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AN ANALYSIS OF THE CSNI GREST CORE CONCRETE INTERACTION CHEMICAL THERMODYNAMIC BENCHMARK EXERCISE USING THE MPEC2 COMPUTER CODE

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An Analysis of the CSNI/GREST Core Concrete Interaction Chemical Thermodynamic Benchmark Exercise Using the MPEC2 Computer Code

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Fission product (FP) release during a core concrete interaction (CCI) is an important factor of the uncertainty associated with a source term estimation for an LWR severe accident. An analysis was made on the CCI Chemical Thermodynamic Benchmark Exercise organized by OECD/NEA/CSNI Group of Experts on Source Terms (GREST) for investigating the uncertainty in thermodynamic modeling for CCI.

The benchmark exercise was to calculate the equilibrium FP vapor pressure for given systems of temperature, pressure, and debris composition. The benchmark consisted of two parts, A and B. Part A was a simplified problem intended to test the numerical techniques. In Part B, the participants were requested to use their own best estimate thermodynamic data base to examine the variability of the results due to the difference in thermodynamic data base.

JAERI participated in this benchmark exercise with use of the MPEC2 code. Chemical thermodynamic data base needed for analysis of Part B was taken from the VENESA code.

This report describes the computer code used, inputs to the code, and results from the calculation by JAERI.

The present calculation indicates that the FP vapor pressure depends strongly on temperature and Oxygen potential in core debris and the pattern of dependency may be different for different FP elements.

Keywords: CSNI/GREST, MPEC2, Fission Product, Core-Concrete Interaction, Source Term, LWR, Severe Accident, VANESA

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MPEC 2コードによるCSNI/GREST炉心－コンクリート反応化学熱力学ベンチマーク問題の解析

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（1988年12月5日受理）

軽水炉のシビアアクシデント時ソースタームを評価する上で，炉心―コンクリート反応（CCI）によるFPの放出は，重要な不確実さ要因となっている。そこで，OECD/NEA/CSNIのソースターム専門家グループ（GREST）がCCI解析モデルに伴う不確実さについて検討するために実施しているCCI化学熱力学ベンチマーク問題の解析を行なった。

このベンチマーク問題は，与えられた温度，圧力，デブリ組成に対するFPの平衡蒸気圧を求めるものであり，Part A，Part Bの2部からなる。Part Aは，解析コードの数値解法の相違の影響をみるために単純化した問題であり，Part Bでは，解析に使用する熱力学データの相違による解析結果への影響を調べるために，各解析者は夫々最良と判断する熱力学データを用いることを要求されている。

原研では，MPEC 2を用いてこのベンチマーク計算に参加した。熱力学データとしては，VANESAコードの内蔵データを用いた。

本報告書は，原研が行なった計算のモデル，入力データ，及び計算結果について記述したものである。

解析の結果，FPの平衡蒸気圧は，炉心デブリの温度と酸素ポテンシャルによって大きく変化し，その変化の傾向は，元素により異なることが示唆された。

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1. Introduction

One of the largest uncertainties associated with the estimation of fission product source terms of an LWR severe accident is the release of radionuclides from molten core interaction with concrete in the containment following reactor vessel melt-through. In estimating the release of radioactive aerosols from core concrete interaction (CCI), the analysis of chemical reactions among the constituents of the core debris and concrete plays an important role of determining (1) the chemical forms of fission products, (2) the vapor pressure of chemical species that contain the important fission products, and (3) the chemical reaction heat source in the core debris.

Considering the importance of the chemical analysis, the OECD/NEA (Organization for Economic Cooperation and Development / Nuclear Energy Agency) CSNI/GREST (Committee on the Safety of Nuclear Installations / Group of Experts on Source Terms) has proposed an international cooperative benchmark exercise[1] on the chemical thermodynamic modeling, aiming at establishing the magnitude of the uncertainties associated with the chemical thermodynamic inputs and assessing their significance in relation to the other uncertainty contributors to the overall aerosol release calculation. Proposed benchmark consisted of two parts, Part A and Part B. Part A was a simplified standard problem intended to test the numerical solution techniques involved in defining chemical equilibrium in the codes. Part B was designed to investigate the uncertainties resulting from variability in chemical thermodynamic modeling for core-concrete melts of more realistic composition.

An analysis of this benchmark problem was performed at the Japan Atomic Energy Research Institute (JAERI) using the MPEC2 code[2], which is the second version of MPEC[3] and was developed by Uchida as part of a computer code HORN[4] for analysis of chemical and physical behavior of fission products in an LWR reactor coolant system. The objective for JAERI to perform this analysis was to investigate the uncertainties associated with CCI calculations as well as to contribute to the verification of its computer codes developed for the source term analysis.

The chemical thermodynamic data base needed for the analysis of Part B were taken from the VANESA code[5]. Since VANESA is being used for a source term analysis at JAERI as part of the Source Term Code Package (STCP)[6], it is important for JAERI to assess the uncertainty associated with the data used in VANESA.

This report describes the benchmark problem (section 2), computer code used for the analysis (section 3), input and results of the calculations for Part A (section 4) and Part B (section 5).

2. Specification of Benchmark Exercise

2.1 Aims of the Benchmark Exercise

The benchmark problem consisted of two parts, Part A and Part B. The specific aims of two parts were as follows.

Part A was a simplified standard problem intended to test the numerical solution techniques involved in defining chemical equilibrium in the codes. The aim was to check how well the minimization routines in different codes converge to the same equilibrium for the minor species of main concern in the presence of large excesses of other materials. For this purpose, a limited composition had been chosen, and the chemical speciation and thermodynamic data base are fully specified as input. The output required was the number of moles of each input vapor species present in equilibrium with the condensed phases.

Part B was designed to investigate the uncertainties resulting from variability in chemical thermodynamic treatments for core-concrete melts of more realistic composition. Three melt compositions had been specified, intended to cover the key variables of oxygen potential in the melt, and composition (limestone or basaltic) of the concrete. Two temperatures were specified for each melt. Participants were entirely free to choose their own best estimate approach to both the chemical speciation and the thermodynamic data employed in calculating the equilibria. The output required includes both the equilibrium vapor-phase composition and the thermodynamic basis of the calculations.

In the following two sections, the problems are presented as specified by the organizer of the CSNI/GREST CCI benchmark.

2.2 Benchmark Part A

Input

(1) Specification of the system

The system consists of a gas phase, a liquid oxide solution phase, and a liquid metal solution phase, all in equilibrium.

This report describes the benchmark problem (section 2), computer code used for the analysis (section 3), input and results of the calculations for Part A (section 4) and Part B (section 5).

2. Specification of Benchmark Exercise

2.1 Aims of the Benchmark Exercise

The benchmark problem consisted of two parts, Part A and Part B. The specific aims of two parts were as follows.

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Part B was designed to investigate the uncertainties resulting from variability in chemical thermodynamic treatments for core-concrete melts of more realistic composition. Three melt compositions had been specified, intended to cover the key variables of oxygen potential in the melt, and composition (limestone or basaltic) of the concrete. Two temperatures were specified for each melt. Participants were entirely free to choose their own best estimate approach to both the chemical speciation and the thermodynamic data employed in calculating the equilibria. The output required includes both the equilibrium vapor-phase composition and the thermodynamic basis of the calculations.

In the following two sections, the problems are presented as specified by the organizer of the CSNI/GREST CCI benchmark.

2.2 Benchmark Part A

Input

(1) Specification of the system

The system consists of a gas phase, a liquid oxide solution phase, and a liquid metal solution phase, all in equilibrium.

The components in each phase are as follows:

Gas : O_2, UO_2, UO_3, UOH, H_2, H_2O, Zr, Cr, La, LaO, K, KOH
Oxide solution : UO_2, $U_2O_{4.5}$, ZrO_2, Cr_2O_3, K_2O
Metal solution : U, Zr, Cr, La, K

(2) Thermodynamic data

Expressions for the Gibbs free energy of formation are in the form,

$$\Delta G_0 = A + B \times T \qquad (2.1)$$

where T is in Kelvin. The Gibbs free energies of formation of all elements in their normal physical form at 298.15K are taken to be Zero.

The values for the coefficients A and B for the species are:

Species	A	B
O_2 (g)	0.0	0.0
UO_2 (g)	-5.083560E+5	2.280E+1
UO_3 (g)	-8.368000E+5	8.117E+1
UOH (g)	2.493900E+4	-2.619E+0
H_2 (g)	0.0	0.0
H_2O (g)	-2.464376E+5	5.481E+1
Zr (g)	6.095980E+5	-1.320E+2
Cr (g)	3.794340E+5	-1.318E+2
La (g)	4.208690E+5	-1.142E+2
LaO (g)	-1.477080E+5	-5.272E+1
K (g)	6.886400E+4	-6.976E+1
KOH (g)	-2.40284E+5	1.074E+1
UO_2 (o)	-1.080000E+6	1.690E+2
$U_2O_{4.5}$ (o)	-2.250000E+6	3.914E+2
ZrO_2 (o)	-1.098000E+6	1.940E+2
Cr_2O_3 (o)	-1.120776E+6	2.534E+2
La_2O_3 (o)	-1.790049E+6	2.820E+2
K_2O (o)	-4.547004E+5	2.254E+2
U (m)	0.0	0.0
Zr (m)	0.0	0.0
Cr (m)	0.0	0.0
La (m)	0.0	0.0
K (m)	0.0	0.0

(3) Input amounts in moles

H_2O (g)	5.0E+4
UO_2 (o)	3.0E+5
La_2O_3 (o)	1.0E+2
K_2O (o)	1.5E+4
Zr (m)	1.0E+5
Cr (m)	5.0E+5

(4) Conditions and representation of the melt

The temperature of the system is constant at 2500K and the gas pressure is 1 atmosphere.

The oxide and metal solutions are treated as ideal solutions. The final equilibrium composition that is calculated is such that the gas phase is in equilibrium with the oxide and metal solutions.

Output

The output required is the number of moles of each input vapor species in equilibrium with the melt.

2.3 Benchmark Part B

This is based on three test cases A, B and C of more realistic composition. Participants should use their own chemical thermodynamic data and choice of species in all phases.

Input

(1) In each Case, the system consists of a gas phase, a liquid oxide solution phase, and a liquid metal solution phase, all in equilibrium. The initial components in each phase are as follows:

Gas phase : H_2O, CO_2
Oxide solution : UO_2, SiO_2, SrO, CaO, La_2O_3, CeO_2
Metal solution : Zr, Fe, Mo

The methods adopted to define the final equilibrium in terms of permissible species in each phase, activity coefficients, etc. are entirely at the choice of the participant.

(2) Input amounts

The initial compositions in the three Cases are defined in the following Table:

Components	Amount (moles) Case A 'reducing'	Case B 'not as reducing'	Case C 'CaO/SiO =10'
UO_2	10^5	10^5	10^5
Zr	10^5	10^4	10^4
SiO_2	10^4	10^5	10^4
Fe	10^5	10^5	10^5
SrO	10^2	10^2	10^2
CaO	10^4	10^5	10^5
La_2O_3	10^2	10^2	10^2
CeO_2	10^3	10^3	10^3
Mo	10^2	10^2	10^2
H_2O	10^2	10^2	10^2
CO_2	10^2	10^2	10^2

(3) Conditions

For each Case, the final state should be calculated for the three phases in equilibrium at fixed temperatures of 2000 K and 2500 K in a static system at 1 atmosphere total pressure.

Output

The following should be specified in the output information:

(1) Number of moles of each element in the gas phase at equilibrium.

(2) A complete listing of the final composition of each phase by the species included in the calculation, together with the Gibbs free energies of formation employed. The latter may be supplied in the form of point values at the two temperatures of the calculation, in algorithmic temperature-dependent form, or as an abstract of the data block in the code employed.

3. MPEC2 Code

3.1 Outline of the MPEC2 Code

MPEC2 is FORTRAN-77 code that calculates complex multi-phase chemical equilibria by minimization of total free energy under either constant-pressure or constant-volume conditions. The code was originally developed for use as a subroutine of a larger code HORN[3] which simulates the fission product transport in the primary system during a severe accident in an LWR. Since a transient analysis requires a large number of chemical equilibrium calculations special efforts were made for achieving computational efficiency without losing numerical stability. Main features of the code are:

(1) use of logarithm of gram-moles as independent variable,
(2) initial estimate of composition by the Simplex method,
(3) use of imaginary elements, which contributes particularly to reducing the running time in problems in which many phases are postulated.

3.2 Theory

Here we consider a system consisting of an ideal gas mixture, ideal condensed solutions, and condensed pure phases whole total number is M, consisting altogether of N compounds. Although MPEC2 allows non-ideal solutions as far as the activity coefficients can be treated as constants, the present discussion assumes ideal gas and ideal solutions.

The total Gibbs free energy is given by

$$G_{tot} = \sum_{i}^{N} x_i\{G_i^0 + RT\ln(a_i)\} \tag{3.1}$$

where x_i represents the gram-moles of species i; G_i^0 is the standard partial molar free energy of species i; R is the gas constant, T is temperature; a_i is activity. The usual problem is to determine values of x_i for a given set of gram-atoms of constituent elements, and for a given set of chemical species together with their G_i^0 values. Hence the x_i values must satisfy the conservation constraints for a total of L elements or independent constituents:

$$\sum_{i}^{N} A_{ij}x_i = b_j \quad (j=1, \ldots L) \tag{3.2}$$

where A_{ij} is the stoichiometric coefficient, and b_j is the total number of gram-atoms of element j.

The equilibrium composition in terms of x_i is determined as that which makes the total free energy G_{tot} a minimum. Here the discussion is limited to the constant-pressure problem; modification to the constant-volume case is easy. Minimizing G_{tot} under the constraint equation (3.2) is achieved by applying Lagrange's multipliers to (3.2). By differentiating (3.1) with x_i and applying Lagrange's multipliers to (3.2), the conditions for the equilibrium composition may be written for each species.

For an ideal gaseous mixture, using $g_i^0 = G_i^0/RT$,

$$\sum_{i}^{N} A_{ij}\pi j - [g_i^0 + \ln(P) + \ln(x_i/X_l)] = 0 \qquad (3.3)$$

For a species in a condensed ideal solution m,

$$\sum_{i}^{N} A_{ij}\pi j - [g_i^0 + \ln(x_i/X_m)] = 0 \qquad (3.4)$$

For a species forming a pure phase,

$$\sum_{j}^{L} A_{ij}\pi j - g_i^0 = 0 \qquad (3.5)$$

where πj is Lagrange's multiplier; P is total pressure (atm); X_m is gram-moles of all species that belong to mixture m. Mixture 1 is assigned to the gas phase here. Finally equations are written for the composition of each mixture.

$$X_m = \Sigma\, x_i \text{ (for all i that belong to m).} \qquad (3.6)$$

Equations (3.2) - (3.6) constitute (L+M+N) simultaneous equations whose unknowns are πj, x_i and X_m. By solving above equations, an equilibrium composition can be obtained.

3.3 Numerical Method

The usual procedure for solving equations (3.2) - (3.6) is to expand $\ln(x_i)$ and $\ln(X_m)$ in a Taylor series and to take the first-order terms in order to linearize equations (3.3) and (3.4). In MPEC2, however, $\ln(x_i)$

and $\ln(X_m)$ are adopted as independent variables:

$$z_i = \ln(x_i) \quad \text{and} \quad W_m = \ln(X_m) \tag{3.7}$$

and x_i (=exp(z_i)) and X_m (=exp(W_m)) are expanded in Taylor's series of z_i and W_m around the initial estimates. Then equations (3.2) and (3.6) are transformed into

$$\sum_i A_{ij} x_{i0} z_i = \sum_i A_{ij} x_i \quad (Z_{i0}-1) + b_j \tag{3.8}$$

and

$$\sum_i x_{i0} z_i - X_{m0} W_m = \sum_i x_{i0} z_{i0} - X_{m0} W_{m0} \tag{3.9}$$

where x_{i0}, z_{i0}, X_{m0}, W_{m0}, are the initial (or previous-step) values of x_i, z_i, X_m, and W_m, respectively, and hence are known quantities.

