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Modeling of Thermal Plasma Arc Technology FY 1994 Report

**Grant L. Hawkes
Hoa D. Nguyen
Seungho Paik
Michael G. McKellar**

Lockheed
Idaho Technologies Company

MASTER

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Thermal Plasma Arc Technology
FY 1994 Report**

**Grant L. Hawkes
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**Idaho National Engineering Laboratory
Lockheed Idaho Technologies Company
Idaho Falls, Idaho 83415**

**Prepared for the
U.S. Department of Energy
Assistant Secretary for Environmental Management
Under DOE Idaho Operations Office
Contract DE-AC07-94ID13223**

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ABSTRACT

The thermal plasma arc process is under consideration to thermally treat hazardous and radioactive waste. A computer model for the thermal plasma arc technology was designed as a tool to aid in the development and use of the plasma arc-Joule heating process. The value of this computer model is to: (a) aid in understanding the plasma arc-Joule heating process as applied to buried waste or exhumed buried waste, (b) help design melter geometry and electrode configuration, (c) calculate the process capability of vitrifying waste (i.e., tons/hour), (d) develop efficient plasma and melter operating conditions to optimize the process and/or reduce safety hazards, (e) calculate chemical reactions during treatment of waste to track chemical composition of off-gas products, and composition of final vitrified waste form and (f) help compare the designs of different plasma-arc facilities.

A steady-state model of a two-dimensional axisymmetric transferred plasma arc has been developed and validated. A parametric analysis was performed that studied the effects of arc length, plasma gas composition, and input power on the temperatures and velocity profiles of the slag and plasma gas. A two-dimensional transient thermo-fluid model of the U.S. Bureau of Mines plasma arc melter has been developed. This model includes the growth of a slag pool. The thermo-fluid model is used to predict the temperature and pressure fields within a plasma arc furnace. An analysis was performed to determine the effects of a molten metal pool on the temperature, velocity, and voltage fields within the slag. A robust and accurate model for the chemical equilibrium calculations has been selected to determine chemical composition of final waste form and off-gas based on the temperatures and pressures within the plasma-arc furnace. A chemical database has been selected. The database is based on the materials to be processed in the plasma arc furnaces. This material includes hazardous and radioactive waste as well as additives like soil.

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ACKNOWLEDGMENTS

The authors thank Mr. R. B. Nielson for figures throughout this document. Valuable comments from Dr. P. C. Kong are gratefully acknowledged. The work was performed under the auspices of the U.S. Department of Energy, contract DE-AC07-94ID13223, and was supported by the Buried Waste Integrated Demonstration Program.

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NOMENCLATURE

B	magnetic field	ρ	global density
C_p	specific heat at constant pressure	τ	stress tensor
e	elementary charge	σ	electrical conductivity
E	energy		
E	electric field	Subscripts	
g	gravity acceleration vector	i	ions
h	specific enthalpy	m	soil melt
I	total current	P	plasma
j	current vector	r	radial coordinate
k	Boltzmann constant	x	axial coordinate
L_m	latent heat of soil		
n	number density		
p	pressure		
q	heat flux		
r	radial coordinate		
r	position vector		
r₀	radius of cathode spot		
S	radiation energy loss		
T	temperature		
T_{melt}	soil melt temperature (= 1,473 K)		
T₀	reference temperature(= 273 K)		
u	velocity vector		
u	axial velocity		
v	radial velocity		
V	volume		
V_{drop}	Voltage specified by input power		
x	axial coordinate		

Greek symbols

α	current distribution
ϕ	electric potential
γ	surface tension
κ	thermal conductivity
μ	viscosity
μ_0	magnetic permeability at vacuum (= 1.26×10^{-6} H/m)

1. INTRODUCTION

1.1 Background

Thermal plasma arc technology is a promising method for high-temperature treatment of transuranic (TRU) and mixed hazardous wastes. This technology uses a plasma arc to pyrolyze and combust organic materials and melt residual inorganic materials. The resulting molten slag, upon cooling, produces a durable vitrified cast form that may be safely disposed. This technology offers several advantages over conventional thermal processing methods, including high temperatures, high enthalpies, choice of inert or chemically active torch gases, and operation with low gas volumes. Although these advantages have been utilized in metallurgical processes during the past two decades, only recently has there been efforts to evaluate the feasibility of plasma applications to waste treatment. These efforts are motivated in part by the potential for high efficiency destruction of organics, permanent encapsulation of heavy metals and radio nuclides in a non-leachable final product, and the low cost of downstream equipment for gas handling and cleanup.

Pilot-scale testing projects have been funded by DOE to demonstrate the use of plasma technology to treat simulated TRU and mixed hazardous wastes. Although pilot-scale testing programs are an indispensable component of any technology evaluation, they lend themselves to added expense by using the systems to examine technical issues that could otherwise be resolved using less expensive computer simulations. For example, parametric simulation studies can be performed to quantify the observed effects of changing process variables and thus provide an economical means for optimizing the quality of the final product.

Even though technology development has been affected in the past without recourse to mathematical modeling, the increased use of the mathematical modeling in combination with pilot-scale testing has made modern research and development efforts much more cost effective and timely.

1.2 Purpose

There are three primary purposes for developing a computer model of the plasma arc treatment process:

1. The model will simulate a variety of plasma arc waste treatment facilities.

2. The model may be used as a tool to aid designers in modifying current designs or developing new designs. By performing parametric analyses within the model and combining with optimization techniques, designers can modify or develop designs that reduce the construction and operating costs of the facilities.
3. The model can aid engineers and scientists in understanding the causes and effects of the physical processes occurring within the plasma arc facilities. The model will determine the migration of contaminants to the off-gas and into the equipment, and which contaminants may be encapsulated within the final waste slag. The effects of molten metal pooling on the chemistry and heat transfer can be determined. The effects of convection within the molten slag and melts can be determined. The thicknesses of the different layers within the waste during treatment can be found.

1.3 Code Development

This project uses a simple-to-complex modeling approach that modifies existing codes to develop a working model of the process. In future years, the model can be developed further to account for some of the higher-order effects, if the need arises. The primary tasks of the code development for are fourfold.

Task 1	Review and modify existing plasma arc codes to model the plasma arc for melters.
Task 2	Modify the existing thermal code, FIDAP, to model the heat transfer and fluid flow within the slag, metal pool, untreated waste, and surrounding equipment to optimize the melter design configurations.
Task 3	Modify an existing code to determine the chemical equilibrium within the waste, slag, metal pool, surrounding equipment, and off-gas to optimize containment dissolution within the slag.
Task 4	Compare the results from the integrated code with experimental data from the Buried Waste Integrated Demonstration (BWID) melter demonstrations, benchmark numerical data, and analytical solutions to verify and validate the codes.

During FY 1994, two plasma arc facilities were simulated. The first facility simulated was the lab-scale melter located at the Idaho National Engineering Laboratory (INEL). A two-dimensional, direct current, axisymmetric, steady-state, transferred-arc model of the facility was simulated. The temperature, velocity, and electric fields of the slag and the plasma were determined. Parametric studies were performed in which the plasma gas, arc length, and power input were adjusted. Chapter two discusses the development of this model as well as the results from the parametric studies.

The second facility was the U.S. Bureau of Mines facility. The model is two dimensional and transient. The temperature, velocity, and electric fields of the slag were simulated. The plasma was simulated as a heat source based on the power input. The effects of a molten metal pool were also simulated. Chapter four presents this information

A chemical equilibrium program was selected to simulate the chemistry of the simulations. Simulations were performed and the results are presented in chapter three.

2. PLASMA ARC MODEL

2.1 Literature Review

The increased use of the plasma arc in metallurgical and waste minimization processes has prompted researchers to optimize the process. Understanding these processes requires detailed information on both the plasma arc and the molten pool. Research on the plasma arc has been performed by various researchers (Hsu 1983; Tsai 1990; Pfender 1980; Gonzalez 1993). Because of the complex nature of the plasma, experimental work is limited to measuring temperatures and global heat transfer rates rather than obtaining local measurements that may be important for finding the optimum operating conditions in the plasma reactor. Instead, numerical models of the processes have been successfully used to obtain detailed information. Earlier work concentrated on modeling the near electrode regions (both anode and cathode) where the major focus of the models was the sheath layers formed near the electrodes (Hsu 1983). The non equilibrium effects near the electrodes were studied numerically. Good agreement between spectrometric measurements and numerical predictions was found. Tsai and Kou (Tsai 1990) studied the cathode-geometry effect on the flow and temperature fields of welding arcs. They found that the calculated flow and temperature fields were sensitive to the current density distribution along the cathode tip. Pfender (1980) discussed the various heat transfer modes in the plasma arc. The recent work of Gonzalez et al. (1993) focused on the effects of the metal vapor on the heat transfer mechanism during metal scraping by way of a transferred arc. For the moderate current intensities, they concluded that the presence of the metal vapor significantly affects the radiation heat transfer. Heat conduction in the anode region was considered in their work. The use of the plasma arc for refractory metal oxides has been considered by Taniuchi (1993). For this application, the plasma interaction with the processing material was the most important factor to optimize the design of a processing reactor.

For the melt pool, much research is found in the literature, mostly related to metal welding. A large portion of the numerical work is focused on the metal pool flow and heat transfer. A comprehensive review on this subject was performed by Szekely (1979). For the melt pool composed of soil, Hawkes (1991) considered the effect of natural convection on the soil-melt shape during the in situ vitrification process. By considering Joule heating inside the melt, the temperature and flow fields were obtained inside the melt.

To date, most of the previous studies on this subject consider either the plasma region or molten material domain only. However, information on the interaction between the plasma arc and molten material are crucial to understand the process. Gu et al. (1993) studied the plasma arc and molten metal pool interaction with vapor contaminant effect. The metal pool is treated as an anodic

liquid in their work. Inclusion of the liquid pool convection was considered without the phase change of the soil in their work. This study is focused on the plasma arc reactor for the waste minimization process. The interaction of the plasma and the molten pool (usually composed of contaminated soils) is studied by considering the flow, temperature, and electromagnetic fields inside the reactor. The molten liquid and solid soil interface is treated by using the algorithm described by Basu and Date (Basu, 1990).

In the following section, the mathematical model and assumptions are presented. The numerical validation studies are performed for both the plasma and the molten pool regions by comparing results with previously published ones. Finally, results and discussions on the present work are presented.

2.2 Mathematical Model

The geometry considered in this study is shown in Figure 1. The calculation domain is divided into the plasma and the soil (either liquid or solid) regions. The dimension of the soil volume is fixed, while the plasma arc length or gap (the distance between the cathode tip and the soil surface) is varied for the calculations. The dimensions of the reactor used in this study resemble the experimental thermal waste treatment facility of Kong et al. (1993).

2.2.1 Assumptions.

In this study, we have made the following assumptions:

1. Steady-state, two-dimensional (2-D), axisymmetric, and laminar plasma and molten pool flows prevail. The transient behavior of the reactor is not an objective of this study. Even though there are many factors that may disturb the axisymmetric nature of the problem, we believe the 2-D calculation may yield proper information for present purposes. The laminar flow assumption is reasonable for the high-viscosity region of the plasma and the molten pool.
2. Local thermodynamic equilibrium (LTE) is used to simplify mathematical formulations. The effect of non equilibrium as addressed by Hsu and Pfender (Hsu 1983) is not considered in this study. As a consequence, the plasma is treated as a single continuous fluid with only one representative temperature for the flow. Likewise, the molten material is treated as a homogeneous liquid whose thermophysical properties are functions of temperature only.
3. No interface deformation is considered. The interface between the plasma arc and the molten pool is fixed as a flat surface. This is the most serious restriction, considering the fact that a

strong plasma jet impinges on the molten pool surface, and boiling of the melt occurs at the location of arc root attachment. However, this assumption is made to simplify the model.

