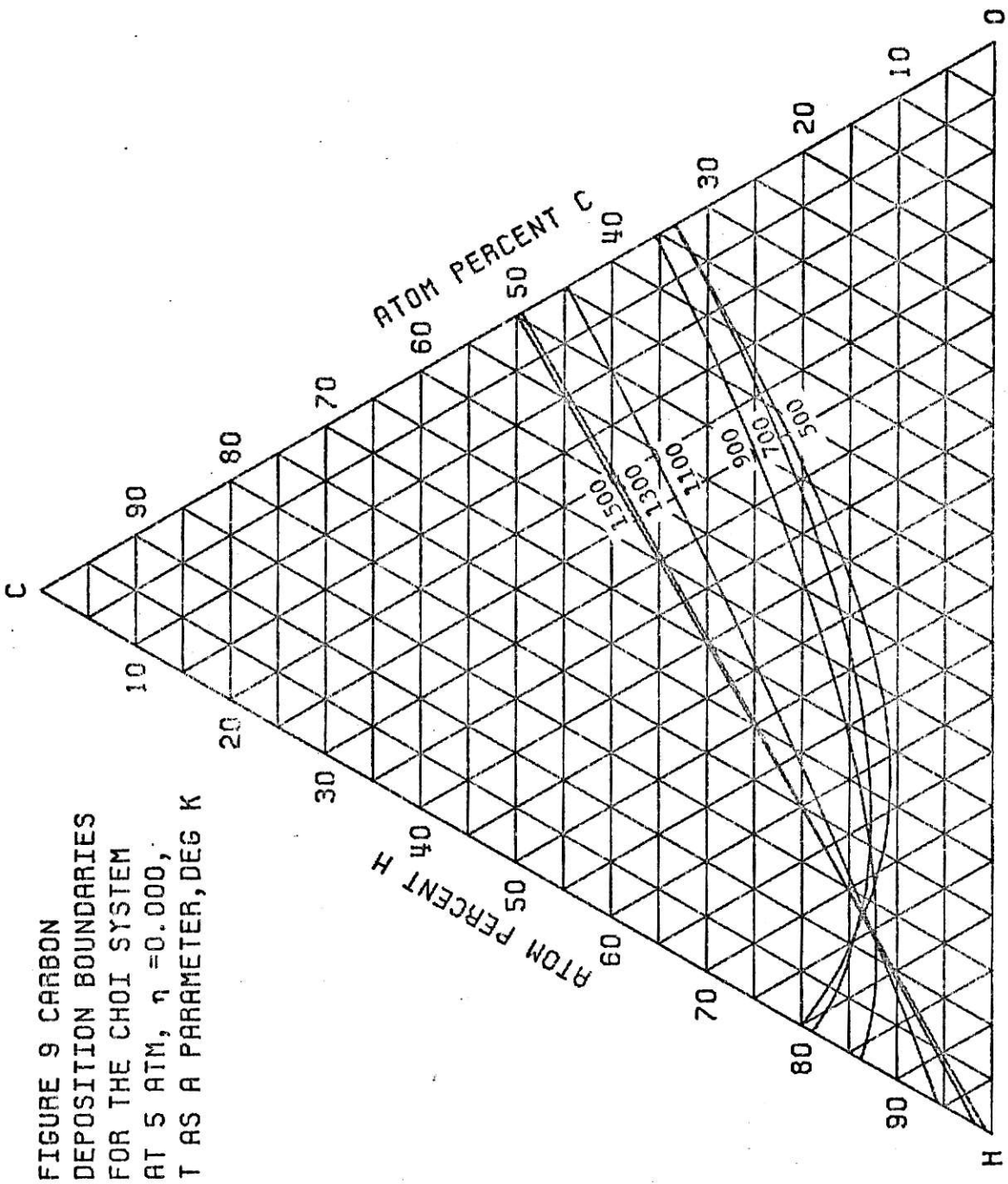


FIGURE 9 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =0.000,
T AS A PARAMETER, DEG K

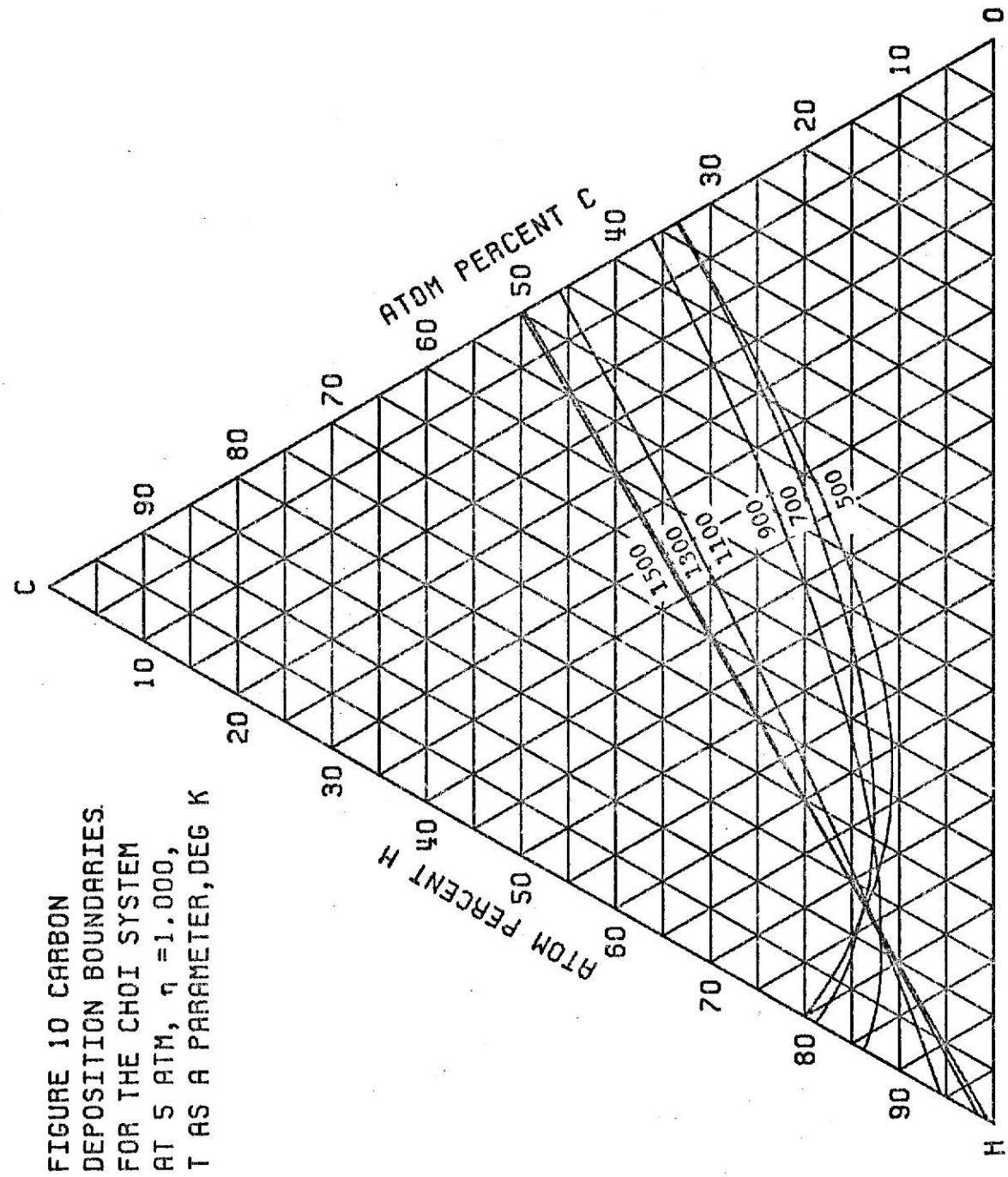


FIGURE 10 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =1.000,
T AS A PARAMETER, DEG K

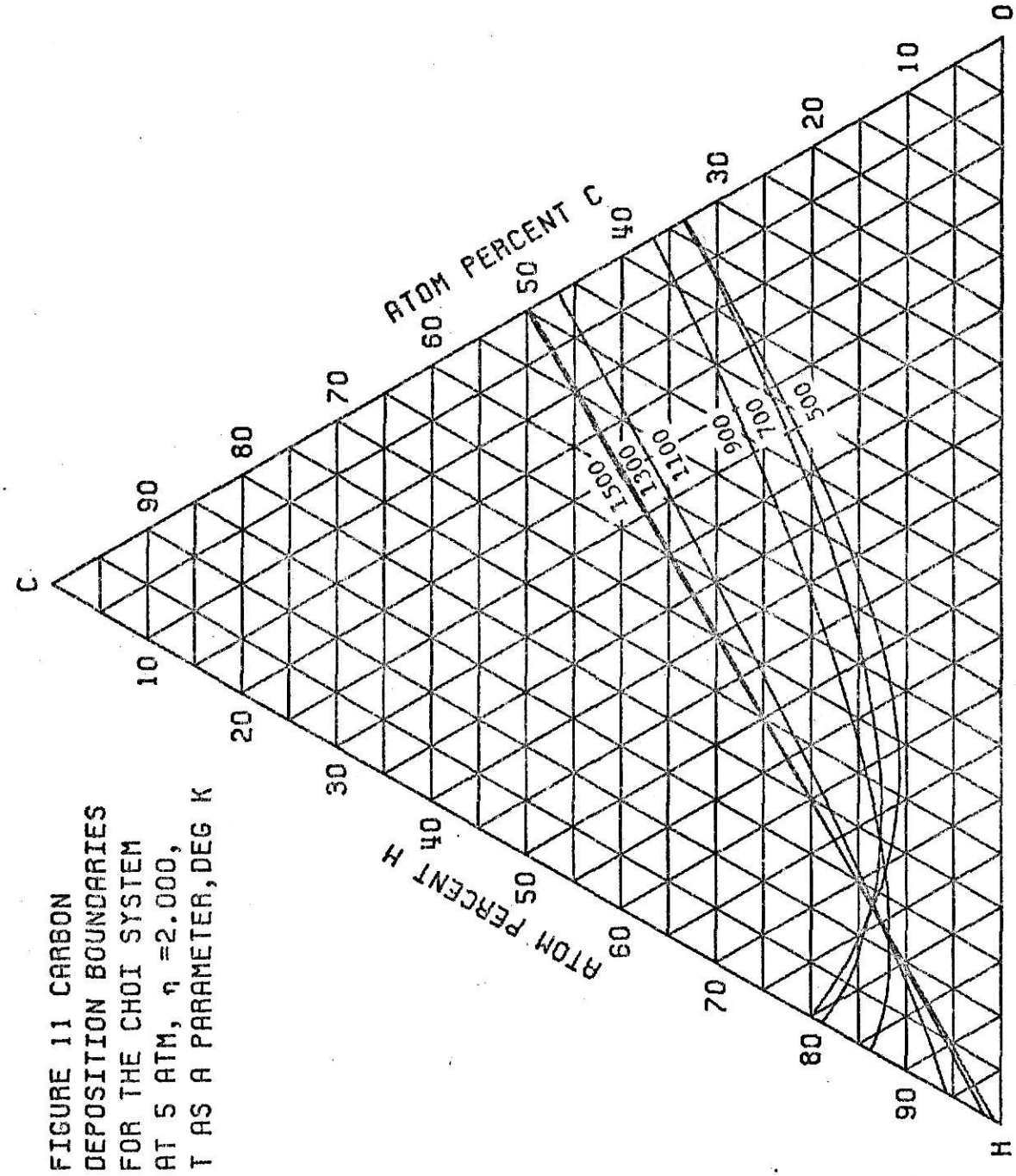


FIGURE 11 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =2.000,
T AS A PARAMETER, DEG K

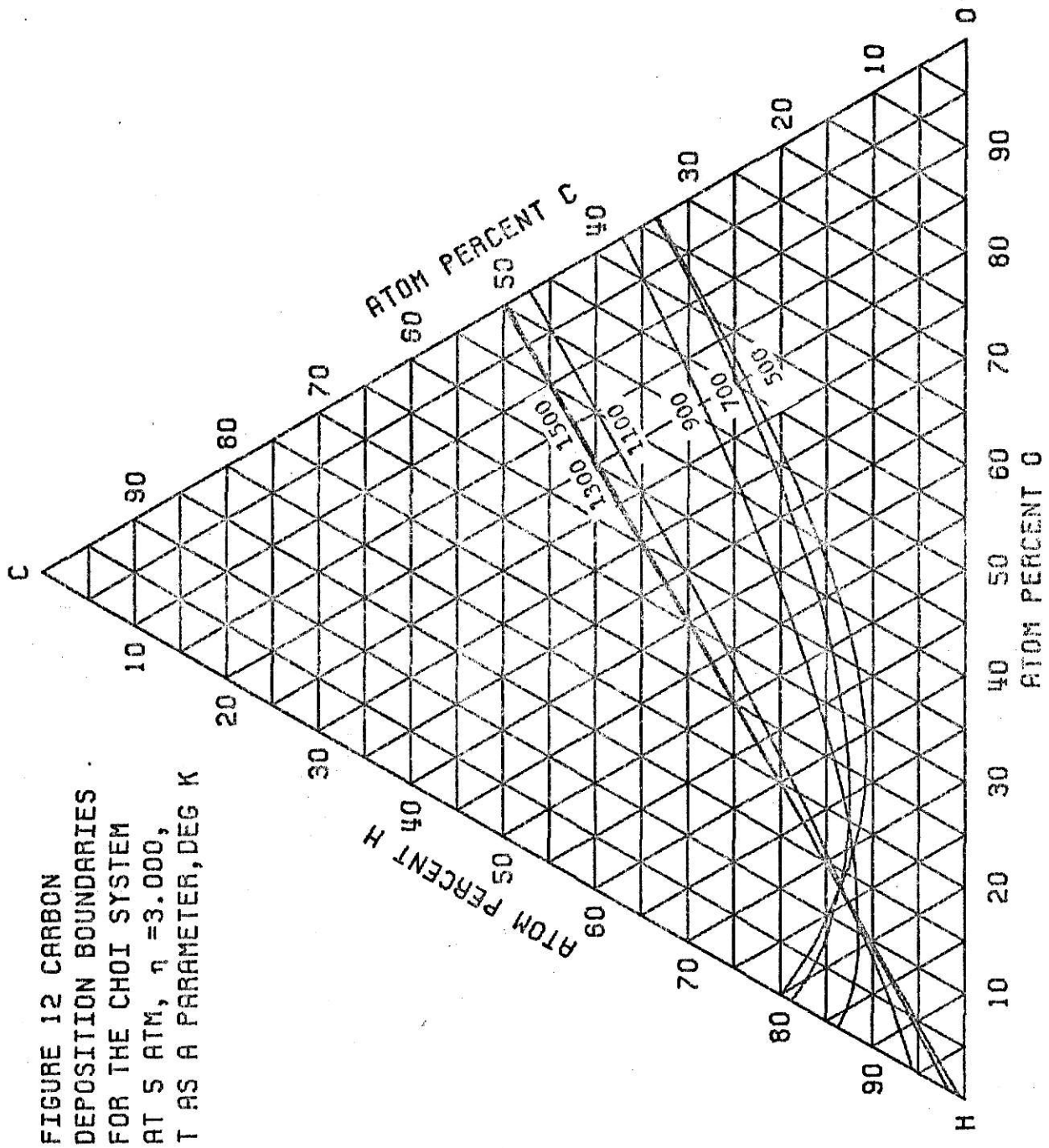


FIGURE 12 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =3.000,
T AS A PARAMETER, DEG K

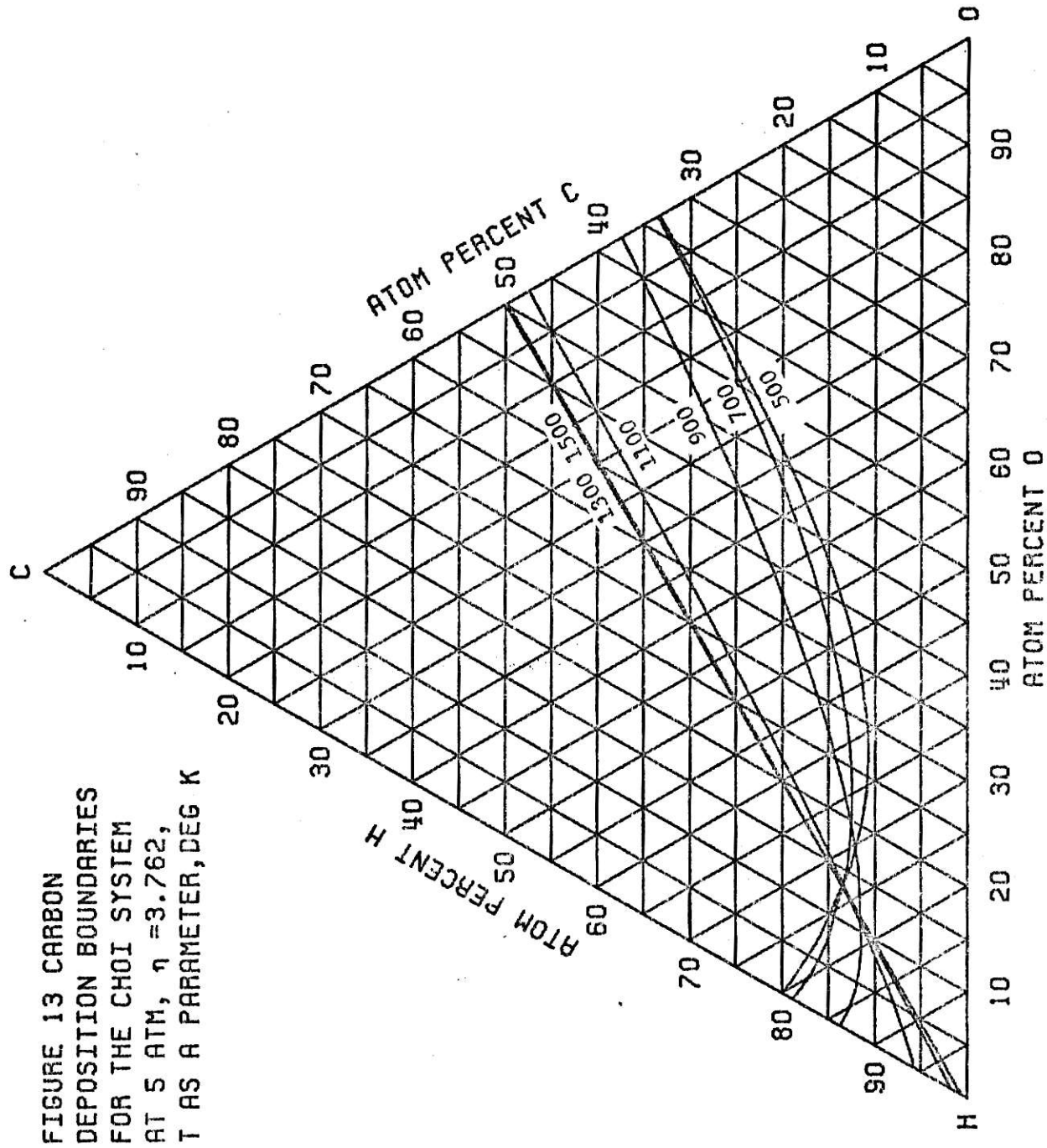


FIGURE 13 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =3.762,
T AS A PARAMETER, DEG K

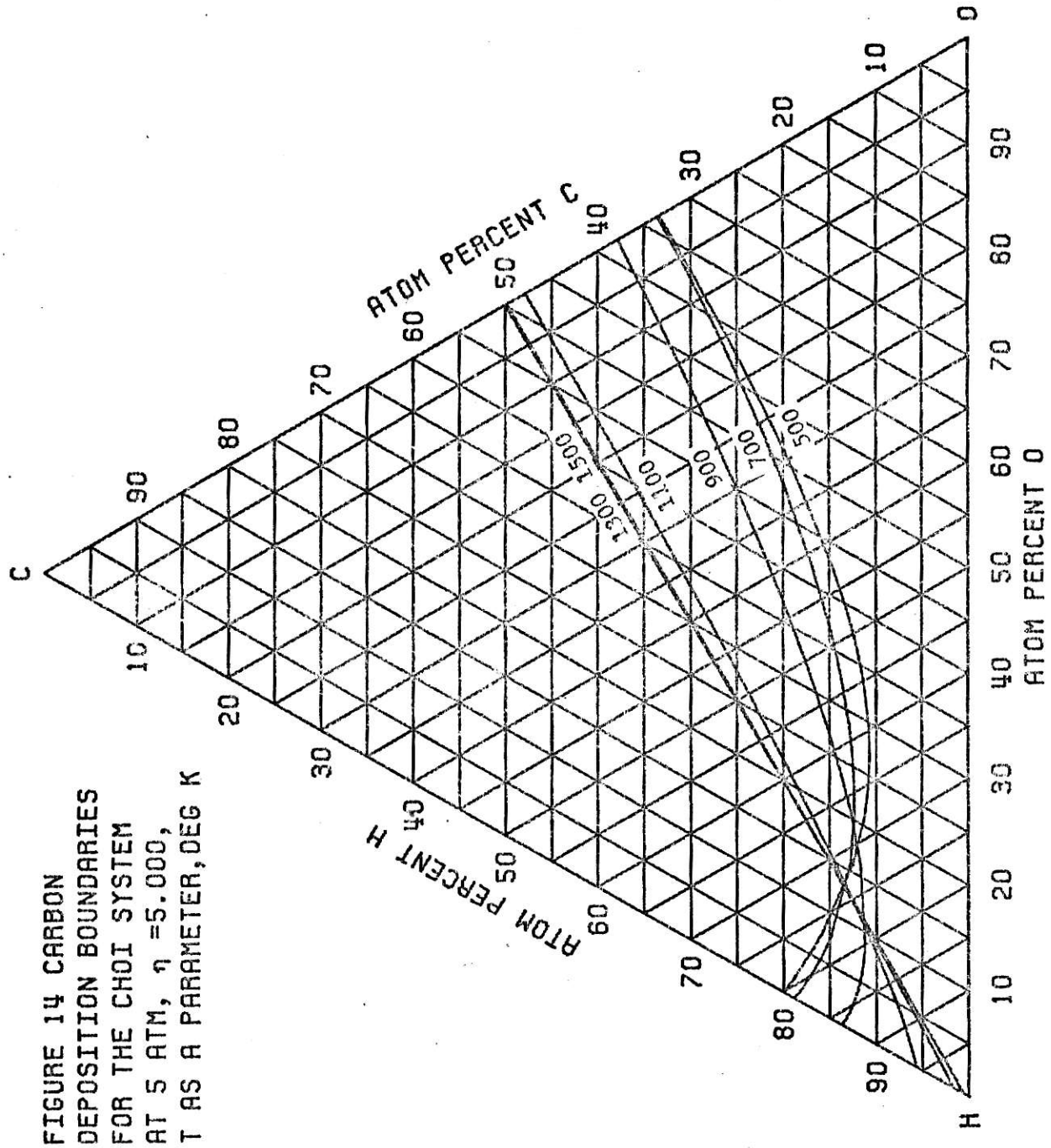


FIGURE 14 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =5.000,
T AS A PARAMETER, DEG K

