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

January 1989

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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

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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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 exercise¹⁾ 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 code²⁾, which is the second version of MPEC³⁾ and was developed by Uchida as part of a computer code HORN⁴⁾ 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 code⁵⁾. 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.

The components in each phase are as follows:

Gas : O₂, UO₂, UO₃, UOH, H₂, H₂O, Zr, Cr, La, LaO, K, KOH

Oxide solution : UO₂, U₂O_{4.5}, ZrO₂, Cr₂O₃, K₂O

Metal solution : U, Zr, Cr, La, K

(2) Thermodynamic data

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

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

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 ₂ O (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 ₂ O _{4.5} (o)	-2.250000E+6	3.914E+2
ZrO ₂ (o)	-1.098000E+6	1.940E+2
Cr ₂ O ₃ (o)	-1.120776E+6	2.534E+2
La ₂ O ₃ (o)	-1.790049E+6	2.820E+2
K ₂ O (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 ₂ O (g)	5.0E+4
UO ₂ (o)	3.0E+5
La ₂ O ₃ (o)	1.0E+2
K ₂ O (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 : H₂O, CO₂
 Oxide solution : UO₂, SiO₂, SrO, CaO, La₂O₃, CeO₂
 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 ₂ O ₃	10 ²	10 ²	10 ²
CeO ₂	10 ³	10 ³	10 ³
Mo	10 ²	10 ²	10 ²
H ₂ O	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 HORN³⁾ 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 whose 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

$$G_{\text{tot}} = \sum_i^N x_i \{G_i^0 + RT \ln(a_i)\} \quad (3.1)$$

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:

$$\sum_i^N A_{ij} x_i = b_j \quad (j=1, \dots, L) \quad (3.2)$$

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 $g_i^0 = G_i^0/RT$,

$$\sum_i^N A_{ij} \pi_j - [g_i^0 + \ln(P) + \ln(x_i/X_1)] = 0 \quad (3.3)$$

For a species in a condensed ideal solution m ,

$$\sum_i^N A_{ij} \pi_j - [g_i^0 + \ln(x_i/X_m)] = 0 \quad (3.4)$$

For a species forming a pure phase,

$$\sum_j^L A_{ij} \pi_j - g_i^0 = 0 \quad (3.5)$$

where π_j 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.

$$X_m = \sum x_i \text{ (for all } i \text{ that belong to } m\text{)}. \quad (3.6)$$

Equations (3.2) - (3.6) constitute $(L+M+N)$ simultaneous equations whose unknowns are π_j , 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:

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

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

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

and

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

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,

$$z_i = \sum_j^L A_{ij} \pi_j + W_m - g_i^0 \quad (3.10)$$

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 π_j and W_m ($=z_i$ for pure phase). These simultaneous equations are solved by the Gauss' elimination method. The iterative 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.

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

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 code⁴⁾, 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

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

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 are 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.

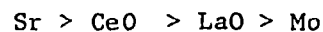
Before discussing the results of the present analysis, it should be pointed out that the number of moles in the gas phase calculated by the present analysis is not proportional to the FP release rate in a severe accident. The FP release is influenced not only by chemical equilibrium but also by mass 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

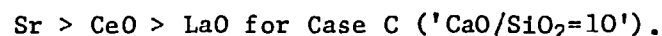
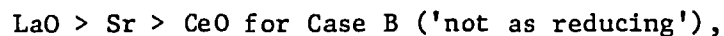
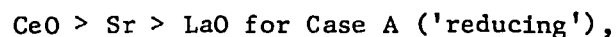
In Table 5.4 it should be noted that the most volatile form (the species that is most abundant in gas phase) of FP elements Mo, Sr, La, and Ce are Mo, Sr, LaO, and CeO. These are common to Cases A, B, and C at both 2000 K and 2500 K.

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



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



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 ' $\text{CaO/SiO}_2=10$ ', which means that the oxygen potential is in the order of

$$\text{Case B} > \text{Case C} > \text{Case A.}$$

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

$$\mu_{\text{O}_2} = RT(\ln P_{\text{O}_2}), \quad (5.2)$$

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

$$\text{Case A} > \text{Case C} > \text{Case B.}$$

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

$$\text{Case B} > \text{Case C} > \text{Case A.}$$

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 oxygen. Therefore the oxygen 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 oxygen 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 MoO₃ which is stable only at very high oxygen potential. In the present cases, the oxygen potential is not high enough to make MoO₃ 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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- 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

O ₂ (G)	3.0118E-08
UO ₂ (G)	3.5081E+00
UO ₃ (G)	1.3505E-02
UOH(G)	6.9720E-04
H ₂ (G)	4.9993E+04
H ₂ O(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

UO ₂ (O)	2.7550E+05
U ₂ O ₄ (O)	2.1692E+01
ZrO ₂ (O)	5.6996E+04
Cr ₂ O ₃ (O)	8.0494E-04
La ₂ O ₃ (O)	5.9338E+01
K ₂ O(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 ₂ O,	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,
SiO₂,
UO₂,
ZrO₂,
SrO,
La₂O₃,
CeO₂.

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
<u>Gas Phase</u>			<u>Gas Phase (Continued)</u>		
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	<u>Oxide Phase</u>		
MOO2(OH)2	-856305.2	209.9412	FEO(L)	-254098.5	52.8420
(MOO3)2	-572461.1	148.6599	CAO(L)	-687974.9	158.4201
(MOO3)3	-652717.9	184.1623	SiO2(L)	-929720.7	189.1358
CA	0.0	0.0	UO2(L)	-933112.1	122.5321
CAO	-129326.1	35.9236	ZRO2(L)	-1017459.4	159.4476
CAOH	-349212.6	78.5473	SRO(L)	-640530.1	149.9929
CA(OH)2	-760548.9	188.6878	LA2O3(L)	-1777233.0	271.8740
SI	395028.2	-113.2433	CEO2(L)	-1086935.0	212.2707
SiO	-162614.9	-46.6569			
SiO2	-359269.2	30.6646	<u>Metal Phase</u>		
SiOH	-9438.3	-3.5211	FE(L)	0.0	0.0
Si(OH)2	-526150.9	141.5432	MO(L)	0.0	0.0
U	497157.4	-112.1183	ZR(L)	0.0	0.0
UO	-21771.4	-49.4042			
UO2	-495160.2	11.7230			
UO3	-834291.1	78.7118			
UO2(OH)2	-1272129.0	229.9977			
ZR	600324.3	-127.8879			
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
Benchmark Part B