4. Material volatilization effects at the plasma-molten pool interface are not included. The effects of cathode material contaminating the plasma properties are not considered. Because of the high temperatures encountered at the interface, it is expected that there is mass transfer from the molten pool to the gas environment. However, the mass transfer at the interface is highly dependent on the material properties of the soil. In this parametric study, the basic soil composition at INEL is used.
5. The plasma is optically thin, which implies that re absorption of radiation by the plasma compared with the total radiative loss over all wavelengths is insignificant. The radiation from the molten pool surface is also neglected.
6. Viscous dissipation is neglected in both the plasma arc and the molten pool regions.

2.2.2 Governing Equations and Thermophysical Properties.

Based on the above assumptions, the governing equations are written in vector notations. Neglecting the effects of electrode erosion and material volatilization at the melt pool surface, the global mass conservation equation becomes

$$\nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

where

ρ is the global density

$\mathbf{u}$ is the velocity vector.

The currents, $\mathbf{j}$, generated by the cathode emission are conserved as $\nabla \cdot \mathbf{j} = 0$. By use of electric potential, ϕ , defined as $\mathbf{j} = \sigma \nabla \phi$, the current conservation equation can be written as

$$\nabla \cdot (\sigma \nabla \phi) = 0 \quad (2)$$

where

σ is the electrical conductivity.

Besides the gravity field, the only body force exerted on the arc is a net magnetic force or Lorentz force, generated in the arc column by an asymmetric interaction between the arc current and self-induced magnetic field. The conservation equations of momentum with the Lorentz force acting as a body force can be expressed as

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \mathbf{j} \times \mathbf{B} + \rho \mathbf{g}, \quad (3)$$

where

p is the pressure

ρg is the gravitational force

B is the self-generated magnetic field because of the current flow.

Total specific enthalpy for the plasma (h_p) is defined as

$$h_p = \left(\frac{5}{2} n k T + n_i E_i \right) / \rho_p, \quad (4)$$

where

n is the total number density

k is the Boltzman constant

n_i is the ion species number density

E_i is the ionization energy.

By using the enthalpy formulation, the governing energy conservation equation becomes

$$\nabla \cdot (\rho_p u h_p) = \nabla \cdot \left(\frac{\kappa_p}{C_{pp}} \nabla h_p \right) + \frac{\mathbf{j} \cdot \mathbf{j}}{\sigma_p} + \frac{5}{2} \frac{k}{e C_{pp}} (\mathbf{j} \cdot \nabla h_p) - S_r \quad (5)$$

where

κ_p is the plasma thermal conductivity

C_{pp} is the specific heat at constant pressure

S_r is the optically thin radiation energy loss

e is the elementary charge.

The subscript P represents the plasma quantity. Equation (5) contains the convection, the conduction, the Joule heating, the transport of electron enthalpy because of the drift of the electrons, and the radiation loss terms in respective order.

The molten pool domain requires the same set of governing equations as the plasma domain. The electrically conducting molten pool is subjected to the gravity and the electromagnetic fields; therefore, Equations (1), (2), and (3) can be used for the molten pool. For the energy conservation, the radiant energy and the electron drift energy contribution to the molten pool is ignored. The specific enthalpy of the soil (h_m) can be defined as

$$\begin{aligned}
h_m &= C_{pm} (T - T_0) & \text{for } T < T_{melt} \\
h_m &= C_{pm} (T_{melt} - T_0) + L_m & \text{for } T = T_{melt} \\
h_m &= C_{pm} (T - T_0) + L_m & \text{for } T > T_{melt}
\end{aligned} \tag{6}$$

where

T_{melt} is the melt temperature

L_m is the latent heat of melting for the soil.

By using the specific enthalpy of Equation (6), the energy conservation equation for the molten pool domain can be written as

$$\nabla \cdot (\rho_m \mathbf{u} h_m) = \nabla \cdot \left(\frac{\kappa_m}{C_{pm}} \nabla h_m \right) + \frac{\mathbf{j} \cdot \mathbf{j}}{\sigma_m} \tag{7}$$

The Joule heating term is kept with convection and conduction terms due to the electrically conducting property of the molten soil. The transport of electron enthalpy due to electron drift is small compared to the high enthalpy of the soil, and therefore can be neglected.

Equations (1-3,5,7) are the physical governing equations used in this study for the plasma and the soil region. The governing equations can be solved with any established elliptic partial differential equation solver. To solve the governing equations, supplementary information about the current and the magnetic fields is needed. The current density may be calculated using Ohm's law:

$$\mathbf{j} = \sigma(\mathbf{E} + \mathbf{u} \times \mathbf{B}) \tag{8}$$

where

$\mathbf{E}$ is the electric field

$\mathbf{B}$ is the magnetic field

$\mathbf{u}$ is the drift velocity of the charged particles.

In the absence of externally applied magnetic field, the induced current density by the motion of the charged particles across the magnetic field, the $\mathbf{u} \times \mathbf{B}$ term, is comparably small. Thus only the electric field contribution to the current is considered in this study. The self-induced magnetic field can be expressed by using the Biot-Savart law (Jackson 1975) expressed as

$$\mathbf{B} = \frac{\mu_0}{4\pi} \oint \frac{\mathbf{j} \times \mathbf{r}}{r^3} dV \tag{9}$$

where

μ_0 is the magnetic permeability of vacuum ($= 1.26 \times 10^{-6}$ H/m)

dV is the differential volume.

In case of the free burning arc, the magnetic field is dominated by the strong axial current. Thus the inclusion of the radial current contribution does not change the obtained temperature solution fields significantly (Hsu 1982).

The thermodynamic and transport properties of argon at one atmospheric pressure are taken from Hsu (1982). The data of the radiation energy loss are taken from the experimental work of Evans and Tankin (Evans 1967). All the plasma property data are provided in a tabulated form with every 1,000 K temperature intervals from 1,000K to 25,000K. The properties between the specified temperature intervals are linearly interpolated. The density and the viscosity of the soil are taken from Buelt et al. (1987) which are shown in Figure 2. The other thermophysical properties of the soil used for this study are from Henderson and Taylor (Henderson 1993) and shown in Table 1. Due to the lack of data points for the thermophysical properties of soil, linear interpolation is used in the calculation for the properties between the data points.

2.2.3 Boundary Conditions.

At the wall, the constant temperature boundary condition and no slip boundary condition for the velocity fields are used in this study. High electrical conductivity with a floating current condition for the electric field are imposed at the bottom anodic wall surface. For the centerline ($r=0$), symmetry boundary condition with zero normal velocity component is specified. Since no interface deformation between the molten pool and plasma phase is considered in this study, normal velocity at the interface is set to zero with shear stress continuity requirement across the interface. The usual boundary condition for the tangential velocity at the interface in welding problems considers the surface tension driving force (Marangoni force) only. However, the surface tension is a complicated function of material composition, and the information about the thermal

Table 1. Soil thermophysical properties.

Temperature (K)	C_{pm} (J/kg-K)	k_m (W/m-K)	s_m (1/Ohm-m)
0.0	881	0.2	0.001
673	1,096	0.23	0.001
1,073	1,166	0.45	0.016
1,428	1,284	8.5	0.98
1,773	1,284	18	5.6
2,173	1,284	50	20
2,573	1,284	80	44
5,000	1,284	80	88

behavior of the surface tension is not available for the present problem. Moreover, for the free burning arc problem, the induced convective flow is much stronger and tends to overcome the surface-tension-induced force (Jensen 1993). Thus, the Marangoni effect is not considered in this study. The heat flux continuity at the interface is used for the energy conservation. No shielding gas is used in this study. The above-mentioned boundary conditions can be translated into mathematical expressions as follows:

At the wall:

$$u_P = v_P = u_m = v_m = 0, \quad (10a)$$

$$T = 1,000K, \quad (10b)$$

$$\left. \frac{\partial \phi}{\partial r} \right|_{r=R} = 0, \quad \left. \frac{\partial^2 \phi}{\partial x^2} \right|_{x=0} = 0. \quad (10c)$$

At the interface:

$$u_P \Big|_{x=3.55 \text{ cm}} = u_m \Big|_{x=3.55 \text{ cm}} = 0, \quad (11a)$$

$$\tau_{Px} \Big|_{x=3.55 \text{ cm}} = \tau_{mx} \Big|_{x=3.55 \text{ cm}}, \quad (11b)$$

$$q_{Px} \Big|_{x=3.55 \text{ cm}} = q_{mx} \Big|_{x=3.55 \text{ cm}}, \quad (11c)$$

$$j_{Px} \Big|_{x=3.55 \text{ cm}} = j_{mx} \Big|_{x=3.55 \text{ cm}}. \quad (11d)$$

where

τ is the stress tensor

q is the heat flux,

which are defined in (Bird 1960).

At the center:

$$\frac{\partial u_p}{\partial r} = \frac{\partial u_m}{\partial r} = \frac{\partial T_p}{\partial r} = \frac{\partial T_m}{\partial r} = \frac{\partial \phi}{\partial r} = v_p = v_m = 0. \quad (12)$$

At the top of the reactor (open boundary):

$$\frac{\partial u_p}{\partial x} = \frac{\partial u_m}{\partial x} = \frac{\partial T_p}{\partial x} = \frac{\partial T_m}{\partial x} = v_p = v_m = 0, \quad \phi = V_{\text{drop}}, \quad (13)$$

where

V_{drop} is the voltage specified by the input power.

At the cathode tip, the current boundary condition is imposed, which represents cathode emission of electrons. The current is specified at 1 mm below the cathode with an exponential function as

$$j_x \Big|_{x=3\text{mm}} = j_{x_{\text{max}}} \exp(-r/r_0) \quad (14)$$

where

$j_{x_{\text{max}}}$ is the maximum current at the cathode tip

r_0 is the cathode spot radius.

Both $j_{x_{\text{max}}}$ and r_0 vary with the operating condition and the cathode shape and can be determined from experimental observation (Hsu 1982).

2.3 Numerical Method and Validation Test

The momentum and the mass conservation equations are solved by using the SIMPLEC algorithm (Vandoormal 1984). The energy and the electron conservation equations are solved by using the same procedure described by Patankar (1980). For the solid/liquid boundary, the approach used by Basu and Date (Basu 1990) is adopted in this study. Details of the solid/liquid boundary treatment is referred to Basu and Date. In the solid domain, the viscosity is set to 10^{16} kg/m/s to ensure no flow is allowed.

To validate our physical model and computer code, comparison is made on the temperature profile for the argon plasma arc region. Hsu (1982) makes a similar comparison to verify their

model on the free burning arc. Figure 3 shows the isotherms in the plasma domain. The same boundary conditions and the operating conditions as those of Hsu are also shown to compare with the experimental data. The results are slightly different from Hsu's results near the anode region, which can be explained by the different grid resolution (32×22) for the present calculation. By increasing the axial direction resolution, we obtained stiff temperature gradients near the anode surface. Reasonable agreement with the experimental data is found for the isotherms of the plasma arc.