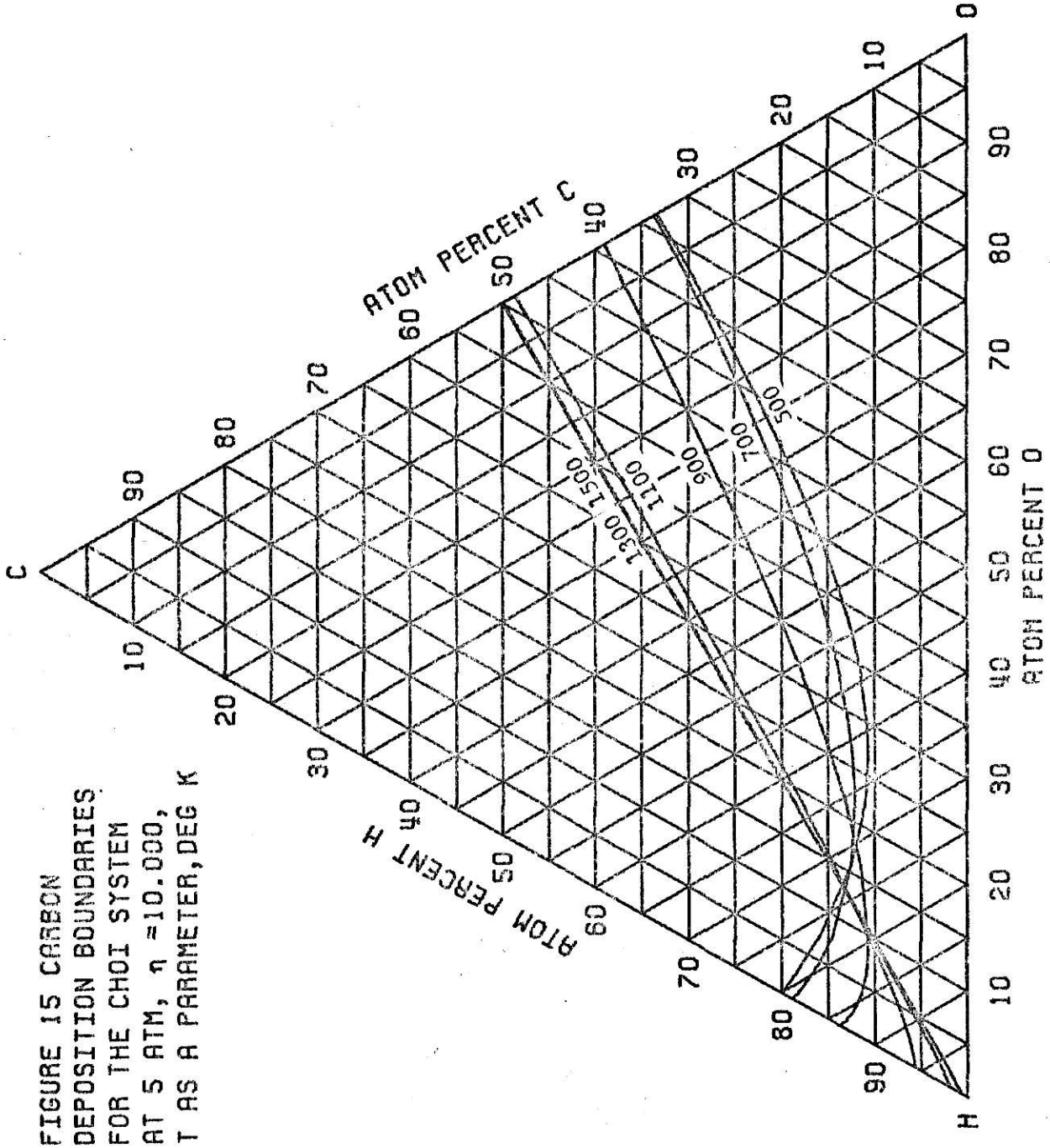


FIGURE 15 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 5 ATM, η =10.000, T AS A PARAMETER, DEG K

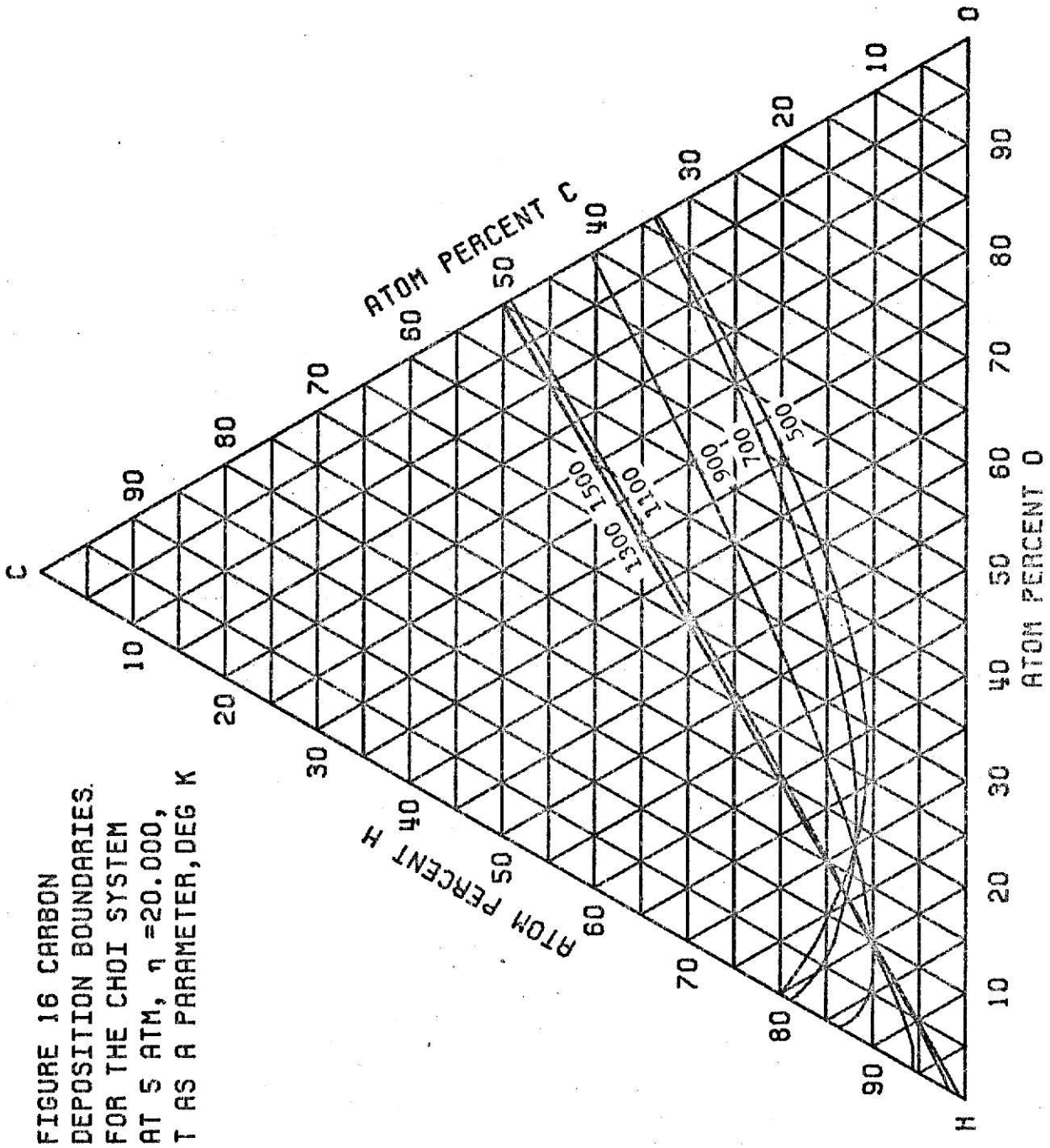


FIGURE 16 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 5 ATM, η =20.000,
T AS A PARAMETER, DEG K

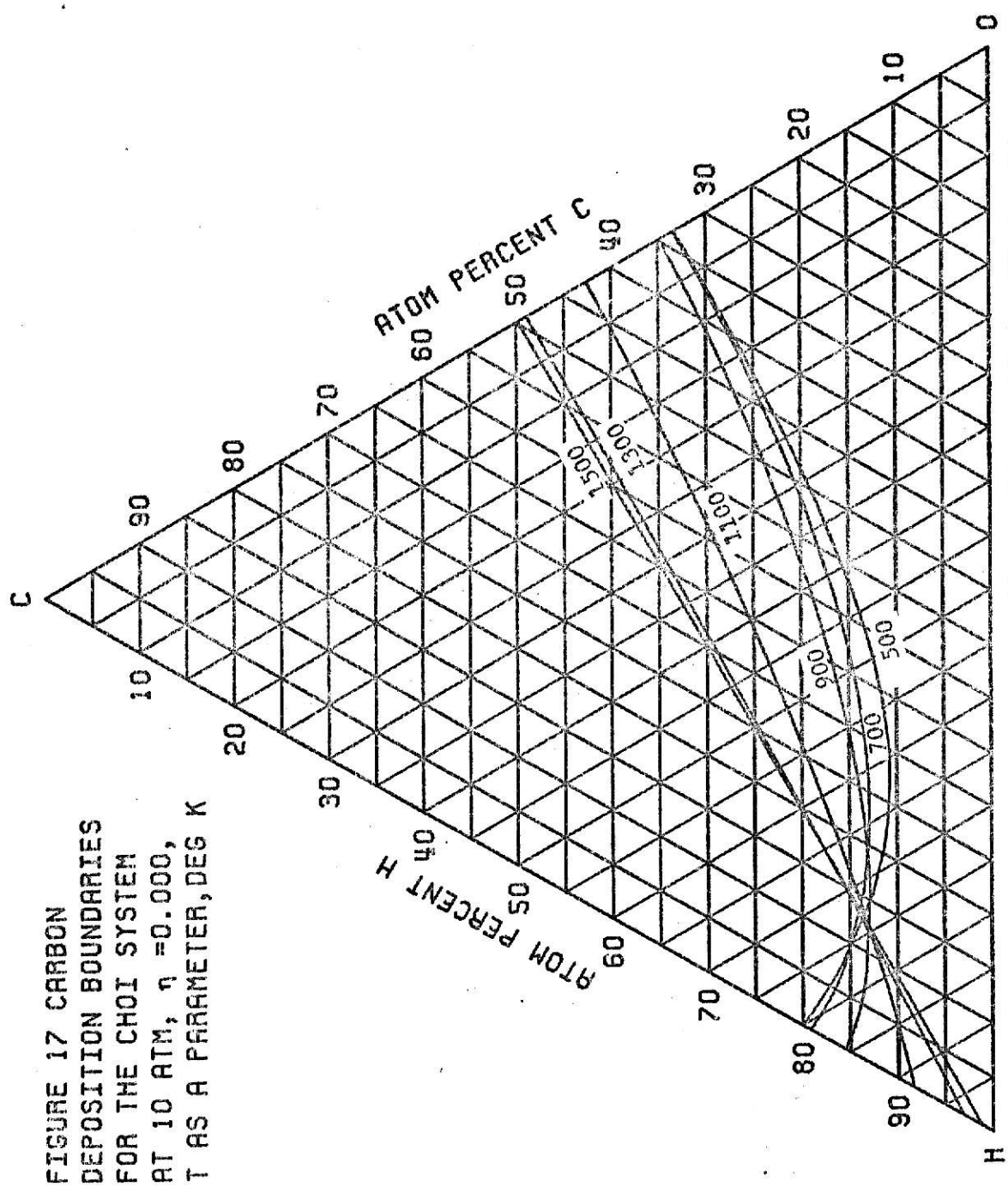


FIGURE 17 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =0.000,
T AS A PARAMETER, DEG K

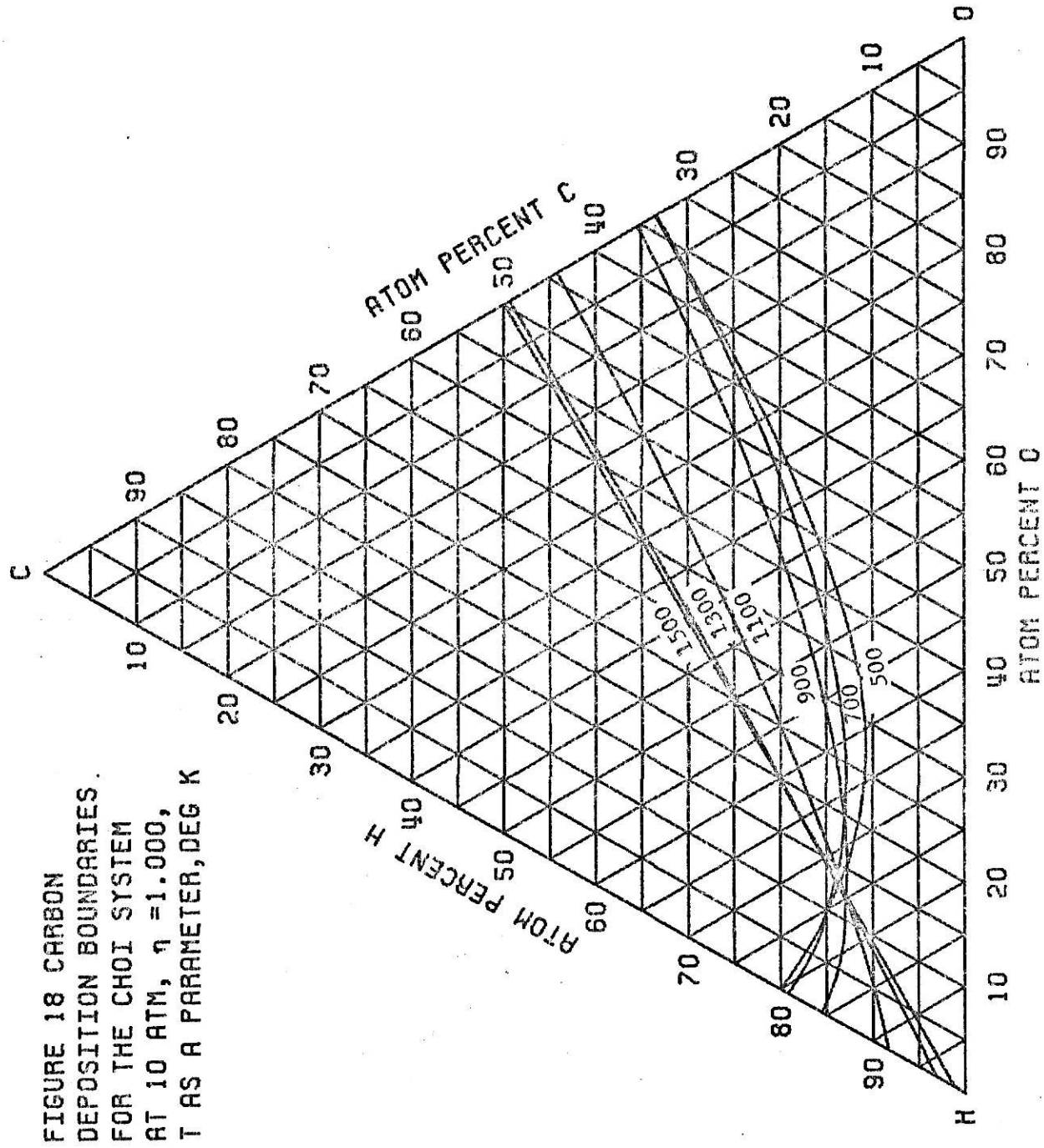


FIGURE 18 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =1.000,
T AS A PARAMETER, DEG K

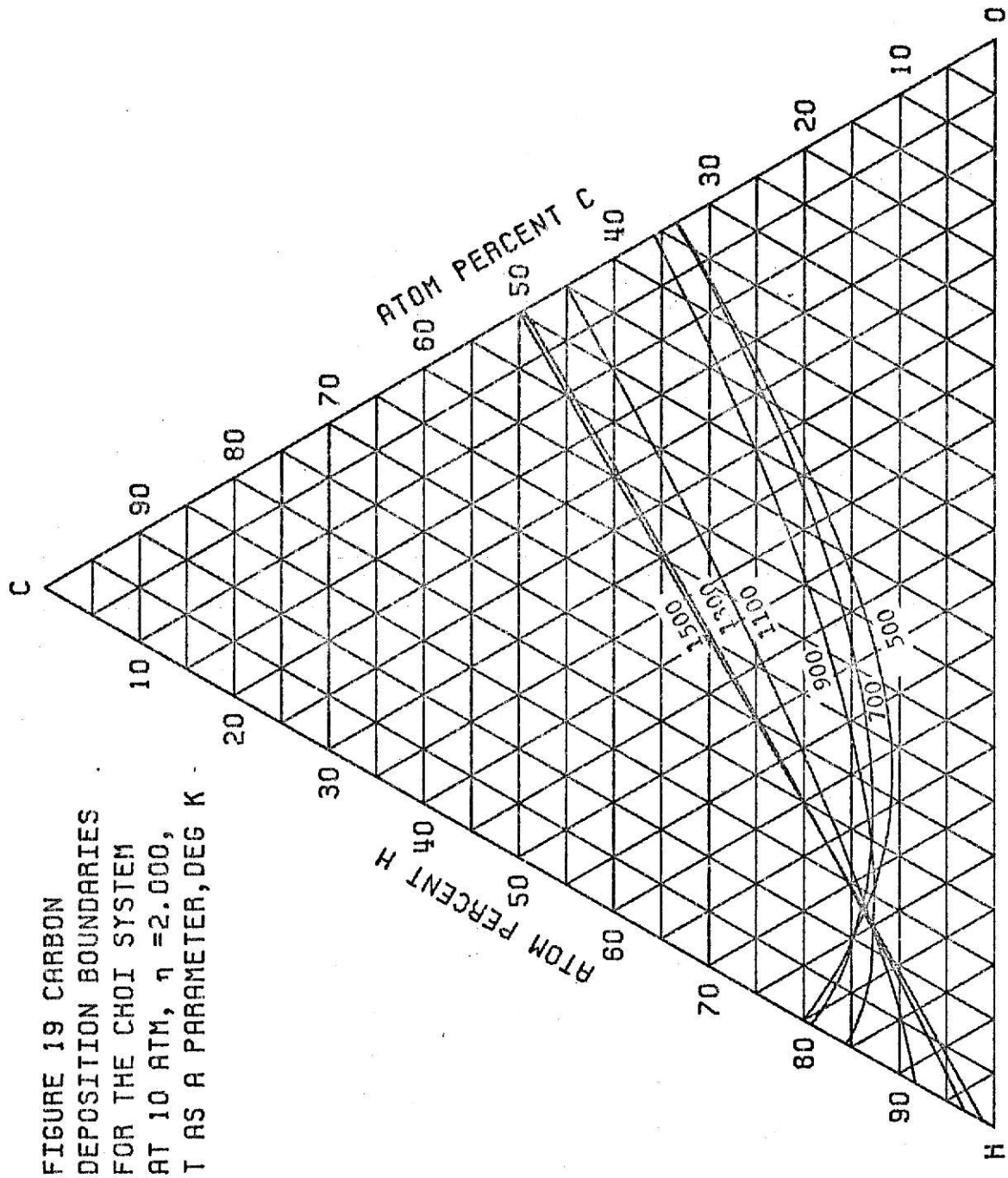


FIGURE 19 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =2.000,
T AS A PARAMETER, DEG K

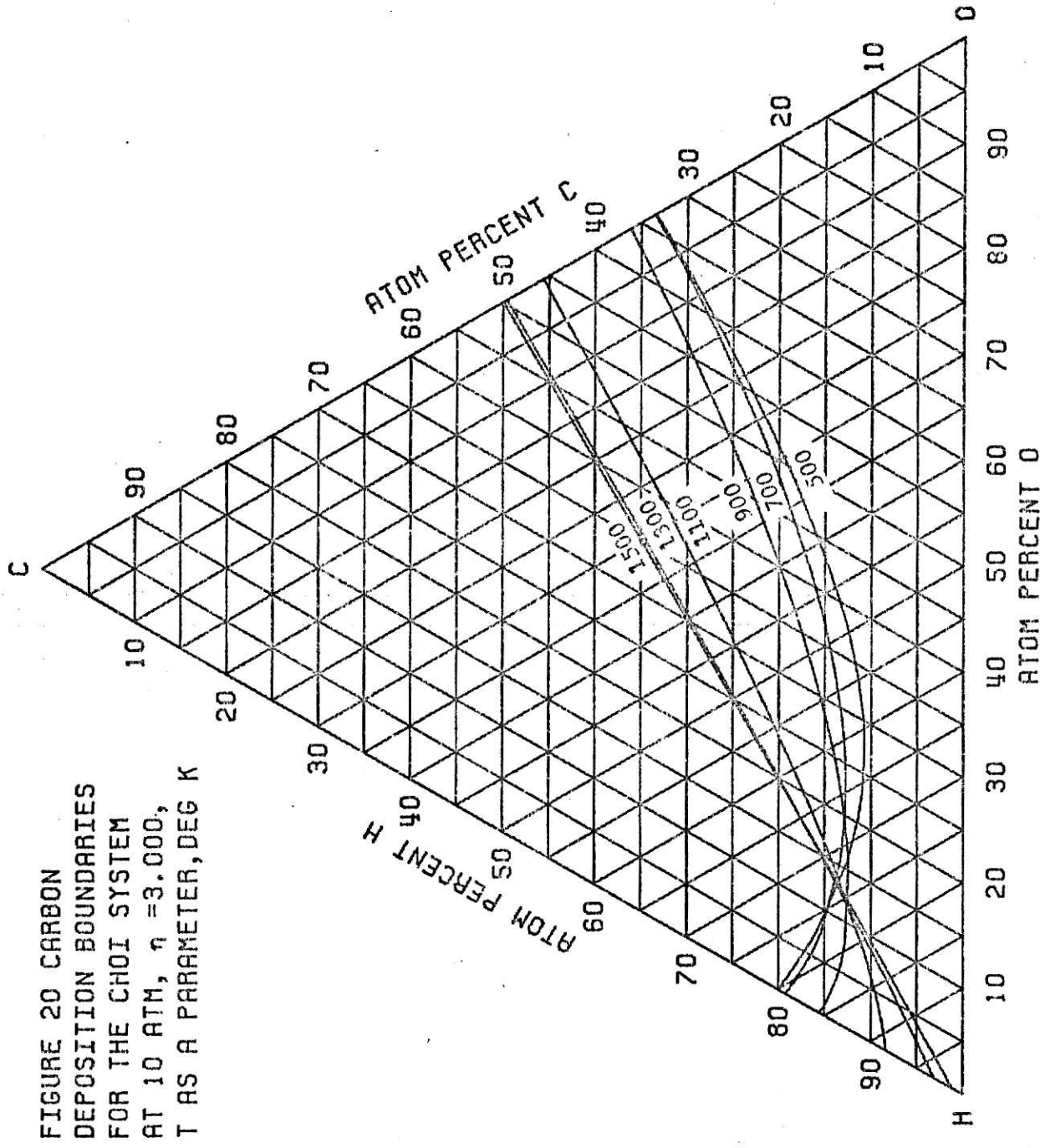


FIGURE 20 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =3.000,
T AS A PARAMETER, DEG K