	Case A (2000K)	Case A (2500K)	Case B
<u>Gas Phase</u>			
H	1.5987E+00	2.8506E+01	
OH	2.5239E-16	1.4294E-11	
O	7.3217E-09	5.1242E-04	
O2	4.9723E-16	2.5356E-10	
CO2	1.8081E-05	3.5113E-04	
CO	9.9998E+01	9.9999E+01	
FE	1.6338E+00	2.2905E+02	
FEO	2.6907E-08	2.6938E-04	
FEOH	7.2793E-09	1.2252E-05	
FE(OH)2	2.5484E-14	9.8111E-11	
MO	1.4758E-09	5.2106E-06	
MOO	1.0895E-14	7.9964E-10	
MOO2	4.0828E-17	1.4319E-11	
MOO3	1.2354E-22	4.2999E-16	
MOO2(OH)2	1.4546E-19	8.0576E-16	
(MOO3)2	0.0	0.0	
(MOO3)3	0.0	0.0	
CA	7.0168E+02	4.5203E+03	
CAO	5.0211E-06	3.9072E-03	
CAOH	1.6597E-03	6.8332E-02	
CA(OH)2	3.6826E-09	4.5913E-07	
SI	3.1092E+02	4.9420E+02	
SiO	8.4945E+03	9.4586E+03	
SiO2	2.3986E-05	1.4358E-03	
SiOH	4.8003E-04	2.5094E-03	
Si(OH)2	9.0163E-09	4.0202E-08	
U	1.3297E-02	1.9045E+00	
UO	5.6444E-02	9.0213E+00	
UO2	1.8767E-02	5.7867E+00	
UO3	9.6314E-07	2.8788E-03	
UO2(OH)2	7.5360E-15	3.6913E-11	
Zr	4.7889E-06	1.0044E-02	
ZrO	2.4444E-04	3.2635E-01	
ZrO2	6.0798E-08	6.4189E-04	
ZrOH	3.5694E-07	2.2439E-05	
Zr(OH)2	2.9629E-11	2.0026E-08	
SR	3.2193E+01	7.4516E+01	
SrO	3.0683E-06	5.3552E-04	
SrOH	9.7254E-05	1.2310E-03	
Sr(OH)2	1.1874E-10	6.5730E-09	
LA	1.1932E-04	7.5911E-02	
LAO	3.3949E-02	1.5364E+01	
LAOH	7.1056E-08	4.8689E-05	
LA(OH)2	1.5749E-09	4.5120E-07	
CE	7.4430E-02	1.8233E+01	
CEO	1.0620E+00	1.5154E+02	
CEOH	2.6739E-05	6.2059E-03	
CE(OH)2	2.2198E-09	9.0889E-07	
CEO2	4.2331E-16	2.6569E-10	
(CEO)2	3.6038E-16	2.7840E-10	
H2O	7.7749E-05	1.8543E-03	
H2	9.9199E+01	8.5666E+01	
<u>Oxide Phase</u>			
FeO(L)	1.0132E-01	2.7063E+00	
CAO(L)	9.2982E+03	5.4967E+03	
SiO2(L)	1.1945E+03	4.7133E+01	
UO2(L)	9.9999E+04	9.9982E+04	
ZrO2(L)	5.0257E+03	7.7194E+03	
SrO(L)	6.7815E+01	2.5482E+01	
LA2O3(L)	9.9978E+01	9.2277E+01	
CEO2(L)	9.9885E+02	8.3029E+02	
<u>Metal Phase</u>			
Fe(L)	9.9998E+04	9.9768E+04	
MD(L)	1.0000E+02	1.0000E+02	
Zr(L)	9.4974E+04	9.2280E+04	