On the other hand, free energy equations (3.3) and (3.4) are linearized and can be solved for z_i. In equation (3.4), for example,

$$z_i = \sum_j^L A_{ij} \pi j + W_m - g_i^0 \tag{3.10}$$

Inserting (3.10) and the corresponding equation obtained from (3.3) into (3.8) and (3.9), we finally have (L+M) equations (3.5), (3.8) and (3.9) with (L+M) unknowns πj and W_m (=z_i for pure phase). These simultaneous equations are solved by the Gauss' elimination method. The interative use of the solutions as initial values in the next step constitutes a Newton-Raphson process.

The principal advantages of using the logarithms as independent variables is that the non-negative condition for gram-mole values is automatically satisfied by this transformation. The second advantage is that a small increment of z_i results in a large jump of x_i, hence fast convergence. This advantage, however, can easily result in a disadvantage in that the iterative process may become unstable. To avoid instability, the size of increments of z_i needs to be restricted, particularly for principal species and in early steps.

4. Analysis of Benchmark Part A

4.1 Input for Part A

Input to MPEC2 for Part A analysis was made from information given in section 2.2. Since specification for Part A included a complete description of the system, there was no arbitrary choice for the participant to make, except for a parameter CONV for numerical error control.

The parameter CONV is used to judge the convergence of iteration by the following criteria.

$$ABS(\ln(x_i) - \ln(x_i^{old})) < CONV \qquad (4.1)$$

where the superscript 'old' denotes the value obtained in the preceding iteration. The given value for CONV was 0.1, which was the default value in MPEC. This value does not need to be very small because the species that becomes critical in convergence judgment is usually the species of least amount. A complete listing of the input and output for Part A is given in Appendix A.

4.2 Results from Analysis of Part A

The required output is the number of moles of each input vapor species and is given in Table 4.1 and Fig. 4.1. A complete listing of output for Part A is included in Appendix A.

4.3 Sensitivity Analysis and Discussion on Part A

Part A was aimed at examining the uncertainty associated with numerical solution techniques. The basic equations solved by MPEC2, which have been described in section 3.2, are based on fundamental laws of thermodynamics and should be common to computer codes that solve the thermodynamic equilibrium. Therefore, if the iterative calculations to solve the basic equations, described in section 3.3, are performed until a sufficient degree of convergence is obtained, the results of the calculation should be identical to those of other codes.

In order to examine the effect of convergence requirement, a sensitivity analysis was made. In MPEC2 the convergence of the iterative process is judged by Eq. (4.1) using an input variable CONV. MPEC2 was

run for five different values of CONV, 1.0, 0.1, 0.01, 0.001, and 0.0001, where 0.1 was used for the base case calculation shown in section 4.2. The calculated number of moles of each species are shown in Table 4.2 together with the number of iterations needed for convergence.

In this table the results for CONV=0.1 and CONV=0.01 are identical because the same number of iterations (5) was needed for both CONV=0.1 and CONV=0.01. Only 6 iterations were needed to obtain the convergence for CONV=0.001 which corresponds to a relative error of 0.1%. Considering that the convergence was obtained very quickly and the relative difference between the results for CONV=0.1 and CONV=0.001 is less than 1% for each species in Table 4.2, the results for CONV=0.1 seems to have reached to the exact solution within an error of 1% or less. It was impossible to obtain a solution for CONV=0.0001. The reason for this was attributed to the effect of rounding error.

5. Analysis of Benchmark Part B

5.1 Input for Part B

The benchmark specification in section 2.3 included following information.

- phases existing in the system (gas, oxide solution, and metal solution phases),
- initial amount of materials,
- pressure,
- temperature.

The participants were requested to use their best estimate data for:

- chemical species existing in each phase,
- Gibbs free energy of formation for each species,
- activity coefficients and fugacity coefficients.

In the present analysis, the chemical thermodynamic data used in the VANESA code[4], which was included in the USNRC Source Term Code Package (STCP)[5], was used for this purpose.

Following information were taken from VANESA.

run for five different values of CONV, 1.0, 0.1, 0.01, 0.001, and 0.0001, where 0.1 was used for the base case calculation shown in section 4.2. The calculated number of moles of each species are shown in Table 4.2 together with the number of iterations needed for convergence.

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5. Analysis of Benchmark Part B

5.1 Input for Part B

The benchmark specification in section 2.3 included following information.

- phases existing in the system (gas, oxide solution, and metal solution phases),
- initial amount of materials,
- pressure,
- temperature.

The participants were requested to use their best estimate data for:

- chemical species existing in each phase,
- Gibbs free energy of formation for each species,
- activity coefficients and fugacity coefficients.

In the present analysis, the chemical thermodynamic data used in the VANESA code[4], which was included in the USNRC Source Term Code Package (STCP)[5], was used for this purpose.

Following information were taken from VANESA.

(1) Species in each phase

The elements involved in the system are O, H, C, U, Si, Sr, Ca, La, Ce, Zr, Fe, and Mo. VANESA considers 62 chemical forms for above elements, which are shown in Table 5.1.

(2) Gibbs free energy of formation

In VANESA, the Gibbs free energy of formation is calculated as a linear function of temperature as

$$\Delta G_0 = A + B \times T \qquad (5.1)$$

where ΔG_0 is in cal/mol and T is in Kelvin. The values of constants A and B are stored as DATA statements for variable BARR in FORTRAN program of VANESA, which was received from USNRC as a part of STCP Mod 1.1. The values of A and B taken from VANESA are shown in Table 5.2.

(3) Activity constants and fugacity constants

In VANESA, nearly all constituents of the metallic and oxidic phases are treated as ideal. The only exceptions and Na_2O and K_2O, which are not involved in the present benchmark. Therefore all the activity coefficients were assumed to be one in the present analysis. VANESA also assumes that the gas species are all ideal and the fugacity coefficients are one.

A complete listing of input and output for Part B is shown in Appendix B.

5.2 Results from Analysis of Part B

The requested results are the number of moles of each element in the gas phase at equilibrium and a complete listing of final composition of each phase, which are shown in Tables 5.3 and 5.4, respectively. A graphical presentation of the results is given in Fig. 5.1.

A complete listing of the output from analysis of Part B is given in Appendix B.

5.3 Discussion of Part B

Part B was aimed at investigating the uncertainty associated with thermodynamic data base. The thermodynamic data used in the present

calculation was taken from the VANESA code, for which an extensive discussion on thermodynamic data base is given in reference (4).

Although the comparison of calculations with different data base can not be made in this report, it would be useful to summarize the qualitative insights that can be gained from the present analysis.

Before discussing the results of the present analysis, it should be pointed out that the number of moles in the gas phase calculated by the present analysis is not proportional to the FP release rate in a severe accident. The FP release is influenced not only by chemical equilibrium but also by mass transfer and other rate processes. Therefore the calculated vapor pressure is not more than a indicator of driving force for release of FP.

(1) Characteristic behavior of FP elements

In Table 5.4 it should be noted that the most volatile form (the species that is most abundant in gas phase) of FP elements Mo, Sr, La, and Ce are Mo, Sr, LaO, and CeO. These are common to Cases A, B, and C at both 2000 K and 2500 K.

The number of moles in gas phase of these species are shown in Table 5.5. This table indicates the following:

- Amount of Mo in the gas phase is always much less than other three elements.
- At 2000 K, the number of moles in the gas phase are in the order of

  Sr > CeO > LaO > Mo

  for all cases. This is, however, not the case at 2500 K, where the order is

  CeO > Sr > LaO for Case A ('reducing'),
  LaO > Sr > CeO for Case B ('not as reducing'),
  Sr > CeO > LaO for Case C ('CaO/SiO_2=10').

  Therefore the relative volatility of FP elements can be significantly changed by both temperature and oxygen potential and the effect of oxygen potential becomes more significant at a higher temperature.

(2) Effect of temperature

The rate of FP release is generally believed to increase with the temperature. The results of present analysis indicate that this is true for most cases but there may be some exceptions. In Case B the number of moles of Sr in gas phase at 2000 K is 1.58, which is about three times larger than the value for 2500 K, 0.49.

(3) Effect of oxygen potential

Cases A, B, and C are characterized as 'reducing', 'not as reducing' and 'CaO/SiO_2=10', which means that the oxygen potential is in the order of

Case B > Case C > Case A.

The actual values of oxygen potential for each case, defined as

$$\mu_{O2} = RT(\ln P_{O2}) \ , \qquad (5.2)$$

is shown in Table 5.6.

The comparison of results for these three cases gives an insight for the effect of oxygen potential. In Table 5.5 it is indicated that Sr, La, and Ce have the same pattern of dependency on oxygen potential. For these elements, the number of moles in the gas phase is in the order of

Case A > Case C > Case B.

These elements seem to become more volatile in reducing condition. However Mo has a different tendency. The number of moles of Mo in the gas phase is in the order of

Case B > Case C > Case A.

Above observations are qualitatively explained as follows.

The amount of each element in gas phase is, in principle, determined by the relative stability of the species in gas phase and the species in condensed phase.

For most elements in the present cases, the gas-phase species are simple substances and the condensed species are oxides. For such elements, the stability of each oxide becomes the controlling parameter. Considering the condition that the oxygen potential in the present cases are not fixed but are dependent on stability of each oxides, the essential parameter is the relative stability of oxides of each element.

As temperature goes higher, oxides generally become less stable than simple substances and release oxigen. Therefore the oxigen partial

pressure becomes higher at a higher temperature. However the degree of unstabilization is different between elements and the oxides of some elements, such as Sr and Ba, do not become so unstable as oxides of other elements. Therefore the oxides of such elements can be even stabilized by the oxigen released from oxides of other elements at a higher temperature. Therefore the number of moles of Sr in the gas phase in Case B become higher at 2500 K than at 2000 K.

The behavior of Mo is different. Mo has very high boiling point temperature (4800°C) and the oxide form of high vapor pressure is limited to MoO_3 which is stable only at very high oxygen potential. In the present cases, the oxygen potential is not high enough to make MoO_3 stable. Therefore the amount of Mo in the gas phase is very low for all cases.

In summary, the present calculation indicates that the equilibrium number of moles of FP elements in the gas phase is strongly dependent on temperature and oxygen potential in the core debris and the pattern of dependency may be different for different FP elements.

6. Conclusion

An analysis of the CSNI/GREST Chemical Thermodynamic Benchmark was made at JAERI using the MPEC2 computer code with the use of chemical thermodynamic data in the VANESA code. The computer code used, the input, and the results of the analysis have been presented. The present calculation indicated that the equilibrium number of moles of FP elements in the gas phase is strongly dependent on temperature and oxygen potential in the core debris and the pattern of dependency may be different for different FP elements.

The results of the present analysis will be compared with the analyses using other computer codes and data base by the CSNI/GREST member countries.

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The results of the present analysis will be compared with the analyses using other computer codes and data base by the CSNI/GREST member countries.

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1) Powers, D.A., "Submission for the CSNI/GREST Benchmark Exercise on Chemical Thermodynamic Modeling in Core-Concrete Interaction Releases of Radionuclides," NUREG/CR-5196, SAND88-1920.

2) Uchida, M., "MPEC2: A Code for Multi-Phase Chemical Equilibria," Comput. Chem. Vol. 11, No. 1, pp. 19-24, 1987.

3) Uchida, M., "MPEC: Multi-Phase Equilibrium Chemical Code by Free Energy Minimization Method," JAERI-M 84-143, 1984.

4) Uchida, M., "HORN: A Computer Code to Analyze the Gas-Phase Transport of Fission Products in Reactor Cooling System under Severe Accidents," JAERI-M 86-158, 1986.

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6) Gieseke J. A., et al., "Source Term Code Package: A User's Guide (Mod 1)," NUREG/CR-4587, 1986.

Table 4.1 Calculated number of moles of species in gas, metal, and oxide phases

Gas Phase

O2(G)	3.0118E-08
UO2(G)	3.5081E+00
UO3(G)	1.3505E-02
UOH(G)	6.9720E-04
H2(G)	4.9993E+04
H2O(G)	5.7192E+00
ZR(G)	9.4717E-03
CR(G)	6.8078E+03
LA(G)	1.7352E-02
LAO(G)	4.7655E+00
K(G)	2.8817E+04
KOH(G)	2.3419E+00

Oxide Phase

UO2(O)	2.7550E+05
U2O45(O)	2.1692E+01
ZRO2(O)	5.6996E+04
CR2O3(O)	8.0494E-04
LA2O3(O)	5.9338E+01
K2O(O)	4.6531E-09

Metal Phase

U(M)	2.4451E+04
ZR(M)	4.3003E+04
CR(M)	4.9319E+05
LA(M)	7.6536E+01
K(M)	1.1811E+03

Table 4.2 Sensitivity of calculated number of moles to the convergence parameter CONV

Species	CONV				
	1.0	0.1	0.01	0.001	0.0001
	Number of moles				
O2(G)	3.0143E-08	3.0118E-08	3.0118E-08	3.0120E-08	
UO2(G)	3.5147E+00	3.5081E+00	3.5081E+00	3.5081E+00	
UO3(G)	1.3524E-02	1.3505E-02	1.3505E-02	1.3506E-02	
UOH(G)	6.9822E-04	6.9720E-04	6.9720E-04	6.9717E-04	
H2(G)	4.9993E+04	4.9993E+04	4.9993E+04	4.9993E+04	N/C
H2O(G)	5.7162E+00	5.7192E+00	5.7192E+00	5.7194E+00	
ZR(G)	9.4989E-03	9.4717E-03	9.4717E-03	9.4713E-03	
CR(G)	6.8221E+03	6.8078E+03	6.8078E+03	6.8079E+03	
LA(G)	1.7401E-02	1.7352E-02	1.7352E-02	1.7351E-02	
LAO(G)	4.7764E+00	4.7655E+00	4.7655E+00	4.7654E+00	
K(G)	2.8972E+04	2.8817E+04	2.8817E+04	2.8816E+04	
KOH(G)	2.3511E+00	2.3419E+00	2.3419E+00	2.3420E+00	
UO2(O)	2.7551E+05	2.7550E+05	2.7550E+05	2.7550E+05	
U2O45(O)	2.1687E+01	2.1692E+01	2.1692E+01	2.1692E+01	
ZRO2(O)	5.6994E+04	5.6996E+04	5.6996E+04	5.6998E+04	
CR2O3(O)	8.0408E-04	8.0494E-04	8.0494E-04	8.0504E-04	
LA2O3(O)	5.9358E+01	5.9338E+01	5.9338E+01	5.9339E+01	
K2O(O)	4.6835E-09	4.6531E-09	4.6531E-09	4.6533E-09	
U(M)	2.4470E+04	2.4451E+04	2.4451E+04	2.4449E+04	
ZR(M)	4.3035E+04	4.3003E+04	4.3003E+04	4.3001E+04	
CR(M)	4.9318E+05	4.9319E+05	4.9319E+05	4.9319E+05	
LA(M)	7.6588E+01	7.6536E+01	7.6536E+01	7.6532E+01	
K(M)	1.1850E+03	1.1811E+03	1.1811E+03	1.1811E+03	
Number of iterations needed	4	5	5	6	—

N/C : Convergence was not reached.

Table 5.1 Chemical species considered in the present analysis (based on reference 4, Table 56)

Gas Phase (52 species)

H,	OH,	O,	O_2,	CO_2,	CO,	H_2O,	H_2,
Fe,	FeO,	FeOH,	$Fe(OH)_2$,				
Mo,	MoO,	MoO_2,	MoO_3,	$MoO_2(OH)_2$,	$(MoO_3)_2$,	$(MoO_3)_3$,	
Ca,	CaO,	CaOH,	$Ca(OH)_2$,				
Si,	SiO,	SiO_2,	SiOH,	$Si(OH)_2$,			
U,	UO,	UO_2,	UO_3,	$UO_2(OH)_2$,			
Zr,	ZrO,	ZrO_2,	ZrOH,	$Zr(OH)_2$,			
Sr,	SrO,	SrOH,	$Sr(OH)_2$,				
La,	LaO,	LaOH,	$La(OH)_2$,				
Ce,	CeO,	CeO_2,	CeOH,	$Ce(OH)_2$,	$(CeO)_2$		

Oxide Phase (8 species)

FeO,
CaO,
SiO_2,
UO_2,
ZrO_2,
SrO,
La_2O_3,
CeO_2.

Metal Phase (3 species)

Fe,
Mo,
Zr.