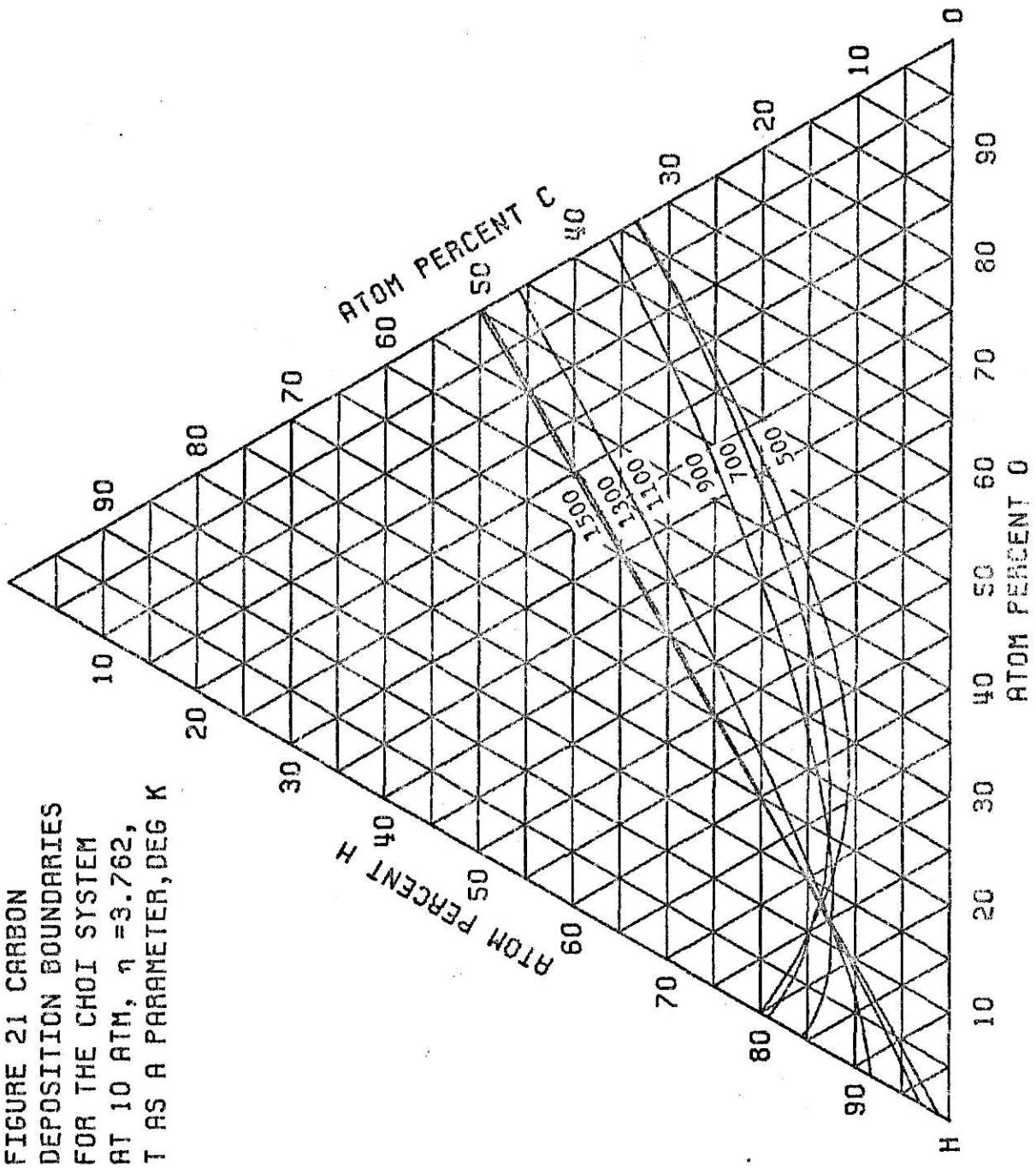


FIGURE 21 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =3.762,
T AS A PARAMETER, DEG K

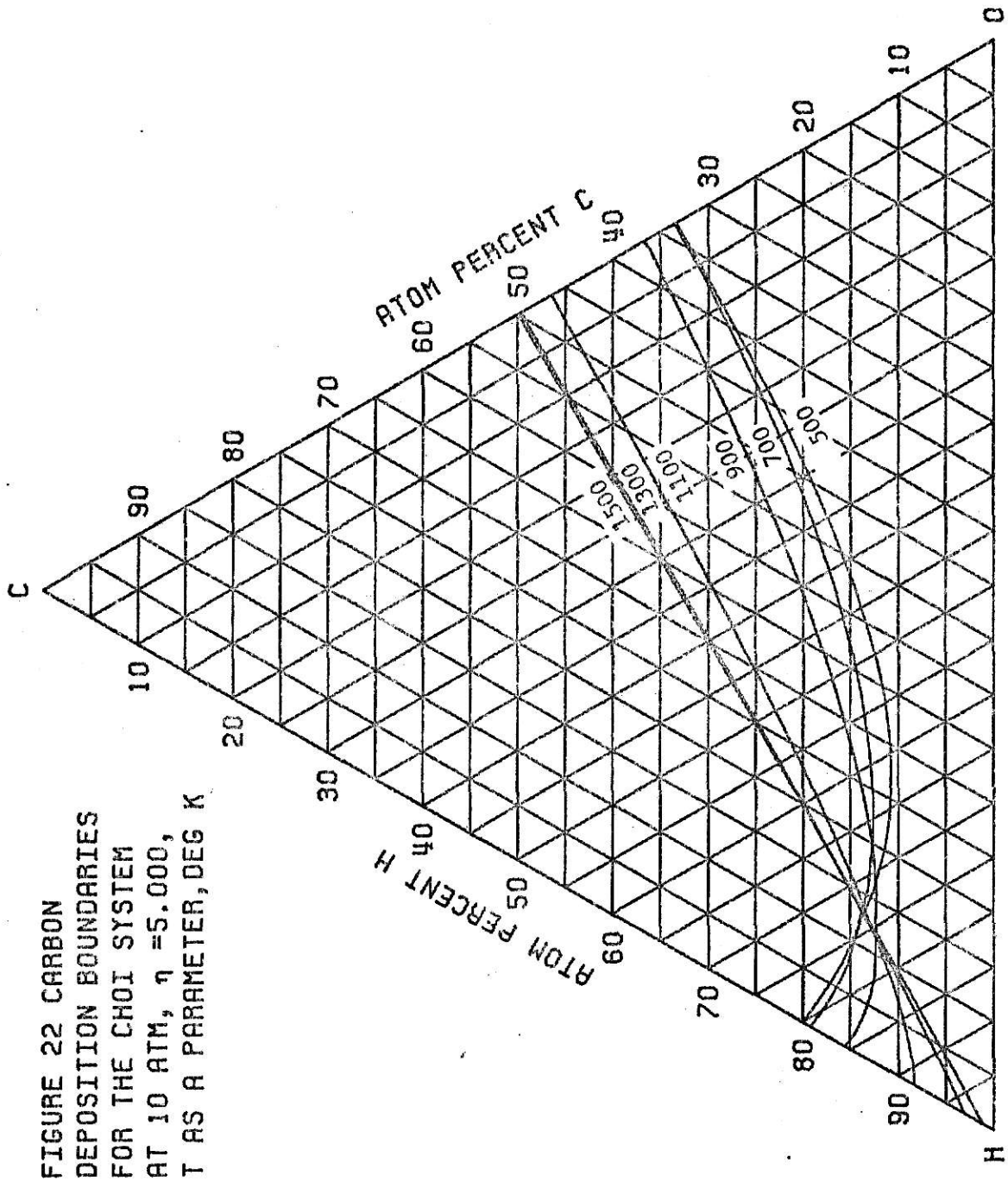


FIGURE 22 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =5.000,
T AS A PARAMETER, DEG K

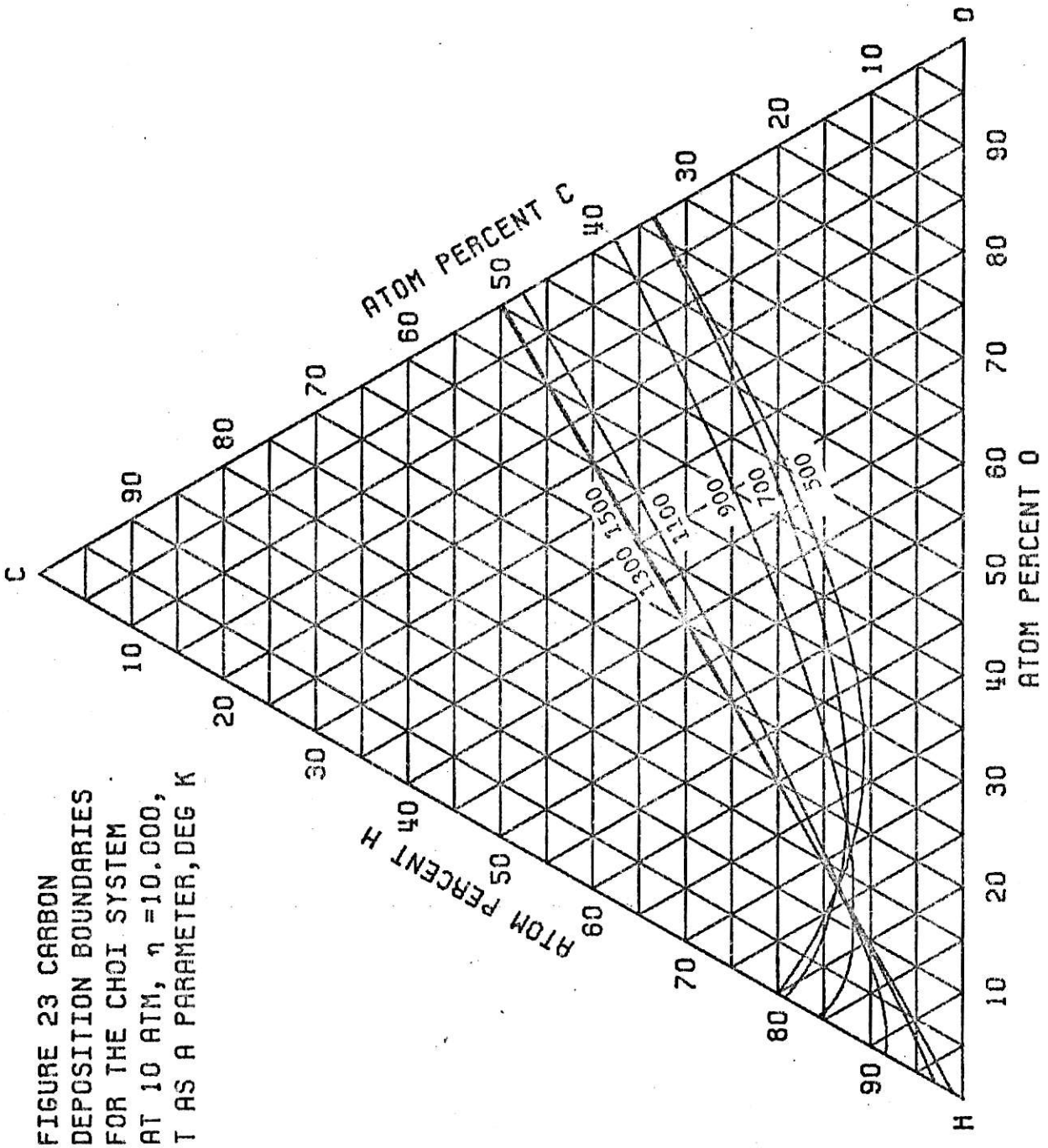
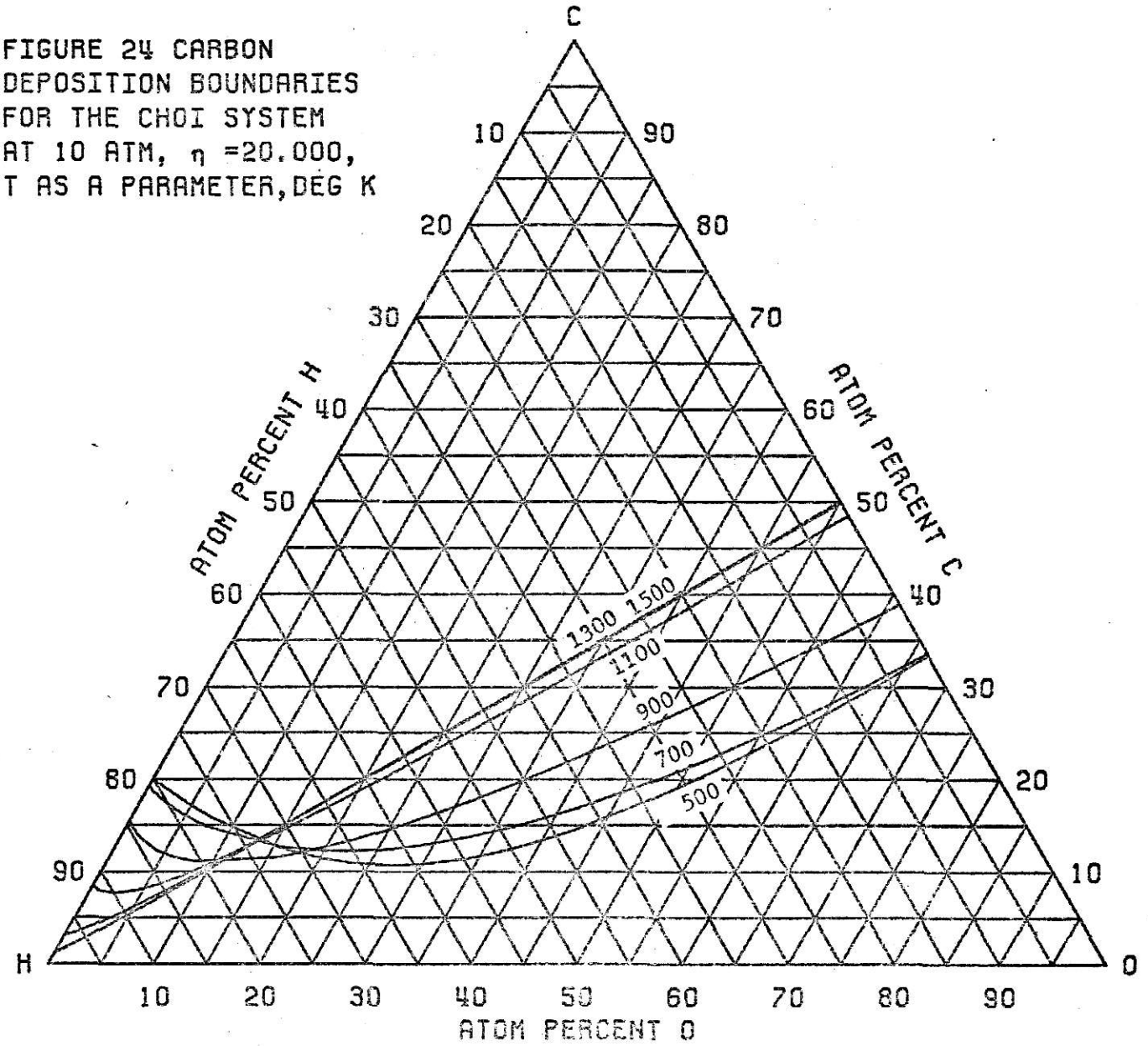


FIGURE 23 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 10 ATM, η =10.000,
T AS A PARAMETER, DEG K

FIGURE 24 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 10 ATM, η =20.000, T AS A PARAMETER, DEG K



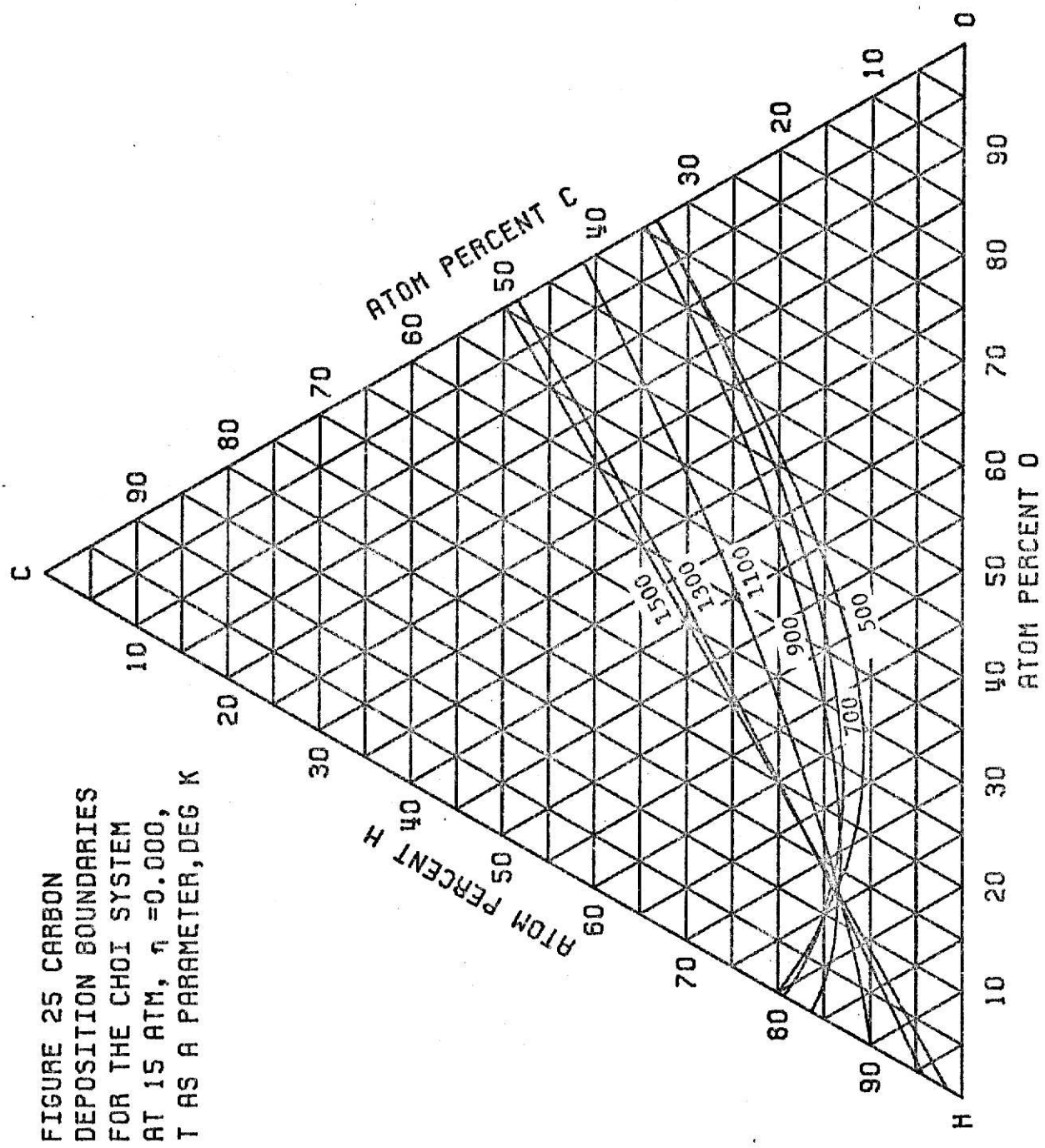


FIGURE 25 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, r_1 =0.000,
T AS A PARAMETER, DEG K

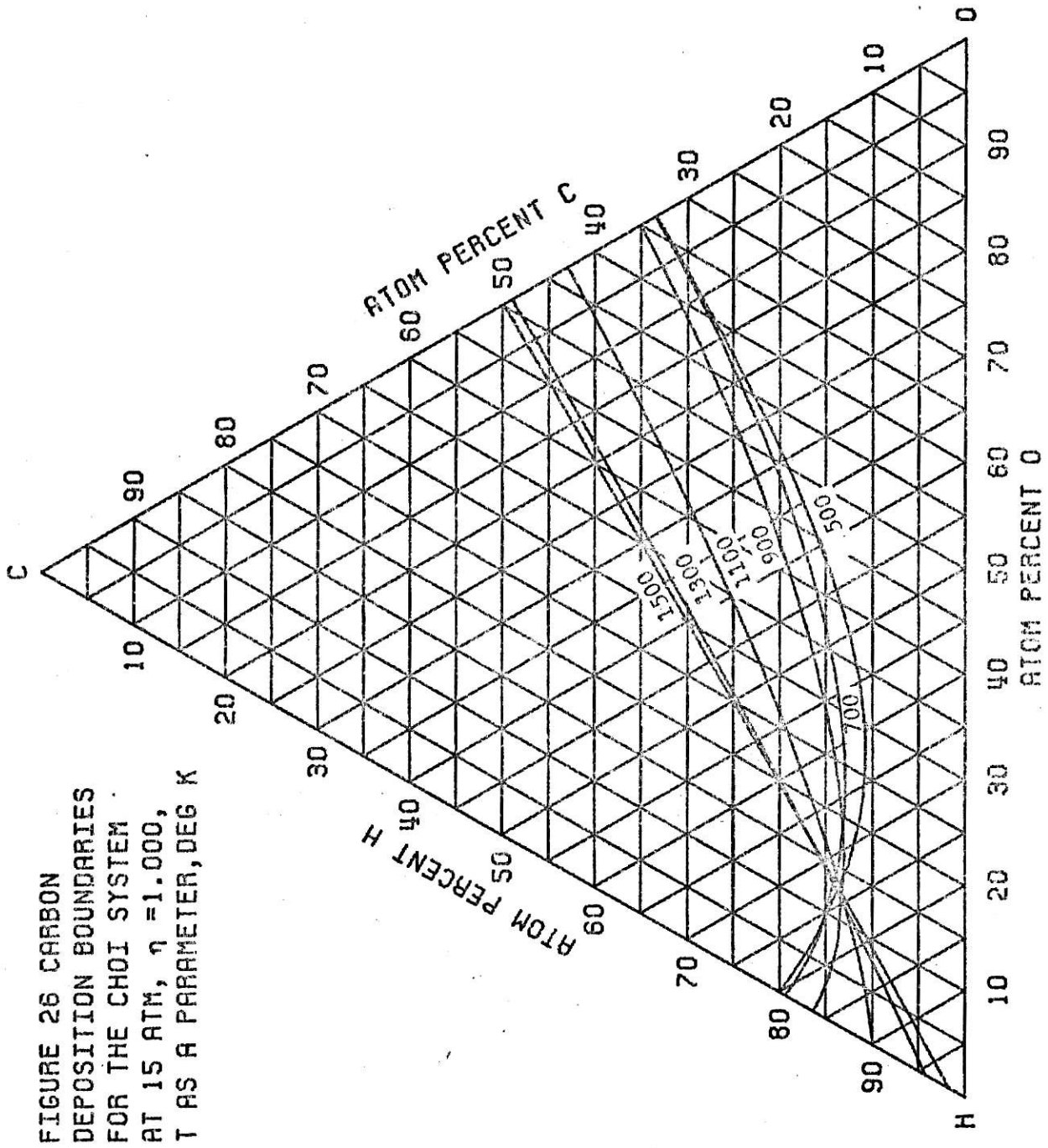


FIGURE 26 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, η =1.000,
T AS A PARAMETER, DEG K