n gas, oxide, and metal phases calculated for

(2000K)	Case B (2500K)	Case C (2000K)	Case C (2500K)
1.2784E+00	3.6434E+01	1.4704E+00	3.1532E+01
1.6870E-15	7.3881E-09	4.7199E-16	9.8159E-11
1.6040E-07	2.5808E-01	1.2585E-08	3.9646E-03
1.9111E-13	7.1853E-05	1.7378E-15	1.2213E-08
1.3669E-04	1.4219E-01	3.6764E-05	2.1858E-03
1.9999E+01	9.9857E+01	9.9999E+01	9.9996E+01
1.4853E+00	7.5936E+02	2.5437E+00	5.4316E+02
1.5794E-06	3.6216E-01	8.5174E-08	3.9768E-03
1.8794E-07	1.2184E-02	2.5069E-08	1.6053E-04
2.8848E-11	2.9262E-05	1.9414E-13	7.1024E-09
5.8590E-09	1.8364E-05	2.2977E-09	1.2402E-05
1.0446E-12	1.1428E-06	3.4489E-14	1.1848E-08
7.4542E-14	8.2985E-06	2.6279E-16	1.3208E-09
5.9088E-18	1.0105E-07	1.6167E-21	2.4691E-13
3.9774E-15	1.0360E-07	2.2531E-18	3.6447E-13
0.0	9.6000E-24	0.0	0.0
0.0	0.0	0.0	0.0
2.5428E+02	1.3675E+02	1.7352E+03	8.4809E+03
4.3945E-05	4.7934E-02	2.5246E-05	4.5635E-02
1.0157E-02	6.2004E-01	9.0784E-03	7.0833E-01
3.8057E-07	1.2496E-03	4.4559E-08	2.6296E-05
2.9349E+01	3.2269E+00	1.1120E+02	7.9733E+01
1.9365E+04	2.5046E+04	6.1768E+03	9.5001E+03
1.3206E-03	1.5418E+00	3.5463E-05	8.9776E-03
7.6518E-04	4.9146E-03	3.7974E-04	2.2369E-03
2.4270E-07	2.3615E-05	1.5778E-08	1.9800E-07
1.8599E-05	7.8213E-06	1.5302E-03	3.4478E-02
1.9069E-03	1.5024E-02	1.3208E-02	1.0167E+00
1.5311E-02	3.9080E+00	8.9287E-03	4.0598E+00
1.8978E-05	7.8842E-01	9.3171E-07	1.2573E-02
1.7534E-12	2.2427E-06	1.7544E-14	7.9058E-10
1.3241E-08	5.3426E-08	4.5752E-07	2.1589E-04
1.6322E-05	7.0397E-04	4.7482E-05	4.3669E-02
9.8047E-08	5.6149E-04	2.4013E-08	5.3469E-04
1.6666E-08	3.5802E-08	7.5433E-08	2.6649E-06
2.3362E-11	9.5833E-09	1.3851E-11	1.3141E-08
1.5783E+00	4.8456E-01	1.0001E+01	2.4800E+01
3.6331E-06	1.4122E-03	1.9382E-06	1.1095E-03
8.0521E-05	2.4010E-03	6.6834E-05	2.2636E-03
1.6602E-09	1.8452E-06	1.8050E-10	6.6780E-08
1.2965E-06	1.0416E-05	2.6103E-05	4.6799E-03
8.9091E-03	8.5489E-01	1.5101E-02	5.8963E+00
1.3038E-08	2.0039E-06	3.4385E-08	1.6585E-05
4.8801E-09	6.0635E-04	1.6858E-09	9.2442E-07
1.0423E-04	9.0145E-05	8.5733E-03	3.8933E-01
3.5916E-02	3.0382E-01	2.4872E-01	2.0143E+01
6.3230E-07	9.2029E-06	6.8129E-06	7.3218E-04
8.8646E-10	4.0426E-07	1.2511E-09	5.9247E-07
3.4575E-16	2.1602E-10	2.0158E-16	2.1987E-10
2.0223E-19	6.4942E-16	2.3382E-17	3.9582E-12
1.8712E-03	7.0888E-01	1.5818E-04	1.1301E-02
9.8853E+01	8.0759E+01	9.9260E+01	8.3868E+01
1.1906E+01	5.3881E+03	6.7416E-01	5.6953E+01
9.9745E+04	9.9860E+04	9.8263E+04	9.1518E+04
8.0605E+04	7.4949E+04	3.7118E+03	4.2011E+02
9.9999E+04	9.9995E+04	9.9998E+04	9.9994E+04
9.9337E+03	9.9998E+03	4.1720E+03	9.1665E+03
9.8421E+01	9.9510E+01	9.0036E+01	7.5262E+01
9.9994E+01	9.9570E+01	9.9988E+01	9.7047E+01
9.9995E+02	9.9969E+02	9.9973E+02	9.7946E+02
9.9982E+04	9.3852E+04	9.9997E+04	9.9400E+04
1.0000E+02	1.0000E+02	1.0000E+02	1.0000E+02
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

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

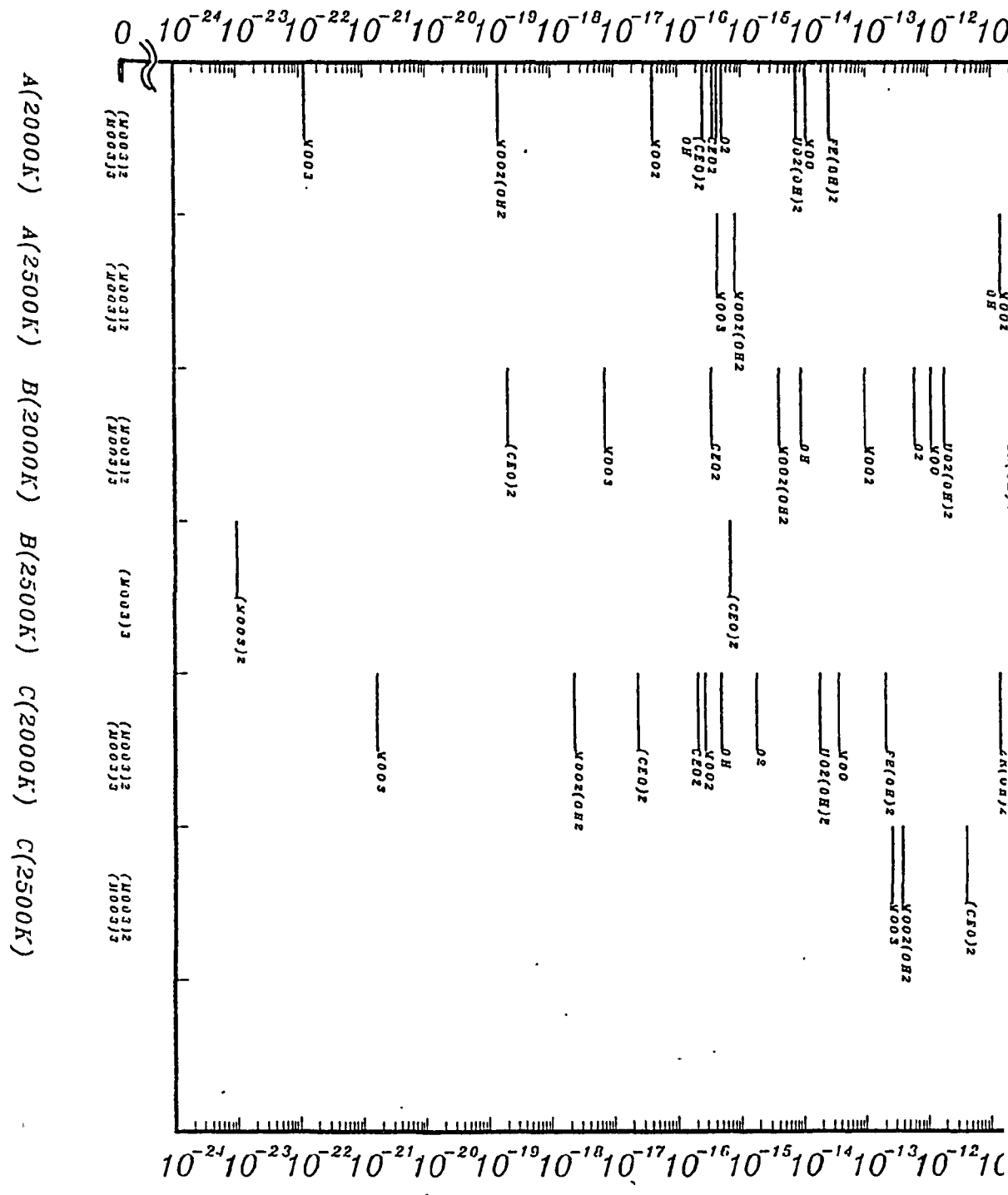


Fig. 5.1 Graphical pre: species calcu.