Table 5.2 Parameters for calculation of Gibbs free energy of formation, taken from VENESA (reference 4)

Species	A	B	Species	A	B
Gas Phase			**Gas Phase (Continued)**		
H	227474.7	-60.3301	LA	405856.6	-112.0618
OH	369828.4	-13.6243	LAO	-150515.4	-65.5988
O	362870.7	-133.9805	LAOH	-91451.0	-5.4470
O2	0.0	0.0	LA(OH)2	-660396.5	106.9057
CO2	-395375.4	-0.5234	CE	403327.0	-105.0108
CO	-114033.7	-85.5949	CEO	-169665.9	-25.3469
FE	373116.3	-119.8137	CEOH	-104644.9	11.1394
FEO	200081.3	-68.9679	CE(OH)2	-560918.1	113.6239
FEOH	76346.2	-15.3028	CEO2	0.0	0.0
FE(OH)2	-358328.6	102.7143	(CEO)2	0.0	0.0
MO	641250.2	-138.1321	H2O	-252053.7	58.2296
MOO	365570.4	-86.7421	H2	0.0	0.0
MOO2	-32389.7	-26.0239			
MOO3	-369560.4	63.5297			
MOO2(OH2	-856305.2	209.9412			
(MOO3)2	-572461.1	148.6599	**Oxide Phase**		
(MOO3)3	-652717.9	184.1623			
CA	0.0	0.0	FEO(L)	-254098.5	**52.8420**
CAO	-129326.1	35.9236	CAO(L)	-687974.9	**158.4201**
CAOH	-349212.6	78.5473	SIO2(L)	-929720.7	189.1358
CA(OH)2	-760548.9	188.6878	UO2(L)	-933112.1	122.5321
SI	395028.2	-113.2433	ZRO2(L)	-1017459.4	159.4476
SIO	-162614.9	-46.6569	SRO(L)	-640530.1	149.9929
SIO2	-359269.2	30.6646	LA2O3(L)	-1777233.0	271.8740
SIOH	-9438.3	-3.5211	CEO2(L)	-1086935.0	212.2707
SI(OH)2	-526150.9	141.5432			
U	497157.4	-112.1183			
UO	-21771.4	-49.4042	**Metal Phase**		
UO2	-495160.2	11.7230			
UO3	-834291.1	78.7118	FE(L)	0.0	0.0
UO2(OH)2	-1272129.0	229.9977	MO(L)	0.0	0.0
ZR	600324.3	-127.8879	ZR(L)	0.0	0.0
ZRO	34716.9	-62.5177			
ZRO2	-321346.6	-0.1884			
ZROH	-194866.2	87.5008			
ZR(OH)2	-500820.8	114.8271			
SR	0.0	0.0			
SRO	-168518.7	33.9856			
SROH	-362179.9	82.9958			
SR(OH)2	-742947.6	182.8204			

Note: Gibbs free energy of formation is calculated as $\Delta G_0 = A + B * T$, where ΔG_0 is in J/mol and T is in Kelvin. A unit conversion has been made to the original values of A and B in VANESA from cal/mol and cal/mol.K to J/mol and J/mol.K.

Table 5.3 Number of moles of each element in gas phase

Element	Case A		Case B		Case C	
	2000K	2500K	2000K	2500K	2000K	2500K
H	2.000E+2	2.000E+2	2.000E+2	2.000E+2	2.000E+2	2.000E+2
C	1.000E+2	1.000E+2	1.000E+2	1.000E+2	1.000E+2	1.000E+2
O	8.594E+3	9.759E+3	1.946E+4	2.515E+4	6.277E+3	9.600E+3
Fe	1.634E+0	2.291E+2	6.485E+0	7.594E+2	2.544E+0	5.432E+2
Mo	1.476E-9	5.211E-6	5.859E-9	1.836E-5	2.298E-9	1.240E-5
Ca	7.017E+2	4.520E+3	2.543E+2	1.368E+2	1.735E+3	8.481E+3
Si	8.805E+3	9.953E+3	1.939E+4	2.505E+4	6.288E+3	9.580E+3
U	8.851E-2	1.671E+1	1.724E-2	3.923E+0	2.367E-2	5.124E+0
Zr	2.492E-4	3.363E-1	1.634E-5	1.266E-3	4.804E-5	4.442E-2
Sr	3.219E+1	7.452E+1	1.578E+0	4.884E-1	1.000E+1	2.480E+1
La	3.420E-2	1.536E+1	8.909E-3	8.549E-1	1.510E-2	5.896E+0
Ce	1.171E+1	1.698E+2	3.604E-2	3.039E-1	2.573E-1	2.053E+1

Table 5.4 Number of moles of species in gas, oxide, and metal phases calculated for Benchmark Part B

	Case A (2000K)	Case A (2500K)	Case B (2000K)	Case B (2500K)	Case C (2000K)	Case C (2500K)
Gas Phase						
H	1.5987E+00	2.8586E+01	2.2784E+00	3.6434E+01	1.4704E+00	3.1532E+01
OH	2.5239E-16	1.4294E-11	8.6870E-15	7.3881E-09	4.7199E-16	9.8159E-11
O	7.3217E-09	5.1242E-04	3.6040E-07	3.5808E-01	1.2585E-08	3.9646E-03
O2	4.9723E-16	2.5356E-10	5.9111E-13	7.1853E-05	1.7378E-15	1.2213E-08
CO2	1.8081E-05	3.5113E-04	4.3669E-04	1.4219E-01	3.6764E-05	2.1858E-03
CO	9.9998E+01	9.9999E+01	9.9999E+01	9.9857E+01	9.9999E+01	9.9996E+01
FE	1.6338E+00	2.2905E+02	6.4853E+00	7.5936E+02	2.5437E+00	5.4316E+02
FEO	2.6907E-08	2.6938E-04	2.5794E-06	3.6216E-01	8.5174E-08	3.9768E-03
FEOH	7.2793E-09	1.2252E-05	4.8794E-07	1.2184E-02	2.5069E-08	1.6053E-04
FE(OH)2	2.5484E-14	9.8111E-11	2.8848E-11	2.9262E-05	1.9414E-13	7.1024E-09
MO	1.4758E-09	5.2106E-06	5.8590E-09	1.8364E-05	2.2977E-09	1.2402E-05
MOO	1.0895E-14	7.9964E-10	1.0446E-12	1.1428E-06	3.4489E-14	1.1848E-08
MOO2	4.0828E-17	1.4319E-11	9.4542E-14	8.2985E-06	2.6279E-16	1.3208E-09
MOO3	1.2354E-22	4.2999E-16	6.9088E-18	1.0105E-07	1.6167E-21	2.4691E-13
MOO2(OH2	1.4546E-19	8.0576E-16	3.9774E-15	1.0360E-07	2.2531E-18	3.6447E-13
(MOO3)2	0.0	0.0	0.0	9.6000E-24	0.0	0.0
(MOO3)3	0.0	0.0	0.0	0.0	0.0	0.0
CA	7.0168E+02	4.5203E+03	2.5428E+02	1.3675E+02	1.7352E+03	8.4809E+03
CAO	5.0211E-06	3.9072E-03	4.3945E-05	4.7934E-02	2.5246E-05	4.5635E-02
CAOH	1.6597E-03	6.8332E-02	1.0157E-02	6.2004E-01	9.0784E-03	7.0833E-01
CA(OH)2	3.6826E-09	4.5913E-07	3.8057E-07	1.2496E-03	4.4559E-08	2.6296E-05
SI	3.1092E+02	4.9420E+02	2.9349E+01	3.2269E+00	1.1120E+02	7.9733E+01
SIO	8.4945E+03	9.4586E+03	1.9365E+04	2.5046E+04	6.1768E+03	9.5001E+03
SIO2	2.3986E-05	1.4358E-03	1.3206E-03	1.5418E+00	3.5463E-05	8.9776E-03
SIOH	4.8003E-04	2.5094E-03	7.6518E-04	4.9146E-03	3.7974E-04	2.2369E-03
SI(OH)2	9.0163E-09	4.0202E-08	2.4270E-07	2.3615E-05	1.5778E-08	1.9800E-07
U	1.3297E-02	1.9045E+00	1.8599E-05	7.8213E-06	1.5302E-03	3.4478E-02
UO	5.6446E-02	9.0213E+00	1.9069E-03	1.5024E-02	1.3208E-02	1.0167E+00
UO2	1.8767E-02	5.7867E+00	1.5311E-02	3.9080E+00	8.9287E-03	4.0598E+00
UO3	9.6314E-07	2.8788E-03	1.8978E-05	7.8842E-01	9.3171E-07	1.2573E-02
UO2(OH)2	7.5360E-15	3.6913E-11	1.7534E-12	2.2427E-06	1.7544E-14	7.9058E-10
ZR	4.7889E-06	1.0044E-02	1.3241E-08	5.3426E-08	4.5752E-07	2.1589E-04
ZRO	2.4444E-04	3.2635E-01	1.6322E-05	7.0397E-04	4.7482E-05	4.3669E-02
ZRO2	6.0798E-08	6.4189E-04	9.8047E-08	5.6149E-04	2.4013E-08	5.3469E-04
ZROH	3.5694E-07	2.2439E-05	1.6666E-08	3.5802E-08	7.5433E-08	2.6649E-06
ZR(OH)2	2.9629E-11	2.0026E-08	2.3362E-11	9.5833E-09	1.3851E-11	1.3141E-08
SR	3.2193E+01	7.4516E+01	1.5783E+00	4.8456E-01	1.0001E+01	2.4800E+01
SRO	3.0683E-06	5.3552E-04	3.6331E-06	1.4122E-03	1.9382E-06	1.1095E-03
SROH	9.7254E-05	1.2310E-03	8.0521E-05	2.4010E-03	6.6834E-05	2.2636E-03
SR(OH)2	1.1874E-10	6.5730E-09	1.6602E-09	3.8452E-06	1.8050E-10	6.6780E-08
LA	1.1932E-04	7.5911E-02	1.2965E-06	1.0416E-05	2.6103E-05	4.6799E-03
LAO	3.3949E-02	1.5364E+01	8.9091E-03	8.5489E-01	1.5101E-02	5.8963E+00
LAOH	7.1056E-08	4.8689E-05	1.3038E-08	2.0039E-06	3.4385E-08	1.6585E-05
LA(OH)2	1.5749E-09	4.9120E-07	4.8801E-09	6.0635E-06	1.6858E-09	9.2442E-07
CE	7.4430E-02	1.8233E+01	1.0423E-04	9.0145E-05	8.5733E-03	3.8933E-01
CEO	1.0620E+00	1.5154E+02	3.5916E-02	3.0382E-01	2.4872E-01	2.0143E+01
CEOH	2.6739E-05	6.2059E-03	6.3230E-07	9.2029E-06	6.8129E-06	7.3218E-04
CE(OH)2	2.2198E-09	9.0889E-07	8.8646E-10	4.0426E-07	1.2511E-09	5.9247E-07
CEO2	4.2331E-16	2.6569E-10	3.4575E-16	2.1602E-10	2.0158E-16	2.1987E-10
(CEO)2	3.6038E-16	2.7840E-10	2.0223E-19	6.4942E-16	2.3382E-17	3.9582E-12
H2O	7.7749E-05	1.8543E-03	1.8712E-03	7.0888E-01	1.5818E-04	1.1301E-02
H2	9.9199E+01	8.5666E+01	9.8853E+01	8.0759E+01	9.9260E+01	8.3868E+01
Oxide Phase						
FEO(L)	1.0132E-01	2.7063E+00	1.1906E+01	5.3881E+03	6.7416E-01	5.6953E+01
CAO(L)	9.2982E+03	5.4967E+03	9.9745E+04	9.9860E+04	9.8263E+04	9.1518E+04
SIO2(L)	1.1945E+03	4.7133E+01	8.0605E+04	7.4949E+04	3.7118E+03	4.2011E+02
UO2(L)	9.9999E+04	9.9982E+04	9.9999E+04	9.9995E+04	9.9998E+04	9.9994E+04
ZRO2(L)	5.0257E+03	7.7194E+03	9.9337E+03	9.9998E+03	4.1720E+03	9.1665E+03
SRO(L)	6.7815E+01	2.5482E+01	9.8421E+01	9.9510E+01	9.0036E+01	7.5262E+01
LA2O3(L)	9.9978E+01	9.2277E+01	9.9994E+01	9.9570E+01	9.9988E+01	9.7047E+01
CEO2(L)	9.9885E+02	8.3029E+02	9.9995E+02	9.9969E+02	9.9973E+02	9.7946E+02
Metal Phase						
FE(L)	9.9998E+04	9.9768E+04	9.9982E+04	9.3852E+04	9.9997E+04	9.9400E+04
MO(L)	1.0000E+02	1.0000E+02	1.0000E+02	1.0000E+02	1.0000E+02	1.0000E+02
ZR(L)	9.4974E+04	9.2280E+04	6.6142E+01	1.3928E-01	5.8279E+03	8.3335E+02

Table 5.5 Number of moles in gas phase of most volatile species of FP elements at 2000 K and 2500 K

At 2000 K

Species	Case A	Case B	Case C
Mo	1.48×10^{-9}	5.86×10^{-9}	2.30×10^{-9}
Sr	3.22×10^{1}	1.58×10^{0}	1.00×10^{1}
LaO	3.39×10^{-2}	8.91×10^{-3}	1.51×10^{-2}
CeO	1.06×10^{0}	3.59×10^{-2}	2.49×10^{-1}

At 2500 K

Species	Case A	Case B	Case C
Mo	5.21×10^{-6}	1.84×10^{-5}	1.24×10^{-5}
Sr	7.45×10^{1}	4.85×10^{-1}	2.48×10^{1}
LaO	1.53×10^{1}	8.55×10^{-1}	5.90×10^{0}
CeO	1.52×10^{2}	3.04×10^{-1}	2.01×10^{1}

Table 5.6 Oxygen potential in Cases A, B, and C

	Oxygen Potential (kJ/mole)		
Temperature	Case A	Case B	Case C
2000 K	-738.3	-632.4	-714.7
2500 K	-659.1	-409.5	-583.1

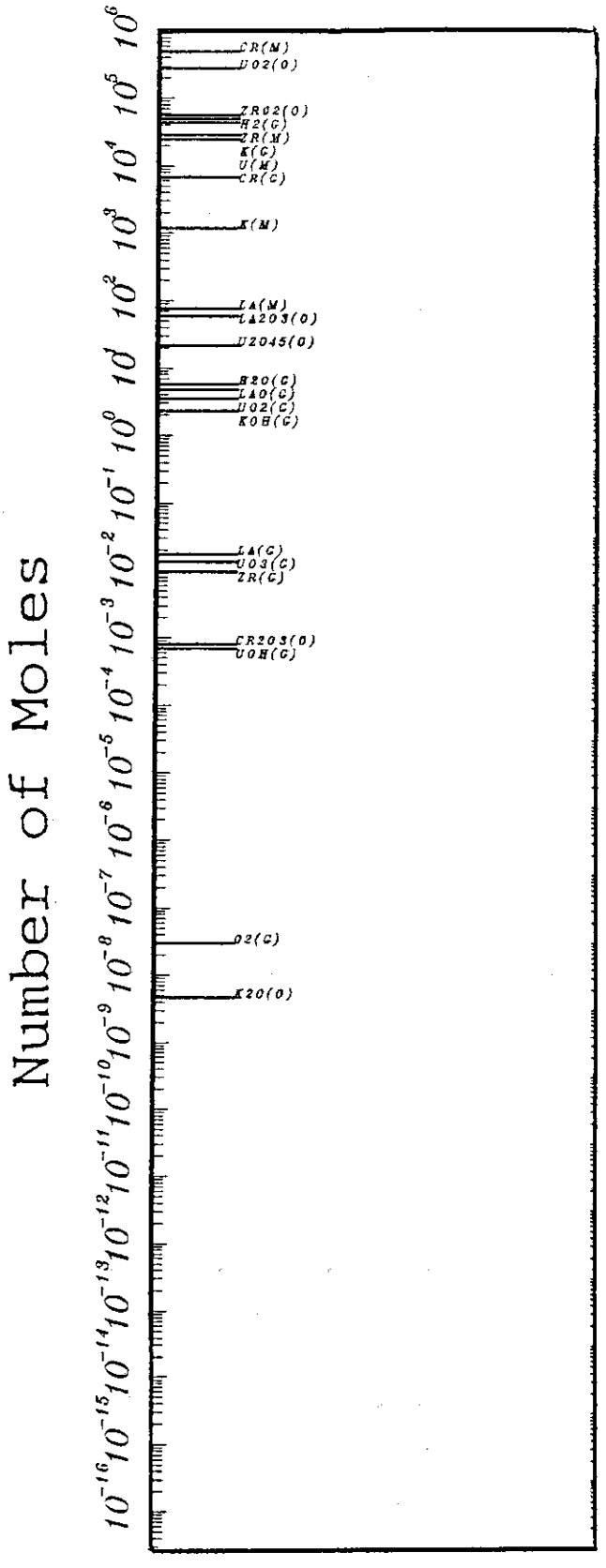

Fig. 4.1 Graphical presentation of number of moles of species calculated for Benchmark Part A