Another comparison is made for the molten pool region calculation. For this validation test, we selected the validation test performed by Basu and Date (Basu 1990). In their calculation, the surface is assumed to be driven by the surface-tension gradient, which results in replacing the boundary condition, i.e., equation (11b), with the Marangoni force, which can be written as

$$\mu_m \frac{\partial v}{\partial x} = -\frac{\partial \gamma}{\partial T} \frac{\partial T}{\partial r} \quad (15)$$

where

γ is the surface tension.

The melt depth and width resulting from laser welding for Al-4.5% Cu is compared. The beam diameter is 1.0 mm and the predicted depth and width is compared with the experimental results obtained by Sekhar (1982). The physical properties used for this comparison can be found in (Basu 1990) and (Sekhar 1982). The Lorentz force term as well as the Ohmic heating term in the momentum and energy conservation equations were not used for the simulation. Table 2 shows the compared results. In general, good agreement is found with the numerical results of Basu and Date.

Table 2. Comparison of the melt widths and depths with previous results.

$q \times 10^8$ (W/m ²)	Width (mm)			Depth (mm)		
	Sekhar (exp.)	Basu & Date	Present Results	Sekhar (exp.)	Basu & Date	Present Results
2.43	0.238	0.294	0.287	0.146	0.049	0.053
3.12	0.410	0.443	0.441	0.175	0.130	0.135
3.97	0.470	0.494	0.495	0.201	0.198	0.198
4.10	0.500	0.520	0.524	0.230	0.239	0.236
5.00	0.577	0.579	0.581	0.264	0.398	0.351
5.60	0.600	0.610	0.621	0.500	0.453	0.427

2.4 Results and Discussion

Many issues need to be addressed concerning the design of the arc melter for waste minimization (Donaldson 1992). One of the primary purposes of the present study is to determine the effect of the distance between the cathode and the melt pool surface. Arc length is an important factor in determining steady-state operating conditions for an arc reactor (Kong 1993) which can practically be operated from as close as the cathode submerged into the melt pool to as far from the interface as the arc can be sustained. When the cathode is submerged into the melt pool, the heating is primarily via the Joule heating between the electrodes. Another consideration is given to the arc current variation. Two different arc current cases, 200 A and 300 A, are considered with different arc powers (ranges from 5 to 15 kW) in this study. The same cathode tip radius of 200 A (Hsu 1983), (Hsu 1982) is used for the 300 A case for the calculation.

Figure 4 shows isotherms in the arc reactor for the arc current $I = 200$ A and 5 kW input power with different arc lengths. The melt front in the soil region shows a bowl shape with the maximum temperature occurring at the bottom of the reactor because of the high current density collected at the bottom. In Figure 4, the maximum temperature near the bottom of the reactor increases as the arc length becomes shorter. However, for the higher input power (i.e. 7.5 kW in Figure 5), the maximum temperature near the bottom of the reactor remains the same for different arc length cases; instead, the surface temperature near the melt core increases for short arc case. In Figure 6, high current density is found near the core region of the soil because of the relatively high

electrical conductivity of the soil at the high temperatures. The high current density induces the high Joule heat dissipation, which results in the higher temperatures in that region. Figure 7 shows that the induced flow fields in the molten soil region have strong clockwise convection occurring on the right-hand side of the reactor. There are two factors for this convection. One factor is because of the shear stress-induced flow at the interface. The arc jet, after impinging on the interface, makes a sharp radially outward turn, which induces high radially outflow at the interface. The other factor is due to the buoyancy force induced by the high temperature at the bottom of the reactor. Because of the large density difference caused by the temperature gradient inside the molten soil, the induced natural convection force contributes to the clockwise convection in the melt pool. For the cases considered in this study, the effect of the electromagnetic force in the melt pool is not causing major changes for the flow directions as found by Gu et al. (1993) for the metal pool case because of the low electrical conductivity of the soil. The ratio of the electromagnetic force to the buoyancy force is defined (Oreper 1984) as

$$\text{Ratio} = \frac{\mu_0 I^2 C L_R^2 \alpha_j^4}{\rho \pi^2 L g \beta \Delta T} \quad (16)$$

where

I is the total current

α_j is the current distribution over the melt surface

L_R is the melt pool radius

C is the constant depending on the arc operating mode.

In this study, the cathode spot mode is considered. Thus $C=8$ is used. Values of the Ratio in Equation (16) based on the parameters considered in this study are on the order of 0.1. Thus, the contribution of the Lorentz force on the melt pool convection is not significant compared to that of the buoyancy force. Besides, the strong tangential shear at the interface intensifies the clockwise convection in the melt pool. Oreper and Szekely (1984) have noticed that the clockwise circulation (i.e., radially outward convection at the melt surface) may yield a shallow melt pool in traditional welding. However, in their study the Joule heating through the melt is not considered. The Joule heating effect on the melt pool shape was shown experimentally by Kou and Sun (1985). The current arriving at the melt surface penetrates vertically through the melt and generates a deeper melt pool than without the current. These combined effects of the convection and the Joule heat transfer yields an efficient way of melting the soil in the arc melter.

The effect of the arc length is shown in Figures 4–7. For the arc length of 3 cm and total current 200 Amps (Figure 4), the melted volume of the soil is about 10% less than for the arc length of 1 cm. However, for the long arc, a larger volume of the environment gas is heated up to 2,000 K, which may give favorable conditions for the off-gas emitting from the melt surface during contaminated waste treatment. Treatment of the off-gas, especially high volatile pressure materials

from the melt, is one of the major concerns of the waste treatment process (Donaldson 1992). For the efficient treatment of the volatile gases, longer residence time of the off-gas in the hot stream is desirable. During the process, this effect should be considered to determine the arc length. Similar effects on the temperature of the environment gas are found for the increased arc current. For the high current case, the gas temperature is higher than that of low arc current. Thus, the melt pool volume and the heated gas volume should be considered during the process.

Figures 8–10 show the interfacial temperature, current, and velocities for different operating conditions. For the short arc, the temperature at the interface is higher than for the long arc. Likewise, the maximum currents at the interface for the short arc are higher than those of the long arc. For the long arc, slightly higher currents than those of short arc can be found far from the arc core since the electrical conductivities of the plasma and the melt pool are relatively evenly distributed over the interface. This effect becomes noticeable for the high input power case. For the higher input power case (7.5 kw), the currents and the temperatures at the interface far from the arc core show a slight increase for the longer arc case. This is because that for the high input power with long arc, the increased gas temperatures are more uniform above the molten pool and increase the molten pool surface temperature and electrical conductivity. The tangential velocity (i.e., radial direction velocity) at the interface shows that the maximum velocity can be as high as 20 m/s. The maximum velocity increases as the current increases since the electromagnetically induced plasma flow increases as the current increases. The velocity increases as the distance from the stagnant point increases initially and reaches maximum in magnitude, and decreases because the viscosity increases as temperature decreases.

Finally, soil heating efficiency is calculated for different arc operating conditions and listed in Table 3. The efficiency is defined as the ratio between the power absorbed by the melt pool to the total power of the reactor. The melted soil volume percentage to the total soil volume is also listed in Table 3. By comparing the melted volume percentage, increasing the voltage for the same current does not affect the melt volume significantly. Rather, increasing the arc current has significant effects on producing a large melted volume. This is mainly due to the fact that the heating mechanism of the soil is Joule heating. By increasing the arc current, heat is transferred to the soil more efficiently. However, when material volatility is a major concern of operation, the selection of high current flow may increase volatility of the materials in the reactor. Besides, high current results in fast electrode erosion, which may lead to short life time of the electrodes. The absorbed power by the soil decreases as the arc length increases for the same power. This is in qualitative agreement with the results by Qian et al. (1993)

Table 3. Percentage of the power absorbed by the melt pool to the total power for different operating conditions.

Total Power (kW)	Gap = 1 cm		Gap = 3 cm	
	I = 200 A	I = 300 A	I = 200 A	I = 300 A
5	38.3(28.50)*	46.7(37.53)	35.2(27.68)	42.8(38.28)
7.5	27.5(28.82)	37.4(37.75)	26.0(27.69)	35.9(41.43)
10	20.9(28.95)	33.9(38.05)	19.4(28.68)	29.7(43.47)
15	16.9(29.21)	27.1(38.43)	15.3(29.18)	22.3(46.32)

*The number in the parenthesis is the percent ratio of the melt volume to the total soil volume.

An arc melter is being used for vitrification of thermally oxidized, buried transuranic (TRU) contaminated wastes by INEL in conjunction with the U.S. Bureau of Mines (USBM) as a part of the BWID project (Oden 1993). One of the interesting features of the USBM arc melter is that air is used as a working gas for the plasma. Different working gases have different heating characteristics on the waste as well as on arc melter operating conditions. Usually inert gases, such as argon, helium, etc., are used for the working gas in the DC plasma arc because they yield stable operating environments. Compared to those inert gases, air is difficult to break into a plasma because more heat is required to sustain the plasma state. It is one of the primary purposes of this study to find out the differences between the air and inert gases. In this study, argon was selected since it is one of the most widely used working gases for the DC arc. Heating efficiency and the melt pool shape are compared with different working gases. A laboratory-scale arc melter is modeled to study the various effects of the different working gases.

Before we discuss the calculated results, the air plasma properties are compared with those of argon. Figure 11 shows the temperature dependence of thermodynamic and transport properties of air and argon. Heat capacity is shown at constant pressure, density, thermal conductivity, electrical conductivity, molecular viscosity, and radiation heat loss. These properties are taken from Paik (1987). Since the air is treated as a mixture of diatomic gases, the thermodynamic and transport properties show two peaks on the temperature ranges considered in this study. The first peak, around 7,000 K in heat capacity and thermal conductivity, is due to the dissociation of the nitrogen gas, and the second peak is due to the ionization of the nitrogen. One of the unique differences between air and argon is that the air properties show two peaks while the argon has only one peak in the

temperature ranges we considered. This is because the argon is a monatomic gas. The peak occurring in argon properties is due to the ionization of the argon at that temperature. It should be noted here that air has substantially higher heat capacity, thermal conductivity, and radiation energy loss than the argon at the same temperature. The density and the viscosity of the soil are taken from Buelt (1987). The other thermophysical properties of the soil used for this study are from Henderson and Taylor (1993).