APPENDIX A

INPUT AND OUTPUT LISTING OF PART A ANALYSIS

INPUT DATA LIST

CARD NO.	1	2	3	4	5	6	7	8
1.	GSNI/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)= 5H02(G),							
6.	TEXT(02)= 6HU02(G),							
7.	TEXT(03)= 6HU03(G),							
8.	TEXT(04)= 6HU0H(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)= 6HLA0(G),							
15.	TEXT(11)= 4HK(G),							
16.	TEXT(12)= 6HKOH(G),							
17.	TEXT(13)= 6HU02(O),							
18.	TEXT(14)= 8HU2O45(O),							
19.	TEXT(15)= 7HZR02(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.	LA0(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.	ZR02(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		

INPUT DATA LIST

CARD NO.	1	2	3	4	5	6	7	8
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.	U2O4(O)		-2250000.	391.4				
66.	ZR2O(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	U2O4(O)	2	4.500	2.000	0.0	0.0	0.0	0.0	0.0
15	ZR2O(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	U2O4(O)	2	-61.153	2.1690E+01	6.5223E-05	0.0
15	ZR2(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	0.0
2	UO2(G)	0.0	-5.0836E+05	2.2800E+00	0.0	0.0	0.0	0.0
3	UO3(G)	0.0	-8.3680E+05	8.1170E+01	0.0	0.0	0.0	0.0
4	UOH(G)	0.0	2.4939E+04	-2.6190E+00	0.0	0.0	0.0	0.0
5	H2(G)	0.0	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	0.0
7	ZR(G)	0.0	6.0960E+05	-1.3200E+02	0.0	0.0	0.0	0.0
8	CR(G)	0.0	3.7943E+05	-1.3180E+02	0.0	0.0	0.0	0.0
9	LA(G)	0.0	4.2087E+05	-1.1420E+02	0.0	0.0	0.0	0.0
10	LAO(G)	0.0	-1.4771E+05	-5.2720E+01	0.0	0.0	0.0	0.0
11	K(G)	0.0	6.8864E+04	-6.9760E+01	0.0	0.0	0.0	0.0
12	KOH(G)	0.0	-2.4028E+05	1.0740E+01	0.0	0.0	0.0	0.0
13	UO2(O)	0.0	-1.0800E+06	1.6900E+02	0.0	0.0	0.0	0.0
14	U2O45(O)	0.0	-2.2500E+06	3.9140E+02	0.0	0.0	0.0	0.0
15	ZRO2(O)	0.0	-1.0980E+06	1.9400E+02	0.0	0.0	0.0	0.0
16	CR2O3(O)	0.0	-1.1208E+06	2.5340E+02	0.0	0.0	0.0	0.0
17	LA2O3(O)	0.0	-1.7900E+06	2.8200E+02	0.0	0.0	0.0	0.0
18	K2O(O)	0.0	-4.5470E+05	2.2540E+02	0.0	0.0	0.0	0.0
19	U(M)	0.0	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	0.0
21	CR(M)	0.0	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	0.0
23	K(M)	0.0	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.	1	2	3	4	5	6	7	8
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,2HS1,1HU,2HZR,2HSR,2HLA,2HCE, IPC=1,							00250003
4.	IFEF=1, IOM=1,							00260003
5.	TEXT(1)=BHH / IPC=1,							00270001
6.	TEXT(2)=BHOH / IPC=1,							00280001
7.	TEXT(3)=BHO / IPC=1,							00290001
8.	TEXT(4)=BHQ2 / IPC=1,							00300001
9.	TEXT(5)=BHCO2 / IPC=1,							00310001
10.	TEXT(6)=BHCO / IPC=1,							00320001
11.	TEXT(7)=BHFE / IPC=1,							00330001
12.	TEXT(8)=BHFE0 / IPC=1,							00340001
13.	TEXT(9)=BHFE0H / IPC=1,							00350003
14.	TEXT(10)=BHFF(OH)2 / IPC=1,							00360001
15.	TEXT(11)=BHMO / IPC=1,							00370001
16.	TEXT(12)=BHMO0 / IPC=1,							00380001
17.	TEXT(13)=BHMO02 / IPC=1,							00390003
18.	TEXT(14)=BHMO03 / IPC=1,							00400003
19.	TEXT(15)=BHMO02(OH)2 / IPC=1,							00410003
20.	TEXT(16)=BH(MO03)2 / IPC=1,							00420003
21.	TEXT(17)=BH(MO03)3 / IPC=1,							00430003
22.	TEXT(18)=BHCA / IPC=1,							00440001
23.	TEXT(19)=BHCAO / IPC=1,							00450001
24.	TEXT(20)=BHCAOH / IPC=1,							00460003
25.	TEXT(21)=BHCA(OH)2 / IPC=1,							00470003
26.	TEXT(22)=BHS1 / IPC=1,							00480001
27.	TEXT(23)=BHS10 / IPC=1,							00490003
28.	TEXT(24)=BHS102 / IPC=1,							00500003
29.	TEXT(25)=BHS1OH / IPC=1,							00510003
30.	TEXT(26)=BHS1(OH)2 / IPC=1,							00520003
31.	TEXT(27)=BHU / IPC=1,							00530001
32.	TEXT(28)=BHU0 / IPC=1,							00540003
33.	TEXT(29)=BHU02 / IPC=1,							00550003
34.	TEXT(30)=BHU03 / IPC=1,							00560003
35.	TEXT(31)=BHU02(OH)2 / IPC=1,							00570003
36.	TEXT(32)=BHZR / IPC=1,							00580001
37.	TEXT(33)=BHZRO / IPC=1,							00590001
38.	TEXT(34)=BHZRO2 / IPC=1,							00600001
39.	TEXT(35)=BHZROH / IPC=1,							00610003
40.	TEXT(36)=BHZR(OH)2 / IPC=1,							00620003
41.	TEXT(37)=BHSR / IPC=1,							00630001
42.	TEXT(38)=BHSRO / IPC=1,							00640001
43.	TEXT(39)=BHSROH / IPC=1,							00650003
44.	TEXT(40)=BHSR(OH)2 / IPC=1,							00660003
45.	TEXT(41)=BHLA / IPC=1,							00670001
46.	TEXT(42)=BHLAO / IPC=1,							00680001
47.	TEXT(43)=BHLAOH / IPC=1,							00690003
48.	TEXT(44)=BHLA(OH)2 / IPC=1,							00700003
49.	TEXT(45)=BHCE / IPC=1,							00710001
50.	TEXT(46)=BHCEO / IPC=1,							00720001