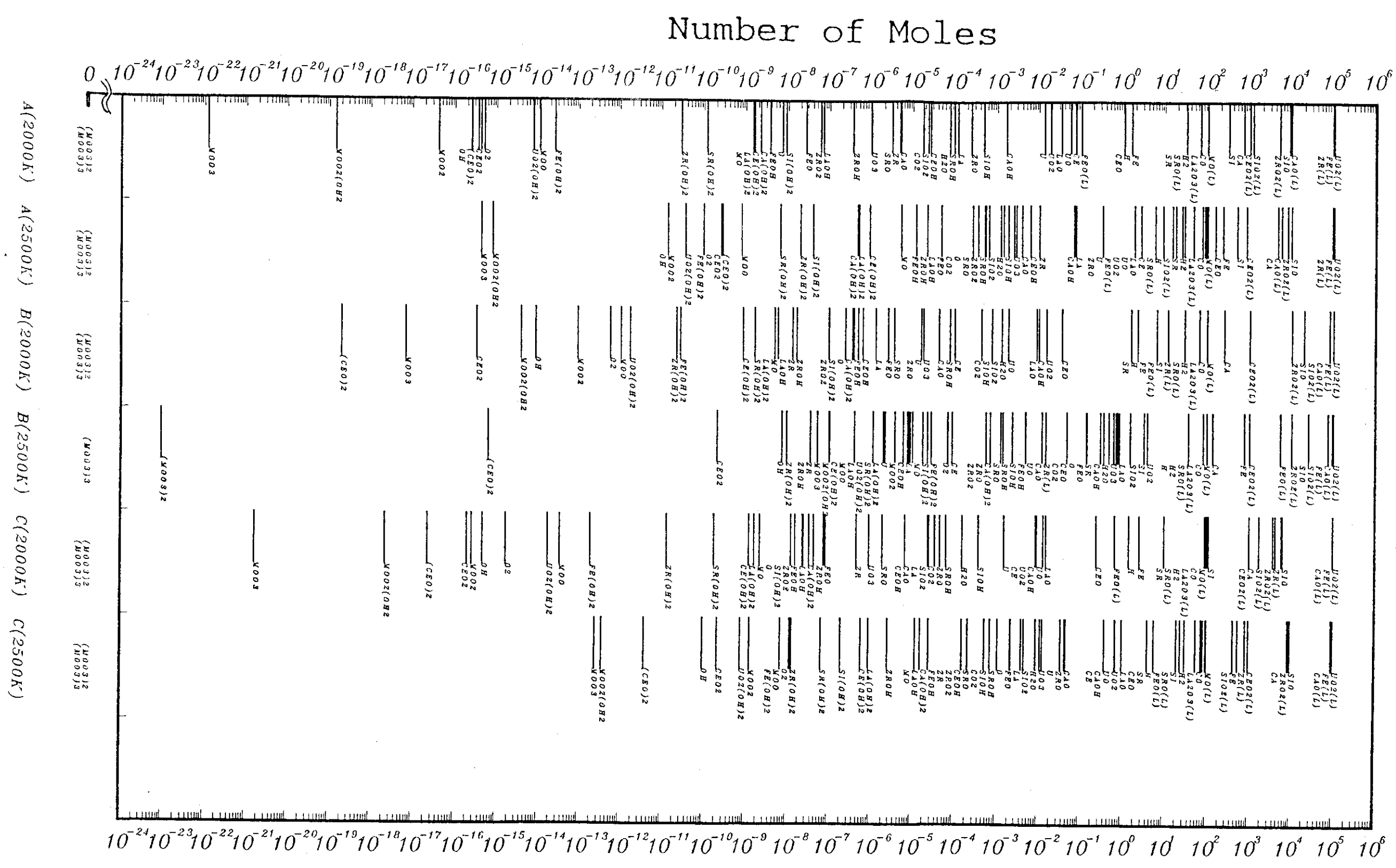

Fig. 5.1 Graphical presentation of number of moles of species calculated for Benchmark Part B

APPENDIX A

INPUT AND OUTPUT LISTING OF PART A ANALYSIS

INPUT DATA LIST

```
                1         2         3         4         5         6         7         8
CARD NO. ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
      1.  CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART A (REV.1)         00001300
      2.  &COND1  L=7, NN=23, MP=3, MR=0, ML(1)=12,6,5,                          00001400
      3.   EL(1)=1HO,1HU,1HH,2HZR,2HCR,2HLA,1HK,
      4.   IPC=1, IFEF=1, IOM=1,
      5.   TEXT(01)= 5HO2(G),
      6.   TEXT(02)= 6HUO2(G),
      7.   TEXT(03)= 6HUO3(G),
      8.   TEXT(04)= 6HUOH(G),
      9.   TEXT(05)= 5HH2(G),
     10.   TEXT(06)= 6HH2O(G),
     11.   TEXT(07)= 5HZR(G),
     12.   TEXT(08)= 5HCR(G),
     13.   TEXT(09)= 5HLA(G),
     14.   TEXT(10)= 6HLAO(G),
     15.   TEXT(11)= 4HK(G),
     16.   TEXT(12)= 6HKOH(G),
     17.   TEXT(13)= 6HUO2(O),
     18.   TEXT(14)= 8HU2O45(O),
     19.   TEXT(15)= 7HZRO2(O),
     20.   TEXT(16)= 8HCR2O3(O),
     21.   TEXT(17)= 8HLA2O3(O),
     22.   TEXT(18)= 6HK2O(O),
     23.   TEXT(19)= 4HU(M),
     24.   TEXT(20)= 5HZR(M),
     25.   TEXT(21)= 5HCR(M),
     26.   TEXT(22)= 5HLA(M),
     27.   TEXT(23)= 4HK(M),
     28.   IGT=0,1,        &END
     29. O2(G)          2
     30. UO2(G)         2    1
     31. UO3(G)         3    1
     32. UOH(G)         1    1    1
     33. H2(G)                   2
     34. H2O(G)         1        2
     35. ZR(G)                        1
     36. CR(G)                             1
     37. LA(G)                                  1
     38. LAO(G)         1                       1
     39. K(G)                                        1
     40. KOH(G)         1              1            1
     41. UO2(O)         2    1
     42. U2O45(O)     4.5    2
     43. ZRO2(O)        2              1
     44. CR2O3(O)       3                   2
     45. LA2O3(O)       3                        2
     46. K2O(O)         1                             2
     47. U(M)                 1
     48. ZR(M)                        1
     49. CR(M)                             1
     50. LA(M)                                  1
         ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
```

I N P U T   D A T A   L I S T

```
                          1         2         3         4         5         6         7         8
CARD NO.  ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
   51. K(M)                                                1
   52. O2(G)                            0.0       0.0
   53. UO2(G)                     -508356.0       22.8
   54. UO3(G)                     -836800.0       81.17
   55. UOH(G)                       24939.0       -2.619
   56. H2(G)                            0.0       0.0
   57. H2O(G)                     -246437.6       54.81
   58. ZR(G)                       609598.0     -132.0
   59. CR(G)                       379434.0     -131.8
   60. LA(G)                       420869.0     -114.2
   61. LAO(G)                     -147708.0      -52.72
   62. K(G)                         68864.0      -69.76
   63. KOH(G)                     -240284.0       10.74
   64. UO2(O)                    -1080000.       169.0
   65. U2045(O)                  -2250000.       391.4
   66. ZRO2(O)                   -1098000.       194.0
   67. CR2O3(O)                  -1120776.       253.4
   68. LA2O3(O)                  -1790049.       282.0
   69. K2O(O)                     -454700.4      225.4
   70. U(M)                             0.0       0.0
   71. ZR(M)                            0.0       0.0
   72. CR(M)                            0.0       0.0
   73. LA(M)                            0.0       0.0
   74. K(M)                             0.0       0.0
   75.  &COND2         TEMP=2500.0,
   76.  PRESS=1.0,
   77.  BB(1)=6.653E+5,
   78.  BB(2)=3.000E+5,
   79.  BB(3)=1.000E+5,
   80.  BB(4)=1.000E+5,
   81.  BB(5)=5.000E+5,
   82.  BB(6)=2.000E+2,
   83.  BB(7)=3.000E+4,
   84.  IEND=1,
   85.  MDEBUG=0,    &END
```

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART A (REV.1)

MPEC CODE CALCULATION ** FIXED CONDITIONS**
NUMBER OF ELEMENTS (L) = 7 NO. OF MIXTURE = 3 NO. OF PURE SUBSTANCES = 0
TOTAL NO. OF PHASES = 3 TOTAL NO. OF SPECIES= 23

STOICHIOMETRY COEFFICIENTS

NO.	SPECIES	MIXTURE	O	U	H	ZR	CR	LA	K
1	O2(G)	1	2.000	0.0	0.0	0.0	0.0	0.0	0.0
2	UO2(G)	1	2.000	1.000	0.0	0.0	0.0	0.0	0.0
3	UO3(G)	1	3.000	1.000	0.0	0.0	0.0	0.0	0.0
4	UOH(G)	1	1.000	1.000	1.000	0.0	0.0	0.0	0.0
5	H2(G)	1	0.0	0.0	2.000	0.0	0.0	0.0	0.0
6	H2O(G)	1	1.000	0.0	2.000	0.0	0.0	0.0	0.0
7	ZR(G)	1	0.0	0.0	0.0	1.000	0.0	0.0	0.0
8	CR(G)	1	0.0	0.0	0.0	0.0	1.000	0.0	0.0
9	LA(G)	1	0.0	0.0	0.0	0.0	0.0	1.000	0.0
10	LAO(G)	1	1.000	0.0	0.0	0.0	0.0	1.000	0.0
11	K(G)	1	0.0	0.0	0.0	0.0	0.0	0.0	1.000
12	KOH(G)	1	1.000	0.0	1.000	0.0	0.0	0.0	1.000
13	UO2(O)	2	2.000	1.000	0.0	0.0	0.0	0.0	0.0
14	U2O45(O)	2	4.500	2.000	0.0	0.0	0.0	0.0	0.0
15	ZRO2(O)	2	2.000	0.0	0.0	1.000	0.0	0.0	0.0
16	CR2O3(O)	2	3.000	0.0	0.0	0.0	2.000	0.0	0.0
17	LA2O3(O)	2	3.000	0.0	0.0	0.0	0.0	2.000	0.0
18	K2O(O)	2	1.000	0.0	0.0	0.0	0.0	0.0	2.000
19	U(M)	3	0.0	1.000	0.0	0.0	0.0	0.0	0.0
20	ZR(M)	3	0.0	0.0	0.0	1.000	0.0	0.0	0.0
21	CR(M)	3	0.0	0.0	0.0	0.0	1.000	0.0	0.0
22	LA(M)	3	0.0	0.0	0.0	0.0	0.0	1.000	0.0
23	K(M)	3	0.0	0.0	0.0	0.0	0.0	0.0	1.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART A (REV.1)

CASE 1 TEMPERATURE (K)= 2500.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 1.761E+04
INPUT GRAM-ATOMS OF ELEMENTS

O	U	H	ZR	CR	LA	K
6.653E+05	3.000E+05	1.000E+05	1.000E+05	5.000E+05	2.000E+02	3.000E+04

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	O2(G)	1	0.0	3.0136E-08	3.5175E-13	3.5175E-13
2	UO2(G)	1	-24.175	4.1381E+01	4.8300E-04	4.8300E-04
3	UO3(G)	1	-30.486	1.3512E-02	1.5772E-07	1.5772E-07
4	UOH(G)	1	0.885	6.9732E-04	8.1390E-09	8.1390E-09
5	H2(G)	1	0.0	4.9993E+04	5.8352E-01	5.8352E-01
6	H2O(G)	1	-5.262	5.7195E+00	6.6758E-05	6.6758E-05
7	ZR(G)	1	13.447	9.4765E-03	1.1061E-07	1.1061E-07
8	CR(G)	1	2.402	6.8113E+03	7.9500E-02	7.9500E-02
9	LA(G)	1	6.511	1.7360E-02	2.0263E-07	2.0263E-07
10	LAO(G)	1	-13.443	4.7680E+00	5.5651E-05	5.5651E-05
11	K(G)	1	-5.076	2.8817E+04	3.3635E-01	3.3635E-01
12	KOH(G)	1	-10.265	2.3415E+00	2.7330E-05	2.7330E-05
13	UO2(O)	2	-31.622	2.7547E+05	8.2836E-01	0.0
14	U2O5(O)	2	-61.153	2.1690E+01	6.5223E-05	0.0
15	ZRO2(O)	2	-29.482	5.6996E+04	1.7140E-01	0.0
16	CR2O3(O)	2	-23.435	8.0500E-04	2.4207E-09	0.0
17	LA2O3(O)	2	-52.185	5.9339E+01	1.7844E-04	0.0
18	K2O(O)	2	5.233	4.6484E-09	1.3978E-14	0.0
19	U(M)	3	0.0	2.4448E+04	4.3509E-02	0.0
20	ZR(M)	3	0.0	4.3003E+04	7.6532E-02	0.0
21	CR(M)	3	0.0	4.9319E+05	8.7772E-01	0.0
22	LA(M)	3	0.0	7.6533E+01	1.3621E-04	0.0
23	K(M)	3	0.0	1.1806E+03	2.1010E-03	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -2.2903E+11 JOULE
END OF DISSPLA 10.0 -- 32926 VECTORS IN 2 PLOTS.
RUN ON 6/9/88 USING SERIAL NUMBER 1 AT ISSCO SD
PROPRIETARY SOFTWARE PRODUCT OF ISSCO, SAN DIEGO, CALIF.
2822 VIRTUAL STORAGE REFERENCES; 7 READS; 0 WRITES.