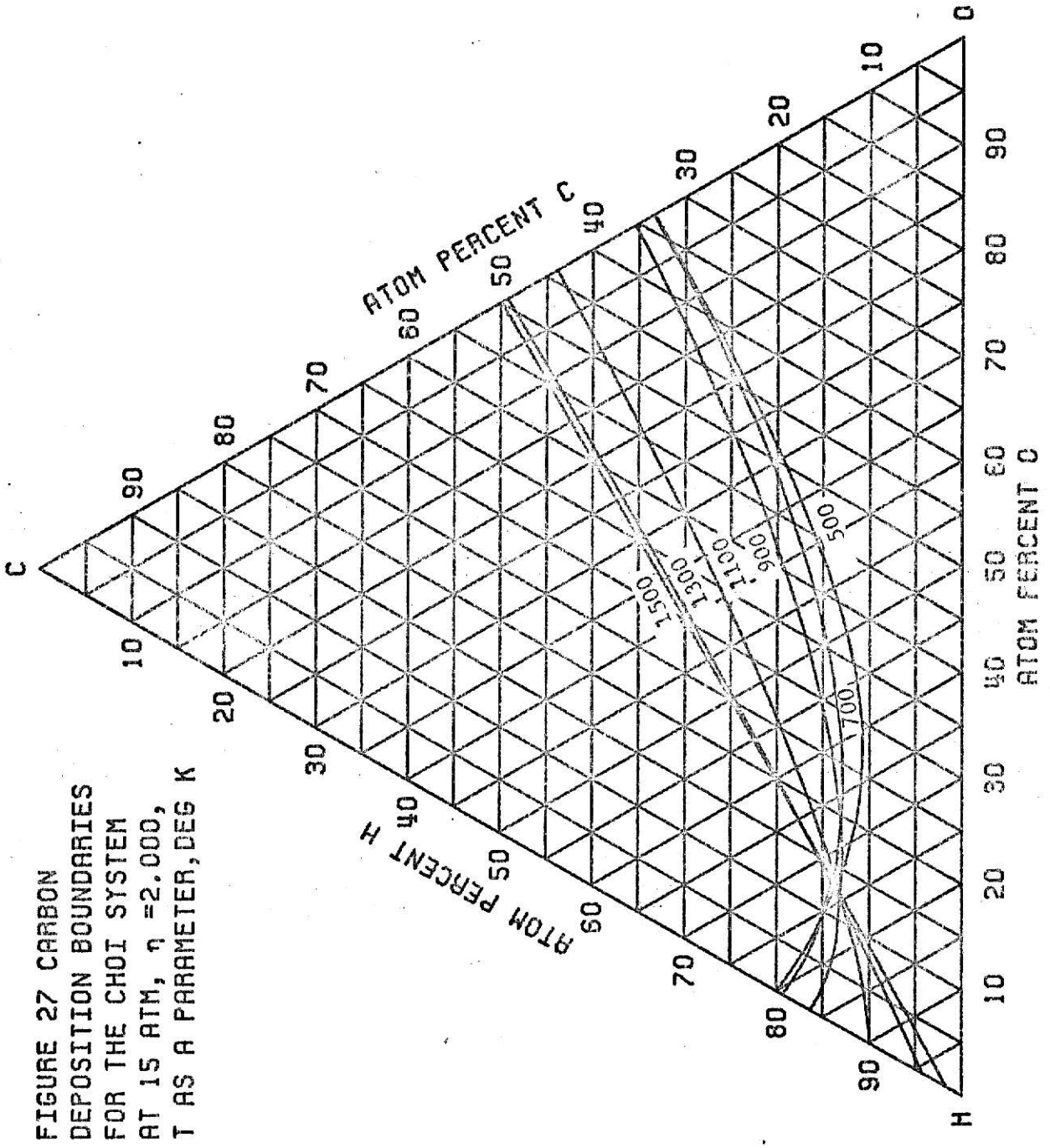


FIGURE 27 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, η =2.000,
T AS A PARAMETER, DEG K

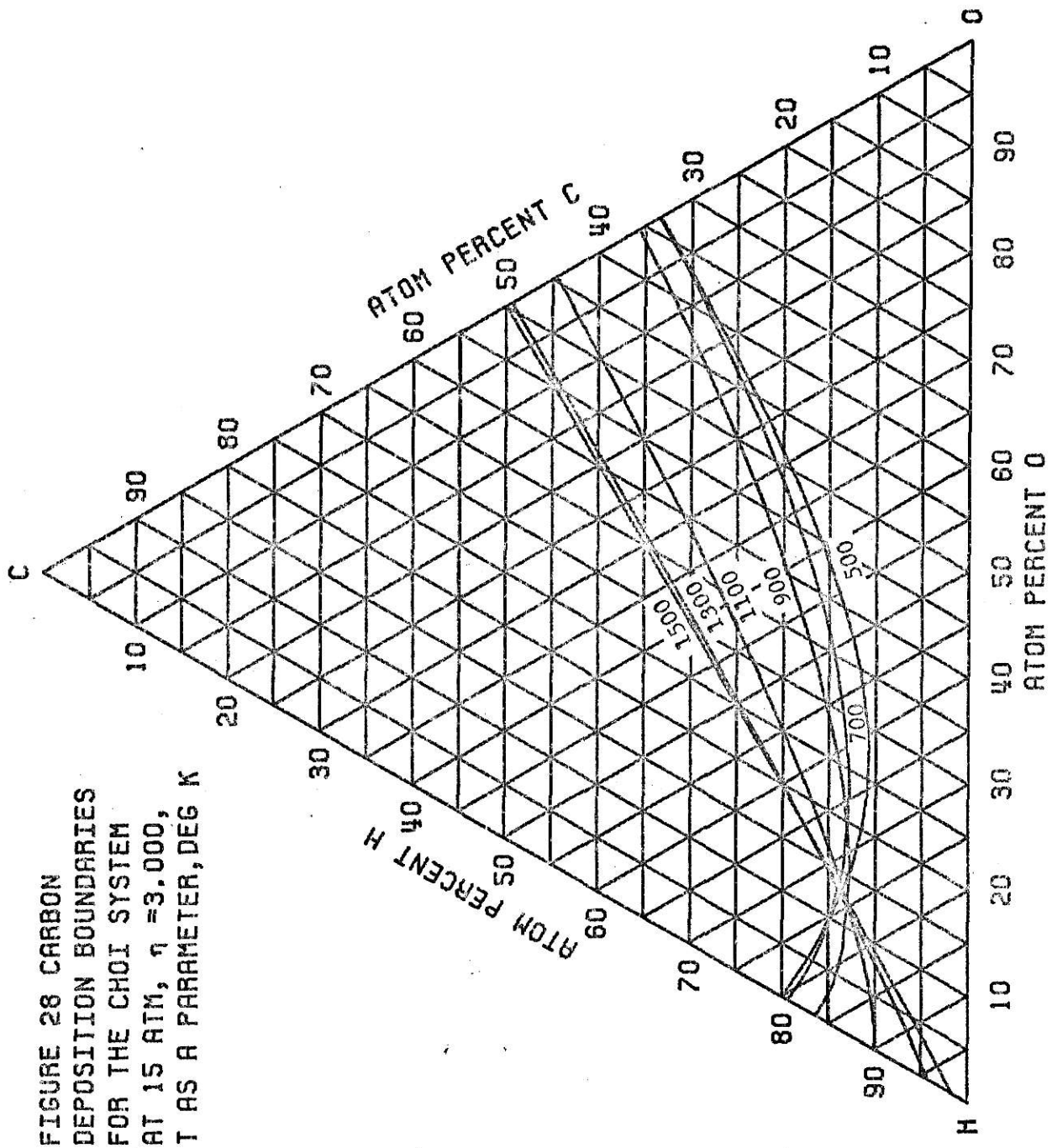


FIGURE 28 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, η =3.000,
T AS A PARAMETER, DEG K

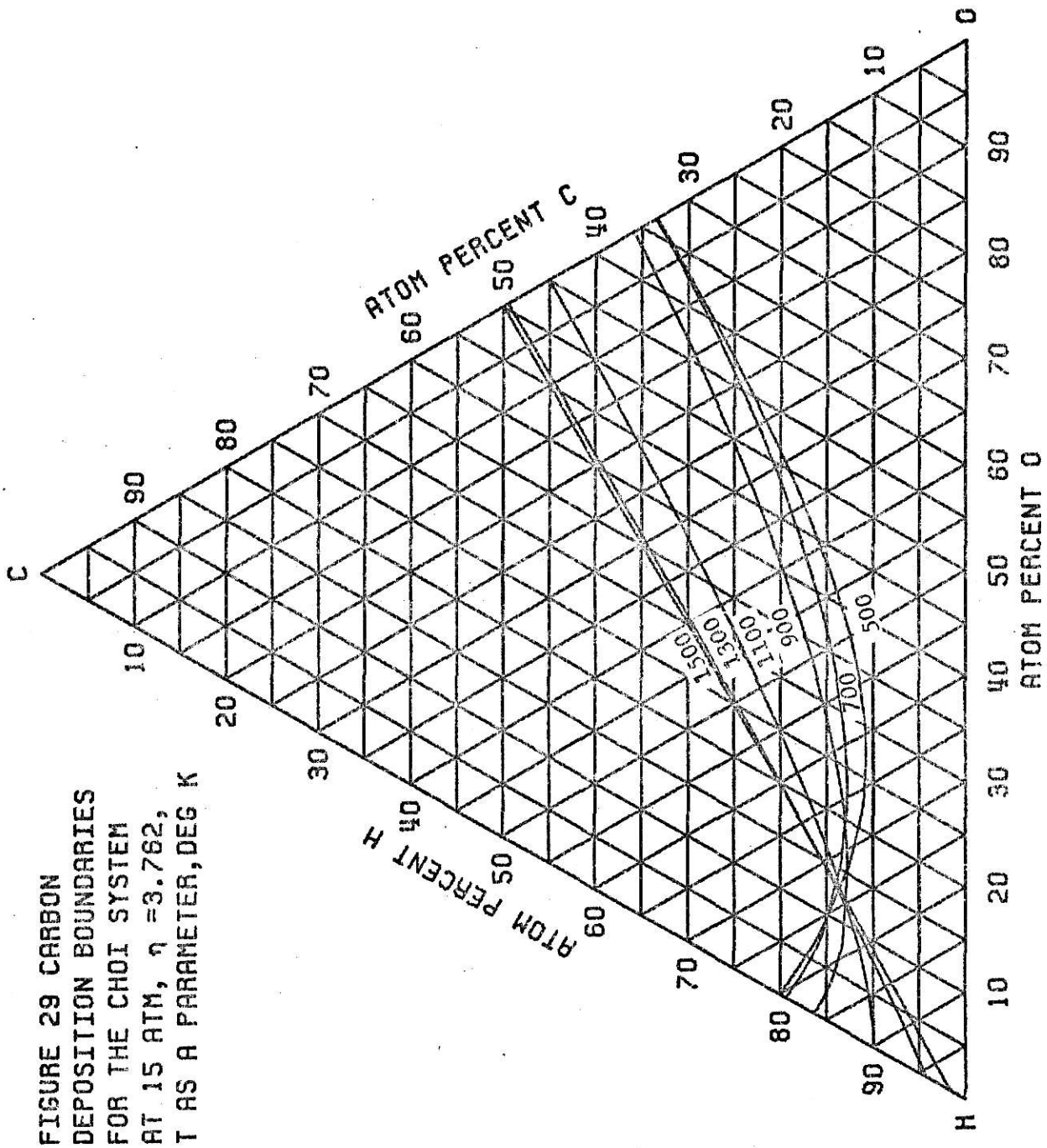


FIGURE 29 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, η =3.782,
T AS A PARAMETER, DEG K

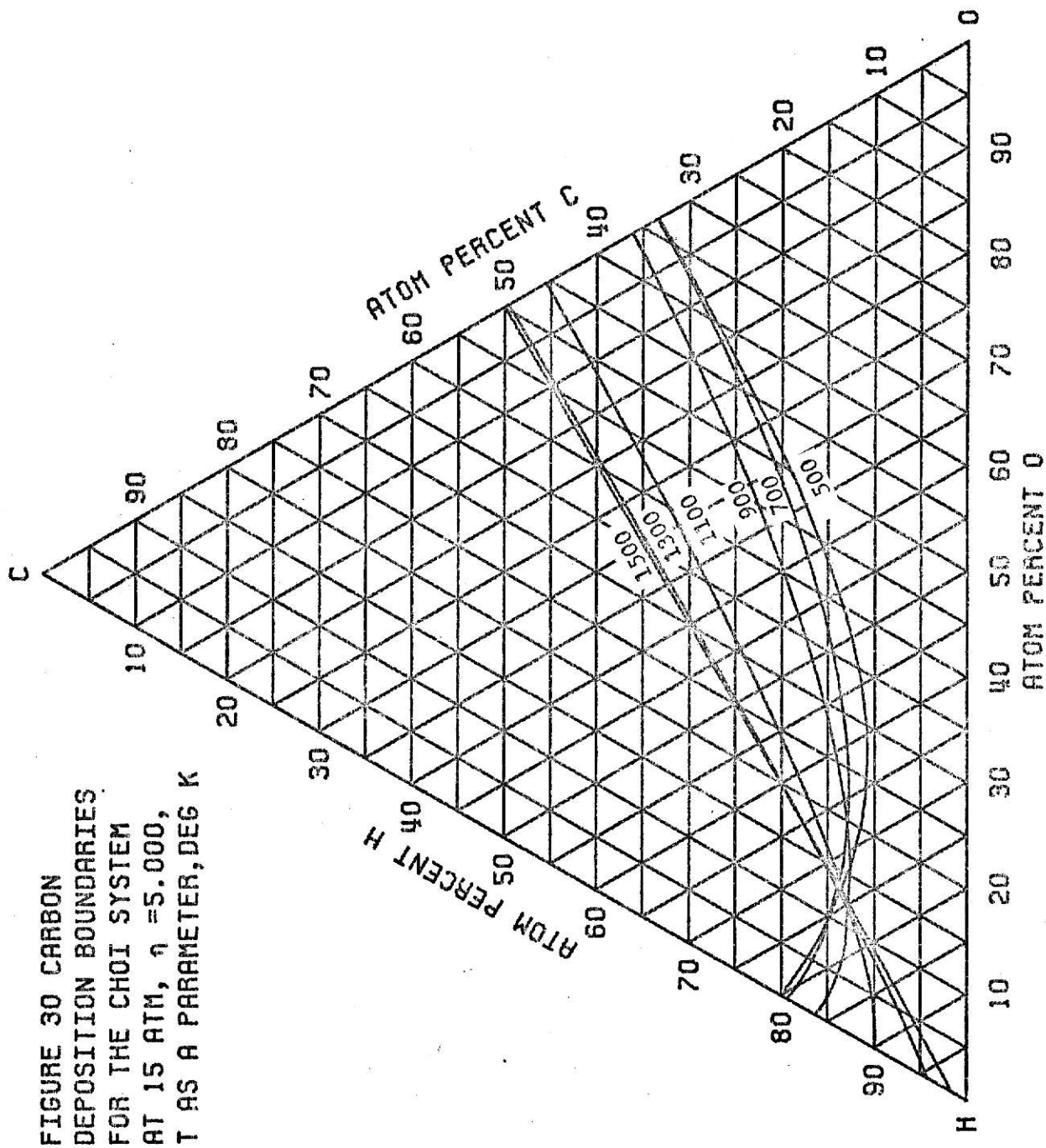


FIGURE 30 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, η =5.000,
T AS A PARAMETER, DEG K

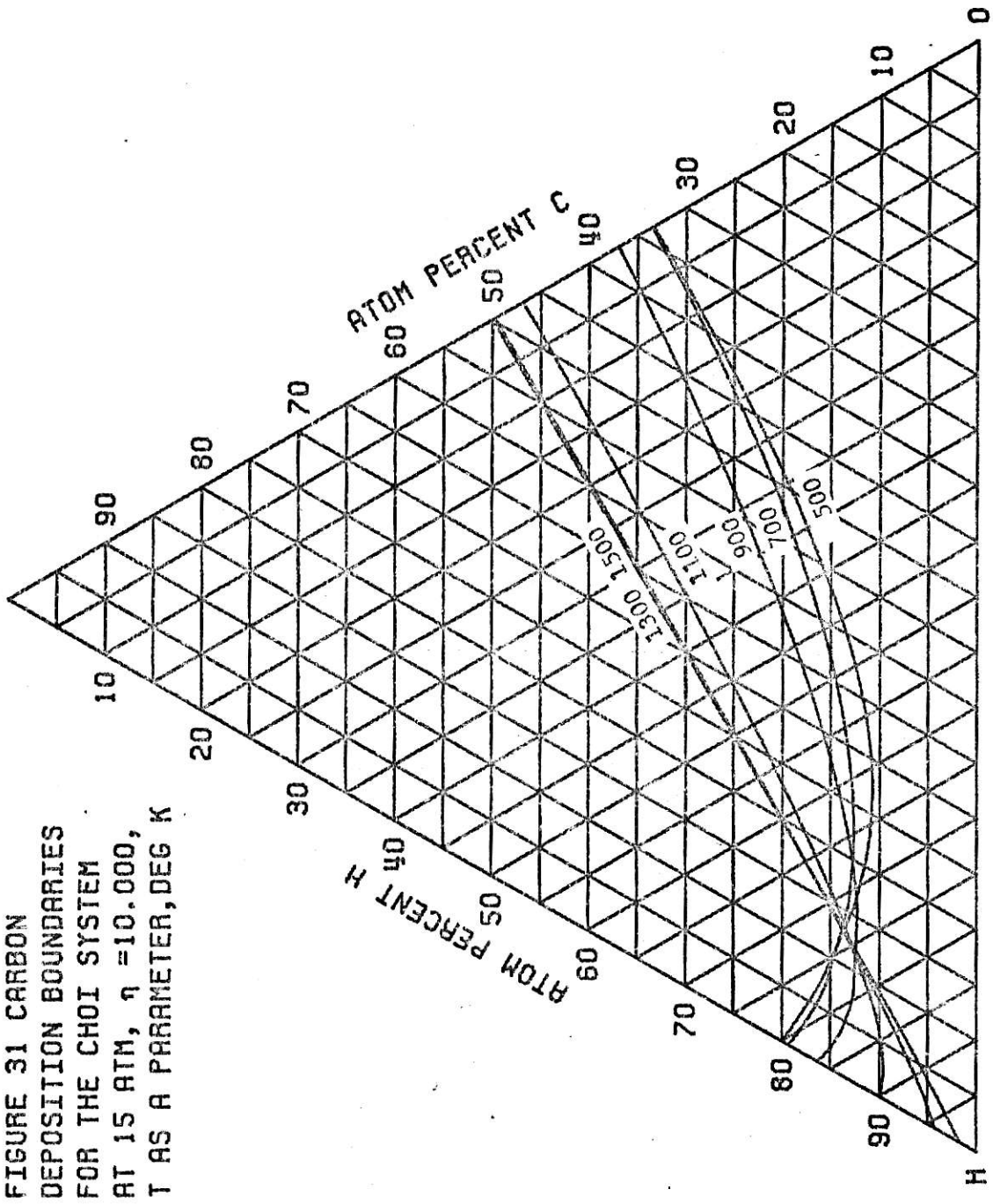
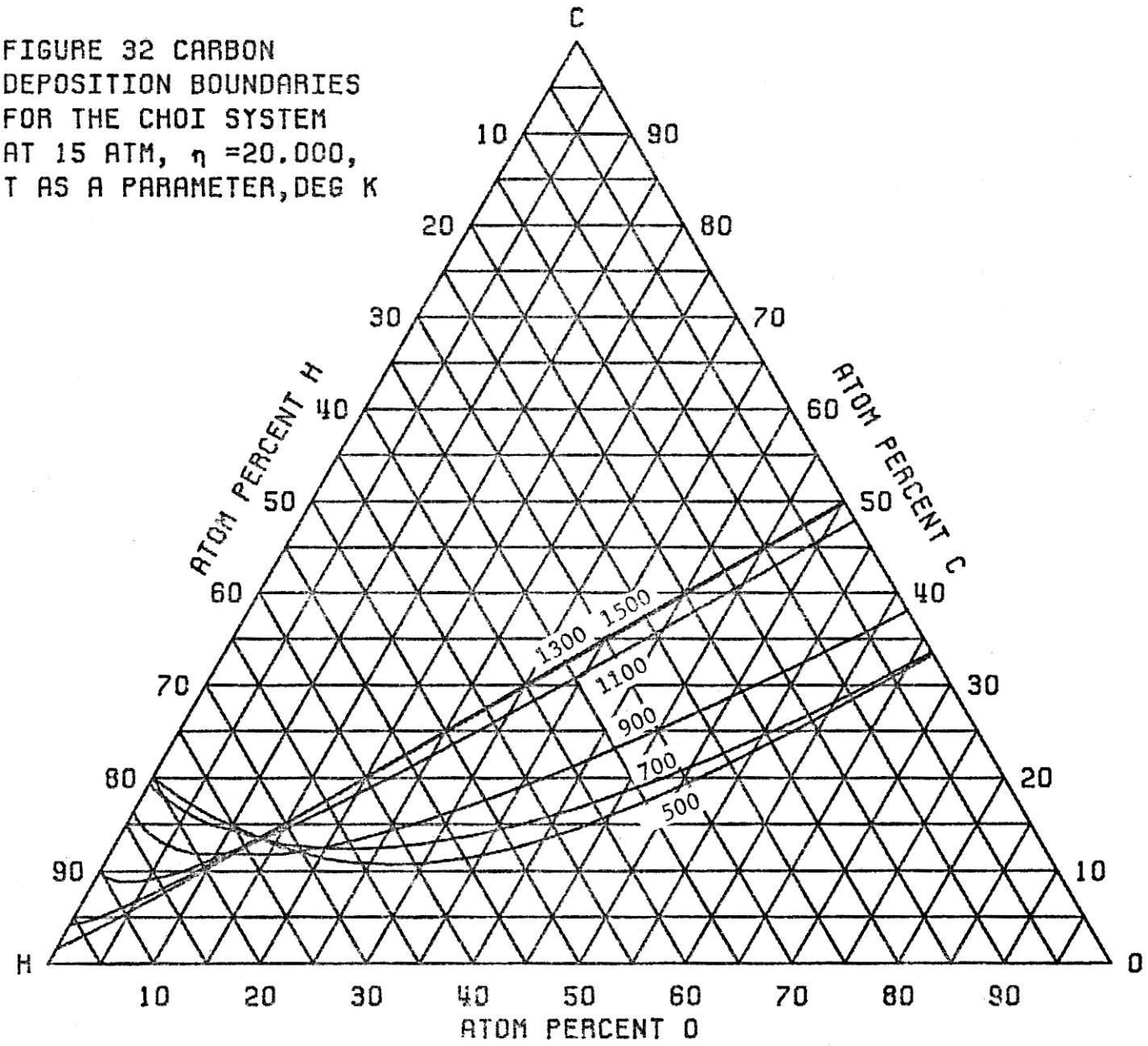


FIGURE 31 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 15 ATM, η =10.000,
T AS A PARAMETER, DEG K

FIGURE 32 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 15 ATM, η =20.000, T AS A PARAMETER, DEG K