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CARD NO.	1	2	3	4	5	6	7	8
51.	TEXT(47)=BHCEOH	IPC=1						00740003
52.	TEXT(48)=BHCE(OH)2	IPC=1						00750003
53.	TEXT(49)=BHCEO2	IPC=1						00751003
54.	TEXT(50)=BH(CED)2	IPC=1						00752003
55.	TEXT(51)=BHH2O	IPC=1						00760003
56.	TEXT(52)=BHH2	IPC=1						00770003
57.	TEXT(53)=BHFE(O(L))	IPC=1						00780003
58.	TEXT(54)=BHCAO(L)	IPC=1						00790003
59.	TEXT(55)=BHSIO2(L)	IPC=1						00800003
60.	TEXT(56)=BHUO2(L)	IPC=1						00810003
61.	TEXT(57)=BHZRO2(L)	IPC=1						00820003
62.	TEXT(58)=BHSRO(L)	IPC=1						00830003
63.	TEXT(59)=BHLA2O3(L)	IPC=1						00840003
64.	TEXT(60)=BHCEO2(L)	IPC=1						00850003
65.	TEXT(61)=BHFE(L)	IPC=1						00860003
66.	TEXT(62)=BHMO(L)	IPC=1						00870003
67.	TEXT(63)=BHZR(L)	IPC=1						00880003
68.	IGT=0,1, &END							00890003
69.	H	0	1	0	0	0	0	00900003
70.	OH	1	1	0	0	0	0	00910001
71.	O	1	0	0	0	0	0	00920001
72.	O2	2	0	0	0	0	0	00930001
73.	CO2	2	0	0	0	0	0	00940001
74.	CO	1	0	1	0	0	0	00950001
75.	FE	0	0	0	0	0	0	00960001
76.	FE0	1	0	0	0	0	0	00970001
77.	FE0H	1	1	0	0	0	0	00980003
78.	FE(OH)2	2	2	0	0	0	0	00990003
79.	MO	0	0	0	0	0	0	01000001
80.	MO0	1	0	0	0	0	0	01010001
81.	MO02	2	0	0	0	0	0	01020003
82.	MO03	3	0	0	0	0	0	01030003
83.	MO02(OH)2	3	2	0	0	0	0	01040003
84.	(MO03)2	6	0	0	0	0	0	01050003
85.	(MO03)3	9	0	0	0	0	0	01060003
86.	CA	0	0	0	1	0	0	01070001
87.	CAO	1	1	0	0	0	0	01080001
88.	CAOH	1	1	0	0	0	0	01090003
89.	CA(OH)2	2	2	0	0	0	0	01100003
90.	SI	0	0	0	1	0	0	01110001
91.	SiO	1	0	0	0	0	0	01120003
92.	SiO2	2	0	0	0	0	0	01130003
93.	SiOH	1	1	0	0	0	0	01140003
94.	Si(OH)2	2	2	0	0	0	0	01150003
95.	U(G)	0	0	0	0	0	0	01160003
96.	U0	1	0	0	0	0	0	01170003
97.	U02	2	0	0	0	0	0	01180003
98.	U03	3	0	0	0	0	0	01190003
99.	U02(OH)2	4	2	0	0	0	0	01200003
100.	ZR	0	0	0	0	0	0	01210001
		5	0	5	0	5	0	0

CARD NO.	1	2	3	4	5	6	7	8
101. ZRD	1	0	0	0	0	0	0	01220001
102. ZRD2	2	0	0	0	0	0	0	01230001
103. ZROH	1	1	0	0	0	0	0	01240003
104. ZR(OH)2	2	2	0	0	0	0	0	01250003
105. SR	0	0	0	0	0	0	0	01260001
106. SRD	1	0	0	0	0	0	0	01270001
107. SROH	1	1	0	0	0	0	0	01280003
108. SR(OH)2	2	2	0	0	0	0	0	01290003
109. LA	0	0	0	0	0	0	0	01300001
110. LAO	1	0	0	0	0	0	0	01310001
111. LAOH	1	1	0	0	0	0	0	01320003
112. LA(OH)2	2	2	0	0	0	0	0	01330003
113. CE	0	0	0	0	0	0	0	01340001
114. CED	1	0	0	0	0	0	0	01350001
115. CEDH	1	1	0	0	0	0	0	01370003
116. CE(OH)2	2	2	0	0	0	0	0	01380103
117. CE02	2	0	0	0	0	0	0	01381003
118. (CEO)2	2	0	0	0	0	0	2	01390001
119. H2O	1	2	0	0	0	0	0	01400001
120. H2	0	2	0	0	0	0	0	01410003
121. FED(L)	1	0	0	0	0	0	0	01420003
122. CAD(L)	1	0	0	0	0	0	0	01430003
123. SIO2(L)	1	0	0	0	0	0	0	01440003
124. UO2(L)	2	0	0	0	0	0	0	01450003
125. ZRO2(L)	2	0	0	0	0	0	0	01460003
126. SRO(L)	1	0	0	0	0	0	0	01470003
127. LA2O3(L)	3	0	0	0	0	0	0	01480003
128. CE02(L)	2	0	0	0	0	0	1	01490003
129. FE(L)	2	0	0	0	0	0	0	01500003
130. MO(L)	0	0	0	0	0	0	0	01510003
131. ZR(L)	0	0	0	0	0	0	0	01520000
132. H	0	0	0	0	0	0	0	01530000
133. OH	0	0	0	0	0	0	0	01540000
134. O	0	0	0	0	0	0	0	01550000
135. O2	0	0	0	0	0	0	0	01560000
136. CO2	0	0	0	0	0	0	0	01570000
137. CO	0	0	0	0	0	0	0	01580000
138. FE	0	0	0	0	0	0	0	01590000
139. FED	0	0	0	0	0	0	0	01600000
140. FE(OH)	0	0	0	0	0	0	0	01610000
141. FE(OH)2	0	0	0	0	0	0	0	01620000
142. MO	0	0	0	0	0	0	0	01630000
143. MOO	0	0	0	0	0	0	0	01640000
144. MOO2	0	0	0	0	0	0	0	01650000
145. MOO3	0	0	0	0	0	0	0	01660000
146. MOO2(OH)2	0	0	0	0	0	0	0	01670000
147. (MOO3)2	0	0	0	0	0	0	0	01680000
148. (MOO3)3	0	0	0	0	0	0	0	01690000
149. CA	0	0	0	0	0	0	0	01700000
150. CAD	0	0	0	0	0	0	0	01700000