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART A (REV.1)

THERMODYNAMIC DATA ** IFEF= 1(IF MINUS, FREE ENERGY FUNCTION IS GIVEN BY TDDATA)

NO.	SPECIES	GF298(J/MOL)		TDDATA				
			T**I	0	1	0	0	0
1	O2(G)	0.0		0.0	0.0	0.0	0.0	0.0
2	UO2(G)	0.0		-5.0836E+05	2.2800E+00	0.0	0.0	0.0
3	UO3(G)	0.0		-8.3680E+05	8.1170E+01	0.0	0.0	0.0
4	UOH(G)	0.0		2.4939E+04	-2.6190E+00	0.0	0.0	0.0
5	H2(G)	0.0		0.0	0.0	0.0	0.0	0.0
6	H2O(G)	0.0		-2.4644E+05	5.4810E+01	0.0	0.0	0.0
7	ZR(G)	0.0		6.0960E+05	-1.3200E+02	0.0	0.0	0.0
8	CR(G)	0.0		3.7943E+05	-1.3180E+02	0.0	0.0	0.0
9	LA(G)	0.0		4.2087E+05	-1.1420E+02	0.0	0.0	0.0
10	LAO(G)	0.0		-1.4771E+05	-5.2720E+01	0.0	0.0	0.0
11	K(G)	0.0		6.8864E+04	-6.9760E+01	0.0	0.0	0.0
12	KOH(G)	0.0		-2.4028E+05	1.0740E+01	0.0	0.0	0.0
13	UO2(O)	0.0		-1.0800E+06	1.6900E+02	0.0	0.0	0.0
14	U2O45(O)	0.0		-2.2500E+06	3.9140E+02	0.0	0.0	0.0
15	ZRO2(O)	0.0		-1.0980E+06	1.9400E+02	0.0	0.0	0.0
16	CR2O3(O)	0.0		-1.1208E+06	2.5340E+02	0.0	0.0	0.0
17	LA2O3(O)	0.0		-1.7900E+06	2.8200E+02	0.0	0.0	0.0
18	K2O(O)	0.0		-4.5470E+05	2.2540E+02	0.0	0.0	0.0
19	U(M)	0.0		0.0	0.0	0.0	0.0	0.0
20	ZR(M)	0.0		0.0	0.0	0.0	0.0	0.0
21	CR(M)	0.0		0.0	0.0	0.0	0.0	0.0
22	LA(M)	0.0		0.0	0.0	0.0	0.0	0.0
23	K(M)	0.0		0.0	0.0	0.0	0.0	0.0

** CONVERGED, ITERATION= 5 (LIMIT= 2) TIME (MS)= 19.000 TIME FOR INITIAL GUESS (MS)= 5.000

APPENDIX B

INPUT AND OUTPUT LISTING OF PART B ANALYSIS

INPUT DATA LIST

```
CARD NO. ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
      1.  CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B                    00230003
      2.  &COND1  L=12, NN=63, MP=3, MR=0, ML(1)=52,8,3,                            00240003
      3.  EL(1)=1HO,1HH,1HC,2HFE,2HMO,2HCA,2HSI,1HU,2HZR,2HSR,2HLA,2HCE, IPC=1,     00250003
      4.  IFEF=1, IOM=1,                                                            00260003
      5. TEXT( 1)=8HH         , IPC=1,                                              00270001
      6. TEXT( 2)=8HOH        , IPC=1,                                              00280001
      7. TEXT( 3)=8HO         , IPC=1,                                              00290001
      8. TEXT( 4)=8HO2        , IPC=1,                                              00300001
      9. TEXT( 5)=8HCO2       , IPC=1,                                              00310001
     10. TEXT( 6)=8HCO        , IPC=1,                                              00320001
     11. TEXT( 7)=8HFE        , IPC=1,                                              00330001
     12. TEXT( 8)=8HFEO       , IPC=1,                                              00340001
     13. TEXT( 9)=8HFEOH      , IPC=1,                                              00350003
     14. TEXT(10)=8HFE(OH)2   , IPC=1,                                              00360003
     15. TEXT(11)=8HMO        , IPC=1,                                              00370001
     16. TEXT(12)=8HMOO       , IPC=1,                                              00380001
     17. TEXT(13)=8HMOO2      , IPC=1,                                              00390003
     18. TEXT(14)=8HMOO3      , IPC=1,                                              00400003
     19. TEXT(15)=8HMOO2(OH2, IPC=1,                                                00410003
     20. TEXT(16)=8H(MOO3)2   , IPC=1,                                              00420003
     21. TEXT(17)=8H(MOO3)3   , IPC=1,                                              00430003
     22. TEXT(18)=8HCA        , IPC=1,                                              00440001
     23. TEXT(19)=8HCAO       , IPC=1,                                              00450001
     24. TEXT(20)=8HCAOH      , IPC=1,                                              00460003
     25. TEXT(21)=8HCA(OH)2   , IPC=1,                                              00470003
     26. TEXT(22)=8HSI        , IPC=1,                                              00480001
     27. TEXT(23)=8HSIO       , IPC=1,                                              00490003
     28. TEXT(24)=8HSIO2      , IPC=1,                                              00500003
     29. TEXT(25)=8HSIOH      , IPC=1,                                              00510003
     30. TEXT(26)=8HSI(OH)2   , IPC=1,                                              00520003
     31. TEXT(27)=8HU         , IPC=1,                                              00530001
     32. TEXT(28)=8HUO        , IPC=1,                                              00540003
     33. TEXT(29)=8HUO2       , IPC=1,                                              00550003
     34. TEXT(30)=8HUO3       , IPC=1,                                              00560003
     35. TEXT(31)=8HUO2(OH)2, IPC=1,                                                00570003
     36. TEXT(32)=8HZR        , IPC=1,                                              00580001
     37. TEXT(33)=8HZRO       , IPC=1,                                              00590001
     38. TEXT(34)=8HZRO2      , IPC=1,                                              00600001
     39. TEXT(35)=8HZROH      , IPC=1,                                              00610003
     40. TEXT(36)=8HZR(OH)2   , IPC=1,                                              00620003
     41. TEXT(37)=8HSR        , IPC=1,                                              00630001
     42. TEXT(38)=8HSRO       , IPC=1,                                              00640001
     43. TEXT(39)=8HSROH      , IPC=1,                                              00650003
     44. TEXT(40)=8HSR(OH)2   , IPC=1,                                              00660003
     45. TEXT(41)=8HLA        , IPC=1,                                              00670001
     46. TEXT(42)=8HLAO       , IPC=1,                                              00680001
     47. TEXT(43)=8HLAOH      , IPC=1,                                              00690003
     48. TEXT(44)=8HLA(OH)2   , IPC=1,                                              00700003
     49. TEXT(45)=8HCE        , IPC=1,                                              00710001
     50. TEXT(46)=8HCEO       , IPC=1,                                              00720001
         ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
```

INPUT DATA LIST

```
                1         2         3         4         5         6         7         8
CARD NO. ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
     51. TEXT(47)=8HCEOH     , IPC=1,                                              00740003
     52. TEXT(48)=8HCE(OH)2  , IPC=1,                                              00750003
     53. TEXT(49)=8HCEO2     , IPC=1,                                              00751003
     54. TEXT(50)=8H(CEO)2   , IPC=1,                                              00752003
     55. TEXT(51)=8HH2O      , IPC=1,                                              00760003
     56. TEXT(52)=8HH2       , IPC=1,                                              00770003
     57. TEXT(53)=8HFEO(L)   , IPC=1,                                              00780003
     58. TEXT(54)=8HCAO(L)   , IPC=1,                                              00790003
     59. TEXT(55)=8HSIO2(L)  , IPC=1,                                              00800003
     60. TEXT(56)=8HUO2(L)   , IPC=1,                                              00810003
     61. TEXT(57)=8HZRO2(L)  , IPC=1,                                              00820003
     62. TEXT(58)=8HSRO(L)   , IPC=1,                                              00830003
     63. TEXT(59)=8HLA2O3(L), IPC=1,                                               00840003
     64. TEXT(60)=8HCEO2(L)  , IPC=1,                                              00850003
     65. TEXT(61)=8HFE(L)    , IPC=1,                                              00860003
     66. TEXT(62)=8HMO(L)    , IPC=1,                                              00870003
     67. TEXT(63)=8HZR(L)    , IPC=1,                                              00880003
     68.  IGT=0,1,       &END                                                      00890003
     69. H                0    1    0    0    0    0    0    0    0    0    0    00900003
     70. OH               1    1    0    0    0    0    0    0    0    0    0    00910001
     71. O                1    0    0    0    0    0    0    0    0    0    0    00920001
     72. O2               2    0    0    0    0    0    0    0    0    0    0    00930001
     73. CO2              2    0    1    0    0    0    0    0    0    0    0    00940001
     74. CO               1    0    1    0    0    0    0    0    0    0    0    00950001
     75. FE               0    0    0    1    0    0    0    0    0    0    0    00960001
     76. FEO              1    0    0    1    0    0    0    0    0    0    0    00970001
     77. FEOH             1    1    0    1    0    0    0    0    0    0    0    00980003
     78. FE(OH)2          2    2    0    1    0    0    0    0    0    0    0    00990003
     79. MO               0    0    0    0    1    0    0    0    0    0    0    01000001
     80. MOO              1    0    0    0    1    0    0    0    0    0    0    01010001
     81. MOO2             2    0    0    0    1    0    0    0    0    0    0    01020003
     82. MOO3             3    0    0    0    1    0    0    0    0    0    0    01030003
     83. MOO2(OH2         3    2    0    0    1    0    0    0    0    0    0    01040003
     84. (MOO3)2          6    0    0    0    2    0    0    0    0    0    0    01050003
     85. (MOO3)3          9    0    0    0    3    0    0    0    0    0    0    01060003
     86. CA               0    0    0    0    0    1    0    0    0    0    0    01070001
     87. CAO              1    0    0    0    0    1    0    0    0    0    0    01080001
     88. CAOH             1    1    0    0    0    1    0    0    0    0    0    01090003
     89. CA(OH)2          2    2    0    0    0    1    0    0    0    0    0    01100003
     90. SI               0    0    0    0    0    0    1    0    0    0    0    01110001
     91. SIO              1    0    0    0    0    0    1    0    0    0    0    01120003
     92. SIO2             2    0    0    0    0    0    1    0    0    0    0    01130003
     93. SIOH             1    1    0    0    0    0    1    0    0    0    0    01140003
     94. SI(OH)2          2    2    0    0    0    0    1    0    0    0    0    01150003
     95. U(G)             0    0    0    0    0    0    0    1    0    0    0    01160003
     96. UO               1    0    0    0    0    0    0    1    0    0    0    01170003
     97. UO2              2    0    0    0    0    0    0    1    0    0    0    01180003
     98. UO3              3    0    0    0    0    0    0    1    0    0    0    01190003
     99. UO2(OH)2         4    2    0    0    0    0    0    1    0    0    0    01200003
    100. ZR               0    0    0    0    0    0    0    0    1    0    0    01210001
         ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
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INPUT DATA LIST

CARD NO.		1	2	3	4	5	6	7	8
101.	ZRO	1	0	0	0	0	1	0	01220001
102.	ZRO2	2	0	0	0	0	1	0	01230001
103.	ZROH	1	1	0	0	0	1	0	01240003
104.	ZR(OH)2	2	2	0	0	0	1	0	01250003
105.	SR	0	0	0	0	0	0	1	01260001
106.	SRO	1	0	0	0	0	0	1	01270001
107.	SROH	1	1	0	0	0	0	1	01280003
108.	SR(OH)2	2	2	0	0	0	0	1	01290003
109.	LA	0	0	0	0	0	0	1	01300001
110.	LAO	1	0	0	0	0	0	1	01310001
111.	LAOH	1	1	0	0	0	0	1	01320003
112.	LA(OH)2	2	2	0	0	0	0	1	01330003
113.	CE	0	0	0	0	0	0	1	01340001
114.	CEO	1	0	0	0	0	0	1	01350001
115.	CEOH	1	1	0	0	0	0	1	01370003
116.	CE(OH)2	2	2	0	0	0	0	1	01380003
117.	CEO2	2	0	0	0	0	0	1	01380103
118.	(CEO)2	2	0	0	0	0	0	2	01381003
119.	H2O	1	2	0	0	0	0	0	01390001
120.	H2	0	2	0	0	0	0	0	01400001
121.	FEO(L)	1	0	0	1	0	0	0	01410003
122.	CAO(L)	1	0	0	0	1	0	0	01420003
123.	SIO2(L)	2	0	0	0	0	1	0	01430003
124.	UO2(L)	2	0	0	0	0	1	0	01440003
125.	ZRO2(L)	2	0	0	0	0	1	0	01450003
126.	SRO(L)	1	0	0	0	0	0	1	01460003
127.	LA2O3(L)	3	0	0	0	0	0	2	01470003
128.	CEO2(L)	2	0	0	0	0	0	1	01480003
129.	FE(L)	0	0	0	0	0	0	0	01490003
130.	MO(L)	0	0	0	1	0	0	0	01500003
131.	ZR(L)	0	0	0	0	0	1	0	01510003
132.	H			227474.7	-60.3301				01520000
133.	OH			369828.4	-13.6243				01530000
134.	O			362870.7	-133.9805				01540000
135.	O2			0.0	0.0				01550000
136.	CO2			-395375.4	-0.5234				01560000
137.	CO			-114033.7	-85.5949				01570000
138.	FE			373116.3	-119.8137				01580000
139.	FEO			200081.3	-68.9679				01590000
140.	FEOH			76346.2	-15.3028				01600000
141.	FE(OH)2			-358328.6	102.7143				01610000
142.	MO			641250.2	-138.1321				01620000
143.	MOO			365570.4	-86.7421				01630000
144.	MOO2			-32389.7	-26.0239				01640000
145.	MOO3			-369560.4	63.5297				01650000
146.	MOO2(OH2			-856305.2	209.9412				01660000
147.	(MOO3)2			-572461.1	148.6599				01670000
148.	(MOO3)3			-652717.9	184.1623				01680000
149.	CA			0.0	0.0				01690000
150.	CAO			-129326.1	35.9236				01700000

INPUT DATA LIST

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                1         2         3         4         5         6         7         8
CARD NO. ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
     151. CAOH                -349212.6   78.5473                              01710000
     152. CA(OH)2             -760548.9  188.6878                              01720000
     153. SI                   395028.2 -113.2433                              01730000
     154. SIO                 -162614.9  -46.6569                              01740000
     155. SIO2                -359269.2   30.6646                              01750000
     156. SIOH                  -9438.3   -3.5211                              01760000
     157. SI(OH)2             -526150.9  141.5432                              01770000
     158. U                    497157.4 -112.1183                              01780000
     159. UO                   -21771.4  -49.4042                              01790000
     160. UO2                 -495160.2   11.7230                              01800000
     161. UO3                 -834291.1   78.7118                              01810000
     162. UO2(OH)2           -1272129.0  229.9977                              01820000
     163. ZR                   600324.3 -127.8879                              01830000
     164. ZRO                   34716.9  -62.5177                              01840000
     165. ZRO2                -321346.6   -0.1884                              01850000
     166. ZROH                -194866.2   87.5008                              01860000
     167. ZR(OH)2             -500820.8  114.8271                              01870000
     168. SR                        0.0    0.0                                 01880000
     169. SRO                 -168518.7   33.9856                              01890000
     170. SROH                -362179.9   82.9958                              01900000
     171. SR(OH)2             -742947.6  182.8204                              01910000
     172. LA                   405856.6 -112.0618                              01920000
     173. LAO                 -150515.4  -65.5988                              01930000
     174. LAOH                 -91451.0   -5.4470                              01940000
     175. LA(OH)2             -660396.5  106.9057                              01950000
     176. CE                   403327.0 -105.0108                              01960000
     177. CEO                 -169665.9  -25.3469                              01970000
     178. CEOH                -104644.9   11.1394                              01980000
     179. CE(OH)2             -560918.1  113.6239                              01990000
     180. CEO2                      0.0    0.0                                 01991003
     181. (CEO)2                    0.0    0.0                                 02000003
     182. H2O                 -252053.7   58.2296                              02010003
     183. H2                        0.0    0.0                                 02020003
     184. FEO(L)              -254098.5   52.8420                              02040003
     185. CAO(L)              -687974.9  158.4201                              02060003
     186. SIO2(L)             -929720.7  189.1358                              02070003
     187. UO2(L)              -933112.1  122.5321                              02080003
     188. ZRO2(L)            -1017459.4  159.4476                              02090003
     189. SRO(L)              -640530.1  149.9929                              02090103
     190. LA2O3(L)           -1777233.0  271.8740                              02090203
     191. CEO2(L)            -1086935.0  212.2707                              02090303
     192. FE(L)                     0.0    0.0                                 02091003
     193. MO(L)                     0.0    0.0                                 02092003
     194. ZR(L)                     0.0    0.0                                 02100003
     195.  &COND2       TEMP=2000.0,                                            02770003
     196.  PRESS=1.0,                                                           02780003
     197.  BB(1)=2.327E+5, IEND=0,                                              02790003
     198.  BB(2)=2.000E+2, IEND=0,                                              02800003
     199.  BB(3)=1.000E+2, IEND=0,                                              02810003
     200.  BB(4)=1.000E+5, IEND=0,                                              02820003
           ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
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INPUT DATA LIST

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CARD NO. ....5....0....5....0....5....0....5....0....5....0....5....0....5....0....5....0
    201. BB(5)=1.000E+2, IEND=0,                                                  02830003
    202. BB(6)=1.000E+4, IEND=0,                                                  02840003
    203. BB(7)=1.000E+4,  IEND=0,                                                 02850003
    204. BB(8)=1.000E+5,  IEND=0,                                                 02860003
    205. BB(9)=1.000E+5,  IEND=0,                                                 02870003
    206. BB(10)=1.000E+2, IEND=0,                                                 02880003
    207. BB(11)=2.000E+2, IEND=0,                                                 02890003
    208. BB(12)=1.000E+3, IEND=0,                                                 02900003
    209. IEND=0,                                                                  02910003
    210. MDEBUG=0,   &END                                                         02920003
    211. &COND2    TEMP=2500.,                                        &END        02930003
    212. &COND2    TEMP=2000.,                                                    02940003
    213.          BB(1)=5.027E+5,    IEND=0,                                      02950003
    214.          BB(6)=1.000E+5,    IEND=0,                                      02960003
    215.          BB(7)=1.000E+5,    IEND=0,                                      02970003
    216.          BB(9)=1.000E+4,    IEND=0,                            &END      02980003
    217. &COND2    TEMP=2500.,                                        &END        02990003
    218. &COND2    TEMP=2000.,                                                    03000003
    219.          BB(1)=3.227E+5,    IEND=0,                                      03010003
    220.          BB(6)=1.000E+5,    IEND=0,                                      03020003
    221.          BB(7)=1.000E+4,    IEND=0,                                      03030003
    222.          BB(9)=1.000E+4,    IEND=0,                             &END     03040003
    223. &COND2    TEMP=2500.,                          IEND=1,        &END      03050003
```