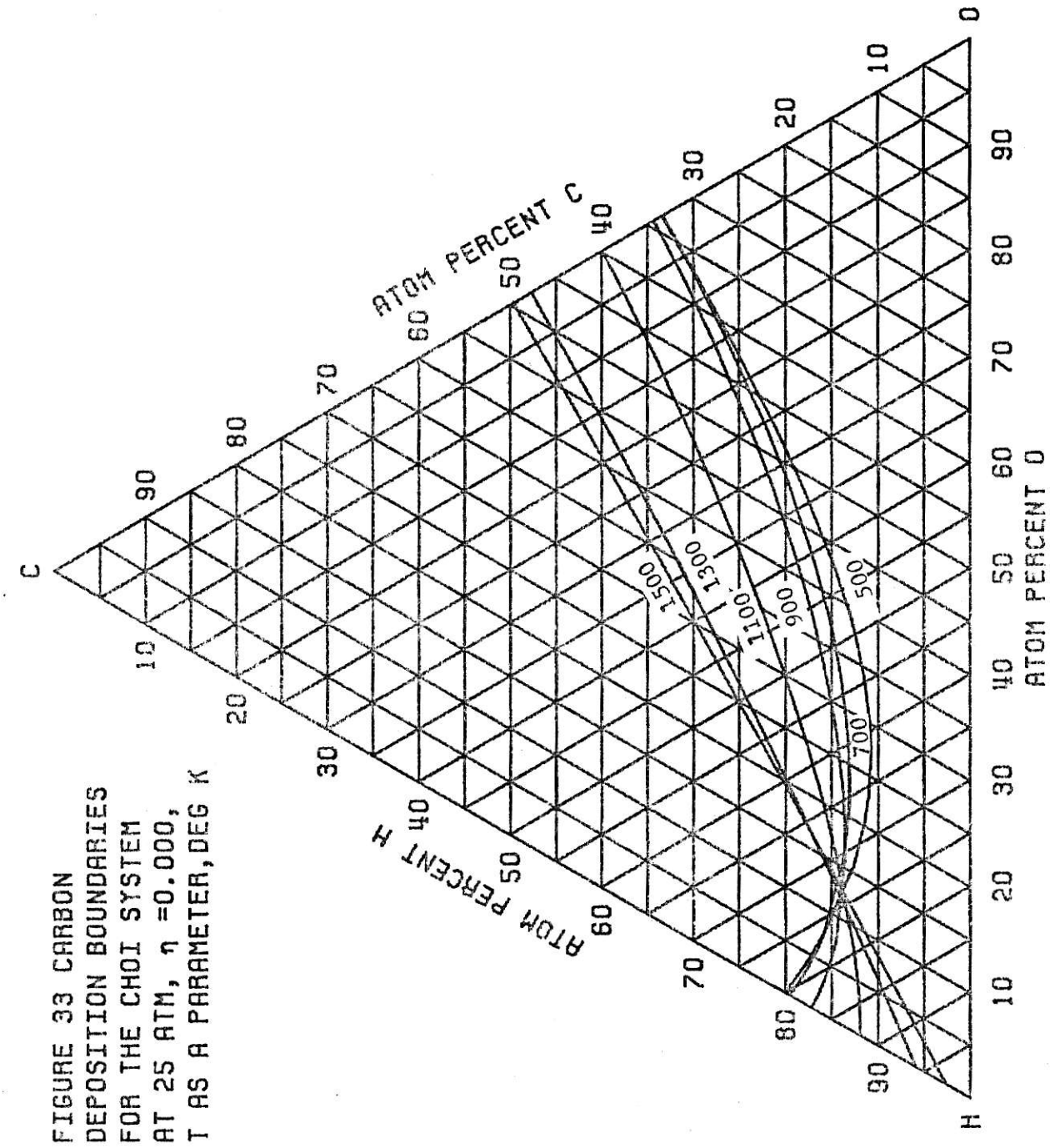


FIGURE 33 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 25 ATM, η =0.000,
T AS A PARAMETER, DEG K

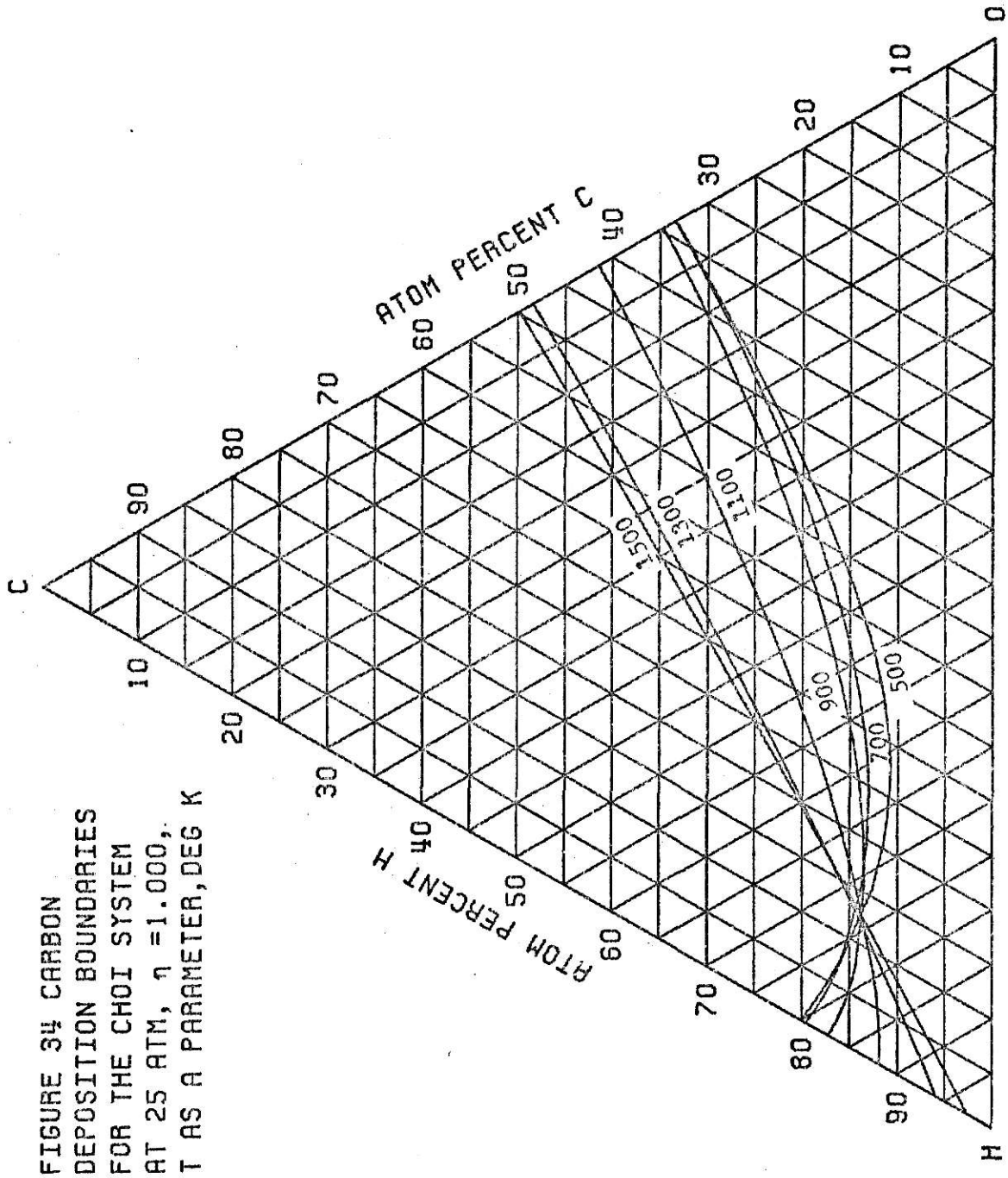
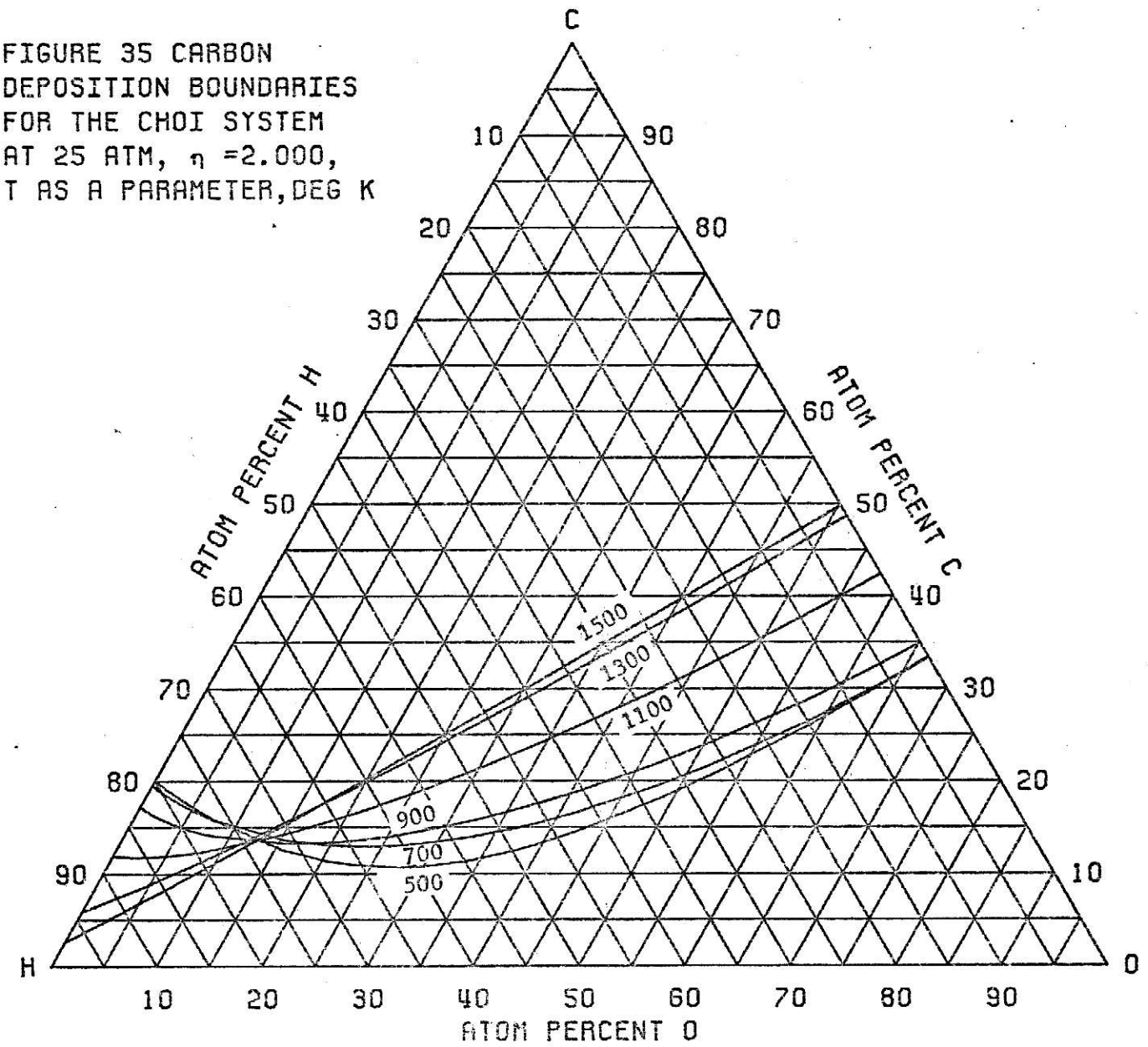


FIGURE 34 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 25 ATM, η =1.000,
T AS A PARAMETER, DEG K

FIGURE 35 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 25 ATM, η =2.000, T AS A PARAMETER, DEG K



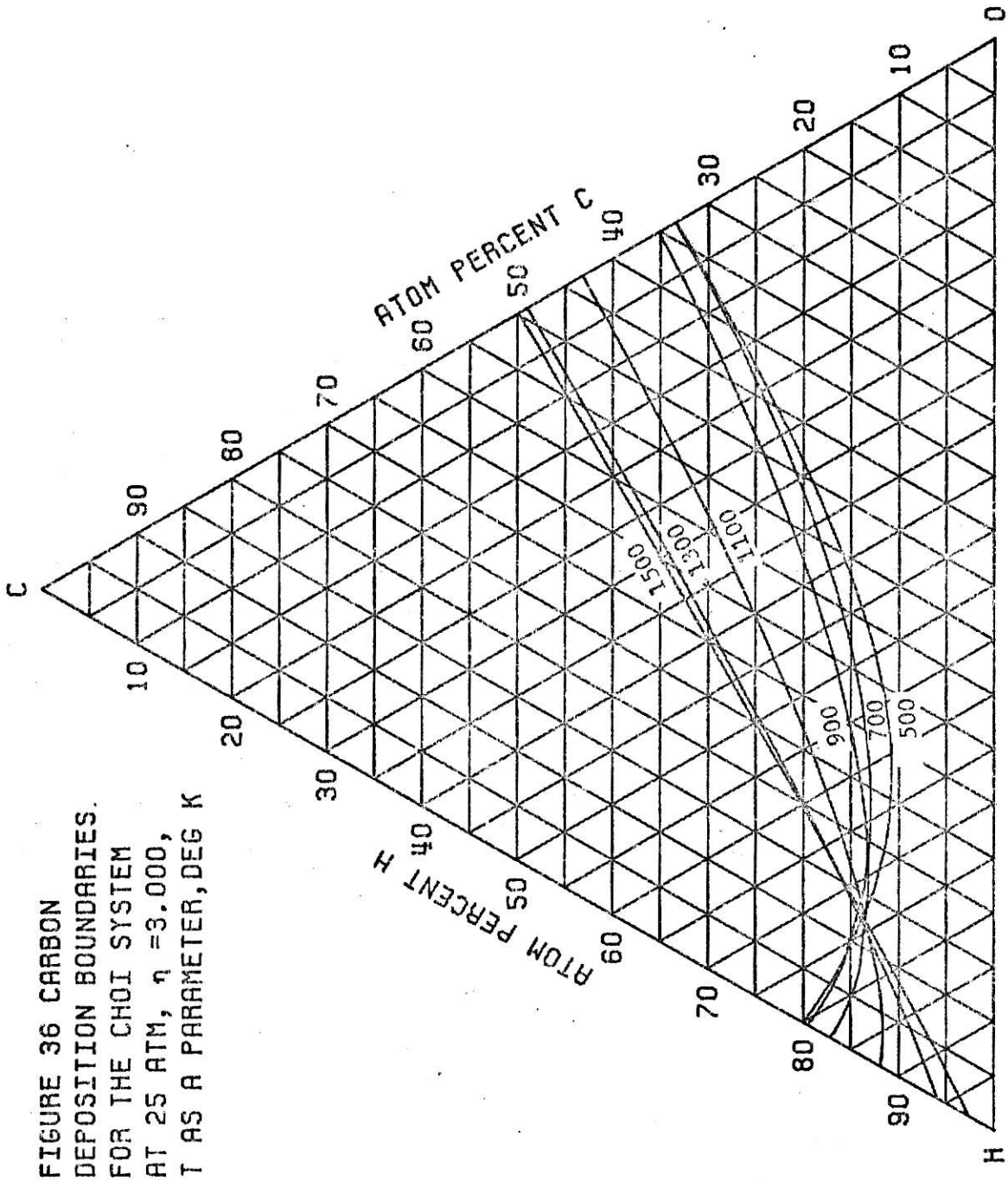
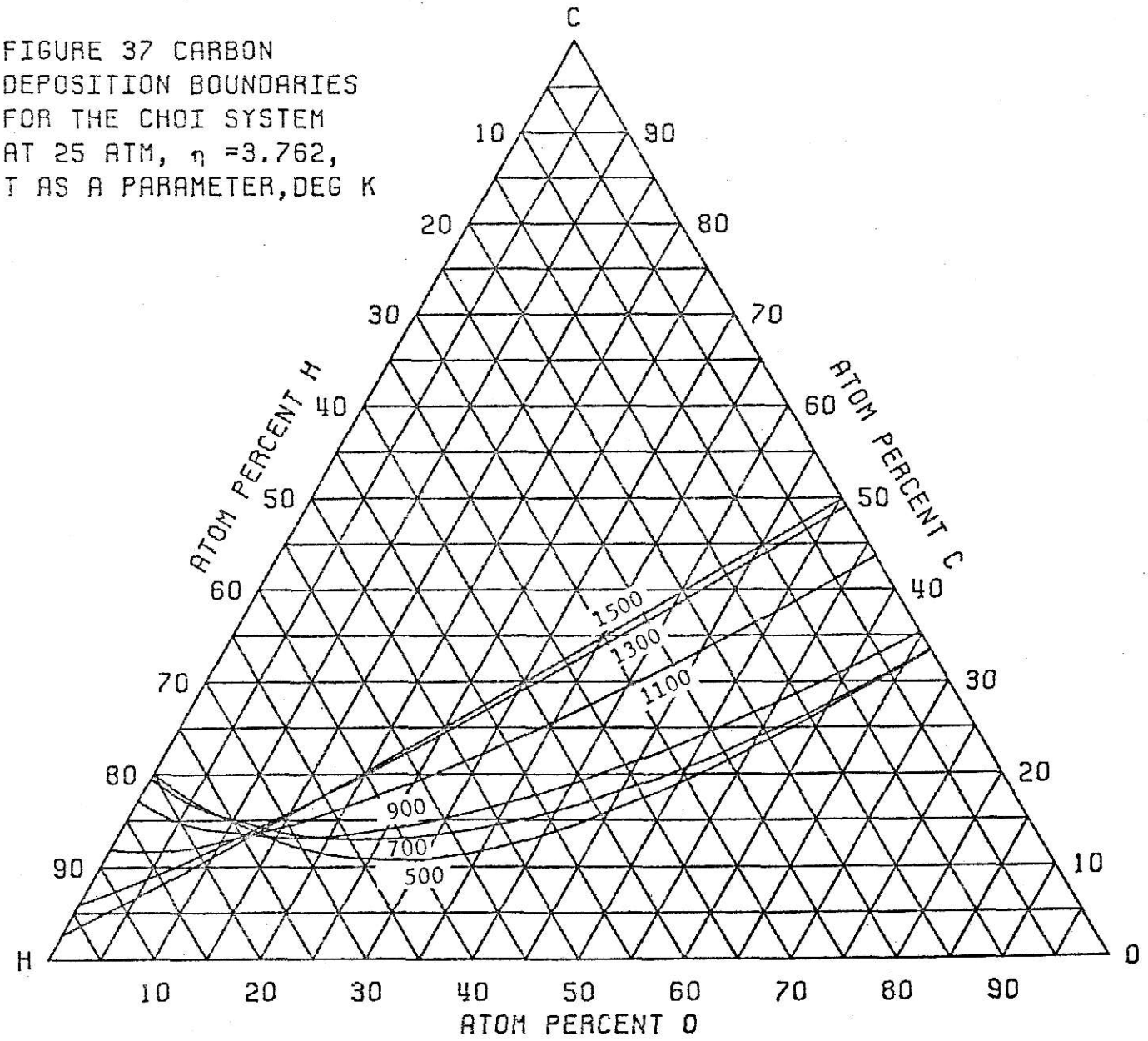


FIGURE 36 CARBON
DEPOSITION BOUNDARIES.
FOR THE CHOI SYSTEM
AT 25 ATM, η =3.000,
T AS A PARAMETER, DEG K

FIGURE 37 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 25 ATM, η =3.762, T AS A PARAMETER, DEG K



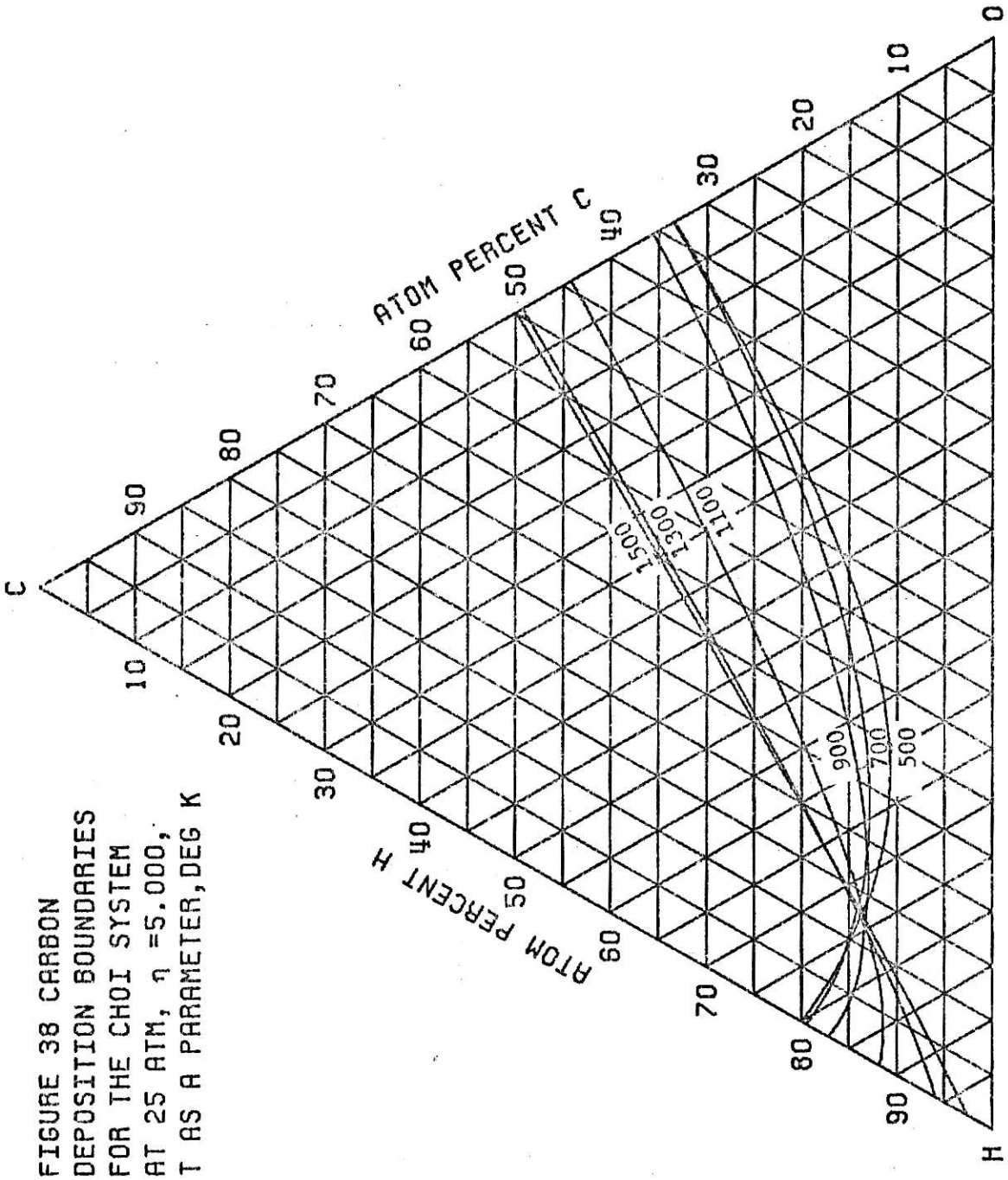
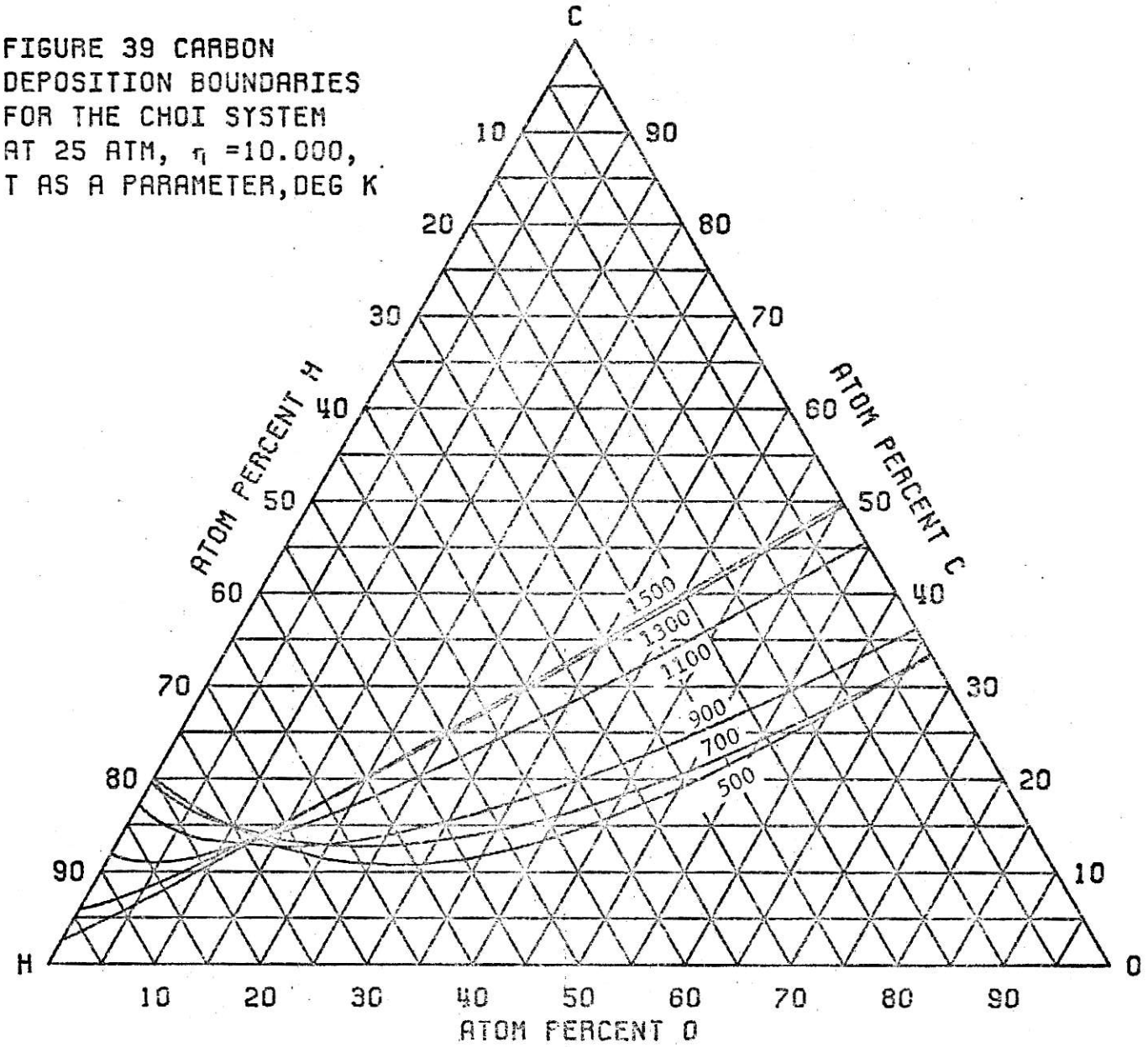