INPUT DATA LIST							
1	2	3	4	5	6	7	8
151. CADH		-349212.6	.78.5473				01710000
152. CA(OH)2		-760548.9	188.6078				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. MD(L)		0.0	0.0				02092003
194. ZR(L)		0.0	0.0				02100003
195. ECOND2	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

INPUT DATA LIST								
CARD NO.	1	2	3	4	5	6	7	8
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** = 3 NO. OF PURE SUBSTANCES = 0
 NUMBER OF ELEMENTS (L) = 12 NO. OF MIXTURE = 3
 TOTAL NO. OF PHASES = 3 TOTAL NO. OF SPECIES = 63

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(OH)2	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

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

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

NO.	SPECIES	GF298KJ/MOL	T**1	0	TDDATA	1	0	0	0	0	0
1	H	0.0	0.0	0.0	-2.2747E+05	-6.0330E+01	0.0	0.0	0.0	0.0	0.0
2	OH	0.0	0.0	0.0	3.6983E+05	-1.3624E+01	0.0	0.0	0.0	0.0	0.0
3	O	0.0	0.0	0.0	3.6287E+05	-1.3398E+02	0.0	0.0	0.0	0.0	0.0
4	O2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	CO2	0.0	0.0	0.0	-3.9538E+05	-5.2340E-01	0.0	0.0	0.0	0.0	0.0
6	CO	0.0	0.0	0.0	-1.1403E+05	-8.5595E+01	0.0	0.0	0.0	0.0	0.0
7	FE	0.0	0.0	0.0	3.7312E+05	-1.1981E+02	0.0	0.0	0.0	0.0	0.0
8	FEO	0.0	0.0	0.0	2.0008E+05	-6.8968E+01	0.0	0.0	0.0	0.0	0.0
9	FEOH	0.0	0.0	0.0	7.6346E+04	-1.5303E+01	0.0	0.0	0.0	0.0	0.0
10	FE(OH)2	0.0	0.0	0.0	-3.5833E+05	1.0271E+02	0.0	0.0	0.0	0.0	0.0
11	MO	0.0	0.0	0.0	6.4123E+05	-1.3813E+02	0.0	0.0	0.0	0.0	0.0
12	MDO	0.0	0.0	0.0	3.6557E+05	-8.6742E+01	0.0	0.0	0.0	0.0	0.0
13	MDO2	0.0	0.0	0.0	-3.2390E+04	-2.6024E+01	0.0	0.0	0.0	0.0	0.0
14	MDO3	0.0	0.0	0.0	-3.6956E+05	6.3530E+01	0.0	0.0	0.0	0.0	0.0
15	MDO2(OH)2	0.0	0.0	0.0	-8.5631E+05	2.0994E+02	0.0	0.0	0.0	0.0	0.0
16	(MDO3)2	0.0	0.0	0.0	-5.7246E+05	1.4866E+02	0.0	0.0	0.0	0.0	0.0
17	(MDO3)3	0.0	0.0	0.0	-6.5272E+05	1.8416E+02	0.0	0.0	0.0	0.0	0.0
18	CA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	CAO	0.0	0.0	0.0	-1.2933E+05	3.5924E+01	0.0	0.0	0.0	0.0	0.0
20	CAOH	0.0	0.0	0.0	-3.4921E+05	7.8547E+01	0.0	0.0	0.0	0.0	0.0
21	CA(OH)2	0.0	0.0	0.0	-7.6055E+05	1.8869E+02	0.0	0.0	0.0	0.0	0.0
22	SI	0.0	0.0	0.0	3.9503E+05	-1.1324E+02	0.0	0.0	0.0	0.0	0.0
23	SiO	0.0	0.0	0.0	-1.6261E+05	-4.6657E+01	0.0	0.0	0.0	0.0	0.0
24	SiO2	0.0	0.0	0.0	-3.5927E+05	3.0665E+01	0.0	0.0	0.0	0.0	0.0
25	SiOH	0.0	0.0	0.0	-9.4383E+03	-3.5211E+00	0.0	0.0	0.0	0.0	0.0
26	Si(OH)2	0.0	0.0	0.0	-5.2615E+05	1.4154E+02	0.0	0.0	0.0	0.0	0.0
27	U	0.0	0.0	0.0	4.9716E+05	-1.1212E+02	0.0	0.0	0.0	0.0	0.0
28	UO	0.0	0.0	0.0	-2.1771E+04	-4.9404E+01	0.0	0.0	0.0	0.0	0.0
29	UO2	0.0	0.0	0.0	-4.9516E+05	1.1723E+01	0.0	0.0	0.0	0.0	0.0
30	UO3	0.0	0.0	0.0	-8.3429E+05	7.8712E+01	0.0	0.0	0.0	0.0	0.0
31	UO2(OH)2	0.0	0.0	0.0	-1.2721E+06	2.3000E+02	0.0	0.0	0.0	0.0	0.0
32	ZR	0.0	0.0	0.0	6.0032E+05	-1.2789E+02	0.0	0.0	0.0	0.0	0.0
33	ZRO	0.0	0.0	0.0	3.4717E+04	-6.2518E+01	0.0	0.0	0.0	0.0	0.0
34	ZRO2	0.0	0.0	0.0	-3.2135E+05	-1.8840E-01	0.0	0.0	0.0	0.0	0.0
35	ZROH	0.0	0.0	0.0	-1.9487E+05	8.7501E+01	0.0	0.0	0.0	0.0	0.0
36	ZR(OH)2	0.0	0.0	0.0	-5.0082E+05	1.1483E+02	0.0	0.0	0.0	0.0	0.0
37	SR	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
38	SRO	0.0	0.0	0.0	-1.6852E+05	3.3986E+01	0.0	0.0	0.0	0.0	0.0
39	SROH	0.0	0.0	0.0	-3.6218E+05	8.2996E+01	0.0	0.0	0.0	0.0	0.0
40	SR(OH)2	0.0	0.0	0.0	-7.4295E+05	1.8282E+02	0.0	0.0	0.0	0.0	0.0
41	LA	0.0	0.0	0.0	4.0586E+05	-1.1206E+02	0.0	0.0	0.0	0.0	0.0
42	LAO	0.0	0.0	0.0	-1.5052E+05	-6.5599E+01	0.0	0.0	0.0	0.0	0.0
43	LAOH	0.0	0.0	0.0	-9.1451E+04	-5.4470E+00	0.0	0.0	0.0	0.0	0.0
44	LA(OH)2	0.0	0.0	0.0	-6.6040E+05	1.0691E+02	0.0	0.0	0.0	0.0	0.0
45	CE	0.0	0.0	0.0	4.0333E+05	-1.0501E+02	0.0	0.0	0.0	0.0	0.0