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B

MPEC CODE CALCULATION ** FIXED CONDITIONS**
NUMBER OF ELEMENTS (L) =12 NO. OF MIXTURE = 3 NO. OF PURE SUBSTANCES = 0
TOTAL NO. OF PHASES = 3 TOTAL NO. OF SPECIES= 63

STOICHIOMETRY COEFFICIENTS

NO.	SPECIES	MIXTURE	O	H	C	FE	MO	CA	SI	U	ZR	SR	LA	CE
1	H	1	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	OH	1	1.000	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	O	1	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	O2	1	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	CO2	1	2.000	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	CO	1	1.000	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	FE	1	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	FEO	1	1.000	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
9	FEOH	1	1.000	1.000	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	FE(OH)2	1	2.000	2.000	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
11	MO	1	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
12	MOO	1	1.000	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	MOO2	1	2.000	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	MOO3	1	3.000	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	MOO2(OH2	1	3.000	2.000	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
16	(MOO3)2	1	6.000	0.0	0.0	0.0	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	(MOO3)3	1	9.000	0.0	0.0	0.0	3.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	CA	1	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0
19	CAO	1	1.000	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0
20	CAOH	1	1.000	1.000	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0
21	CA(OH)2	1	2.000	2.000	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0
22	SI	1	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0
23	SIO	1	1.000	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0
24	SIO2	1	2.000	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0
25	SIOH	1	1.000	1.000	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0
26	SI(OH)2	1	2.000	2.000	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0
27	U	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0
28	UO	1	1.000	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0
29	UO2	1	2.000	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0
30	UO3	1	3.000	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0
31	UO2(OH)2	1	4.000	2.000	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0
32	ZR	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0
33	ZRO	1	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0
34	ZRO2	1	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0
35	ZROH	1	1.000	1.000	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0
36	ZR(OH)2	1	2.000	2.000	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0
37	SR	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0
38	SRO	1	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0
39	SROH	1	1.000	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0
40	SR(OH)2	1	2.000	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0
41	LA	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0
42	LAO	1	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0
43	LAOH	1	1.000	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0
44	LA(OH)2	1	2.000	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0
45	CE	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000

46	CEO	1	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000
47	CEOH	1	1.000	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000
48	CE(OH)2	1	2.000	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000
49	CEO2	1	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000
50	(CEO)2	1	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.000
51	H2O	1	1.000	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
52	H2	1	0.0	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
53	FEO(L)	2	1.000	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
54	CAO(L)	2	1.000	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0
55	SIO2(L)	2	2.000	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0
56	UO2(L)	2	2.000	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0
57	ZRO2(L)	2	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0
58	SRO(L)	2	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0
59	LA2O3(L)	2	3.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.000	0.0
60	CEO2(L)	2	2.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000
61	FE(L)	3	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
62	MO(L)	3	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
63	ZR(L)	3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.000	0.0	0.0	0.0

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B

THERMODYNAMIC DATA ** IFEF= 1(IF MINUS, FREE ENERGY FUNCTION IS GIVEN BY TDDATA)

NO.	SPECIES	GF298(J/MOL) T**I	TDDATA 0	1	0	0	0
1	H	0.0	2.2747E+05	-6.0330E+01	0.0	0.0	0.0
2	OH	0.0	3.6983E+05	-1.3624E+01	0.0	0.0	0.0
3	O	0.0	3.6287E+05	-1.3398E+02	0.0	0.0	0.0
4	O2	0.0	0.0	0.0	0.0	0.0	0.0
5	CO2	0.0	-3.9538E+05	-5.2340E-01	0.0	0.0	0.0
6	CO	0.0	-1.1403E+05	-8.5595E+01	0.0	0.0	0.0
7	FE	0.0	3.7312E+05	-1.1981E+02	0.0	0.0	0.0
8	FEO	0.0	2.0008E+05	-6.8968E+01	0.0	0.0	0.0
9	FEOH	0.0	7.6346E+04	-1.5303E+01	0.0	0.0	0.0
10	FE(OH)2	0.0	-3.5833E+05	1.0271E+02	0.0	0.0	0.0
11	MO	0.0	6.4125E+05	-1.3813E+02	0.0	0.0	0.0
12	MOO	0.0	3.6557E+05	-8.6742E+01	0.0	0.0	0.0
13	MOO2	0.0	-3.2390E+04	-2.6024E+01	0.0	0.0	0.0
14	MOO3	0.0	-3.6956E+05	6.3530E+01	0.0	0.0	0.0
15	MOO2(OH2	0.0	-8.5631E+05	2.0994E+02	0.0	0.0	0.0
16	(MOO3)2	0.0	-5.7246E+05	1.4866E+02	0.0	0.0	0.0
17	(MOO3)3	0.0	-6.5272E+05	1.8416E+02	0.0	0.0	0.0
18	CA	0.0	0.0	0.0	0.0	0.0	0.0
19	CAO	0.0	-1.2933E+05	3.5924E+01	0.0	0.0	0.0
20	CAOH	0.0	-3.4921E+05	7.8547E+01	0.0	0.0	0.0
21	CA(OH)2	0.0	-7.6055E+05	1.8869E+02	0.0	0.0	0.0
22	SI	0.0	3.9503E+05	-1.1324E+02	0.0	0.0	0.0
23	SIO	0.0	-1.6261E+05	-4.6657E+01	0.0	0.0	0.0
24	SIO2	0.0	-3.5927E+05	3.0665E+01	0.0	0.0	0.0
25	SIOH	0.0	-9.4383E+03	-3.5211E+00	0.0	0.0	0.0
26	SI(OH)2	0.0	-5.2615E+05	1.4154E+02	0.0	0.0	0.0
27	U	0.0	4.9716E+05	-1.1212E+02	0.0	0.0	0.0
28	UO	0.0	-2.1771E+04	-4.9404E+01	0.0	0.0	0.0
29	UO2	0.0	-4.9516E+05	1.1723E+01	0.0	0.0	0.0
30	UO3	0.0	-8.3429E+05	7.8712E+01	0.0	0.0	0.0
31	UO2(OH)2	0.0	-1.2721E+06	2.3000E+02	0.0	0.0	0.0
32	ZR	0.0	6.0032E+05	-1.2789E+02	0.0	0.0	0.0
33	ZRO	0.0	3.4717E+04	-6.2518E+01	0.0	0.0	0.0
34	ZRO2	0.0	-3.2135E+05	-1.8840E-01	0.0	0.0	0.0
35	ZROH	0.0	-1.9487E+05	8.7501E+01	0.0	0.0	0.0
36	ZR(OH)2	0.0	-5.0082E+05	1.1483E+02	0.0	0.0	0.0
37	SR	0.0	0.0	0.0	0.0	0.0	0.0
38	SRO	0.0	-1.6852E+05	3.3986E+01	0.0	0.0	0.0
39	SROH	0.0	-3.6218E+05	8.2996E+01	0.0	0.0	0.0
40	SR(OH)2	0.0	-7.4295E+05	1.8282E+02	0.0	0.0	0.0
41	LA	0.0	4.0586E+05	-1.1206E+02	0.0	0.0	0.0
42	LAO	0.0	-1.5052E+05	-6.5599E+01	0.0	0.0	0.0
43	LAOH	0.0	-9.1451E+04	-5.4470E+00	0.0	0.0	0.0
44	LA(OH)2	0.0	-6.6040E+05	1.0691E+02	0.0	0.0	0.0
45	CE	0.0	4.0333E+05	-1.0501E+02	0.0	0.0	0.0

46	CEO	0.0	-1.6967E+05	-2.5347E+01	0.0	0.0	0.0
47	CEOH	0.0	-1.0464E+05	1.1139E+01	0.0	0.0	0.0
48	CE(OH)2	0.0	-5.6092E+05	1.1362E+02	0.0	0.0	0.0
49	CEO2	0.0	0.0	0.0	0.0	0.0	0.0
50	(CEO)2	0.0	0.0	0.0	0.0	0.0	0.0
51	H2O	0.0	-2.5205E+05	5.8230E+01	0.0	0.0	0.0
52	H2	0.0	0.0	0.0	0.0	0.0	0.0
53	FEO(L)	0.0	-2.5410E+05	5.2842E+01	0.0	0.0	0.0
54	CAO(L)	0.0	-6.8797E+05	1.5842E+02	0.0	0.0	0.0
55	SIO2(L)	0.0	-9.2972E+05	1.8914E+02	0.0	0.0	0.0
56	UO2(L)	0.0	-9.3311E+05	1.2253E+02	0.0	0.0	0.0
57	ZRO2(L)	0.0	-1.0175E+06	1.5945E+02	0.0	0.0	0.0
58	SRO(L)	0.0	-6.4053E+05	1.4999E+02	0.0	0.0	0.0
59	LA2O3(L)	0.0	-1.7772E+06	2.7187E+02	0.0	0.0	0.0
60	CEO2(L)	0.0	-1.0869E+06	2.1227E+02	0.0	0.0	0.0
61	FE(L)	0.0	0.0	0.0	0.0	0.0	0.0
62	MO(L)	0.0	0.0	0.0	0.0	0.0	0.0
63	ZR(L)	0.0	0.0	0.0	0.0	0.0	0.0

*** ELEMENT C WAS REPLACED BY SPECIES CO

** CONVERGED, ITERATION= 5 (LIMIT= 1) TIME (MS)= 109.000 TIME FOR INITIAL GUESS (MS)=20.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B

CASE 1 TEMPERATURE (K)= 2000.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 1.600E+03

INPUT GRAM-ATOMS OF ELEMENTS

O	H	C	FE	MO	CA	SI	U	ZR	SR
2.327E+05	2.000E+02	1.000E+02	1.000E+05	1.000E+02	1.000E+04	1.000E+04	1.000E+05	1.000E+05	1.000E+02

LA	CE
2.000E+02	1.000E+03

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	6.422	1.5987E+00	1.6408E-04	1.6408E-04
2	OH	1	20.595	2.5239E-16	2.5905E-20	2.5905E-20
3	O	1	5.706	7.3217E-09	7.5149E-13	7.5149E-13
4	O2	1	0.0	4.9723E-16	5.1035E-20	5.1035E-20
5	CO2	1	-23.832	1.8081E-05	1.8558E-09	1.8558E-09
6	CO	1	-17.147	9.9998E+01	1.0264E-02	1.0264E-02
7	FE	1	8.025	1.6338E+00	1.6769E-04	1.6769E-04
8	FEO	1	3.736	2.6907E-08	2.7616E-12	2.7616E-12
9	FEOH	1	2.750	7.2793E-09	7.4713E-13	7.4713E-13
10	FE(OH)2	1	-9.192	2.5484E-14	2.6156E-18	2.6156E-18
11	MO	1	21.942	1.4758E-09	1.5147E-13	1.5147E-13
12	MOO	1	11.548	1.0895E-14	1.1182E-18	1.1182E-18
13	MOO2	1	-5.076	4.0828E-17	4.1905E-21	4.1905E-21
14	MOO3	1	-14.579	1.2354E-22	1.2679E-26	1.2679E-26
15	MOO2(OH2	1	-26.237	1.4546E-19	1.4930E-23	1.4930E-23
16	(MOO3)2	1	-16.541	0.0	0.0	0.0
17	(MOO3)3	1	-17.097	0.0	0.0	0.0
18	CA	1	0.0	7.0168E+02	7.2019E-02	7.2019E-02
19	CAO	1	-3.456	5.0211E-06	5.1536E-10	5.1536E-10
20	CAOH	1	-11.550	1.6597E-03	1.7035E-07	1.7035E-07
21	CA(OH)2	1	-23.036	3.6826E-09	3.7797E-13	3.7797E-13
22	SI	1	10.132	3.1092E+02	3.1912E-02	3.1912E-02
23	SIO	1	-15.386	8.4945E+03	8.7186E-01	8.7186E-01
24	SIO2	1	-17.912	2.3986E-05	2.4618E-09	2.4618E-09
25	SIOH	1	-0.991	4.8003E-04	4.9269E-08	4.9269E-08
26	SI(OH)2	1	-14.613	9.0163E-09	9.2542E-13	9.2542E-13
27	U	1	16.408	1.3297E-02	1.3647E-06	1.3647E-06
28	UO	1	-7.249	5.6446E-02	5.7935E-06	5.7935E-06
29	UO2	1	-28.359	1.8767E-02	1.9262E-06	1.9262E-06
30	UO3	1	-40.692	9.6314E-07	9.8855E-11	9.8855E-11
31	UO2(OH)2	1	-48.824	7.5360E-15	7.7348E-19	7.7348E-19
32	ZR	1	20.714	4.7889E-06	4.9152E-10	4.9152E-10
33	ZRO	1	-5.430	2.4444E-04	2.5089E-08	2.5089E-08
34	ZRO2	1	-19.342	6.0798E-08	6.2402E-12	6.2402E-12
35	ZROH	1	-1.194	3.5694E-07	3.6635E-11	3.6635E-11
36	ZR(OH)2	1	-16.302	2.9629E-11	3.0411E-15	3.0411E-15
37	SR	1	0.0	3.2193E+01	3.3042E-03	3.3042E-03
38	SRO	1	-6.045	3.0683E-06	3.1493E-10	3.1493E-10
39	SROH	1	-11.795	9.7254E-05	9.9820E-09	9.9820E-09
40	SR(OH)2	1	-22.683	1.1874E-10	1.2188E-14	1.2188E-14
41	LA	1	10.926	1.1932E-04	1.2247E-08	1.2247E-08
42	LAO	1	-16.936	3.3949E-02	3.4845E-06	3.4845E-06

43	LAOH	1	-6.153	7.1056E-08	7.2931E-12	7.2931E-12
44	LA(OH)2	1	-26.848	1.5749E-09	1.6165E-13	1.6165E-13
45	CE	1	11.621	7.4430E-02	7.6393E-06	7.6393E-06
46	CEO	1	-13.248	1.0620E+00	1.0900E-04	1.0900E-04
47	CEOH	1	-4.952	2.6739E-05	2.7444E-09	2.7444E-09
48	CE(OH)2	1	-20.060	2.2198E-09	2.2784E-13	2.2784E-13
49	CEO2	1	0.0	4.2331E-16	4.3448E-20	4.3448E-20
50	(CEO)2	1	0.0	3.6038E-16	3.6989E-20	3.6989E-20
51	H2O	1	-8.152	7.7749E-05	7.9800E-09	7.9800E-09
52	H2	1	0.0	9.9199E+01	1.0182E-02	1.0182E-02
53	FEO(L)	2	-8.922	1.0132E-01	8.6837E-07	0.0
54	CAO(L)	2	-22.312	9.2982E+03	7.9687E-02	0.0
55	SIO2(L)	2	-33.152	1.1945E+03	1.0237E-02	0.0
56	UO2(L)	2	-41.364	9.9999E+04	8.5701E-01	0.0
57	ZRO2(L)	2	-41.997	5.0257E+03	4.3071E-02	0.0
58	SRO(L)	2	-20.473	6.7815E+01	5.8119E-04	0.0
59	LA2O3(L)	2	-74.155	9.9978E+01	8.5683E-04	0.0
60	CEO2(L)	2	-39.822	9.9885E+02	8.5603E-03	0.0
61	FE(L)	3	0.0	9.9998E+04	5.1262E-01	0.0
62	MO(L)	3	0.0	1.0000E+02	5.1263E-04	0.0
63	ZR(L)	3	0.0	9.4974E+04	4.8687E-01	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -8.2831E+10 JOULE
*** ELEMENT C WAS REPLACED BY SPECIES CO
** CONVERGED, ITERATION= 4 (LIMIT= 1) TIME (MS)= 92.000 TIME FOR INITIAL GUESS (MS)=21.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART 8