Two different cases are simulated with different gaps between the cathode and the molten surface. Figure 12 shows the comparisons of the temperature fields of the argon and air plasmas over the molten soil field. In the case of air plasma, the plasma volume is smaller than that of argon plasma at the same input power (5 kW input power is used for both argon and air cases). There are three factors for this small plasma volume for air. One is significant radiation energy loss of air plasma at the high temperatures (see Figure 11f). This is one reason that the air plasma has low energy efficiencies as described below (see Table 4). The second factor is that the heat capacity of the air is an order higher than that of argon (see Figure 11a) so that more energy is absorbed by the air at the same temperature. The third is because of the high thermal conductivity of the air plasma is higher than that of argon (see Figure 11c). Owing to the high thermal conductivity of the air, heat conduction plays an important part on heating the soil surface. The melt front in the soil region shows a bowl shape with maximum temperature occurring at the bottom of the reactor because of the high current density collected at the bottom. In Figure 12, the maximum temperature near the bottom of the reactor increases as the arc length becomes shorter. Soil heating efficiency is calculated for different arc operating conditions and listed in Table 4. The efficiency is defined as the ratio between the power absorbed by the melt pool to the total power of the reactor. The melted soil volume percentage to the total soil volume is also listed in Table 4. We found that increasing the voltage for the same current does not affect the melt volume significantly; thus, we made no attempts to reveal the effects of different voltages on the plasma. By comparing the energy absorbed in the soil, the argon plasma cases show better energy efficiency than that of air at the same operating conditions. However, the fraction of the melted volume to the total soil volume shows that the air plasma case has more molten soil than that of argon. This can be explained by the fact that in the case of argon plasma, the joule heating is concentrated near the center of the molten pool, which locally heats the soil near the center of the reactor. In case of the air plasma, the current arriving at the molten surface is more radially spread, which results in more uniform heating of the soil. To show this effect, interfacial temperatures and currents are shown in Figure 13. For the air plasma case, the interface shows higher temperatures than that of argon toward the wall. The difference between the temperatures becomes significant as the arc length increases. For the short arc, the temperature at the interface is higher than for the long arc, as expected. The maximum currents at the interface for the short arc are higher than those of the long arc. For the longer arc, slightly higher currents than those of short arc can be found far from the arc core, since the electrical conductivity of the plasma and the melt pool is relatively evenly distributed over the interface.

Table 4. Percentage of the power absorbed by the melt pool to the total power for different operating conditions.

Total Power (kW)	Gap = 1 cm		Gap = 1.5 cm	
	Argon I = 200 A	Air I = 200 A	Argon I = 200 A	Air I = 200 A
5	38.3(28.50)*	36.2(30.13)	40.2(31.03)	38.8(32.75)
7.5	27.5(28.82)	27.2(31.45)	26.0(27.69)	37.1(33.96)

*The number in parentheses is the percent ratio of the melt volume to the total soil volume.

Figure 14 shows that the induced flow fields in the molten soil region have strong clockwise convection occurring on the right-hand side of the reactor. This convection is a result of the combined effects of the shear and buoyancy induced force. For the air plasma case, the center of the circulation is far from the centerline compared to the argon plasma case. As shown in the Figures 12 and 13, the steep temperature gradient occurs near the center of the reactor for the argon plasma. Thus the magnitude of the buoyancy force is higher near the center for the argon plasma case while the recirculation occurs far from the centerline in the air plasma case. Because of the large density difference caused by the temperature gradient inside the molten soil, the induced natural convection force contributes to the clockwise convection in the melt pool.

2.5 Conclusions

1. A computer model for simulating steady-state, 2-D axisymmetric heat, fluid flow, and electromagnetic fields is developed for the calculation of the arc plasma and molten pool regions for the waste treatment process. The interaction between the plasma and the pool regions is treated in a consistent manner by using the interface physical quantity continuity assumption.
2. The convective heat transfer and the joule heating mechanisms are responsible for heating the molten soil for the waste minimization process.
3. For the different lengths of the arc at the same total power and currents, the currents arriving at the melt pool surface make little difference with respect to heating the melt pool. Instead, the convective heat transfer from the surface causes different melt shapes in the pool.
4. For the same currents, the longer arc heats up a larger volume of the gas environment while the melt pool volume is smaller than that of short arc. With respect to off-gas treatment, a larger volume of high temperature gas may be a favorable environment.

5. Inside the melt pool, a short arc induces strong convection which may lead to uniform mixing of materials inside the pool. If the localized gas heating effect is not desirable, the short arc mode operation is recommended for thermal waste treatment.
6. Increasing power via increasing voltage drop dissipates more heat to the environment gas than to the soil. If a large volume of melted soil is desired, increasing the power by increasing current is a more efficient way of heating the soil. However, the fact that the high currents induce fast electrode erosion should be considered for finding the optimum operating conditions.
7. At the same input power, the volume of air plasma is significantly less than that of argon plasma because of the high heat capacity, radiation loss, and thermal conductivity of the air.
8. The maximum temperature inside the melt pool is higher in an argon plasma arc melter than that in an air plasma owing to the concentrated currents arriving at the melt pool surface.
9. Total melted volume of the air plasma arc melter is larger than that of argon plasma since the heat is dissipated more uniformly inside the melt pool for the air plasma.

Figure 1. Geometry of the plasma arc melter considered in this study.

Figure 2. Temperature dependence of the soil's density and viscosity at Idaho National Engineering Laboratory (Buel 1987).

Figure 3. Comparison of the free burning arc (200 A) isotherms with the experimental measurements performed by Hsu and Pfender (1983).

Figure 4. Isotherms inside the plasma arc melter for current of 200 A and 5 kW power. Results on the left are for the 1-cm gap.

Figure 5. Isotherms inside the plasma arc melter for current of 300 A and 7.5 kW power. Results on the left are for the 1-cm gap.

Figure 6. Current vectors inside the plasma arc melter for current of 200 A and 5 kW power. Results on the left are for the 1-cm gap.

Figure 7. Velocity vectors inside the plasma arc melter for current of 200 A and 5 kW power. Results on the left are for the 1-cm gap.

Figure 8. Plasma-soil interfacial temperature profile.

Figure 9. Plasma-soil interfacial normal current profile.

Figure 10. Plasma-soil interfacial tangential velocity profile.

Figure 11. Plasma thermodynamic and transport properties used in this study: (a) heat capacity, (b) density, (c) thermal conductivity, (d) electrical conductivity, (e) viscosity, (f) radiation loss.

Figure 12.

Isotherms inside the plasma arc melter (from 1,473K to 18,473K with 20,00K increment) for a current density of 200 A and 5 kW input power. Results on the left-hand side are the argon plasma case and those on the right-hand side are the air plasma case (a) for the 1-cm arc length case (Gap = 1 cm), and (b) for 1.5-cm arc length case (Gap = 1.5 cm).

Figure 13. (a) Plasma-soil interfacial temperature profile. (b) Plasma-soil interfacial normal current profile

Figure 14.

Velocity vector inside the plasma arc melter for a current density of 1-cm gap, 200 A, and 5 kW input power. The loops inside the melt represent streamlines. Results on the left-hand side are for the argon plasma case and those on the right-hand side are for the air plasma case.

3. CHEMISTRY MODEL

3.1 Introduction

The purpose of this task is to develop a model to predict the chemical composition that prevails during thermal plasma treatment of the wastes. Both equilibrium and non equilibrium calculations will be considered, but the former was the main focus in FY-94. This route was chosen considering the facts that (a) the temperature in the plasma furnace is very high so that chemical reactions take place at very rapid rates; thereby, equilibrium state can be attained instantaneously, and (b) the thermodynamic database for equilibrium chemistry analyses is readily available and is much more extensive than that of the kinetics. However, there may be a need for kinetic-based calculations, especially when the flow velocity is sufficiently low to prevent low-temperature fluid regions to be mixed with the high-temperature regions. Under this circumstance, the equilibrium assumption may break down, and equilibrium chemistry calculations are therefore inappropriate.

Three subtasks are involved in the equilibrium chemistry modeling. First, chemical species that would exist during processing are identified, and a data search is conducted for those not included in existing databases. Second, an assessment of a number of equilibrium computer codes is performed to determine the code best suited for our purpose. Finally, a sample calculation is made using INEL soil to demonstrate the capability of the software chosen. A review of the underlying principle of chemical equilibrium follows. Then, each of the subtasks will be discussed in detail.

3.2 Theoretical Background

Consider a system consisting of a gas phase, liquid and solid mixtures, and pure condensed phases, in which each chemical specie is made up from a set of L elements. The total free energy of this multiphase system is given by

$$g = \sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} n_{p,i} \mu_{p,i}, \quad (17)$$

where

n is the mole number

μ is the chemical potential

M is the number of species

NQ is the number of species in the liquid phase

NS is the number of species in the solid phase.

The subscripts p and i pertain to phase and specie number, respectively.

From thermodynamics, the chemical potential has been shown to be a function of temperature and pressure as

$$\mu_{p,i} = \begin{cases} \mu_{p,i}^0 + RT \left[\ln P + \ln \left(n_{p,i} / N_p \right) \right] & p = 1 \text{ (gas phase)} \\ \mu_{p,i}^0 + RT \left[\ln \gamma_{p,i} + \ln \left(n_{p,i} / N_p \right) \right] & p = 2, \dots, NQ + 1 \\ \mu_{p,i}^0 & p = NQ + 2, \dots, NQ + NS + 1 \end{cases} \quad (18)$$

where

P is the total pressure of the system

R is the universal gas constant

T is the temperature

N_p is the total mole numbers in phase p

γ is the activity coefficient having a value of one for ideal mixture and less than one

otherwise

$\mu_{p,i}^0$ is the chemical potential at standard state.

It should be remarked that the gas has been assumed ideal or else an additional term must be included to account for non ideal gas behavior.

At equilibrium, the free energy is minimum; hence, our problem reduces to an optimization problem, with g in equation (17) being the objective function subjected to the following mass conservation constraints:

$$\sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} A_{p,ij} n_{p,i} = b_j \quad j = 1, \dots, L. \quad (19)$$

where

$A_{p,ij}$ is the number of atoms of the j element in a molecule i in phase p

b_j is the total number of moles of the j element.

In the framework of the Lagrange's method, minimizing equation (17) is equivalent to minimizing

$$G = g + \sum_{j=1}^L \lambda_j \left\{ \sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} A_{p,ij} n_{p,i} - b_j \right\}, \quad (20)$$

where $\{\lambda_j, j=1,\dots,L\}$ is a set of the so-called Lagrangian multipliers to be determined. It is known from elementary calculus that the function G is minimum when its first derivative vanishes. By differentiating equation (20), we obtain

$$dG = \sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} \left\{ \mu_{p,i} + \sum_{j=1}^L \lambda_j A_{p,ij} \right\} dn_{p,i} + \sum_{j=1}^L \left\{ \sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} A_{p,ij} n_{p,i} - b_j \right\} d\lambda_j, \quad (21)$$

and upon setting $dG=0$ and noting that $dn_{p,i}$ and $d\lambda_j$ are independent for all p, i , and j , there follows

$$\begin{aligned} \mu_{p,i} + \sum_{j=1}^L \lambda_j A_{p,ij} &= 0 & p = 1, \dots, 1+NQ+NS \\ & & i = 1, \dots, M_p \end{aligned} \quad (22)$$

and

$$\sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} A_{p,ij} n_{p,i} = b_j \quad j = 1, \dots, L. \quad (23)$$

Equations (22) and (23) constitute a system of $L + M_1 + \dots + M_{1+NQ+NS}$ equations with an identical number of unknowns (mole numbers); hence a unique solution exists. However, because they are nonlinear, the solution must be obtained by an iterative procedure such as the Newton-Raphson method.

For a given nonlinear system represented by

$$F_i(x_1, x_2, \dots, x_N) = 0 \quad i = 1, \dots, N, \quad (24)$$

the Newton-Raphson formula is

$$\frac{\partial F_i^{\text{old}}}{\partial x_j} \Delta x_j^{\text{new}} = -F_i^{\text{old}}, \quad (25)$$

where $\Delta x_j^{\text{new}} = x_j^{\text{new}} - x_j^{\text{old}}$.