46	CEO	0.0	-1.6967E+05	-2.5347E+01	0.0	0.0	0.0	0.0
47	CEOH	0.0	-1.0464E+05	1.1139E+01	0.0	0.0	0.0	0.0
48	CE(OH)2	0.0	-5.6092E+05	1.1362E+02	0.0	0.0	0.0	0.0
49	CEO2	0.0	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	0.0
51	H2O	0.0	-2.5205E+05	5.8230E+01	0.0	0.0	0.0	0.0
52	H2	0.0	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	0.0
54	CAO(L)	0.0	-6.8797E+05	1.5842E+02	0.0	0.0	0.0	0.0
55	SiO2(L)	0.0	-9.2972E+05	1.8914E+02	0.0	0.0	0.0	0.0
56	UO2(L)	0.0	-9.3311E+05	1.2253E+02	0.0	0.0	0.0	0.0
57	ZrO2(L)	0.0	-1.0175E+06	1.5945E+02	0.0	0.0	0.0	0.0
58	SrO(L)	0.0	-6.4053E+05	1.4999E+02	0.0	0.0	0.0	0.0
59	LA2O3(L)	0.0	-1.7772E+06	2.7187E+02	0.0	0.0	0.0	0.0
60	CEO2(L)	0.0	-1.0869E+06	2.1227E+02	0.0	0.0	0.0	0.0
61	Fe(L)	0.0	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	0.0
63	Zr(L)	0.0	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


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** 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+05  1.000E+05  1.000E+02
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  FEOH)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(OH)2  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

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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	UD2(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 B

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/R/T	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	FE0	1	1.330	2.6938E-04	1.7730E-08	1.7730E-08
9	FE0H	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(OH)2	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	FE(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	SI02(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	ZR02(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	CE02(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(OH)2	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 B

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(OH)2	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	CAD	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	SIO(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	SI02(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++S)= 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	FE0	1	3.736	8.5174E-08	1.0341E-11	1.0341E-11
9	FE0H	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	MO0	1	11.548	3.4489E-14	4.1873E-18	4.1873E-18
13	MO02	1	-5.076	2.6279E-16	3.1904E-20	3.1904E-20
14	MO03	1	-14.579	1.6167E-21	1.9628E-25	1.9628E-25
15	MO02(OH)2	1	-26.237	2.2531E-18	2.7354E-22	2.7354E-22
16	(MO03)2	1	-16.541	0.0	0.0	0.0
17	(MO03)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	CA0	1	-3.456	2.5246E-05	3.0650E-09	3.0650E-09
20	CA0H	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	SI0	1	-15.386	6.1768E+03	7.4991E-01	7.4991E-01
24	SI02	1	-17.912	3.5463E-05	4.3054E-09	4.3054E-09
25	SI0H	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	U0	1	-7.249	1.3208E-02	1.6036E-06	1.6036E-06
29	U02	1	-28.359	8.9287E-03	1.0840E-06	1.0840E-06
30	U03	1	-40.692	9.3171E-07	1.1312E-10	1.1312E-10
31	U02(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	ZR0	1	-5.430	4.7482E-05	5.7647E-09	5.7647E-09
34	ZR02	1	-19.342	2.4013E-08	2.9153E-12	2.9153E-12
35	ZR0H	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	LA0	1	-16.936	1.5101E-02	1.8333E-06	1.8333E-06