FIGURE 38 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 25 ATM, η =5.000,
T AS A PARAMETER, DEG K

FIGURE 39 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 25 ATM, η =10.000, T AS A PARAMETER, DEG K



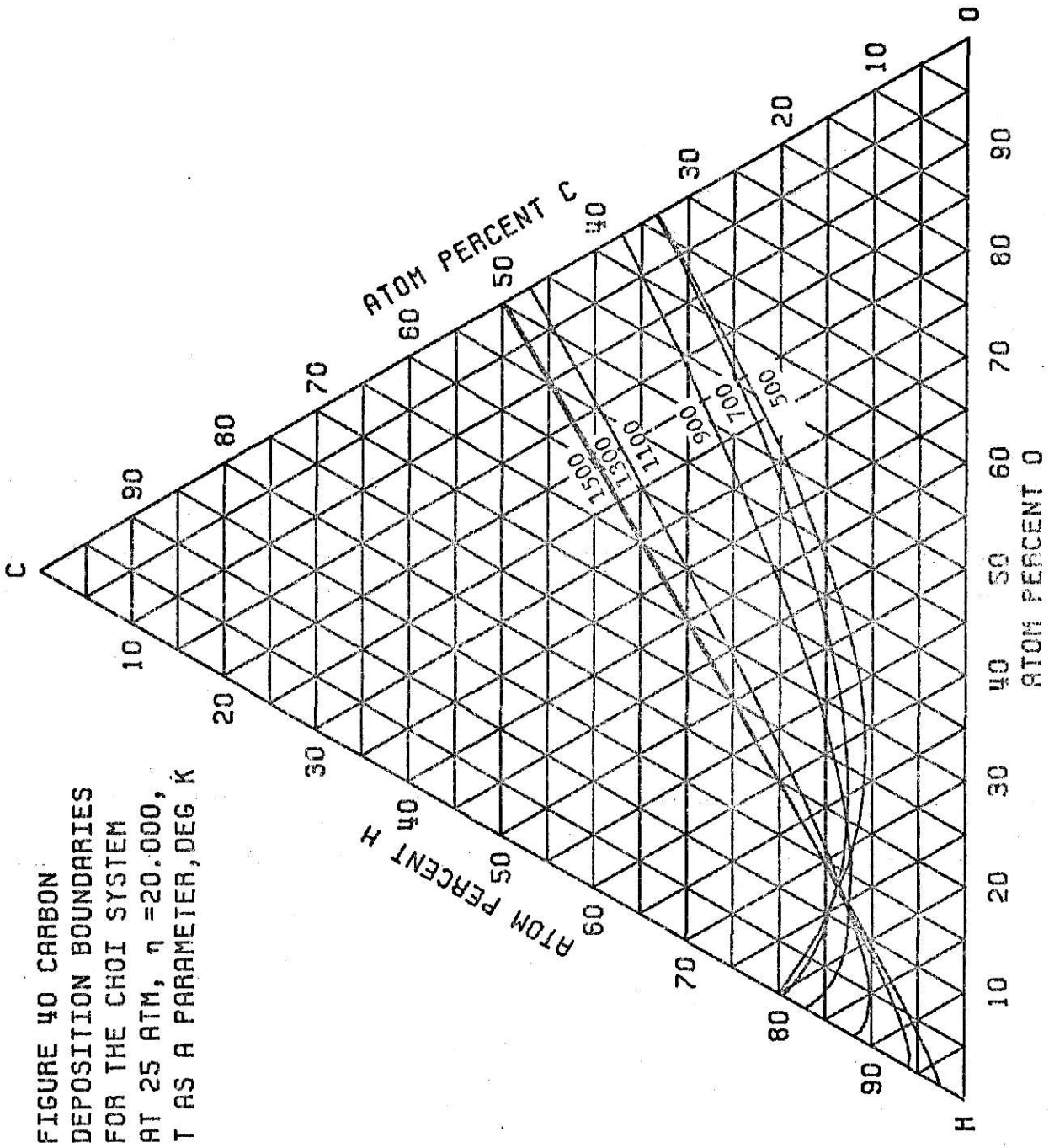


FIGURE 40 CARBON
DEPOSITION BOUNDARIES
FOR THE CHOI SYSTEM
AT 25 ATM, η =20.000,
T AS A PARAMETER, DEG K

CHAPTER V

DISCUSSIONS

5.1 GAS-PHASE IDEALITY ASSUMPTION

Since the gas-phase non-ideality effect is maximum at the highest pressure and the lowest temperature, the calculations of equilibrium mole fractions of the gas-phase were redone, using the fugacity data from Deming (6, 7, 8, 9) and Zwolinski (12), at 25 atm and 500° K. The fugacity data are used in the expression for c_i, in equation (2-11). The calculations were performed for N/O = 0, 3, and 10 and for O/H = 10^{-3} to 10^{3} and the results compared with those obtained under the ideality assumption. For most species, the maximum value of the absolute error in mole fraction was found to be of the order of 10^{-3} which represents a fractional percentage error. In most cases, the absolute error was found to be 10^{-4} or less, corresponding to relative error of 0.1% or less, for the abundant species. However, the maximum relative error was of the order of hundred per cent for species whose mole fractions were in the order of 10^{-4} or less.

Considering these relative small errors and remembering the fact that there is some inherent uncertainty of the results due to the limited accuracy of the free energy and fugacity data, it is concluded that the effect of non-ideality of the gas-phase can be reasonably neglected.

5.2 ABSENCE OF LIQUID WATER, NITROGEN COMPOUNDS, AND HIGHER MOLECULAR WEIGHT HYDROCARBONS

The lowest temperature used for calculation of the equilibrium results in this work was 500° K. It was found that the vapor pressure of liquid water at 500° K exceeds the partial pressure of water in the gas phase at the highest pressure used (25 atm). This explains why the liquid-water phase was not considered in the method of calculation.

In the gas-phase, only six species have been considered to be significant. The mole fraction of any other gaseous specie composed of one or more of the elements from C, H, O, and N can be calculated using the equilibrium constants of formation and the previously calculated mole fractions of other six abundant species, or using the values of Lagrangian multipliers and equation (2-17).

For example, the mole fraction of O_2 is calculated from the following reaction whose equilibrium constant of formation is denoted by K_{CO_2}:

$$C(s) + O_2 = CO_2$$

Therefore,

$$y_{O_2} = y_{CO_2} / K_{CO_2}$$

then, for any other compound, $C_\alpha H_\beta O_\gamma N_\theta$, the mole fraction can be found from its formation reaction:

$$\alpha\ C + \frac{\beta}{2} H_2 + \frac{\gamma}{2} O_2 + \frac{\theta}{2} N_2 = C_\alpha H_\beta O_\gamma N_\theta$$

$$\Delta G_f^\circ = -RT \ln K_f$$

$$K_f = \frac{p_{C_\alpha H_\beta O_\gamma N_\theta}}{\sqrt{p_{H_2}^{\beta} \; p_{O_2}^{\gamma} \; p_{N_2}^{\theta}}} = \frac{P \; y_{C_\alpha H_\beta O_\gamma N_\theta}}{P^{\frac{\beta+\gamma+\theta}{2}} \sqrt{y_{H_2}^{\beta} \; y_{O_2}^{\gamma} \; y_{N_2}^{\theta}}}$$

or, $$y_{C_\alpha H_\beta O_\gamma N_\theta} = K_f \; P^{(\beta+\gamma+\theta)/2} \sqrt{y_{H_2}^{\beta} \; y_{O_2}^{\gamma} \; y_{N_2}^{\theta}}$$

By calculation, it was found that even the most common nitrogen compounds, e.g., N_2O, NO, NO_2, HCN, $(CN)_2$, and NH_3 had equilibrium mole fractions less than 10^{-5}.

Higher molecular weight hydrocarbons were also tested for their presence in trace quantities and their mole fractions were found to be, generally, of the order of 10^{-5} or less except in the region of small O/H values. Under some conditions, their presence in greater than trace amounts was indicated, however, their estimated mole fractions were still below 10^{-4} and thus too low to warrant their inclusion in a recalculation of the equilibrium gas phase compositions.

5.3 EFFECT OF TEMPERATURE ON CARBON DEPOSITION BOUNDARIES

A typical characteristic observed in the Figures 1 through 40 is that an increase in temperature causes a shift in equilibrium gas-phase compositions towards more CO and H_2. This is why at temperatures around 1500° K, the carbon deposition boundaries are very close to a straight line joining H_2 and CO. Conversely, at low temperatures, CH_4 and CO_2 are present in larger amounts.

Therefore, at high temperatures, the carbon deposition

boundary can be used to graphically predict the equilibrium gas-phase compositions. At lower temperatures, the other species namely CH_4, CO_2, and H_2O become increasingly important and the gas-phase composition may no longer be determined simply by graphical calculations.

5.4 EFFECT OF PRESSURE AND INERT ON THE CARBON DEPOSITION BOUNDARIES

To illustrate the effects of inert and pressure on the carbon deposition boundaries, the results were plotted with η or P as a parameter on the triangular CHO diagrams. Figure 41 shows how the carbon deposition boundary shifts with a change of N/O ratio, at 1000° K and 1 atm. The effect is found to be much less at very low and at very high temperatures.

Similarly, Figures 42 and 43 are plotted to illustrate the effect of pressure for different values of η, at 1000° K. Again, it was observed that the effects were pronounced at medium temperatures.

The insignificant effect of P and η on the carbon deposition boundaries at low and at high temperatures can be explained by a simple thermodynamic analysis for the binary element systems represented by the C-O and C-H sides of the triangular diagram.

When $\eta = 0$, these binary elemental systems will consist of only three species, either C, H_2, and CH_4 or C, CO, and CO_2. The effect of pressure for these systems is considered here separately.

For the C-H system, the relevant reaction is:

FIGURE 41 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 1000°K, P=1 WITH n AS A PARAMETER: 0,2,3.76,10

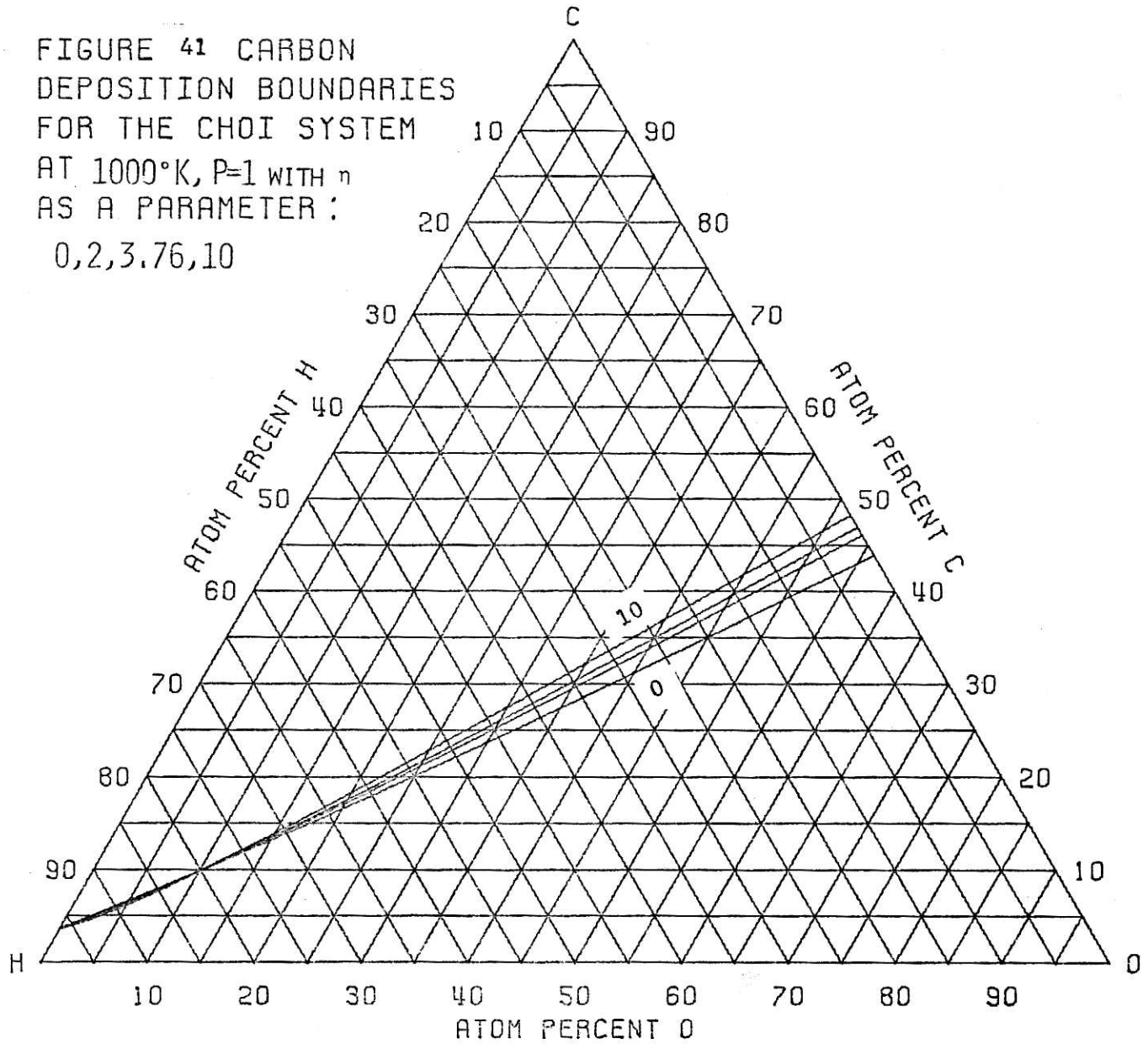
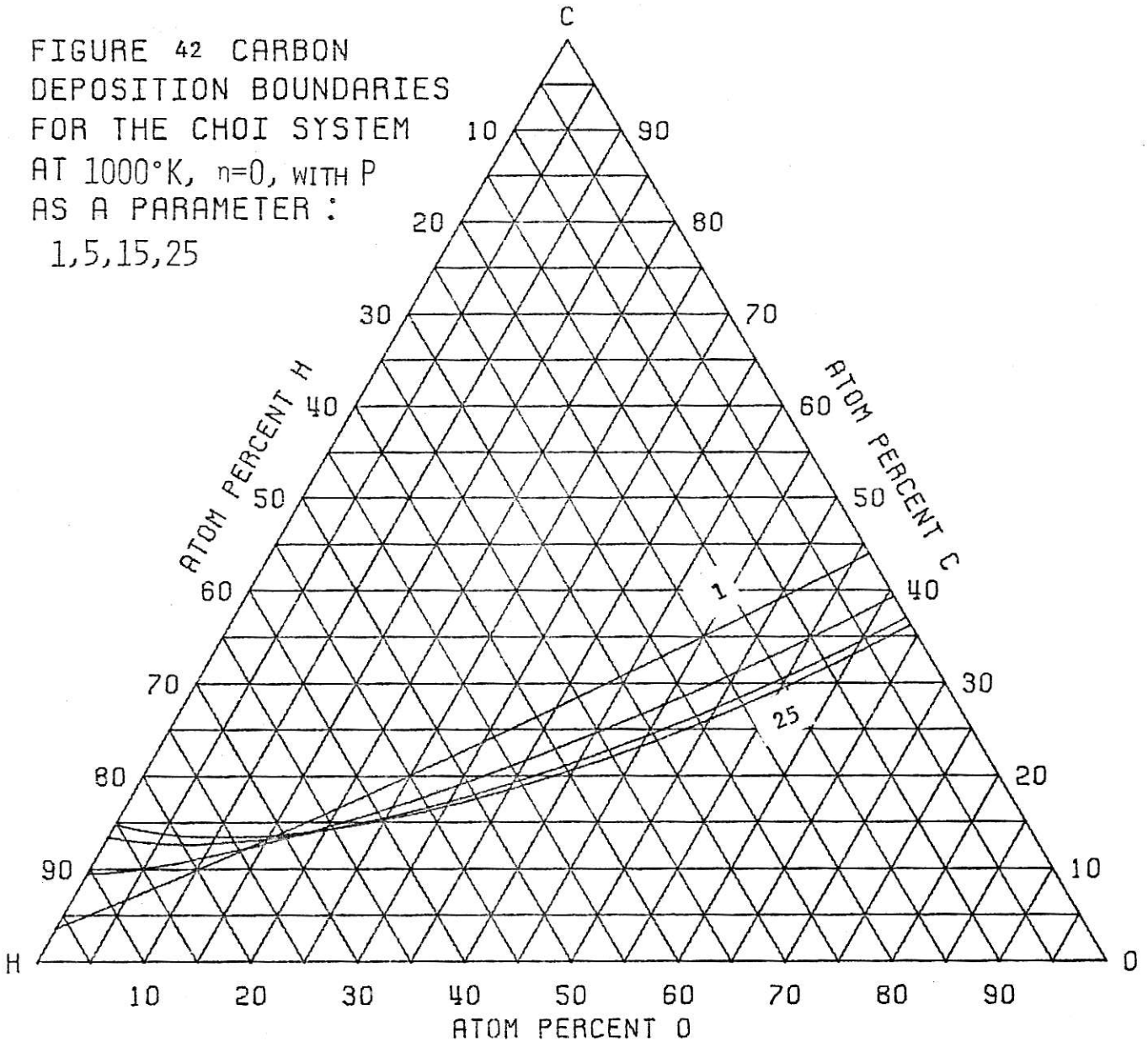


FIGURE 42 CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 1000°K, n=0, WITH P AS A PARAMETER : 1,5,15,25



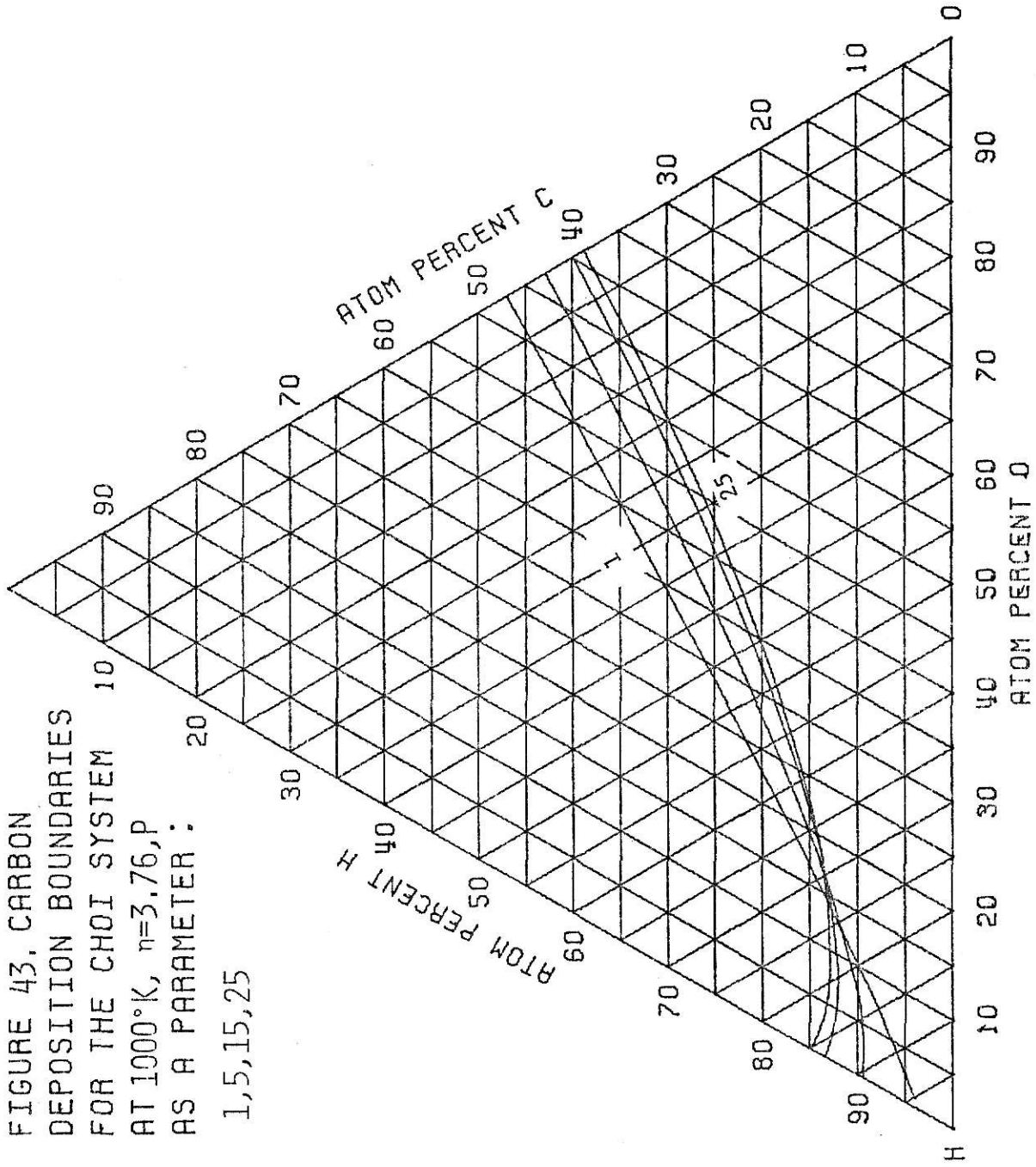


FIGURE 43. CARBON DEPOSITION BOUNDARIES FOR THE CHOI SYSTEM AT 1000°K, n=3.76,P AS A PARAMETER: 1,5,15,25

$$C(s) + 2H_2 = CH_4$$

In the presence of solid carbon and under the perfect gas assumption, the relation among the equilibrium constant for this reaction, K_1, the total pressure, P, and the mole fraction of hydrogen, y, is given by:

$$K_1 = \frac{P(1-y)}{(Py)^2}$$

or:

$$K_1 P y^2 + y - 1 = 0$$

By differentiation, the following relation is obtained:

$$\left(\frac{\partial y}{\partial P} \right)_T = \frac{K_1 y^2}{1 + 2 K_1 P y}$$

At 500° K, $K_1 = 2675$, and y varies in the order of 10^{-2} to 10^{-3} as P changes from 1 to 25 atm.