The solution process starts with an initial guess, which is subsequently refined by solving equation (25) repeatedly until Δx_j^{new} satisfies a prescribed convergence criteria. When applying to our system, equation (25) becomes

$$\left(\Delta \ln n_{p,i}\right)^{new} - \left(\Delta \ln N_p\right)^{new} = - \left[\frac{\mu_{p,i}}{RT} + \sum_{j=1}^L \frac{\lambda_j}{RT} A_{p,ij} \right]^{old}, \quad \begin{matrix} p = 1, \dots, 1+NQ+NS \\ i = 1, \dots, M_p \end{matrix}, \quad (26)$$

$$\sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} A_{p,ij} n_{p,i}^{old} \left(\Delta \ln n_{p,i}\right)^{new} = - \sum_{p=1}^{1+NQ+NS} \sum_{i=1}^{M_p} A_{p,ij} n_{p,i}^{old} - b_j \quad (27)$$

which are now linear and can be solved easily. Equations (26) and (27) form a standard mathematical basis for chemical equilibrium calculations and have been used widely since it requires only thermodynamic data that are undoubtedly much easier to obtain.

3.3 Species Identification and Data Search

There are a number of organizations that can provide the type of information we need, including MSE (Mountain State Energy Inc. in Montana), PNL (Pacific Northwest Laboratory in Washington), MIT (Massachusetts Institute of Technology in Massachusetts), and IRC (Idaho Research Center at the INEL in Idaho). However, the IRC work was chosen because of the easy access to the data.

The on going efforts at IRC to develop and construct a bench-scale arc melter for mixed wastes treatments have resulted in a good database on the final waste form composition and are well documented in the report by Grandy et al. (1993). Table 5 summarizes the species generated for a number of different waste streams containing hydrated metal oxide sludges, alkalines, oils, cleaning agents, and salts. A major assumption associated with this data source is that all organic materials are completely converted to CO₂ and H₂O; thereby implying an uncertainty in the composition of the gas phase. It is not clear at this point how the missing information would affect our modeling effort since the off-gas has never been analyzed. However, this uncertainty may not create much difficulty for the calculations unless the gas mixture contains uncommon species that could not be identified because of the lack of data in the database. From Table 5, a list of major elements, tabulated in Table 6, can be deduced.

Table 5. Major species produced from non radioactive wastes.

Al	Ce	Fe ₂ O ₃	Mn	P	TiO ₂
Al ₂ O ₃	CO	H ₂ O	N ₂	Pb	Zn
As	CO ₂	Hg	Na ₂ O	SiO ₂	
CaO	Cu	K ₂ O	Ni	SO ₂	
Cd	FeO	MgO	NO _x	Ta	

Table 6. Major elements present in non radioactive wastes.

Al	Cu	Mg	P	Zn
As	Fe	Mn	Pb	
Ca	H	Na	Si	
Ce	Hg	Ni	Ta	
Cd	K	O	Ti	

The above Tables were derived from hypothetical feeds, which are free of radioactive materials, used to test the IRC melter. Real wastes, such as those at the SDA at the RWMC, contain several nuclides in a wide range of half-lives from a few years to several thousand years. Table 7 gives the identity of those found at the RWMC.

Table 7. Radio nuclides at the RWMC

Am	Cm	Pu
U		

Although these species were listed in their elemental form, it should be understood that each can have several daughters (isotopes), and because no chemical equilibrium software is able to distinguish the isotopes from their parent, they are not listed. Other species such as Ni-59, Co-60, Sr-90, Cs-137 are also present, but were not taken into account due to the same reason.

As mentioned above, the required input data for the free energy minimization calculation approach is the free energy function. The most comprehensive source of the thermophysical data has been the JANAF table, which compiles the Gibbs free energy data for a wide range of temperatures. However, be aware that old versions may leave out some of the species due to the lack of an update. Fortunately, the version used at the INEL contains all the above-tabulated species

except for most radioactive elements. Our fruitful data search has discovered another database that contains the data for Am, Pu, and U, as well as their oxides (Roine 1993). Because their database is so large, no attempt is given to reproduce it here, and interested readers are referred to the cited reference for further information.

3.4 Codes Selection

The main objective of this subtask is to determine a code which satisfies our needs the most. Four criteria are used in the selection:

1. Completeness of the database
2. Code reliability
3. Code robustness
4. Code accessibility.

The first is given the highest priority.

After an initial screening of a pool of codes including SOLGASMIX (Besmann 1977), FACT (Thompson 1985), HSC (Roin 1993), and MIXTURE-PV (Tseng 1989) the last three were selected for further consideration. MIXTURE-PV has been used extensively by researchers at the University of Minnesota for chemistry calculations concerning plasma synthesis. On the other hand, FACT is being used for a variety of applications at McGill University in Canada and it appears to contain the most comprehensive thermodynamic database. Unlike MIXTURE-PV, FACT is a proprietary code, and therefore no source code is available to the public. To use FACT, an user must apply for an account to get on McGill's computer facility and charges are based on the computing time used. The code may not produce good results at low and high temperature, but it is a common problem to all codes because at low temperature, the equilibrium assumption becomes questionable, and at high temperature, the data are unreliable. From past experience, MIXTURE-PV is very robust, and the correctness of the results have been confirmed for simple problems (Nguyen 1991). Based on our priorities set forth earlier, MIXTURE-PV is eliminated. The remaining codes are now FACT and HSC, which both suffer the same disadvantage of being commercial codes. Despite the fact that the FACT database could be broader, it is unsure how much broader it is compared to HSC database, because no information is given in the FACT manual. However, our preliminary examination indicates that HSC database is reasonably adequate for our purpose. Based on the easy access to HSC and the potentially high cost associated with the use of FACT, HSC is adopted for the chemistry calculations.

3.5 Validation

Having selected HSC as a code for chemistry modeling in thermal plasma arc technology, we performed several tests to ensure its reliability and to provide confidence to the results reported in the Applications section to follow.

As a first test, we determined the equilibrium compositions of a gaseous mixture resulting from 2 moles of CH_4 reacted with 3 moles of H_2O at 1,000K and 1 bar. The product gas is assumed to contain only the following species: CH_4 , H_2O , CO , CO_2 , and H_2 . The calculated result is given in Table 8 along with the data of Smith and Van Ness (1987). Clearly, the two results agree exceptionally well.

Table 8. Equilibrium mole fraction of 2 mol. CH_4 + 3 mol. H_2O at 1,000K and 1 bar.

	H_2	CO	CO_2	CH_4	H_2O
HSC	0.6701	0.1741	0.0369	0.0201	0.0987
Smith & Van Ness (1987)	0.6705	0.1740	0.0372	0.0200	0.0983

The second example is a two-phase system involving solids and gases. Here, a coal bed (assumed to be carbon) in a gasifier is oxidized by a stream of air and steam in 2.38:1 mole proportion, i.e., 1 mole of steam and 2.38 moles of air. The air is assumed to consist of 79% N_2 and 21% O_2 on the molar basis. With the given feed information, one is interested in searching for an optimum temperature that gives the least amount of carbon monoxide in the gas phase. The desired operating condition is between 1,000K and 1,500K for temperature with the pressure fixed at 20 bar.

One way to comprehend this problem is to perform a parametric study, in which the temperature is varied incrementally so as to narrow the desired temperature range. As an example, 6 runs were performed to narrow the range, and the results are shown in Table 9. It is apparent from Table 9 that the amount of CO gas produced is a monotonic function of temperature; therefore, one should keep the temperature as low as possible to minimize the production of such a poisoning gas. To demonstrate the validity of our conclusion, our results are compared with those of Smith and Van Ness (1987) as shown in the same table. Again, the match is quite good even though their data were obtained based on the equilibrium-constant approach. Note that the discrepancy in this test problem is within the rounding errors.

Table 9. Mole fraction of CO in the product gas at 20 bar.

	1,000K	1,100K	1,200K	1,300K	1,400K	1,500K
HSC	0.1117	0.2259	0.3268	0.3783	0.3896	0.4047
Smith & Van Ness (1987)	0.112	0.226	0.327	0.378	0.398	0.405

The third example is the oxidation of a mixture of Si and Pb with O₂. The unreacted state contains 1 mole of Si, 1 mole of Pb, and 2.5 moles of O₂. After equilibrium is reached, the product gas has the composition listed in Table 10. In this Table, the results are compared with those predicted by SOLGAS. Even though the discrepancy is obvious, its magnitude is probably unimportant because it may very well be within the errors associated with the fitting of the thermodynamic correlations. Nonetheless, the values are in the same range.

Table 10. Equilibrium mole numbers in the gas phase for Si + Pb + 2.5 O₂.

Species	Temperature							
	3,500 K		4,000 K		4,500 K		5,000 K	
	HSC	SOLGAS	HSC	SOLGAS	HSC	SOLGAS	HSC	SOLGAS
O	1.147	1.174	2.650	2.674	3.601	3.610	3.942	3.936
O ₂	1.224	1.286	0.597	0.616	0.179	1.833	0.052	0.053
O ₃	1.4(-6)	1.5(-6)	7.6(-7)	8.6(-7)	1.8(-7)	2.1(-7)	3.6(-8)	4.8(-8)
Pb	0.638	0.788	0.856	0.918	0.956	0.973	0.986	0.991
PbO	0.362	0.212	0.144	0.082	0.044	0.026	0.0136	9.2(-3)
Pb ₂	1.7(-5)	1.0(-4)	1.5(-5)	7.7(-5)	1.0(-5)	5.3(-5)	6.2(-6)	3.8(-5)
Si	2.8(-5)	2.7(-4)	5.2(-4)	4.9(-4)	7.0(-3)	6.3(-3)	0.061	0.053
SiO	0.957	0.957	0.987	0.987	0.989	0.990	0.938	0.946
SiO ₂	0.043	0.042	0.013	0.012	3.7(-3)	3.4(-3)	1.2(-3)	1.1(-3)
Si ₂	1.4(-11)	1.3(-11)	1.1(-9)	9.5(-10)	6.0(-8)	4.9(-8)	1.8(-6)	1.4(-6)
Si ₃	1.2(-17)	1.1(-17)	2.5(-15)	2.1(-15)	7.6(-14)	3.3(-13)	3.8(-11)	2.5(-11)

3.6 Applications

With the confidence gained in the preceding section, we now attempt to simulate the INEL soil. Because the composition of the soil-waste mixture is not fixed, but rather varies from one location to another, we shall construct a waste stream according to the information summarized in Table 11 as suggested by Bates (1993).

Table 11. Composition of nominal waste stream.^{††}

Material	Weight %
Soil: SiO ₂ (71.23%), Al ₂ O ₃ (13.2%), Fe ₂ O ₃ (4.7%), CaO (4.11%), K ₂ O (3.34%), MgO (1.92%), Na ₂ O (1.5%).	59.5
Metals: Fe (90.5%), Al (5%), Zr (2.5%), Cu (1.5%), Pb (0.5%)	15
Solid combustible: Assume C ₆ H ₁₀ O ₅ (100%)	10
741 & 742 sludge: Al(OH) ₃ (11.5%), Ca(OH) ₂ (6.6%), Fe(OH) ₃ (10.8%), KOH (7.4%), Mg(OH) ₂ (7.9%), H ₂ O (44.2%), Portland cement [†] (11.6%)	4
743 sludge: assume C ₂₀ H ₄₀ (100%)	9
Nitrate salts: NaNO ₃ (60%), KNO ₃ (40%)	2
Radio nuclide: UO ₂ (100%)	0.5

[†]Assumed to be SiO₂ (25%), Al₂O₃ (15%), CaO (60%)

^{††}Other species also exist but are in small quantities; hence neglected.