CASE 2 TEMPERATURE (K)= 2500.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 3.184E+03

INPUT GRAM-ATOMS OF ELEMENTS

O	H	C	FE	MO	CA	SI	U	ZR	SR
2.327E+05	2.000E+02	1.000E+02	1.000E+05	1.000E+02	1.000E+04	1.000E+04	1.000E+05	1.000E+05	1.000E+02

LA	CE
2.000E+02	1.000E+03

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	3.686	2.8586E+01	1.8815E-03	1.8815E-03
2	OH	1	16.149	1.4294E-11	9.4083E-16	9.4083E-16
3	O	1	1.343	5.1242E-04	3.3727E-08	3.3727E-08
4	O2	1	0.0	2.5356E-10	1.6689E-14	1.6689E-14
5	CO2	1	-19.078	3.5113E-04	2.3111E-08	2.3111E-08
6	CO	1	-15.776	9.9999E+01	6.5818E-03	6.5818E-03
7	FE	1	3.539	2.2905E+02	1.5076E-02	1.5076E-02
8	FEO	1	1.330	2.6938E-04	1.7730E-08	1.7730E-08
9	FEOH	1	1.832	1.2252E-05	8.0644E-10	8.0644E-10
10	FE(OH)2	1	-4.884	9.8111E-11	6.4575E-15	6.4575E-15
11	MO	1	14.232	5.2106E-06	3.4295E-10	3.4295E-10
12	MOO	1	7.152	7.9964E-10	5.2632E-14	5.2632E-14
13	MOO2	1	-4.687	1.4319E-11	9.4246E-16	9.4246E-16
14	MOO3	1	-10.135	4.2999E-16	2.8301E-20	2.8301E-20
15	MOO2(OH2	1	-15.941	8.0576E-16	5.3034E-20	5.3034E-20
16	(MOO3)2	1	-9.658	0.0	0.0	0.0
17	(MOO3)3	1	-9.249	0.0	0.0	0.0
18	CA	1	0.0	4.5203E+03	2.9752E-01	2.9752E-01
19	CAO	1	-1.901	3.9072E-03	2.5717E-07	2.5717E-07
20	CAOH	1	-7.351	6.8332E-02	4.4975E-06	4.4975E-06
21	CA(OH)2	1	-13.891	4.5913E-07	3.0219E-11	3.0219E-11
22	SI	1	5.383	4.9420E+02	3.2527E-02	3.2527E-02
23	SIO	1	-13.431	9.4586E+03	6.2255E-01	6.2255E-01
24	SIO2	1	-13.592	1.4358E-03	9.4505E-08	9.4505E-08
25	SIOH	1	-0.877	2.5094E-03	1.6516E-07	1.6516E-07
26	SI(OH)2	1	-8.286	4.0202E-08	2.6460E-12	2.6460E-12
27	U	1	10.430	1.9045E+00	1.2535E-04	1.2535E-04
28	UO	1	-6.987	9.0213E+00	5.9377E-04	5.9377E-04
29	UO2	1	-22.405	5.7867E+00	3.8087E-04	3.8087E-04
30	UO3	1	-30.661	2.8788E-03	1.8948E-07	1.8948E-07
31	UO2(OH)2	1	-33.529	3.6913E-11	2.4296E-15	2.4296E-15
32	ZR	1	13.496	1.0044E-02	6.6106E-07	6.6106E-07
33	ZRO	1	-5.847	3.2635E-01	2.1480E-05	2.1480E-05
34	ZRO2	1	-15.478	6.4189E-04	4.2249E-08	4.2249E-08
35	ZROH	1	1.149	2.2439E-05	1.4769E-09	1.4769E-09
36	ZR(OH)2	1	-10.280	2.0026E-08	1.3181E-12	1.3181E-12
37	SR	1	0.0	7.4516E+01	4.9045E-03	4.9045E-03
38	SRO	1	-4.019	5.3552E-04	3.5247E-08	3.5247E-08
39	SROH	1	-7.440	1.2310E-03	8.1023E-08	8.1023E-08
40	SR(OH)2	1	-13.750	6.5730E-09	4.3262E-13	4.3262E-13
41	LA	1	6.046	7.5911E-02	4.9963E-06	4.9963E-06
42	LAO	1	-15.126	1.5364E+01	1.0112E-03	1.0112E-03

43	LAOH	1	-5.053	4.8689E-05	3.2046E-09	3.2046E-09
44	LA(OH)2	1	-18.908	4.9120E-07	3.2330E-11	3.2330E-11
45	CE	1	6.772	1.8233E+01	1.2001E-03	1.2001E-03
46	CEO	1	-11.208	1.5154E+02	9.9739E-03	9.9739E-03
47	CEOH	1	-3.694	6.2059E-03	4.0847E-07	4.0847E-07
48	CE(OH)2	1	-13.315	9.0889E-07	5.9822E-11	5.9822E-11
49	CEO2	1	0.0	2.6569E-10	1.7487E-14	1.7487E-14
50	(CEO)2	1	0.0	2.7840E-10	1.8324E-14	1.8324E-14
51	H2O	1	-5.121	1.8543E-03	1.2205E-07	1.2205E-07
52	H2	1	0.0	8.5666E+01	5.6384E-03	5.6384E-03
53	FEO(L)	2	-5.867	2.7063E+00	2.3699E-05	0.0
54	CAO(L)	2	-14.040	5.4967E+03	4.8134E-02	0.0
55	SIO2(L)	2	-21.974	4.7133E+01	4.1274E-04	0.0
56	UO2(L)	2	-30.145	9.9982E+04	8.7553E-01	0.0
57	ZRO2(L)	2	-29.763	7.7194E+03	6.7598E-02	0.0
58	SRO(L)	2	-12.771	2.5482E+01	2.2315E-04	0.0
59	LA2O3(L)	2	-52.786	9.2277E+01	8.0806E-04	0.0
60	CEO2(L)	2	-26.753	8.3029E+02	7.2707E-03	0.0
61	FE(L)	3	0.0	9.9768E+04	5.1922E-01	0.0
62	MO(L)	3	0.0	1.0000E+02	5.2043E-04	0.0
63	ZR(L)	3	0.0	9.2280E+04	4.8025E-01	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -7.6547E+10 JOULE
*** ELEMENT C WAS REPLACED BY SPECIES CO
** CONVERGED, ITERATION= 4 (LIMIT= 1) TIME (MS)= 94.000 TIME FOR INITIAL GUESS (MS)=22.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B

CASE 3 TEMPERATURE (K)= 2000.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 3.267E+03

INPUT GRAM-ATOMS OF ELEMENTS

O	H	C	FE	MO	CA	SI	U	ZR	SR
5.027E+05	2.000E+02	1.000E+02	1.000E+05	1.000E+02	1.000E+05	1.000E+05	1.000E+05	1.000E+04	1.000E+02

LA	CE
2.000E+02	1.000E+03

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	6.422	2.2784E+00	1.1473E-04	1.1473E-04
2	OH	1	20.595	8.6870E-15	4.3746E-19	4.3746E-19
3	O	1	5.706	3.6040E-07	1.8149E-11	1.8149E-11
4	O2	1	0.0	5.9111E-13	2.9767E-17	2.9767E-17
5	CO2	1	-23.832	4.3669E-04	2.1990E-08	2.1990E-08
6	CO	1	-17.147	9.9999E+01	5.0357E-03	5.0357E-03
7	FE	1	8.025	6.4853E+00	3.2659E-04	3.2659E-04
8	FEO	1	3.736	2.5794E-06	1.2989E-10	1.2989E-10
9	FEOH	1	2.750	4.8794E-07	2.4571E-11	2.4571E-11
10	FE(OH)2	1	-9.192	2.8848E-11	1.4527E-15	1.4527E-15
11	MO	1	21.942	5.8590E-09	2.9504E-13	2.9504E-13
12	MOO	1	11.548	1.0446E-12	5.2605E-17	5.2605E-17
13	MOO2	1	-5.076	9.4542E-14	4.7609E-18	4.7609E-18
14	MOO3	1	-14.579	6.9088E-18	3.4791E-22	3.4791E-22
15	MOO2(OH2	1	-26.237	3.9774E-15	2.0029E-19	2.0029E-19
16	(MOO3)2	1	-16.541	0.0	0.0	0.0
17	(MOO3)3	1	-17.097	0.0	0.0	0.0
18	CA	1	0.0	2.5428E+02	1.2805E-02	1.2805E-02
19	CAO	1	-3.456	4.3945E-05	2.2130E-09	2.2130E-09
20	CAOH	1	-11.550	1.0157E-02	5.1147E-07	5.1147E-07
21	CA(OH)2	1	-23.036	3.8057E-07	1.9165E-11	1.9165E-11
22	SI	1	10.132	2.9349E+01	1.4779E-03	1.4779E-03
23	SIO	1	-15.386	1.9365E+04	9.7518E-01	9.7518E-01
24	SIO2	1	-17.912	1.3206E-03	6.6501E-08	6.6501E-08
25	SIOH	1	-0.991	7.6518E-04	3.8532E-08	3.8532E-08
26	SI(OH)2	1	-14.613	2.4270E-07	1.2222E-11	1.2222E-11
27	U	1	16.408	1.8599E-05	9.3662E-10	9.3662E-10
28	UO	1	-7.249	1.9069E-03	9.6026E-08	9.6026E-08
29	UO2	1	-28.359	1.5311E-02	7.7104E-07	7.7104E-07
30	UO3	1	-40.692	1.8978E-05	9.5569E-10	9.5569E-10
31	UO2(OH)2	1	-48.824	1.7534E-12	8.8296E-17	8.8296E-17
32	ZR	1	20.714	1.3241E-08	6.6677E-13	6.6677E-13
33	ZRO	1	-5.430	1.6322E-05	8.2195E-10	8.2195E-10
34	ZRO2	1	-19.342	9.8047E-08	4.9374E-12	4.9374E-12
35	ZROH	1	-1.194	1.6666E-08	8.3925E-13	8.3925E-13
36	ZR(OH)2	1	-16.302	2.3362E-11	1.1764E-15	1.1764E-15
37	SR	1	0.0	1.5783E+00	7.9482E-05	7.9482E-05
38	SRO	1	-6.045	3.6331E-06	1.8296E-10	1.8296E-10
39	SROH	1	-11.795	8.0521E-05	4.0549E-09	4.0549E-09
40	SR(OH)2	1	-22.683	1.6602E-09	8.3604E-14	8.3604E-14
41	LA	1	10.926	1.2965E-06	6.5291E-11	6.5291E-11
42	LAO	1	-16.936	8.9091E-03	4.4864E-07	4.4864E-07

43	LAOH	1	-6.153	1.3038E-08	6.5659E-13	6.5659E-13
44	LA(OH)2	1	-26.848	4.8801E-09	2.4575E-13	2.4575E-13
45	CE	1	11.621	1.0423E-04	5.2486E-09	5.2486E-09
46	CEO	1	-13.248	3.5916E-02	1.8086E-06	1.8086E-06
47	CEOH	1	-4.952	6.3230E-07	3.1841E-11	3.1841E-11
48	CE(OH)2	1	-20.060	8.8646E-10	4.4640E-14	4.4640E-14
49	CEO2	1	0.0	3.4575E-16	1.7411E-20	1.7411E-20
50	(CEO)2	1	0.0	2.0223E-19	1.0184E-23	1.0184E-23
51	H2O	1	-8.152	1.8712E-03	9.4229E-08	9.4229E-08
52	H2	1	0.0	9.8853E+01	4.9780E-03	4.9780E-03
53	FEO(L)	2	-8.922	1.1906E+01	4.0844E-05	0.0
54	CAO(L)	2	-22.312	9.9745E+04	3.4219E-01	0.0
55	SIO2(L)	2	-33.152	8.0605E+04	2.7652E-01	0.0
56	UO2(L)	2	-41.364	9.9999E+04	3.4306E-01	0.0
57	ZRO2(L)	2	-41.997	9.9337E+03	3.4079E-02	0.0
58	SRO(L)	2	-20.473	9.8421E+01	3.3764E-04	0.0
59	LA2O3(L)	2	-74.155	9.9994E+01	3.4304E-04	0.0
60	CEO2(L)	2	-39.822	9.9995E+02	3.4305E-03	0.0
61	FE(L)	3	0.0	9.9982E+04	9.9834E-01	0.0
62	MO(L)	3	0.0	1.0000E+02	9.9853E-04	0.0
63	ZR(L)	3	0.0	6.6142E+01	6.6045E-04	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -1.6905E+11 JOULE
*** ELEMENT C WAS REPLACED BY SPECIES CO
** CONVERGED, ITERATION= 5 (LIMIT= 1) TIME (MS)= 111.000 TIME FOR INITIAL GUESS (MS)=22.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART 8

CASE 4 TEMPERATURE (K)= 2500.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 5.363E+03

INPUT GRAM-ATOMS OF ELEMENTS

O	H	C	FE	MO	CA	SI	U	ZR	SR
5.027E+05	2.000E+02	1.000E+02	1.000E+05	1.000E+02	1.000E+05	1.000E+05	1.000E+05	1.000E+04	1.000E+02

LA	CE
2.000E+02	1.000E+03

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	3.686	3.6434E+01	1.3921E-03	1.3921E-03
2	OH	1	16.149	7.3881E-09	2.8229E-13	2.8229E-13
3	O	1	1.343	3.5808E-01	1.3682E-05	1.3682E-05
4	O2	1	0.0	7.1853E-05	2.7454E-09	2.7454E-09
5	CO2	1	-19.078	1.4219E-01	5.4328E-06	5.4328E-06
6	CO	1	-15.776	9.9857E+01	3.8154E-03	3.8154E-03
7	FE	1	3.539	7.5936E+02	2.9014E-02	2.9014E-02
8	FEO	1	1.330	3.6216E-01	1.3838E-05	1.3838E-05
9	FEOH	1	1.832	1.2184E-02	4.6552E-07	4.6552E-07
10	FE(OH)2	1	-4.884	2.9262E-05	1.1180E-09	1.1180E-09
11	MO	1	14.232	1.8364E-05	7.0164E-10	7.0164E-10
12	MOO	1	7.152	1.1428E-06	4.3665E-11	4.3665E-11
13	MOO2	1	-4.687	8.2985E-06	3.1707E-10	3.1707E-10
14	MOO3	1	-10.135	1.0105E-07	3.8611E-12	3.8611E-12
15	MOO2(OH2	1	-15.941	1.0360E-07	3.9583E-12	3.9583E-12
16	(MOO3)2	1	-9.658	9.6000E-24	3.6680E-28	3.6680E-28
17	(MOO3)3	1	-9.249	0.0	0.0	0.0
18	CA	1	0.0	1.3675E+02	5.2251E-03	5.2251E-03
19	CAO	1	-1.901	4.7934E-02	1.8315E-06	1.8315E-06
20	CAOH	1	-7.351	6.2004E-01	2.3691E-05	2.3691E-05
21	CA(OH)2	1	-13.891	1.2496E-03	4.7745E-08	4.7745E-08
22	SI	1	5.383	3.2269E+00	1.2330E-04	1.2330E-04
23	SIO	1	-13.431	2.5046E+04	9.5696E-01	9.5696E-01
24	SIO2	1	-13.592	1.5418E+00	5.8909E-05	5.8909E-05
25	SIOH	1	-0.877	4.9146E-03	1.8778E-07	1.8778E-07
26	SI(OH)2	1	-8.286	2.3615E-05	9.0229E-10	9.0229E-10
27	U	1	10.430	7.8213E-06	2.9884E-10	2.9884E-10
28	UO	1	-6.987	1.5024E-02	5.7405E-07	5.7405E-07
29	UO2	1	-22.405	3.9080E+00	1.4932E-04	1.4932E-04
30	UO3	1	-30.661	7.8842E-01	3.0124E-05	3.0124E-05
31	UO2(OH)2	1	-33.529	2.2427E-06	8.5691E-11	8.5691E-11
32	ZR	1	13.496	5.3426E-08	2.0413E-12	2.0413E-12
33	ZRO	1	-5.847	7.0397E-04	2.6898E-08	2.6898E-08
34	ZRO2	1	-15.478	5.6149E-04	2.1454E-08	2.1454E-08
35	ZROH	1	1.149	3.5802E-08	1.3679E-12	1.3679E-12
36	ZR(OH)2	1	-10.280	9.5833E-09	3.6616E-13	3.6616E-13
37	SR	1	0.0	4.8456E-01	1.8514E-05	1.8514E-05
38	SRO	1	-4.019	1.4122E-03	5.3956E-08	5.3956E-08
39	SROH	1	-7.440	2.4010E-03	9.1737E-08	9.1737E-08
40	SR(OH)2	1	-13.750	3.8452E-06	1.4692E-10	1.4692E-10
41	LA	1	6.046	1.0416E-05	3.9799E-10	3.9799E-10
42	LAO	1	-15.126	8.5489E-01	3.2664E-05	3.2664E-05