Therefore,

$$\left(\frac{\partial y}{\partial P} \right)_T \doteq \frac{y}{2P} \leq 10^{-2}$$

At 1500° K, $K_1 = 0.00256$, and $y > 0.94$.

Therefore,

$$2K_1 Py << 1$$

or,

$$\left(\frac{\partial y}{\partial P} \right)_T \doteq K_1 y^2 \doteq 10^{-3}$$

However, at 1000° K, $K_1 = 0.0983$, and y varies from 0.915 to 0.46 as pressure varies from 1 to 25 atm. Therefore, at 1 atm:

$$\left(\frac{\partial y}{\partial P} \right)_T \doteq 10^{-1}$$

which is significant though it decreases as P increases.

For the C-O system, a similar treatment may be performed with the reaction:

$$C(s) + CO_2 = 2\ CO$$

Let K_2 be the equilibrium constant of this reaction, and y be the mole fraction of CO, at equilibrium. Then,

$$K_2 = \frac{(Py)^2}{P(1-y)}$$

or,

$$K_2(1 - y) - Py^2 = 0$$

and, upon differentiation:

$$\left(\frac{\partial y}{\partial P} \right)_T = - \frac{y^2}{K_2 + 2Py}$$

At low temperatures, K_2 and y are both of the orders of 10^{-4} or less, therefore:

$$\left| \left(\frac{\partial y}{\partial P} \right)_T \right| \leq \frac{y}{2P} \leq 10^{-4}$$

On the other hand, at 1500° K, y is nearly unity, and $K_2 > > 2Py$. Therefore:

$$\left| \left(\frac{\partial y}{\partial P} \right)_T \right| \doteq \frac{y^2}{K_2} \doteq 10^{-3}$$

At 1000° K, however, $K_2 = 1.89$ and y varies around 0.5 to 0.7. Therefore, at P = 1 and y = 0.6,

$$\left(\frac{\partial y}{\partial P} \right)_T \doteq - 10^{-1}$$

which is again very significant.

In the preceding analysis considered at the binary edges of the carbon deposition boundary, there are only two species present in the gas-phase and thus a significant change in the mole fraction y significantly shifts the carbon deposition boundary. However, this sensitivity of carbon deposition boundary to composition is not necessarily found in the interior region of the ternary CHO diagram. Several cases were observed where carbon deposition boundaries superimposed and as much as 20% difference in mole fractions was found. The opposite is, however, necessarily true; that is, a significant shift in the carbon deposition boundary implies significant changes in the mole fractions.

As has been seen in Section 2.5, the effects of P and η can be combined through the use of the term P/n, thus, as expected, an increase in P causes a change in the opposite direction to that due to an increase in n or η . Also, as expected, the maximum effect of η is seen at the lowest pressure, P = 1 atm and accordingly when η = 0 the maximum effect of P is seen. The direction of these effects is determined by Le Chatelier principle as can be seen on Figures 42 and 43. An increased pressure shifts the gas phase composition toward more CH_4 and CO_2. Figure 41 shows that an increase in inerts decreases the effective pressure and causes a shift toward CO. The corresponding shift toward H_2 is not seen on the diagram because as CH_4 and H_2 are approached the quantity of oxygen, hence the effect of N/O elemental ratio, decreases.

APPENDIX A

COMPUTER PROGRAM

AND INPUT DATA

```
      C     ********************************************************************
      C     SHANTY MOHNOT ,MASTER'S RESEARCH  , C H O - INERT(SAY NITROGEN)     *
      C     COMPLEX HETEROGENOUS CHEMICAL EQUILIBRIUM CALCULATIONS AND CARBON   *
      C     DEPOSITION BOUNDARIES AT VARIOUS TEMPERATURES,PRESSURES AND INERT   *
      C     TO OXYGEN RATIOS , CARBON DEPOSITION BOUNDARIES   PRESENTED ON      *
      C     TRIANGULAR  CHO DIAGRAMS                                            *
      C     FOUR DEGREES OF FREEDOM IN THE SYSTEM , PRESSURE, TEMPERATURE, N/O  *
      C     RATIO AND  O/H RATIO                                                *
      C     METHOD OF  CALCULATION IS BASED ON FREE ENERGY MINIMIZATION TECHNIQUE*
      C     OPTIMIZATION COMPUTATIONS ARE BASED ON AN ITERATIVE PROCEDURE WHICH  *
      C     IS GENERATED BY APPLYING THE METHOD OF STEEPEST DESCENT              *
      C     ********************************************************************
0001          IMPLICIT REAL*8(A-H,O-Z)
0002          REAL*8 LOGK,LNK,MF,LAMH,N,NN,LAM,NT,NNT,LL,NCLN
0003          INTEGER P,A,T,PR,TI
0004          LOGICAL CHECK
0005          DIMENSION A(3,7),PI(3),B(3),AA(3,4),BB(3),N(7),NN(7),ETA(10),LNK(7
             *),DEL(7),R(3,3),CLN(7),NCLN(7),C(7),DELH(7),PN(7),MF(7),OMEGA(24)
             *,D(7)  ,LOGK(12,7),P(8),T(12),XXIS(23),YXIS(23)
      C     INPUT DATA                                                          *
0006          ITMAX=125
0007          DELTA=1.0D-8
      C     COEFFICIENT MATRIX                                                  *
0008          READ(5,15)((A(J,I),I=1,7),J=1,3)
0009    15    FORMAT(21I3)
      C     PRESSURE ARRAY                                                      *
0010          READ(5,16) (P(I),I=1,5)
0011    16    FORMAT(5I5)
      C     ETA = N/O ARRAY                                                     *
0012          READ (5,17) (ETA(I),I=1,9)
0013    17    FORMAT( 9F8.0)
      C     TEMPERATURES ARRAY                                                  *
0014          READ(5,18) (T(I),I=1,12)
0015    18    FORMAT(12I5)
      C     OMEGA=O/H ARRAY                                                     *
0016          OMEGA(1)=1.D-3
0017          OMEGA(2)=1.D-2
0018          OMEGA(22)=1.D2
0019          OMEGA(23)=1.D3
0020          OMEGA(24)=1.D4
0021    20    READ(5,25) (OMEGA(I),I=3,21)
0022    25    FORMAT (16F5.0)
      C     EQUILIBRIUM CONSTANTS OF FORMATION OR COMPONENTS AT T               *
0023    30    READ(5,35)((LOGK(J,I),I=1,7),J=1,12)
0024    35    FORMAT(7F10.5)
      C     PRINT DATA                                                          *
0025          WRITE(6,36) ((A(J,I),I=1,7),J=1,3),(P(I),I=1,5),(ETA(I),I=1,9),
             *   (T(I),I=1,12),(OMEGA(I),I=1,23),((LOGK(J,I),I=1,7),J=1,12)
0026    36    FORMAT('1'///,33X,'INPUT DATA',///,10X,'COEFFICIENT MATRIX'/3(//,
             * 8X,7I5),///,10X,'PRESSURE ARRAY',//, 6X,5I7,///10X,'ETA ARRAY',//
             *,10X,9F6.2,///10X,'TEMPERATURE ARRAY',//,10X,12I5,///,10X,'OMEGA A
             *RRAY'//,2(10X,8F7.3,/), 8X,7F7.1,///,10X,'LOG OF EQBM CONST OF FOR
             *MATION ARRAY'//,12(10X,3F5.1,4F10.5/))
0027          B(1)=1.D5
0028          B(3)=50.
      C     START OF DO LOOPS BY SELECTING PRESSURE,ETA=N/O RATIO,OMEGA=O/H RATIO *
      C     AND TEMPERATURE RESPECTIVELY                                        *
0029          ITABLE=0
```

```
0030              IFIG=0
0031              DO 1000 IP=1,5
0032              DO 1000 IE=1,8
0033              ITABLE=ITABLE+1
0034              IFIG=IFIG+1
0035              PR=P(IP)
0036              ETAA=ETA(IE)
                  C     PREPARE TRIANGULAR DIAGRAM WITH  TITLE FOR PLOTTING CARBON DEPOSITION    *
                  C     BOUNDARIES                                                              *
0037              CALL TRIANG (PR,ETAA,IFIG)
0038              WRITE(6,45)ITABLE,PR,ETAA
0039              45  FORMAT('1',// 16X,'TABLE-',I2,' EQUILIBRIUM GAS-PHASE MOLE FRACTIO
                  *NS',/,30X,'P=',I2,' ATM,N/O=',F5.2//,T10,'T, K',3X,'O/H',7X,'N2'
                  *,7X,'H2',7X,'CO',6X,'CH4',6X,'H2O',6X,'CO2')
0040              DO  950 ITEMP=2,12
0041              54  DO  800 IO=1,23
0042              IF(((IO.EQ.2).OR.(IO.EQ.4).OR.(IO.EQ.6).OR.(IO.EQ.8).OR.(IO.EQ.11)
                  *.OR.(IO.EQ.13).OR.(IO.EQ.15).OR.(IO.EQ.18).OR.(IO.EQ.20)).OR.
                  *(((T(ITEMP)-200  )/200.-(T(ITEMP)-200  )/200).GT.1E-2))GO TO 57
0043              GO TO 800
0044              57  TI=T(ITEMP)
0045              OMEGAA=OMEGA(IO)
0046              B(2)=B(3)/OMEGAA
                  C     INITIAL ROUGH GUESS FOR EXIT MOLE NUMBERS
0047              N(2)=B(3)*ETAA/2
0048              N(4)=0.1
0049              IF(OMEGAA    .GT.2.) GO  TO 66
0050              N(5)=0.1
0051              N(6)=0.1
0052              GO TO 70
0053              66  N(5)=0.004
0054              N(6)=0.01
0055              70  N(1)=B(1)-0.5*(B(3)+N(4)-N(6))-N(5)
0056              N(3)=0.5*B(2)-2*N(5)-N(6)
0057              N(7)=0.5*(B(3)-N(4)-N(6))
0058              C1=-DLOG(1D1)
0059              DO 80 I=2,7
0060              LNK(I)=C1*LOGK(ITEMP,I)
0061              PP=PR
0062              80  C(I)=DLOG(PP)+LNK(I)
0063              90  CHECK=.FALSE.
0064              91  DO 95 J=1,3
                  C     CHECKING IF  INITIAL GUESS SATISFIES THE MASS BALANCE CONSTRAINTS       *
0065              92  BCHECK=0.
0066              93  DO 94 I=1,7
0067              94  BCHECK=BCHECK+A(J,I)*N(I)
0068              95  IF(DABS(BCHECK-B(J)).GT.DELTA) CHECK=.TRUE.
0069              96  IF(.NOT.CHECK)  GO TO 100
0070              97  WRITE(6,99)
0071              99  FORMAT(1HO,'BAD INITIAL GUESS , B VECTORS DO NOT CHECK')
                  C     START OF ITERATIVE EVALUATION OF NEW EXIT COMPOSITIONS
0072              100 IT=1
                  C     TOTAL GAS PHASE MOLE NUMBERS
0073              NT=0
0074              DO 120 I=2,7
0075              120 NT=NT+N(I)
                  C     FORM AA COEFF(MATRIX)TO SOLVE 3 SIMULTANEOUS EQUATIONS IN PI(2),        *
                  C     PI(3), AND NNT ,BB IS THE SOLUTION VECTOR
```

```
0076        130   DO 136 I=3,7
0077        132   CLN(I)=C(I)+DLOG(N(I)/NT)
0078        136   NCLN(I)=N(I)*CLN(I)
0079        139   DO 144 L=2,3
0080        140   DO 144 J=1,3
0081        141   R(J,L)=0.
0082        142   DO 143 I=3,7
0083        143   R(J,L)=R(J,L)+A(J,I)*A(L,I)*N(I)
0084        144   CONTINUE
0085              AA(1,4)=-N(2)
0086              AA(2,4)=B(2)
0087              AA(3,4)=B(3)
0088              DO 149 I=3,7
0089              AA(1,4)=AA(1,4)+NCLN(I)
0090              AA(2,4)=AA(2,4)+A(2,I)*NCLN(I)
0091        149   AA(3,4)=AA(3,4)+A(3,I)*NCLN(I)
0092              AA(1,1)=R(2)
0093              AA(1,2)=R(3)
0094              AA(1,3)=-N(2)/NT
0095              AA(2,1)=R(2,2)
0096              AA(2,2)=R(2,3)
0097              AA(2,3)=B(2)/NT
0098              AA(3,1)=R(3,2)
0099              AA(3,2)=R(3,3)
0100              AA(3,3)=B(3)/NT
0101        158   CALL DETSIM(AA,BB,3)
            C     CALCULATING NEW VALUES OF AND CHANGES IN MOLE NUMBERS                    *
0102              PI(2)=BB(1)
0103              PI(3)=BB(2)
0104              NNT=BB(3)
0105              RNT=NNT/NT
0106              NN(1)=B(1)-R(1,2)*PI(2)-R(1,3)*PI(3)-(B(1)-N(1))*RNT
0107              DO 170  I=3,7
0108              NN(1)=NN(1)+A(1,I)*NCLN(I)
0109              NN(I)=N(I)*(RNT+PI(2)*A(2,I)+PI(3)*A(3,I)-CLN(I))
0110              DEL(I)=NN(I)-N(I)
0111        170   CONTINUE
0112              NN(2)=N(2)
0113              DEL(1)=NN(1)-N(1)
0114              DELN=NNT-NT
            C     EVALUATE MAX LAMBDA TO MAKE SURE ALL MOLE NUMBERS ARE POSITIVE - FIRST   *
            C     CONDITION FOR APPROACHING CORRECT OPTIMUM SOLUTION FOR THE PROBLEM       *
0115              LAM=1.0
0116        200   DO 204 I=1,7
0117        201   IF((I.EQ.2).OR.(NN(I).GT.0)) GO TO 204
0118        202   LL= -0.99999*N(I)/DEL(I)
0119        203   IF(LL.LT.LAM) LAM=LL
0120        204   CONTINUE
            C     LAM IS NOW MAX FOR CONDITION 1 . NOW CHECKING 2ND CONDITION THAT         *
            C     MIN G IS NOT PASSED. IF PASSED ,DECREASE LAM BY 10 % AND CHECK           *
            C     AFTER EACH DECREASE.                                                     *
0121              L=1
0122        216   LL=LAM*(1-(L-1)/10.)
0123        220   DFDL=0.
0124              DO 230 I=3,7
0125        230   DFDL     =DFDL     +DEL(I)*(  C(I)+DLOG((N(I)+LL*DEL(I) )/(NT
                 *+LL*DELN)))
0126              IF(DFDL.LE.0) GO TO 310
```

```
0127            L=L+1
0128            IF(L.EQ.11) GO TO 296
0129            GO TO 216
                C     DECREASE LAM OF THE PREVIOUS ITERATION AND RESTART THIS ITERATION        *
                C     WITH DECREASED MOLE NUMBERS                                              *
                C     BECAUSE 2ND CONDITION COULD NOT BE SATISFIED WITH THIS ITERATION         *
0130        296 LLL=LLL+1
0131            DO 298 I=1,7
0132            IF (I.EQ.2) GO TO 298
0133        297 N(I)=PN(I)-LLL*LAMH*DELH(I)/10
0134        298 CONTINUE
0135            NT=PNT-LLL*LAMH*DELNH/10
0136            IF(LLL.NE.10) GO TO 130
0137            WRITE(6,300)
0138        300 FORMAT(2X,'SECOND CONDITION IS NOT BEING SATISFIED.TRY  NEW CALCUL
                1ATION')
0139        310 LAM=LL
0140            LLL=0
0141            DO 330 I=1,7
0142            IF(I.NE.2) N(I)=N(I)+LAM*DEL(I)
0143        330 CONTINUE
0144            NT=NT+LAM*DELN
0145            IT=IT+1
0146            IT1=IT-1
0147        346 IF(N(1).GT.1.0E-10) GO TO 350
0148            WRITE(6,347) PR,TI,ETAA,OMEGAA,IT1
0149        347 FORMAT(I2,I5,F7.3,F7.3,I3,5X,'CARBON WILL NOT BE PRESENT')
0150            GO TO  800
                C     NOW CHECKING FOR CONVERGENCE                                             *
0151        350 IF(IT1.EQ.1) GO TO 400
0152            CHECK=.TRUE.
0153            DO 360 I=1,7
0154            IF(I.EQ.2) GO TO 360
0155             IF (DABS((N(I)-PN(I))/N(I)).GT.DELTA) CHECK=.FALSE.
0156        360 CONTINUE
0157            IF(CHECK) GO TO 510
0158        400 LAMH=LAM
0159            DO 450 I=1,7
0160            IF (I.EQ.2) GO TO  450
0161            PN(I)=N(I)
0162            DELH(I)=DEL(I)
0163        450 CONTINUE
0164            DELNH=DELN
0165            PNT=NT
0166            IF(IT.LT.ITMAX) GO TO 130
0167            WRITE(6,495)
0168        495 FORMAT(//,2X,'ITERATIONS FAILED TO CONVERGE ')
0169        510 DO 520 I=2,7
0170        520 MF(I )=N(I)/NT
                C     CALCULATION OF MINIMUM FREE ENERGY OF THE SYSTEM                         *
0171            GRTM=0.
0172            DO 521 I=2,7
0173            IF((ETAA.EQ.0.0).AND.(I.EQ.2)) GO TO 521
0174            GRTM=GRTM+N(I)*(C(I)+DLOG(N(I)/NT))
0175        521 CONTINUE
                C     TABULATE RESULTS FOR ONLY 9 CHOSEN O/H RATIOS                            *
0176             IF((IO.EQ.2).OR.(IO.EQ.4).OR.(IO.EQ.6).OR.(IO.EQ.8).OR.(IO.EQ.11)
               *.OR.(IO.EQ.13).OR.(IO.EQ.15).OR.(IO.EQ.18).OR.(IO.EQ.20))GO TO 525
```

```
0177              GO TO 730
0178        525   IF((IO   .NE.11).OR.(ITEMP.NE.7)) GO TO 575
0179              WRITE(6,535) ITABLE
0180        535   FORMAT('1',//,30X,'TABLE-',I2,' CONTINUED',//
                 * ,T10,'T, K',3X,'O/H',7X,'N2'
                 *,7X,'H2',7X,'CO',6X,'CH4',6X,'H2O',6X,'CO2')
0181        575   IF(IE.NE.1) GO TO 599
0182              IF(IO   .NE.2) GO TO 590
0183              WRITE(6,580) TI,OMEGAA,(MF(I),I=2,7)
0184        580   FORMAT(9X,I4,1X,F5.2,6X,F3.1,5(1X,F8.5))
0185              GO TO 730
0186        590   WRITE(6,595)    OMEGAA,(MF(I),I=2,7)
0187        595   FORMAT(14X,F5.2,6X,F3.1,5(1X,F8.5))
0188              GO TO 730
0189        599   IF(IO   .NE.2) GO TO 700
0190        600   WRITE(6,601) TI,OMEGAA,(MF(I),I=2,7)
0191        601   FORMAT(9X,I4,1X,F5.2,6(1X,F8.5))
0192              GO TO 730
0193        700   WRITE(6,701)    OMEGAA,(MF(I),I=2,7)
0194        701   FORMAT(14X,F5.2,6(1X,F8.5))
              C     PLOTTING ONLY FOR CHOSEN 6 TEMPERATURES                                    *
0195        730   IF(    ((T(ITEMP)-T (2))/200.-(T(ITEMP)-T (2))/200).GT.1E-2) GO TO
                 *800
              C     GAS PHASE CARBON AND OXYGEN PERCENTAGES FOR PLOTTING ON TRIANGULAR GRAPH *
0196        740   CTOH=(B(1)-N(1))/B(2)
0197              PERC=100*CTOH/(1+CTOH+OMEGAA)
0198              PERO=100*OMEGAA   /(1+CTOH+OMEGAA)
0199        555   XXIS(IO)=(PERO+PERC/2.) *0.065
0200              YXIS(IO)=DSQRT(3.D0)*PERC/2.*0.065
0201              IF(IO.EQ.1) CALL PLOT (XXIS(IO),YXIS(IO),3)
0202              IF(IO.NE.1) CALL PLOT (XXIS(IO),YXIS(IO),2)
0203        800   CONTINUE
0204              DO 805 IX =1,23
0205              IF(IX.EQ.1) CALL PLOT (XXIS(IX),YXIS(IX),3)
0206        805   IF(IX.NE.1) CALL PLOT (XXIS(IX),YXIS(IX),2)
0207        950   CONTINUE
0208        1000  CONTINUE
0209              CALL PLOT(0.,0.,999)
0210              STOP
0211              END
```

```
0001            SUBROUTINE DETSIM(E,X,N)
                C   PROGRAM TO SOLVE LINEAR EQUATIONS BY THE DETERMINANT METHOD--CRAMER'S   *
                C   RULE. VALUE OF A DETERMINANT IS FOUND BY ELIMINATION,THAT IS REDUCING   *
                C   THE DETERMINANT TO ANOTHER DETERMINANT HAVING ONLY DIAGONAL TERMS,BY    *
                C   USE OF DETERMINANT PROPERTIES. THIS MAKES THE DETERMINANT METHOD        *
                C   EFFICIENT IN COMPUTATION.                                               *
0002            IMPLICIT REAL*8(A-H,O-Z)
0003            DIMENSION E(3,4),X(3),DET (5),A(4,4)
                C   N+1 DETERMINANTS NEEDED TO BE EVALUATED FOR N EQUATIONS                *
0004            N1=N+1
0005            DO 100 II=1,N1
0006            IF(II.EQ.N1) GO TO 60
0007            DO 13 J=1,N
0008        13  A(J,II)=E(J,N1)
0009            DO 20 J=1,N
0010            DO 20 K=1,N
0011            IF(K.NE.II) A(J,K)=E(J,K)
0012        20  CONTINUE
0013            GO TO 100
0014        60  DO 70 J=1,N
0015            DO 70 K=1,N
0016        70   A(J,K)=E(J,K)
                C   MATRIX IS STORED FOR IITH DETERMINANT                                 *
0017        100 DET(II)=1.0
0018            NM1=N-1
0019            DO 160 I=1,NM1
0020            IP1=I+1
                C   SET UP THE SEARCH FOR THE LARGEST ELEMENT BELOW A(I,I)                 *
0021            ATOP=DABS(A(I,I))
0022            IPRIME=I
                C   START THE SEARCH                                                       *
0023            DO 110 IP=IP1,N
0024            IF(DABS(A(IP,I)).LE.ATOP) GO TO 110
                C   REMEMBER THIS ELEMENT FOUND TO BE BIGGER                               *
0025            ATOP=DABS(A(IP,I))
0026            IPRIME=IP
0027        110 CONTINUE
                C   SEARCH IS OVER.IPRIME IS THE PIVOT ROW.IS IPRIME EQUAL TO I?           *
0028            IF(IPRIME.EQ.I) GO TO 115
                C   NO.HENCE INTERCHANGE ROWS I & IPRIME.                                  *
0029            DO 112 J=1,N
0030            TEMP=A(IPRIME,J)
0031            A(IPRIME,J)=A(I,J)
0032            A(I,J)=TEMP
0033        112 CONTINUE
                C   PIVOTING DONE.NOW PROCEED AS BEFORE.                                  *
0034        115 DO 140 K=IP1,N
0035            FACTOR=A(K,I)/A(I,I)
0036            A(K,I)=0.0
0037            DO 120 J=IP1,N
0038            A(K,J)=A(K,J)-FACTOR*A(I,J)
0039        120 CONTINUE
0040        140 CONTINUE
                C   STEP NUMBER I FINISHED.                                              *
0041            DET(II)=DET(II)*A(I,I)
0042            IF(IPRIME.NE.I) DET(II)=-DET(II)
0043        160 CONTINUE
                C   NOW MULTIPLY BY THE LAST DIAGONAL ELEMENT.                            *
```

```
0044                DET(II)=DET(II)*A(N,N)
0045          190   CONTINUE
              C     ALL N+1 DETERMINANTS FOUND.NOW THE SOLUTION FOR EQUATIONS..      *
0046                DO 200 I=1,N
0047          200   X(I)=DET(I)/DET(N1)
0048                RETURN
0049                END
```

```
0001            SUBROUTINE TRIANG(IRHO,ETA,IFIG)
                C     THIS SUBROUTINE PREPARES THE TRIANGULAR GRAPH GRIDS AND PRINTS THE       *
                C     TITLE WITH PARAMETER VALUES                                              *
0002            REAL LX(21),LY(21),LAX,LAY
0003            DATA IFIRST/1/,SIDELN/6.5/,C60/.5/,S60/.8660254/,C120/-.5/
0004            DATA S120/.8660254/
0005            DATA HTIT/.1050/,HHCO/.105/,HATOM/.105/,HNUMB/.105/
0006            DATA DHCO/.15/,DATOM/.4/,DNUMB/.2/
0007            DIMENSION BUFF(4000),RX(21),RY(21),BX(21),BY(21)
0008            IF (IFIRST.NE.1) GO TO 10
0009            CALL PLOTS(BUFF,4000)
0010            CALL PLOT(0.,-11.,23)
0011            CALL PLOT(1.,1.50,23)
0012            CALL CYMBOL
0013            DO 5 I=1,21
0014            R=SIDELN*.05*(I-1)
0015            LX(I)=R*C60
0016            LY(I)=R*S60
0017            RX(I)=R*C120+SIDELN
0018            RY(I)=R*S120
0019            BX(I)=R
0020            BY(I)=0.0
0021          5 CONTINUE
0022            IFIRST=0
0023            GO TO 20
0024         10 CALL PLOT(11.,0.,-3)
0025            CALL PLOT(0.,-11.,23)
0026            CALL PLOT(0.,1.5,23)
0027         20 DO 30 I=1,20,2
0028            CALL PLOT(LX(I),LY(I),3)
0029            CALL PLOT(RX(I),RY(I),2)
0030            CALL PLOT(RX(I+1),RY(I+1),3)
0031            CALL PLOT(LX(I+1),LY(I+1),2)
0032         30 CONTINUE
0033            DO 40 I=1,20,2
0034            CALL PLOT(LX(22-I),LY(22-I),3)
0035            CALL PLOT(BX(22-I),BY(22-I),2)
0036            CALL PLOT(BX(21-I),BY(21-I),3)
0037            CALL PLOT(LX(21-I),LY(21-I),2)
0038         40 CONTINUE
0039            DO 50 I=1,20,2
0040            CALL PLOT(BX(I),BY(I),3)
0041            CALL PLOT(RX(22-I),RY(22-I),2)
0042            CALL PLOT(RX(21-I),RY(21-I),3)
0043            CALL PLOT(BX(I+1),BY(I+1),2)
0044         50 CONTINUE
                C     NUMBER THE RIGHT SIDE                                                    *
0045            DO 100 I=3,19,2
0046            CALL POSSYM(RX(I)+DNUMB,RY(I),HNUMB,'CE',0.,2,X,Y)
0047            FNUMB=(I/2)*10
0048            CALL NUMBER(X,Y,HNUMB,FNUMB,0.,-1)
0049        100 CONTINUE
                C     NUMBER THE LEFT SIDE                                                     *
0050            DO 110 I=3,19,2
0051            CALL POSSYM(LX(22-I)-DNUMB,LY(22-I),HNUMB,'CE',0.,2,X,Y)
0052            FNUMB=I/2*10
0053            CALL NUMBER(X,Y,HNUMB,FNUMB,0.,-1)
0054        110 CONTINUE
```

```
      C     NUMBER BOTTOM                                                    *
0055        DO 120 I=3,19,2
0056        CALL POSSYM(BX(I),-DNUMB,HNUMB,'CE',0.,2,X,Y)
0057        FNUMB=(I/2)*10
0058        CALL NUMBER(X,Y,HNUMB,FNUMB,0.,-1)
0059      120 CONTINUE
0060        LAX=-.8660254*DATOM+LX(11)
0061        LAY=DATOM*.5+LY(11)
0062        RAX=DATOM*.8660254+RX(11)
0063        RAY=DATOM*.5+RY(11)
0064        CALL POSSYM(BX(21)+DHCO,0.,HHCO,'CE',0.,1,X,Y)
0065        CALL SYMBOL(X,Y,HHCO,'O',0.,1)
0066        CALL POSSYM(BX(11),-DATOM,HATOM,'CE',0.,14,X,Y)
0067        CALL SYMBOL(X,Y,HATOM,'ATOM PERCENT O',0.,14)
0068        CALL POSSYM(-DHCO,0.,HHCO,'CE',0.,1,X,Y)
0069        CALL SYMBOL(X,Y,HHCO,'H',0.,1)
0070        CALL POSSYM(LAX,LAY,HATOM,'CE',60.,14,X,Y)
0071        CALL SYMBOL(X,Y,HATOM,'ATOM PERCENT H',60.,14)
0072        CALL POSSYM(LX(21),LY(21)+DHCO,HHCO,'CE',0.,1,X,Y)
0073        CALL SYMBOL(X,Y,HHCO,'C',0.,1)
0074        CALL POSSYM(RAX,RAY,HATOM,'CE',-60.,14,X,Y)
0075        CALL SYMBOL(X,Y,HATOM,'ATOM PERCENT C',-60.,14)
0076        X=-.25
0077        Y=LY(21)-HTIT
0078        CALL SYMBOL(X,Y,HTIT,'FIGURE ',0.,7)
0079        FFIG=IFIG
0080        CALL NUMBER(999.,999.,HTIT,FFIG,0.,-1)
0081        CALL SYMBOL(999.,999.,HTIT,' CARBON',0.,7)
0082        Y=Y-2*HTIT
0083        CALL SYMBOL(X,Y,HTIT,'DEPOSITION BOUNDARIES',0.,21)
0084        Y=Y-2*HTIT
0085        CALL SYMBOL(X,Y,HTIT,'FOR THE CHOI SYSTEM',0.,19)
0086        Y=Y-2*HTIT
0087        CALL SYMBOL(X,Y,HTIT,'AT ',0.,3)
0088        FNUMB=IRHO
0089        CALL NUMBER(999.,999.,HTIT,FNUMB,0.,-1)
      C     THE MIDDLE CHAR BETWEEN  THE COMMA AND THE EQUAL SIGN ON THE     *
      C     FOLLOWING SYMBOL CALL IS AN ETA MULTIPLE PUNCH 0-5-8-9   SEE THE *
      C     EXPANDED CHARACTER SET INVOKED BY CYMBOL IN THE PLOTTER GUIDE    *
0090        CALL SYMBOL(999.,999.,HTIT,' ATM,   = ',0.,9)
0091        CALL NUMBER(999.,999.,HTIT,ETA,0.,3)
0092        CALL SYMBOL(999.,999.,HTIT,',',0.,1)
0093        Y=Y-2*HTIT
0094        CALL SYMBOL(X,Y,HTIT,'T AS A PARAMETER,DEG K',0.,22)
0095        RETURN
0096        END
```