From the above Table, the number of species present in the waste stream is 23 and is given in Table 8. These species were made from 15 chemical elements, including Al, C, Ca, Cu, Fe, H, K, Mg, N, Na, O, Pb, Si, U, and Zr. With these elements, HSC predicted a set of 426 possible compounds, which exceeds the capability of the software that is set at 150 maximum. To overcome this problem, Zr and Cu are omitted and their masses are treated as if they were Al. Even with this elimination, there are still 395 compounds left in the set. After further deletion of the minor species, this set of compounds reduces to 130 species. The identity of these species is given in Table 13.

Table 12. Species present in the waste stream (basis 100g).

Species	Amount (g)	Molecular weight	# of moles
Al	0.75	26.98	0.028
Al ₂ O ₃	7.92	101.96	0.078
Al(OH) ₃	0.46	77.98	0.006
C ₂₀ H ₄₀	9	280.2	0.032
C ₆ H ₁₀ O ₅	10	162.06	0.062
CaO	2.73	56.08	0.049
Ca(OH) ₂	0.263	74.08	0.004
Cu	0.224	63.55	0.004
Fe	13.58	55.85	0.243
Fe ₂ O ₃	2.8	159.7	0.006
Fe(OH) ₃	0.43	106.85	0.004
H ₂ O	1.77	18	0.098
K ₂ O	1.99	55.1	0.036
KOH	0.295	56.1	0.005
KNO ₃	0.8	101.17	0.008
MgO	1.44	40.31	0.028
Mg(OH) ₂	0.315	58.31	0.005
Na ₂ O	0.89	62	0.014
NaNO ₃	1.2	85.07	0.014
Pb	0.074	207.2	0.0004
SiO ₂	42.495	90.69	0.469
UO ₂	0.5	266	0.002
Zr	0.374	91.22	0.004
Total	100		1.2

Table 13. Species present at equilibrium.

Species	Phase [†]	Species	Phase [†]	Species	Phase [†]
NH ₃	g	Al ₂ O	g	PbO ₂	c
CH ₄	g	U	g	MgO ₂	c
H ₂ O	g	H ₂ O	c	Na ₂ O	
H ₂	g	CaCO ₃	c	NaN ₃	c
CO ₂	g	SiO ₂	c	UO ₃	c
C ₂ H ₆	g	C	c	UO ₃	c
CO	g	Al ₂ O ₃	c	CaO ₂	c
CH ₃ OH	g	Fe ₃ O ₄	c	Pb ₃ O ₄	c
HCN	g	K ₂ CO ₃	c	K ₂ O	c
C ₂ H ₄	g	Mg(OH) ₂	c	CaH ₂	c
CH ₃	g	Na ₂ CO ₃	c	Mg	c
Pb	g	U ₃ O ₅	c	Na ₂ O ₂	c
KOH	g	Pb	c	Na ₃ UO ₄	c
NH ₂	g	NH ₄ OH	c	KO ₂	c
NaOH	g	Al(OH) ₃	c	NaO ₂	c
C ₂ H ₂	g	Fe ₂ O ₃	c	K ₂ O ₂	c
PbO	g	MgCO ₃	c	Si	c
K	g	Fe(OH) ₂	c	KNO ₃	c
Na	g	FeO	c	Fe(CO) ₅	c
NO	g	NaHCO ₃	c	NaNO ₃	c
Ca(OH) ₂	g	Fe(OH) ₃	c	Al	c
NH	g	MgO	c	NH ₄ NO ₃	
CH ₂	g	Ca(OH) ₂	c	Ca	c
Fe	g	FeCO ₃	c	UO	c
O ₂	g	PbCO ₃	c	UN	c
N	g	PbO	c	HNO ₃	c
MgOH	g	NaFeO ₂	c	Si ₃ N ₄	c
NO ₂	g	NaOH	c	K ₂ O ₃	c
KO	g	Fe	c	KO ₃	c
FeO	g	KOH	c	UC	c
Mg	g	CaO	c	UC ₂	c
SiO	g	KCN	c	U ₃ O ₈	c
SiO ₂	g	HCO ₂ H	c	UH ₃	c
MgO	g	HCOOH	c	U	c

[†]g: gas phase, c: condensed phase

Table 13. Continued.

Species	Phase [†]	Species	Phase [†]	Species	Phase [†]
Ca	g	CH ₃ OH	c	U ₄ O ₉	c
C	g	NaCN	c	UFe ₂	
AlO ₂	g	C ₂ H ₆ O	c	N ₂ O ₄	c
NO ₃	g	N ₂ H ₄	c	Ca(NO ₃) ₂	c
CaO	g	NaH	c	Pb(NO ₃) ₂	c
AlO	g	KH	c	Ca ₃ N ₂	c
Al	g	UO ₂	c	Si ₂ H ₆	c
Si		Na	c	Mg(NO ₃) ₂	c
Al ₂ O ₂	g	K	c	N ₂ O ₅	c
			c	U ₂ C ₃	c

[†]g: gas phase, c: condensed phase

Figures 15 and 16 present the mole fractions of gaseous pollutants as a function of temperature for two different streams of reactants: 100g waste + 32g O₂, and 100g waste + 160g O₂, respectively. With 1 mole of oxygen input, Figure 15 shows a steady increase in quantity of pollutant formation as temperature increases beyond 500K, with the amount of CO being several orders of magnitude larger than Pb, PbO, NO_x, and U. By inspecting the computer outputs, CO concentration is the highest at high temperature. Even though CO is the most dominant specie in the gas phase, lead, lead oxide, and NO_x are present in sufficient amount to be of concern. Throughout the temperature range, 300K to 2,300K, the mole fraction of uranium gas is always below 10⁻²⁴ level. To see the effect of oxygen concentration level in the feed, 100g of waste is now allowed to react with 160g of O₂ (see Figure 16). In contrast to the previous case, the mole fractions of all the gaseous pollutants except uranium are now much closer together. In addition, NO is now the most dominant pollutant instead of CO as before, and that neither pollutant reaches above 10⁻². This is in part due to excess O₂ that dilutes the entire gas phase.

Figure 17 is a plot of gas production as a function of temperature. Clearly, the trend is similar. For the most part, the amount of gas produced increases monotonically with temperature until the temperature reaches about 1,900K, then decreases relatively faster. From this figure, the excess O₂ is responsible for the gap between the two curves.

As another demonstration of what our chemistry model can do, we now present Figure 18, where contours of CO is plotted as a function of temperature and weight of input O₂. One important feature of this contours plot is that it provides information on how to operate the system in order to

minimize the production of undesirable species. For the case being considered, high temperature and high concentration of O_2 in the feed would be desirable if one wants to reduce amount of CO in the gas phase.

Thus far, all the discussion has focused on the pollutants. For details about other species, Appendix should be consulted.

Figure 15. The mole fractions of gaseous pollutants as a function of temperature for 100g waste + 32g O₂.

Figure 16. The mole fractions of gaseous pollutants as a function of temperature 100g waste + 160g O_2 .

Figure 17. Gas production as a function of temperature.

Figure 18. Contours of CO as a function of temperature and weight of input O₂.

4. FIDAP CODE CALCULATIONS

4.1 Introduction

The commercial finite element - heat transfer and computational fluid dynamics code FIDAP was used to model a 2-D melter similar to the U.S. Bureau of Mines melter. A description of the model is shown in Figure 19. The melter is approximately 1 meter wide and 0.3 meters high. The soil entrance is 0.2 meters and the electrode width is 0.1 meters, while the air gaps are 0.1 meters. A flow rate of 0.15 kg/s was used for the flow conditions. The voltage at the electrode was adjusted to obtain a maximum temperature in the melt of between 2,500K to 3,500K.

A steady-state solution to the electric field, mass, momentum, and energy equations was used to simulate melting the soil. A more complete model with the ceramic bricks, feed tubes, exit port, and electrodes is planned to be completed in the future. The purpose of this 2-D model is to learn about the melter and show the capabilities of the code. This section of the report shows the results for the convective heat transfer, fluid flow, and electric field effects in the molten slag portion of a 2-D melter.

4.2 Governing Equations

The governing equation for the steady state electric field calculation is given by

$$\frac{\partial}{\partial x} \left(k_{\phi}(T) \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_{\phi}(T) \frac{\partial \phi}{\partial y} \right) = 0 \quad (28)$$

where

$\phi(x,y)$ is the voltage

$k_{\phi}(T)$ is the temperature-dependent electrical conductivity.

Equation (28) is assumed to hold in the entire domain. Boundary conditions for Equation (28) are constant voltage at the electrodes and zero electric field ($\partial\phi/\partial n=0$) on all other boundaries. The typical electrode voltages were 100V for right electrode and 225V for the left electrode.

The governing equations for steady laminar natural convection are given by

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0 \quad (29)$$

$$\rho \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(\mu(T) \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu(T) \frac{\partial u}{\partial y} \right) \quad (30)$$

$$\rho \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left(\mu(T) \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu(T) \frac{\partial v}{\partial y} \right) - \rho g \beta (T - T_{ref}) \quad (31)$$

$$\rho c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \frac{\partial}{\partial x} \left(k(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k(T) \frac{\partial T}{\partial y} \right) + Q(T) \quad (32)$$

$$Q(T) = k_{\phi}(T) \left[\left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 \right] \quad (33)$$

where

$u(x,y,t)$ is the x velocity

$v(x,y,t)$ is the y velocity

$T(x,y,t)$ is the temperature

ρ is the density

$\mu(T)$ is the viscosity varying with temperature

g is gravity

β is the coefficient of volume expansion

T_{ref} is the buoyancy reference temperature

c_p is the specific heat

$k(T)$ is the thermal conductivity varying with temperature.

Boundary conditions for the momentum equations are no slip at the walls and an inlet velocity for the soil of $1.72e-4$ m/s. A heat transfer coefficient of $50 \text{ W/m}^2\text{-K}$, with a reference temperature of 300K , is applied along the bottom to extract heat from the model as the ceramic bricks do. A heat flux is applied across the top of the model, where the heat comes from radiation and convection of the arcs between the electrodes and the slag. The total heat flow from this is 200 kW . A ramp heat flux profile is applied between the soil entrance area to the electrode, where the heat flux starts at zero and increases to $562e3 \text{ W/m}^2$ at the electrode. The heat flux is constant at $562e3 \text{ W/m}^2$ along the electrodes. A parabolic profile heat flux is imposed between the electrodes, where the heat flux starts at $562e3 \text{ W/m}^2$ at the electrodes and decreases parabolically to $1/3$ of the electrode heat flux at a center point between the electrodes, and then parabolically increases back to the electrode heat flux at the next electrode.

4.3 Results

The results of the FIDAP model are shown in Figures 19 through 44 and in Table 14. Six models were run for this report. The models were created to find the effects of a regular melt, a molten metal pool at the bottom of the melt, and a skull model with and without a molten metal pool. The molten metal pool height is 8 cm. The skull model was created to demonstrate the code's capability to model a solid skull on the outside of the slag. These six models will be referred to as 125wom, 150wom, 125wm, 150wm, skullnm, and skullm; where 125 and 150 mean the voltage drop across the electrodes, wom means without metal, wm means with metal, skullnm means skull no metal, and skullm means skull with metal. The first four models show a parametric study of the different heating rates due to the Joule heating with 125V and 150V voltage drop with and without the molten metal pool. The voltage drop on the skull problems was adjusted several times until the slag exit temperature was around 2,000K. This voltage drop was 300V. A heat transfer coefficient of $5,000 \text{ W/m}^2\text{-K}$ was input as a boundary condition along the bottom of the model to get a skull to form. This is not realistic since ceramic bricks form the bottom of the melter; the only reason this was done was to show the effects of the skull and to show that the code can model a skull-type problem.