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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	FE(O)2	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	SI(O)2(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 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	FE	MO	CA	SI	U	ZR	SR
1	H	1	3.686	3.1532E+01	1.6704E-03	1.6704E-03	1.6704E-03	1.6704E-03	1.6704E-03	1.6704E-03	1.6704E-03
2	OH	1	16.149	9.8159E-11	5.2001E-15	5.2001E-15	5.2001E-15	5.2001E-15	5.2001E-15	5.2001E-15	5.2001E-15
3	O	1	1.343	3.9646E-03	2.1003E-07	2.1003E-07	2.1003E-07	2.1003E-07	2.1003E-07	2.1003E-07	2.1003E-07
4	O2	1	0.0	1.2213E-08	6.4698E-13	6.4698E-13	6.4698E-13	6.4698E-13	6.4698E-13	6.4698E-13	6.4698E-13
5	CO2	1	-19.078	2.1858E-03	1.1580E-07	1.1580E-07	1.1580E-07	1.1580E-07	1.1580E-07	1.1580E-07	1.1580E-07
6	CO	1	-15.776	9.9996E+01	5.2974E-03	5.2974E-03	5.2974E-03	5.2974E-03	5.2974E-03	5.2974E-03	5.2974E-03
7	FE	1	3.539	5.4316E+02	2.8774E-02	2.8774E-02	2.8774E-02	2.8774E-02	2.8774E-02	2.8774E-02	2.8774E-02
8	FE0	1	1.330	3.9768E-03	2.1067E-07	2.1067E-07	2.1067E-07	2.1067E-07	2.1067E-07	2.1067E-07	2.1067E-07
9	FE0H	1	1.832	1.6053E-04	8.5045E-09	8.5045E-09	8.5045E-09	8.5045E-09	8.5045E-09	8.5045E-09	8.5045E-09
10	FE(OH)2	1	-4.884	7.1024E-09	3.7626E-13	3.7626E-13	3.7626E-13	3.7626E-13	3.7626E-13	3.7626E-13	3.7626E-13
11	MO	1	14.232	1.2402E-05	6.5702E-10	6.5702E-10	6.5702E-10	6.5702E-10	6.5702E-10	6.5702E-10	6.5702E-10
12	MOO	1	7.152	1.1848E-08	6.2769E-13	6.2769E-13	6.2769E-13	6.2769E-13	6.2769E-13	6.2769E-13	6.2769E-13
13	MOO2	1	-4.687	1.3208E-09	6.9969E-14	6.9969E-14	6.9969E-14	6.9969E-14	6.9969E-14	6.9969E-14	6.9969E-14
14	MOO3	1	-10.135	2.4691E-13	1.3080E-17	1.3080E-17	1.3080E-17	1.3080E-17	1.3080E-17	1.3080E-17	1.3080E-17
15	MOO2(OH)2	1	-15.941	3.6447E-13	1.9308E-17	1.9308E-17	1.9308E-17	1.9308E-17	1.9308E-17	1.9308E-17	1.9308E-17
16	(MOO3)2	1	-9.658	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	(MOO3)3	1	-9.249	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	CA	1	0.0	8.4809E+03	4.4928E-01	4.4928E-01	4.4928E-01	4.4928E-01	4.4928E-01	4.4928E-01	4.4928E-01
19	CA0	1	-1.901	4.5635E-02	2.4176E-06	2.4176E-06	2.4176E-06	2.4176E-06	2.4176E-06	2.4176E-06	2.4176E-06
20	CA0H	1	-7.351	7.0833E-01	3.7525E-05	3.7525E-05	3.7525E-05	3.7525E-05	3.7525E-05	3.7525E-05	3.7525E-05
21	CA(OH)2	1	-13.891	2.6296E-03	1.3931E-09	1.3931E-09	1.3931E-09	1.3931E-09	1.3931E-09	1.3931E-09	1.3931E-09
22	SI	1	5.383	7.9733E+01	4.2240E-03	4.2240E-03	4.2240E-03	4.2240E-03	4.2240E-03	4.2240E-03	4.2240E-03
23	SI0	1	-13.431	9.5001E+03	5.0328E-01	5.0328E-01	5.0328E-01	5.0328E-01	5.0328E-01	5.0328E-01	5.0328E-01
24	SI02	1	-13.592	8.9776E-03	4.7560E-07	4.7560E-07	4.7560E-07	4.7560E-07	4.7560E-07	4.7560E-07	4.7560E-07
25	SI0H	1	-0.877	2.2369E-03	1.1850E-07	1.1850E-07	1.1850E-07	1.1850E-07	1.1850E-07	1.1850E-07	1.1850E-07
26	SI(OH)2	1	-8.286	1.9800E-07	1.0489E-11	1.0489E-11	1.0489E-11	1.0489E-11	1.0489E-11	1.0489E-11	1.0489E-11
27	U	1	10.430	3.4478E-02	1.8265E-06	1.8265E-06	1.8265E-06	1.8265E-06	1.8265E-06	1.8265E-06	1.8265E-06
28	U0	1	-6.987	1.0167E+00	5.3860E-05	5.3860E-05	5.3860E-05	5.3860E-05	5.3860E-05	5.3860E-05	5.3860E-05
29	U02	1	-22.405	4.0598E+00	2.1507E-04	2.1507E-04	2.1507E-04	2.1507E-04	2.1507E-04	2.1507E-04	2.1507E-04
30	U03	1	-30.661	1.2573E-02	6.6608E-07	6.6608E-07	6.6608E-07	6.6608E-07	6.6608E-07	6.6608E-07	6.6608E-07
31	UO2(OH)2	1	-33.529	7.9058E-10	4.1882E-14	4.1882E-14	4.1882E-14	4.1882E-14	4.1882E-14	4.1882E-14	4.1882E-14
32	ZR	1	13.496	2.1589E-04	1.1437E-08	1.1437E-08	1.1437E-08	1.1437E-08	1.1437E-08	1.1437E-08	1.1437E-08
33	ZR0	1	-5.847	4.3669E-02	2.3134E-06	2.3134E-06	2.3134E-06	2.3134E-06	2.3134E-06	2.3134E-06	2.3134E-06
34	ZR02	1	-15.478	5.3469E-04	2.8326E-08	2.8326E-08	2.8326E-08	2.8326E-08	2.8326E-08	2.8326E-08	2.8326E-08
35	ZR0H	1	1.149	2.6649E-06	1.4118E-10	1.4118E-10	1.4118E-10	1.4118E-10	1.4118E-10	1.4118E-10	1.4118E-10
36	ZR(OH)2	1	-10.280	1.3141E-08	6.9614E-13	6.9614E-13	6.9614E-13	6.9614E-13	6.9614E-13	6.9614E-13	6.9614E-13
37	SR	1	0.0	2.4800E+01	1.3138E-03	1.3138E-03	1.3138E-03	1.3138E-03	1.3138E-03	1.3138E-03	1.3138E-03
38	SR0	1	-4.019	1.1095E-03	5.8778E-08	5.8778E-08	5.8778E-08	5.8778E-08	5.8778E-08	5.8778E-08	5.8778E-08
39	SR0H	1	-7.440	2.2636E-03	1.1992E-07	1.1992E-07	1.1992E-07	1.1992E-07	1.1992E-07	1.1992E-07	1.1992E-07
40	SR(OH)2	1	-13.750	6.6780E-08	3.5377E-12	3.5377E-12	3.5377E-12	3.5377E-12	3.5377E-12	3.5377E-12	3.5377E-12
41	LA	1	6.046	4.6799E-03	2.4792E-07	2.4792E-07	2.4792E-07	2.4792E-07	2.4792E-07	2.4792E-07	2.4792E-07
42	LA0	1	-15.126	5.8963E+00	3.1236E-04	3.1236E-04	3.1236E-04	3.1236E-04	3.1236E-04	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.