INPUT DATA

COEFFICIENT MATRIX (a_{ji})

	C	N_2	H_2	CO	CH_4	H_2O	CO_2
C	1	0	0	1	1	0	1
H	0	0	2	0	4	2	0
O	0	0	0	1	0	1	2

PRESSURE ARRAY (P, atm.)

1 5 10 15 25

ETA ARRAY

0.0 1.00 2.00 3.00 3.76 5.00 10.00 20.00 40.00

TEMPERATURE ARRAY (T, ^{o}K)

298 500 600 700 800 900 1000 1100 1200 1300 1400 1500

OMEGA ARRAY

0.001 0.010 0.025 0.050 0.075 0.100 0.220 0.300
0.350 0.425 0.500 0.625 0.750 0.825 1.000 1.500
2.0 4.0 8.0 10.0 25.0 100.0 1000.0

LOG OF EQBM CONST OF FORMATION ARRAY ($\log_{10} K_i^f$)

C	N_2	H_2	CO	CH_4	H_2O	CO_2	T, ^{o}K
0.0	0.0	0.0	24.04778	8.89850	40.04724	69.09124	298
0.0	0.0	0.0	16.25296	3.42730	22.88604	41.25831	500
0.0	0.0	0.0	14.33598	2.00040	18.63268	34.40082	600
0.0	0.0	0.0	12.96488	0.95290	15.58329	29.50278	700
0.0	0.0	0.0	11.93188	0.15000	13.28854	25.82659	800
0.0	0.0	0.0	11.12555	-0.48810	11.49733	22.96647	900
0.0	0.0	0.0	10.47761	-1.00750	10.05973	20.67680	1000
0.0	0.0	0.0	9.94451	-1.43450	8.88088	18.80244	1100
0.0	0.0	0.0	9.49779	-1.79360	7.89633	17.23996	1200
0.0	0.0	0.0	9.11764	-2.10060	7.06060	15.91649	1300
0.0	0.0	0.0	8.78999	-2.36380	6.34355	14.78164	1400
0.0	0.0	0.0	8.50442	-2.59230	5.72047	13.79867	1500

APPENDIX B

CHOICE OF REFERENCE STATE FOR FREE ENERGY DATA

In the optimization problem for obtaining the equilibrium state of a general system referred to in the third chapter, the free energy function, G, to be minimized is given by

$$g = \frac{G}{RT} = \sum_{i=1}^{s} d_i \, n_i + \sum_{i=s+1}^{c} n_i \left(c_i + \ln \frac{n_i}{n} \right)$$

or

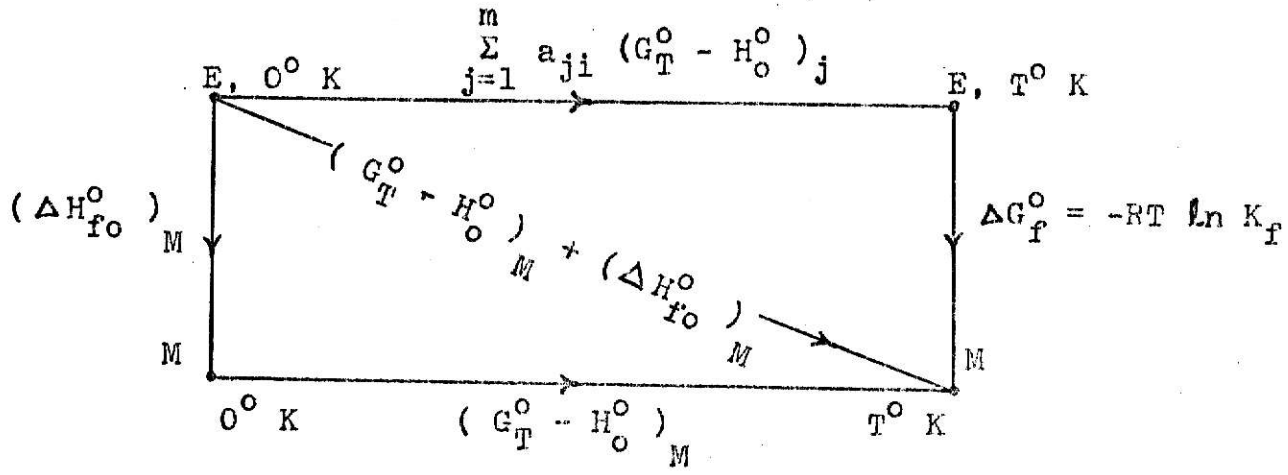
$$G = \sum_{i=1}^{c} \mu_i^o \, n_i + RT \sum_{i=s+1}^{c} n_i \left(\ln f_i + \ln \frac{n_i}{n} \right) \qquad \text{(B-1)}$$

subject to atomic balance constraints

$$\sum_{i=1}^{c} a_{ji} \, n_i = b_j \quad ; \quad 1 \le j \le m \qquad \text{(B-2)}$$

The solution of the problem is obtained by modifying the objective function by including constraint equations with Lagrangian multipliers and setting the partial derivatives equal to zero for each specie. The question here is what data should be used for μ_i^o, since we can never determine an absolute value of it. The two commonly presented and used forms of data are referred to the elements in their standard states at 0° K and T° K, the temperature of the system of concern.

Let E and M represent the elemental and molecular species, respectively. Different kinds of data can be related by use of Hess' law illustrated below:



The superscript ^{o} refers to the standard state and the subscript $_o$ to 0^o K. At absolute zero temperature ,

$$U_o = H_o = G_o = A_o \qquad \text{for every E or M}$$

and for every elemental specie

$$\Delta H_{fo}^o = \Delta H_o^o = \Delta G_o^o = 0$$

It can be easily seen from the diagram that, for any molecular specie, M, at T,

$$\Delta G_f^o = \left[\left(G_T^o - H_o^o \right) + \Delta H_{fo}^o \right] - \sum_{j=1}^{m} a_{ji} G_{Tj}^o$$

The subscript T shall be removed for simplicity of notation, then

$$\Delta G_f^o = \left[\left(G^o - H_o^o \right) + \Delta H_{fo}^o \right] - \sum_{j=1}^{m} a_{ji} G_j^o \qquad \text{(B-3)}$$

Let

$$\mu_i^o = \Delta G_{fi}^o \qquad 1 \leq i \leq c \qquad \text{(B-4)}$$

And, let μ_{io}^o be the free energy referred to the elements at 0^o K.

Then,

$$\mu_i^o = \mu_{io}^o - \sum_{j=1}^{m} a_{ji} G_j^o$$

or,

$$\mu_{io}^o = \mu_i^o + \sum_{j=1}^{m} a_{ji} G_j^o \quad ; \quad 1 \leq i \leq c \tag{B-5}$$

Then, we can compare the expressions for the objective function G and G_o. Using equations (B-1) and (B-5) :

$$G_o = \sum_{i=1}^{c} \mu_{io}^o n_i + RT \sum_{i=s+1}^{c} n_i \left(\ln f_i + \ln \frac{n_i}{n} \right) \tag{B-6}$$

Subtracting (B-1) from this:

$$G_o - G = \sum_{i=1}^{c} \left(\mu_{io}^o - \mu_i^o \right) n_i$$

Using (B-5), it becomes

$$G_o - G = \sum_{i=1}^{c} \left(\sum_{j=1}^{m} a_{ji} G_j^o \right) n_i$$

$$= \sum_{j=1}^{m} \left(\sum_{i=1}^{c} a_{ji} n_i \right) G_i^o$$

and, now using mass balance constraints (B-2)

$$G_o - G = \sum_{j=1}^{m} b_j G_j^o \tag{B-7}$$

For a given problem of minimizing free energy, G, b_j is constant for each j, and G_j^o depends upon the temperature, T. Therefore, $(G_o - G)$ is independent of mole numbers n_i, or

$$\frac{\partial G_o}{\partial n_i} = \frac{\partial G}{\partial n_i} \qquad \text{(B-8)}$$

Therefore, the choice of temperature of elements to which free energy data are referred does not influence the state of equilibrium of a system, though it changes the magnitude or the free energy of the system.

NOMENCLATURE

A_i - Abbreviation for $(c_i + \ln \frac{n_i}{n})$.

a_{ji} - Number of atoms or j-th element in one molecule of i-th component.

B_i - Abbreviation for $n_i A_i$.

b_j - Total number of atoms of j-th element in a system.

C - Number of components, in the sense of phase rule.

c - Number of components (that is, species) present in the system.

c_i - Abbreviation for $(\mu^o + RT \ln f)$ for i-th species in the gas-phase.

d_i - Abbreviation for μ_i^o, for i-th specie in the condensed phase.

E - To represent elements.

F - Number of degrees of freedom, in the section (2.2).

- Abbreviation for $\left(g + \sum_{j=1}^{m} \pi_j \left(b_j - \sum_{i=1}^{c} a_{ji}\, n_i\right)\right)$

f_i - Fugacity of pure i-th species, at total system pressure, P, and temperature, T.

$\hat{f}_i$ - Fugacity of i-th species in the gas mixture.

G, G_o - Total Gibbs free energy of the system with respect to elements in their standard states, taken to be at the system temperature, T^o K, and at 0^o K respectively.

G_j^o - Free energy of formation of j-th element in the standard state, at the system temperature, T^o K.

ΔG_{fi}^o - Standard free energy of formation of i-th specie with reference state being at the system temperature, T^o K.

ΔH_f^o - Standard enthalpy change of formation at T^o K.

K_1 - Equilibrium constant for the reaction $C + 2H_2 = CH_4$.

K_2 - Equilibrium constant for the reaction $C + CO_2 = 2CO$.

K_f - Equilibrium constant of formation of any general compound $C_\alpha H_\beta O_\gamma N_\theta$

K_i^f - Equilibrium constant of formation of i-th species at T^o K.

M - Representing molecular species.

m - Number of atomic species, reactive atomic species.

N - Number of components in the system, in the section (2.2).

N_o - Total number of moles in the gas-phase when there are no inerts.

n - Total number of moles in the gas-phase.

n_i - Number of moles of i-th species.

P - Number of phases, in Section (2.2).

- Pressure of the system, atm.

P_o - Pressure of the system without inerts, atm.

p_i - Partial pressure of i-th species in the gas-phase, atm.

R - Number of independent reactions, in Section (2.2).

- Gas constant.

r_{jl} - Abbreviation for $\sum_i a_{ji}\, a_{li}\, n_i$ for all reactive components i, in the gas-phase.

S - Number of additional restrictions, in Section (2.2).

s - Number of solid species in the system.

T - Temperature of the system, ^oK.

v_s - Specific volume of solid.

y - Mole fraction of CO or H_2.

y_i - Mole fraction of i-th species = n_i/n.

Greek

Δ - Abbreviation for ($n^{\nu+1} - n^{\nu}$), increase in total mole numbers, as calculated by the method of steepest descent.

Δ_i - Abbreviation for increase in mole number of i-th specie = ($n_i^{\nu+1} - n_i^{\nu}$), as calculated by the method of steepest descent.

δ - Specified limit of relative change in mole number, for convergence criterion.

- Error allowed in following mass balance equation.

η - Atomic ratio of inert to oxygen in the system = $2n_2/b_3$, for CHON system.

λ - Fraction of calculated travel, by the method of steepest descent, so that mole numbers are positive and free energy is not increasing.

μ_i - Chemical potential of i-th specie.

μ_i^o, μ_{io}^o - Chemical potential of i-th specie at T^o K, in standard state, referred to elements at T^o K and 0^o K respectively.

π_j - Lagrangian multiplier associated with atomic balance for j-th element.

ω - Atomic ratio, O/H in the system = b_3/b_2.

Subscripts

i, l - For i-th or l-th species in the system; $l \leq i$, $l \leq c$.

j - For atomic species; $l \leq j \leq m$.

α, β, γ and θ - Formula coefficients for any general specie, $C_\alpha H_\beta O_\gamma N_\theta$, in the CHON system.

o - State at 0^o K.

Superscripts

o - To denote standard state.

ν, $\nu+1$ - Number of iteration.

LITERATURE CITED

1. Amundson, N.R., Mathematical Methods in Chemical Engineering - Matrices and their application, pp. 50-54, Prentice Hall Inc. (1966).

2. Balzhiser, R.E., Samuels, M.R., and Eliassen, J.D., Chemical Engineering Thermodynamics, Prentice Hall Inc. (1972).

3. Baron, R.E., Porter, J.H., and Hammond, O.C., Jr., Chemical Equilibria in Carbon-Hydrogen-Oxygen systems, MIT Press (1976).

4. Cairns, E.J. and Tevebaugh, A.D., J. Chem. & Eng. Data 9, No. 3, 453 (1964).

5. Chen, T.C., Global Optimization and Synthesis of Industrial and Process Systems, Ph.D. Dissertation, Kansas State University (1977).

6. Deming, W.E. and Deming, L.E., Phys. Rev. 56, 108 (1939).

7. Deming, W.E. and Shupe, L.E., Phys. Rev. 37, 638 (1931).

8. Ibid., 38, 2245 (1931).

9. Ibid., 40, 848 (1932).

10. Denbigh, K.G., The Principles of Chemical Equilibrium, pp. 184-88, 3rd Ed., Cambridge University Press (1971).

11. White, W.B., Johnson, S.M., and Dantzig, G.B., J. Chem. Phys. 28, 751 (1958).

12. Zwolinski, B.J. et al., "Selected Values of Properties of Hydrocarbons and Related Compounds", American Petroleum Institute Research, Project 44, Carnegie Institute of Technology, Pittsburgh, PA. (1960).

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EQUILIBRIUM GAS-PHASE COMPOSITIONS AND CARBON DEPOSITION BOUNDARIES IN THE CHO-INERT SYSTEM

by

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requirements for the degree

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ABSTRACT

The general technique of free energy minimization has been applied to heterogeneous complex chemical equilibrium calculation. This technique, with the method of steepest descent, has been used to calculate gas-phase compositions in equilibrium with solid carbon over the complete composition range for the system comprised of the elements carbon, hydrogen, oxygen, and nitrogen. The calculations, executed on IBM 370/158 computer with double precision, cover a range of temperatures from 500 to 1500° K, pressures from 1 to 25 atm, O/H elemental ratios from 0.001 to 1000, and N/O elemental ratios from 0 to 20. Also, carbon deposition boundaries are presented on triangular coordinates in terms of atom per cent of the elements C, H, and O.

Under the conditions studied, nitrogen can be considered inert and the species of major interest are C, CO, CO_2, H_2, H_2O, CH_4, and N_2. While the calculations were made with nitrogen as inert, these results can be applied to systems containing C, H, and O plus any inert substances. The effect of gas-phase nonideality was studied and found to be negligible. The carbon deposition boundaries shift significantly by change of pressure and amount of inert at intermediate temperatures, around 1000° K, but the effect is found to be small at low as well as at high temperatures.

Because of the wide range of variables studied this work should be useful for design purposes, for CHOI systems, where the question of carbon deposition is important, or where gas-phase compositions in equilibrium with solid carbon are needed.