The finite element mesh for the model is shown in Figure 19a. The same mesh was used for all of the models. The fine mesh line in the middle-bottom of the mesh was created to capture the effects of the molten metal pool-slag interface. A velocity boundary condition was set so that the molten metal pool could not mix with the slag.

Results for the 125wom model are shown in Figures 20–23, 150wom in Figures 24–27, 125wm in Figures 28–31, 150wm in Figures 32–35, skullnm in Figures 36–39, and skullm in Figures 40–43. Included in each group of figures are the velocity vectors, temperature contours, streamline contours, and voltage contours.

Figure 20 shows the velocity vectors for 125wom. Two large convection cells form because of the temperature difference of the soil. The cold soil enters and is immediately melted within 1–2 cm of the entrance, and on the left side the colder slag goes down along the bottom and is heated in the middle of the model due to the Joule heating. The soil that enters on the right entrance is immediately melted and exits through the exit. The temperature contours for the 125wom model are shown in Figure 21. The bulk of the slag is between contour E and F, or 2,300K. The highest temperatures in the model are the areas of the slag directly beneath the electrodes, since this is where the highest heat flux boundary condition was imposed. Figure 22 shows the streamline contours for model 125wom. The far left streamline enters with the soil entrance, goes down along the left bottom, rises through the center, and stays along the top and goes out the exit. This is the main path

for the soil that enters and exits the melter. Figure 23 shows the voltage contours for model 125wom. The heat generated due to Joule heating is given in Equation 33, where the heat generated is proportional to the voltage gradient squared. This shows the Joule heating is the highest where the contour lines are the closest, mostly right near the electrodes.

The 150wom model figures are very similar to the 125wom, except the temperature is higher and therefore the velocities are higher. Figure 28 shows the velocity vectors for the 125wm model. There are three cells that have formed in the slag and two in the molten metal pool. The temperature is hotter with the metal pool than without. This is because no heat is generated in the metal pool by Joule heating due to the high electrical conductivity of the metal, and thus confines the heat generating to a smaller area, and this raises the temperature. Figure 30 shows the streamline contours for the molten metal pool. As stated earlier, five cells have formed. Figure 31 shows the voltage contours for the molten metal pool model with a voltage drop of 125V. Figures 32–35 are for the 150wm model and are very similar, except the temperature and maximum velocity are higher than the 125wm model.

The results of the skull model without a metal pool are shown in Figures 36–39. The velocities are basically zero for about 1 cm along the bottom edge since the slag is solidified. Contour C in Figure 37 is the melting temperature of the slag shown along the bottom of the model. Figures 40–43 show the results of the skull model with a metal pool. The melting temperature of the metal is 1700K which is between contour C and D in Figure 41. This shows that only the center and upper part of the metal pool is liquid and the rest has solidified. The majority of the slag is at a temperature of 3100K which is extremely hot. Figure 42 shows that six cells have formed in the melter. Figure 43 shows the voltage contours in the model are very close at the edge of the melter where the metal pool-slag interface is. Some heat is being generated in this area that causes the extra cells to form.

Figure 44 shows the effects of the molten metal pool on the temperature along the bottom of the melter for this model. The lower two curves are for the lower voltage drop and the higher curves are for the higher voltage drop. Again the metal pool has the effect of increasing the temperature in the slag and in this case along the bottom of the model. Figure 45 shows the temperature along the bottom of the melter for the skull models. In this case the metal pool has the opposite effect and is cooler than the model without a metal pool. This is due to the high heat transfer coefficient imposed along the bottom boundary which solidifies the metal pool and drastically slows down the heat transfer to a conduction only mode without natural convection.

Table 14 shows the results of the six runs in tabular form. The diffusive heat flow is heat transferred by conduction given by $-k\partial T/\partial n$ where n is normal to the surface. This means that heat lost is positive and heat in is negative. The negative values show that the heat input by the heat flux boundary condition is greater than the heat lost by the convective heat transfer boundary condition.

The convective heat flow is defined as $mc_p(T_{out} - T_{in})$ where m is the mass flow rate and c_p is the specific heat. This is always positive since the temperature out is greater than the temperature in.

Table 14. Results of six models for FIDAP simulation.

Model	Maximum Velocity (m/s)	Maximum Temperature (K)	Average Exit Temperature (K)	Diffusive Heat Flow (kW)	Convective Heat Flow (kW)
125wom	0.33e-1	2,992	1,980	-70	302
125wm	0.53e-1	3,392	2,190	-20	344
150wom	0.25e-1	3,126	2,045	-9	315
150wm	0.30e-1	3,494	2,270	85	360
skullnm	0.71e-1	3,599	1,885	355	282
skullm	0.57e-1	4,374	2,235	13	352

Also included in this report is Appendix B which shows the material properties and boundary conditions of the major portion of a FIDAP input model.

4.4 Conclusions

A model has been created to simulate the electric melting in a 2-D model of a typical melter design. Steady-state heat transfer and fluid flow have been simulated with the computer code FIDAP for the electric melting. Six models were created for the simulations. The effects of the molten metal pool show higher temperatures in the slag for the metal pool than without the metal pool. A parametric study was performed showing the effects of electrode voltage boundary conditions. Two of the six models created were models where a slag skull formed due to high heat loss. The model with a skull with a metal pool showed almost all of the metal pool had been solidified. The results of this work show that the FIDAP code can be used to model these kind of problems.

Figure 20.

Figure 19.

Melter model description.

Figure 21. Velocity vectors without metal pool, $V_d=125$.

Figure 22. Temperature contours without metal pool, $V_d=125$.

Figure 23. Streamline contours without metal pooling, $V_d=125$.

Figure 24. Voltage contours without metal pooling, $V_d=125$.

Figure 25. Velocity vectors without metal pooling, $V_d=150$.

Figure 26. Temperature contours without metal pooling, $V_d=150$.

Figure 27. Streamline contours without metal pooling, $V_d=150$.

Figure 28. Voltage contours without metal pooling, $V_d=150$.

Figure 29. Velocity vectors with metal pooling, $V_d=125$.

Figure 30. Temperature contours with metal pooling, $V_d=125$.

Figure 31. Streamline contours with metal pooling, $V_d=125$.

Figure 32. Voltage contours with metal pooling, $V_d=125$.

Figure 33. Velocity vectors with metal pooling, $V_d=150$.

Figure 34. Temperature contours with metal pooling, $V_d=150$.

Figure 35. Streamline contours with metal pooling, $V_d=150$.

Figure 36. Voltage contours with metal pooling, $V_d=150$.

Figure 37. Velocity vectors skull without metal pooling, Vd=300.

Figure 38. Temperature contours skull without metal pooling, Vd=300.

Figure 39. Streamline contours skull without metal pooling, $V_d=300$.

Figure 40. Voltage contours skull without metal pooling, $V_d=300$.

Figure 41. Velocity vectors skull with metal pooling, Vd=300.

Figure 42. Temperature contours skull with metal pooling, Vd=300.

Figure 43. Streamline contours skull with metal pooling, $V_d=300$.

Figure 44. Voltage contours skull with metal pooling, $V_d=300$.

Figure 45. Temperature along bottom of melter.

Figure 46. Temperature along bottom for skull models.

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APPENDIX A

RESULTS OF CHEMICAL EQUILIBRIUM PROGRAM

APPENDIX A

RESULTS OF CHEMICAL EQUILIBRIUM PROGRAM

GIBBS WINDOWS 8.0 FOR MULTIPHASE EQUILIBRIUM CALCULATIONS
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T.Talonen, T.Syvajarvi and A.Roine

S

Temperature 298.15 K
Pressure 1 bar
Volume 1.315E-01 m3 (NPT)
Reaction enthalpy -9.143E+02 kJ
Reaction entropy -2.910E+02 J/K
Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACT	ACTIVITY	ACTIVITY
O2(g)	7.1550E+00	5.4576E+00	9.299E-01	1.00E+00	9.299E-01
CO2(g)	0.0000E+00	4.1110E-01	7.005E-02	1.00E+00	7.005E-02
H2O(g)	0.0000E+00	1.6630E-09	2.834E-10	1.00E+00	2.834E-10
NO2(g)	0.0000E+00	6.3326E-11	1.079E-11	1.00E+00	1.079E-11
NO(g)	0.0000E+00	2.1080E-11	3.592E-12	1.00E+00	3.592E-12
NO3(g)	0.0000E+00	8.2589E-12	1.407E-12	1.00E+00	1.407E-12
KOH(g)	0.0000E+00	2.4082E-12	4.103E-13	1.00E+00	4.103E-13
H2(g)	9.5000E-01	1.3642E-12	2.325E-13	1.00E+00	2.325E-13
NaOH(g)	0.0000E+00	7.3460E-13	1.252E-13	1.00E+00	1.252E-13
CO(g)	0.0000E+00	6.1022E-13	1.040E-13	1.00E+00	1.040E-13
PbO(g)	0.0000E+00	4.5763E-13	7.798E-14	1.00E+00	7.798E-14
Ca(OH)2(g)	0.0000E+00	9.9640E-15	1.698E-15	1.00E+00	1.698E-15
KO(g)	0.0000E+00	9.4671E-15	1.611E-15	1.00E+00	1.611E-15
K(g)	0.0000E+00	6.5724E-15	1.120E-15	1.00E+00	1.120E-15
Pb(g)	0.0000E+00	5.8570E-15	7.814E-16	1.00E+00	7.814E-16
NH3(g)	0.0000E+00	4.4514E-15	7.595E-16	1.00E+00	7.595E-16
Na(g)	0.0000E+00	3.4591E-15	5.894E-16	1.00E+00	5.894E-16
NH2(g)	0.0000E+00	1.4125E-16	2.407E-17	1.00E+00	2.407E-17
N(g)	0.0000E+00	7.6831E-17	1.309E-17	1.00E+00	1.309E-17
SiO2(g)	0.0000E+00	2.5904E-17	4.414E-18	1.00E+00	4.414E-18
NH(g)	0.0000E+00	2.1139E-17	3.636E-18	1.00E+00	3.636E-18
HgOH(g)	0.0000E+00	7.4227E-18	1.265E-18	1.00E+00	1.265E-18
FeO(g)	0.0000E+00	5.4597E-18	9.301E-19	1.00E+00	9.301E-19
AlO2(g)	0.0000E+00	3.1742E-18	5.409E-19	1.00E+00	5.409E-19
HgO(g)	0.0000E+00	2.2344E-18	3.807E-19	1.00E+00	3.807E-19
HCN(g)	0.0000E+00	5.2188E-20	8.893E-21	1.00E+00	8.893E-21
CH3OH(g)	0.0000E+00	4.2304E-20	7.208E-21	1.00E+00	7.208E-21
SiO(g)	0.0000E+00	2.3738E-20	4.045E-21	1.00E+00	4.045E-21
Fe(g)	0.0000E+00	1.7633E-20	3.005E-21	1.00E+00	3.005E-21
Hg(g)	0.0000E+00	1.1158E-20	1.901E-21	1.00E+00	1.901E-21
CaO(g)	0.0000E+00	2.8271E-21	4.817E-22	1.00E+00	4.817E-22
CH4(g)	0.0000E+00	4.1078E-22	7.000E-23	1.00E+00	7.000E-23
AlO(g)	0.0000E+00	1.0762E-22	1.834E-23	1.00E+00	1.834E-23
Ca(g)	0.0000E+00	5.5186E-23	9.403E-24	1.00E+00	9.403E-24
CH3(g)	0.0000E+00	2.1537E-23	3.670E-24	1.00E+00	3.670E-24
CH2(g)	0.0000E+00	5.6053E-26	9.551E-27	1.00E+00	9.551E-27
C(g)	0.0000E+00	5.3160E-27	9.058E-28	1.00E+00	9.058E-28
Al(g)	0.0000E+00	3.4776E-27	5.926E-28	1.00E+00	5.926E-28
Al2O2(g)	0.0000E+00	1.7651E-29	3.008E-30	1.00E+00	3.008E-30
C2H2(g)	0.0000E+00	4.2556E-31	7.251E-32	1.00E+00	7.251E-32
Si(g)	0.0000E+00	1.8342E-31	3.125E-32	1.00E+00	3.125E-32
SiH4(g)	0.0000E+00	1.2654E-33	2.156E-34	1.00E+00	2.156E-34
Al2O(g)	0.0000E+00	1.0211E-35	1.740E-36	1.00E+00	1.740E-36
C2H6(g)	0.0000E+00	1.3052E-37	2.244E-38	1.00E+00	2.244E-38
U(g)	0.0000E+00	1.9308E-042	3.293E-43	1.00E+00	3.293E-43
Total	8.1050E+00	5.8687E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACT	ACTIVITY	ACTIVITY
H2O	9.8000E-02	1.0535E+00	4.434E-01	1.00E+00	4.434E-01
CaCO3	0.0000E+00	4.9400E-01	2.079E-01	1.00E+00	2.079E-01
SiO2	4.6900E-01	4.6900E-01	1.974E-01	1.00E+00	1.974E-01
Fe2O3	6.0000E-03	1.2950E-01	5.451E-02	1.00E+00	5.451E-02
Al2O3	7.8000E-02	9.9000E-02	4.167E-02	1.00E+00	4.167E-02
NaHCO3	0.0000E+00	4.2000E-02	1.768E-02	1.00E+00	1.768E-02
HgCO3	0.0000E+00	3.3000E-02	1.389E-02	1.00E+00	1.389E-02
K2CO3	0.0000E+00	3.1500E-02	1.326E-02	1.00E+00	1.326E-02
KNO3	8.0000E-03	2.2000E-02	9.260E-03	1.00E+00	9.260E-03
UO3	0.0000E+00	2.0000E-03	8.418E-04	1.00E+00	8.418E-04