43	LAOH	1	-5.053	2.0039E-06	7.6565E-11	7.6565E-11
44	LA(OH)2	1	-18.908	6.0635E-06	2.3168E-10	2.3168E-10
45	CE	1	6.772	9.0145E-05	3.4443E-09	3.4443E-09
46	CEO	1	-11.208	3.0382E-01	1.1608E-05	1.1608E-05
47	CEOH	1	-3.694	9.2029E-06	3.5163E-10	3.5163E-10
48	CE(OH)2	1	-13.315	4.0426E-07	1.5446E-11	1.5446E-11
49	CEO2	1	0.0	2.1602E-10	8.2537E-15	8.2537E-15
50	(CEO)2	1	0.0	6.4942E-16	2.4813E-20	2.4813E-20
51	H2O	1	-5.121	7.0888E-01	2.7085E-05	2.7085E-05
52	H2	1	0.0	8.0759E+01	3.0857E-03	3.0857E-03
53	FEO(L)	2	-5.867	5.3881E+03	1.8491E-02	0.0
54	CAO(L)	2	-14.040	9.9860E+04	3.4270E-01	0.0
55	SIO2(L)	2	-21.974	7.4949E+04	2.5721E-01	0.0
56	UO2(L)	2	-30.145	9.9995E+04	3.4316E-01	0.0
57	ZRO2(L)	2	-29.763	9.9998E+03	3.4318E-02	0.0
58	SRO(L)	2	-12.771	9.9510E+01	3.4150E-04	0.0
59	LA2O3(L)	2	-52.786	9.9570E+01	3.4170E-04	0.0
60	CEO2(L)	2	-26.753	9.9969E+02	3.4308E-03	0.0
61	FE(L)	3	0.0	9.3852E+04	9.9893E-01	0.0
62	MO(L)	3	0.0	1.0000E+02	1.0644E-03	0.0
63	ZR(L)	3	0.0	1.3928E-01	1.4825E-06	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -1.4858E+11 JOULE
*** ELEMENT C WAS REPLACED BY SPECIES CO
** CONVERGED, ITERATION= 6 (LIMIT= 4) TIME (MS)= 128.000 TIME FOR INITIAL GUESS (MS)=21.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B

CASE 5 TEMPERATURE (K)= 2000.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 1.352E+03

INPUT GRAM-ATOMS OF ELEMENTS

O	H	C	FE	MO	CA	SI	U	ZR	SR
3.227E+05	2.000E+02	1.000E+02	1.000E+05	1.000E+02	1.000E+05	1.000E+04	1.000E+05	1.000E+04	1.000E+02

LA	CE
2.000E+02	1.000E+03

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	6.422	1.4704E+00	1.7851E-04	1.7851E-04
2	OH	1	20.595	4.7199E-16	5.7302E-20	5.7302E-20
3	O	1	5.706	1.2585E-08	1.5279E-12	1.5279E-12
4	O2	1	0.0	1.7378E-15	2.1098E-19	2.1098E-19
5	CO2	1	-23.832	3.6764E-05	4.4634E-09	4.4634E-09
6	CO	1	-17.147	9.9999E+01	1.2141E-02	1.2141E-02
7	FE	1	8.025	2.5437E+00	3.0882E-04	3.0882E-04
8	FEO	1	3.736	8.5174E-08	1.0341E-11	1.0341E-11
9	FEOH	1	2.750	2.5069E-08	3.0436E-12	3.0436E-12
10	FE(OH)2	1	-9.192	1.9414E-13	2.3570E-17	2.3570E-17
11	MO	1	21.942	2.2977E-09	2.7895E-13	2.7895E-13
12	MOO	1	11.548	3.4489E-14	4.1873E-18	4.1873E-18
13	MOO2	1	-5.076	2.6279E-16	3.1904E-20	3.1904E-20
14	MOO3	1	-14.579	1.6167E-21	1.9628E-25	1.9628E-25
15	MOO2(OH2	1	-26.237	2.2531E-18	2.7354E-22	2.7354E-22
16	(MOO3)2	1	-16.541	0.0	0.0	0.0
17	(MOO3)3	1	-17.097	0.0	0.0	0.0
18	CA	1	0.0	1.7352E+03	2.1066E-01	2.1066E-01
19	CAO	1	-3.456	2.5246E-05	3.0650E-09	3.0650E-09
20	CAOH	1	-11.550	9.0784E-03	1.1022E-06	1.1022E-06
21	CA(OH)2	1	-23.036	4.4559E-08	5.4098E-12	5.4098E-12
22	SI	1	10.132	1.1120E+02	1.3500E-02	1.3500E-02
23	SIO	1	-15.386	6.1768E+03	7.4991E-01	7.4991E-01
24	SIO2	1	-17.912	3.5463E-05	4.3054E-09	4.3054E-09
25	SIOH	1	-0.991	3.7974E-04	4.6104E-08	4.6104E-08
26	SI(OH)2	1	-14.613	1.5778E-08	1.9156E-12	1.9156E-12
27	U	1	16.408	1.5302E-03	1.8578E-07	1.8578E-07
28	UO	1	-7.249	1.3208E-02	1.6036E-06	1.6036E-06
29	UO2	1	-28.359	8.9287E-03	1.0840E-06	1.0840E-06
30	UO3	1	-40.692	9.3171E-07	1.1312E-10	1.1312E-10
31	UO2(OH)2	1	-48.824	1.7544E-14	2.1299E-18	2.1299E-18
32	ZR	1	20.714	4.5752E-07	5.5546E-11	5.5546E-11
33	ZRO	1	-5.430	4.7482E-05	5.7647E-09	5.7647E-09
34	ZRO2	1	-19.342	2.4013E-08	2.9153E-12	2.9153E-12
35	ZROH	1	-1.194	7.5433E-08	9.1581E-12	9.1581E-12
36	ZR(OH)2	1	-16.302	1.3851E-11	1.6816E-15	1.6816E-15
37	SR	1	0.0	1.0001E+01	1.2142E-03	1.2142E-03
38	SRO	1	-6.045	1.9382E-06	2.3531E-10	2.3531E-10
39	SROH	1	-11.795	6.6834E-05	8.1141E-09	8.1141E-09
40	SR(OH)2	1	-22.683	1.8050E-10	2.1914E-14	2.1914E-14
41	LA	1	10.926	2.6103E-05	3.1691E-09	3.1691E-09
42	LAO	1	-16.936	1.5101E-02	1.8333E-06	1.8333E-06

43	LAOH	1	-6.153	3.4385E-08	4.1745E-12	4.1745E-12
44	LA(OH)2	1	-26.848	1.6858E-09	2.0467E-13	2.0467E-13
45	CE	1	11.621	8.5733E-03	1.0409E-06	1.0409E-06
46	CEO	1	-13.248	2.4872E-01	3.0196E-05	3.0196E-05
47	CEOH	1	-4.952	6.8129E-06	8.2713E-10	8.2713E-10
48	CE(OH)2	1	-20.060	1.2511E-09	1.5190E-13	1.5190E-13
49	CEO2	1	0.0	2.0158E-16	2.4473E-20	2.4473E-20
50	(CEO)2	1	0.0	2.3382E-17	2.8387E-21	2.8387E-21
51	H2O	1	-8.152	1.5818E-04	1.9204E-08	1.9204E-08
52	H2	1	0.0	9.9260E+01	1.2051E-02	1.2051E-02
53	FEO(L)	2	-8.922	6.7416E-01	3.2516E-06	0.0
54	CAO(L)	2	-22.312	9.8263E+04	4.7393E-01	0.0
55	SIO2(L)	2	-33.152	3.7118E+03	1.7902E-02	0.0
56	UO2(L)	2	-41.364	9.9998E+04	4.8230E-01	0.0
57	ZRO2(L)	2	-41.997	4.1720E+03	2.0122E-02	0.0
58	SRO(L)	2	-20.473	9.0036E+01	4.3425E-04	0.0
59	LA2O3(L)	2	-74.155	9.9988E+01	4.8225E-04	0.0
60	CEO2(L)	2	-39.822	9.9973E+02	4.8218E-03	0.0
61	FE(L)	3	0.0	9.9997E+04	9.4404E-01	0.0
62	MO(L)	3	0.0	1.0000E+02	9.4407E-04	0.0
63	ZR(L)	3	0.0	5.8279E+03	5.5020E-02	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -1.1619E+11 JOULE
*** ELEMENT C WAS REPLACED BY SPECIES CO
** CONVERGED, ITERATION= 5 (LIMIT= 1) TIME (MS)= 110.000 TIME FOR INITIAL GUESS (MS)=22.000

** MPEC ** CODE FOR EQUILIBRIUM CHEMICAL COMPOSITION
CSNI/GREST CCI CHEMICAL THERMODYNAMICS BENCHMARK PART B

CASE 6 TEMPERATURE (K)= 2500.00 (CONSTANT PRESSURE) PRESSURE(ATM)= 1.000 GAS VOLUME (M**3)= 3.874E+03
INPUT GRAM-ATOMS OF ELEMENTS

O	H	C	FE	MO	CA	SI	U	ZR	SR
3.227E+05	2.000E+02	1.000E+02	1.000E+05	1.000E+02	1.000E+05	1.000E+04	1.000E+05	1.000E+04	1.000E+02

LA	CE
2.000E+02	1.000E+03

NO.	SPECIES	MIXTURE	G/RT	MOLES	ACTIVITY	PARTIAL PRESSURE(ATM)
1	H	1	3.686	3.1532E+01	1.6704E-03	1.6704E-03
2	OH	1	16.149	9.8159E-11	5.2001E-15	5.2001E-15
3	O	1	1.343	3.9646E-03	2.1003E-07	2.1003E-07
4	O2	1	0.0	1.2213E-08	6.4698E-13	6.4698E-13
5	CO2	1	-19.078	2.1858E-03	1.1580E-07	1.1580E-07
6	CO	1	-15.776	9.9996E+01	5.2974E-03	5.2974E-03
7	FE	1	3.539	5.4316E+02	2.8774E-02	2.8774E-02
8	FEO	1	1.330	3.9768E-03	2.1067E-07	2.1067E-07
9	FEOH	1	1.832	1.6053E-04	8.5045E-09	8.5045E-09
10	FE(OH)2	1	-4.884	7.1024E-09	3.7626E-13	3.7626E-13
11	MO	1	14.232	1.2402E-05	6.5702E-10	6.5702E-10
12	MOO	1	7.152	1.1848E-08	6.2769E-13	6.2769E-13
13	MOO2	1	-4.687	1.3208E-09	6.9969E-14	6.9969E-14
14	MOO3	1	-10.135	2.4691E-13	1.3080E-17	1.3080E-17
15	MOO2(OH2	1	-15.941	3.6447E-13	1.9308E-17	1.9308E-17
16	(MOO3)2	1	-9.658	0.0	0.0	0.0
17	(MOO3)3	1	-9.249	0.0	0.0	0.0
18	CA	1	0.0	8.4809E+03	4.4928E-01	4.4928E-01
19	CAO	1	-1.901	4.5635E-02	2.4176E-06	2.4176E-06
20	CAOH	1	-7.351	7.0833E-01	3.7525E-05	3.7525E-05
21	CA(OH)2	1	-13.891	2.6296E-05	1.3931E-09	1.3931E-09
22	SI	1	5.383	7.9733E+01	4.2240E-03	4.2240E-03
23	SIO	1	-13.431	9.5001E+03	5.0328E-01	5.0328E-01
24	SIO2	1	-13.592	8.9776E-03	4.7560E-07	4.7560E-07
25	SIOH	1	-0.877	2.2369E-03	1.1850E-07	1.1850E-07
26	SI(OH)2	1	-8.286	1.9800E-07	1.0489E-11	1.0489E-11
27	U	1	10.430	3.4478E-02	1.8265E-06	1.8265E-06
28	UO	1	-6.987	1.0167E+00	5.3860E-05	5.3860E-05
29	UO2	1	-22.405	4.0598E+00	2.1507E-04	2.1507E-04
30	UO3	1	-30.661	1.2573E-02	6.6608E-07	6.6608E-07
31	UO2(OH)2	1	-33.529	7.9058E-10	4.1882E-14	4.1882E-14
32	ZR	1	13.496	2.1589E-04	1.1437E-08	1.1437E-08
33	ZRO	1	-5.847	4.3669E-02	2.3134E-06	2.3134E-06
34	ZRO2	1	-15.478	5.3469E-04	2.8326E-08	2.8326E-08
35	ZROH	1	1.149	2.6649E-06	1.4118E-10	1.4118E-10
36	ZR(OH)2	1	-10.280	1.3141E-08	6.9614E-13	6.9614E-13
37	SR	1	0.0	2.4800E+01	1.3138E-03	1.3138E-03
38	SRO	1	-4.019	1.1095E-03	5.8778E-08	5.8778E-08
39	SROH	1	-7.440	2.2636E-03	1.1992E-07	1.1992E-07
40	SR(OH)2	1	-13.750	6.6780E-08	3.5377E-12	3.5377E-12
41	LA	1	6.046	4.6799E-03	2.4792E-07	2.4792E-07
42	LAO	1	-15.126	5.8963E+00	3.1236E-04	3.1236E-04

43	LAOH	1	-5.053	1.6585E-05	8.7859E-10	8.7859E-10
44	LA(OH)2	1	-18.908	9.2442E-07	4.8972E-11	4.8972E-11
45	CE	1	6.772	3.8933E-01	2.0625E-05	2.0625E-05
46	CEO	1	-11.208	2.0143E+01	1.0671E-03	1.0671E-03
47	CEOH	1	-3.694	7.3218E-04	3.8788E-08	3.8788E-08
48	CE(OH)2	1	-13.315	5.9247E-07	3.1387E-11	3.1387E-11
49	CEO2	1	0.0	2.1987E-10	1.1648E-14	1.1648E-14
50	(CEO)2	1	0.0	3.9582E-12	2.0969E-16	2.0969E-16
51	H2O	1	-5.121	1.1301E-02	5.9869E-07	5.9869E-07
52	H2	1	0.0	8.3868E+01	4.4430E-03	4.4430E-03
53	FEO(L)	2	-5.867	5.6953E+01	2.8152E-04	0.0
54	CAO(L)	2	-14.040	9.1518E+04	4.5237E-01	0.0
55	SIO2(L)	2	-21.974	4.2011E+02	2.0766E-03	0.0
56	UO2(L)	2	-30.145	9.9994E+04	4.9427E-01	0.0
57	ZRO2(L)	2	-29.763	9.1665E+03	4.5310E-02	0.0
58	SRO(L)	2	-12.771	7.5262E+01	3.7202E-04	0.0
59	LA2O3(L)	2	-52.786	9.7047E+01	4.7970E-04	0.0
60	CEO2(L)	2	-26.753	9.7946E+02	4.8414E-03	0.0
61	FE(L)	3	0.0	9.9400E+04	9.9070E-01	0.0
62	MO(L)	3	0.0	1.0000E+02	9.9668E-04	0.0
63	ZR(L)	3	0.0	8.3335E+02	8.3059E-03	0.0

***(CONST. PRESSURE) TOTAL GIBBS FREE ENERGY= -1.0282E+11 JOULE
END OF DISSPLA 10.0 -- 250544 VECTORS IN 2 PLOTS.
RUN ON 6/17/88 USING SERIAL NUMBER 1 AT ISSCO SD
PROPRIETARY SOFTWARE PRODUCT OF ISSCO, SAN DIEGO, CALIF.
19944 VIRTUAL STORAGE REFERENCES; 7 READS; 0 WRITES.