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PbCO3	0.0000E+00	4.0000E-004	1.684E-04	1.00E+00	1.684E-04
Al(OH)3	6.0000E-03	1.7548E-009	7.386E-10	1.00E+00	7.386E-10
UO3(G)	0.0000E+00	1.0454E-009	4.400E-10	1.00E+00	4.400E-10
Fe(OH)3	4.0000E-03	9.0500E-010	3.815E-10	1.00E+00	3.815E-10
PbO2	0.0000E+00	8.5153E-010	3.584E-10	1.00E+00	3.584E-10
Na2CO3	0.0000E+00	8.5093E-010	3.582E-10	1.00E+00	3.582E-10
NaNO3	1.4000E-02	6.3855E-010	2.688E-10	1.00E+00	2.688E-10
Mg(OH)2	5.0000E-03	5.8291E-010	2.453E-10	1.00E+00	2.453E-10
U3O5	0.0000E+00	4.0720E-010	1.714E-10	1.00E+00	1.714E-10
PbO	0.0000E+00	3.8336E-010	1.614E-10	1.00E+00	1.614E-10
MgO2	0.0000E+00	3.4524E-010	1.453E-10	1.00E+00	1.453E-10
HgO	2.8000E-02	2.6899E-010	1.132E-10	1.00E+00	1.132E-10
Ca(OH)2	4.0000E-03	2.5487E-010	1.073E-10	1.00E+00	1.073E-10
NaFeO2	0.0000E+00	2.2776E-010	9.586E-11	1.00E+00	9.586E-11
NaOH	0.0000E+00	2.1197E-010	8.922E-11	1.00E+00	8.922E-11
KOH	5.0000E-03	2.0495E-010	8.626E-11	1.00E+00	8.626E-11
KO2	0.0000E+00	1.1469E-010	4.827E-11	1.00E+00	4.827E-11
HNO3	0.0000E+00	8.6772E-011	3.652E-11	1.00E+00	3.652E-11
FeCO3	0.0000E+00	7.7066E-011	3.244E-11	1.00E+00	3.244E-11
Fe3O4	0.0000E+00	7.4243E-011	3.125E-11	1.00E+00	3.125E-11
CaO2	0.0000E+00	5.6283E-011	2.369E-11	1.00E+00	2.369E-11
NaO2	0.0000E+00	5.5240E-011	2.325E-11	1.00E+00	2.325E-11
Ca(NO3)2	0.0000E+00	5.1677E-011	2.175E-11	1.00E+00	2.175E-11
Fe(OH)2	0.0000E+00	5.1627E-011	2.173E-11	1.00E+00	2.173E-11
Pb(NO3)2	0.0000E+00	5.0676E-011	2.133E-11	1.00E+00	2.133E-11
FeO	4.9000E-01	4.5119E-011	1.899E-11	1.00E+00	1.899E-11
CaO	0.0000E+00	3.3298E-011	1.401E-11	1.00E+00	1.401E-11
Pb3O4	2.0000E-03	3.1565E-011	1.329E-11	1.00E+00	1.329E-11
UO2	0.0000E+00	2.8493E-011	1.199E-11	1.00E+00	1.199E-11
U3O8	0.0000E+00	2.3874E-011	1.005E-11	1.00E+00	1.005E-11
KO3	0.0000E+00	7.6616E-012	3.225E-12	1.00E+00	3.225E-12
Hg(NO3)2	0.0000E+00	4.1511E-012	1.747E-12	1.00E+00	1.747E-12
K2O3	0.0000E+00	4.9454E-012	2.082E-12	1.00E+00	2.082E-12
Na2O2	0.0000E+00	1.6340E-012	6.878E-13	1.00E+00	6.878E-13
N2O4	0.0000E+00	1.0140E-012	4.268E-13	1.00E+00	4.268E-13
K2O2	4.0000E-04	1.0136E-012	4.266E-13	1.00E+00	4.266E-13
Pb	0.0000E+00	9.5822E-013	4.033E-13	1.00E+00	4.033E-13
H2O5	0.0000E+00	3.4593E-013	1.456E-13	1.00E+00	1.456E-13
HCO2H	0.0000E+00	3.2470E-013	1.367E-13	1.00E+00	1.367E-13
Na2O	1.4000E-02	1.7755E-013	7.473E-14	1.00E+00	7.473E-14
Na3UO4	0.0000E+00	1.1163E-013	4.698E-14	1.00E+00	4.698E-14
K	0.0000E+00	4.8847E-014	2.056E-14	1.00E+00	2.056E-14
Na	0.0000E+00	4.5890E-014	1.931E-14	1.00E+00	1.931E-14
K2O	3.6000E-02	1.4305E-014	6.021E-15	1.00E+00	6.021E-15
Fe	2.4300E-01	1.3266E-014	5.584E-15	1.00E+00	5.584E-15
C	1.0120E+00	5.4845E-015	2.308E-15	1.00E+00	2.308E-15
U4O9	0.0000E+00	4.6641E-015	1.963E-15	1.00E+00	1.963E-15
NH4OH	0.0000E+00	3.9075E-015	1.645E-15	1.00E+00	1.645E-15
KH	0.0000E+00	2.5833E-015	1.087E-15	1.00E+00	1.087E-15
NaNH	0.0000E+00	2.3562E-015	9.917E-16	1.00E+00	9.917E-16
NH4NO3	0.0000E+00	2.0985E-015	8.832E-16	1.00E+00	8.832E-16
Hg	0.0000E+00	8.9626E-019	3.772E-19	1.00E+00	3.772E-19
NaH3	0.0000E+00	8.1186E-019	3.417E-19	1.00E+00	3.417E-19
UO	0.0000E+00	5.2092E-019	2.193E-19	1.00E+00	2.193E-19
KCN	0.0000E+00	6.9026E-020	2.905E-20	1.00E+00	2.905E-20
CH3OH	0.0000E+00	4.5933E-020	1.929E-20	1.00E+00	1.929E-20
NaCN	0.0000E+00	2.6856E-020	1.130E-20	1.00E+00	1.130E-20
Ca	0.0000E+00	2.2750E-020	9.576E-21	1.00E+00	9.576E-21
N2H4	0.0000E+00	6.3604E-021	2.677E-21	1.00E+00	2.677E-21
Al	3.6000E-02	1.5520E-021	6.532E-22	1.00E+00	6.532E-22
CaH2	0.0000E+00	4.9309E-022	2.075E-22	1.00E+00	2.075E-22
Si	0.0000E+00	1.0094E-022	4.249E-23	1.00E+00	4.249E-23
UN	0.0000E+00	7.4290E-025	3.127E-25	1.00E+00	3.127E-25
U	0.0000E+00	3.0235E-029	1.273E-29	1.00E+00	1.273E-29
C2H6O	0.0000E+00	1.4044E-033	5.911E-34	1.00E+00	5.911E-34
UH3	0.0000E+00	9.2867E-037	3.909E-37	1.00E+00	3.909E-37
UC	0.0000E+00	2.8332E-037	1.192E-37	1.00E+00	1.192E-37
Fe(CO)5	0.0000E+00	2.2274E-045	1.401E-45	1.00E+00	1.401E-45
UC2	0.0000E+00	4.8534E-051	0.000E+00	1.00E+00	0.000E+00
UPe2	0.0000E+00	1.8385E-051	0.000E+00	1.00E+00	0.000E+00
Ca3N2	0.0000E+00	1.2092E-053	0.000E+00	1.00E+00	0.000E+00
Si3N4	0.0000E+00	3.6498E-061	0.000E+00	1.00E+00	0.000E+00
Si2H6	0.0000E+00	6.3239E-092	0.000E+00	1.00E+00	0.000E+00
U2C3	0.0000E+00	4.0000E-178	0.000E+00	1.00E+00	0.000E+00
Total	2.5584E+00	2.3759E+000	1.000E+00		

A-4

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B
Temperature 398.15 K
Pressure 1 bar
Volume 1.561E-01 m3 ( NPT )
Reaction enthalpy -8.332E+02 kJ
Reaction entropy -6.617E+01 J/K
Iterations 80 ( Limit 80 )

INPUT AMOUNT EQUIL AMOUNT MOLE FRACTION ACTIVITY ACTIVITY
      mol      mol
PHASE 1:
O2(g) 7.1550E+00 5.4589E+000 7.837E-01 1.00E+00 7.837E-01
H2O(g) 0.0000E+00 1.0745E+000 1.543E-01 1.00E+00 1.543E-01
CO2(g) 0.0000E+00 4.3210E-01 6.203E-02 1.00E+00 6.203E-02
H2(g) 0.0000E+00 1.5301E-01 2.197E-02 1.00E+00 2.197E-02
H2O(l) 0.0000E+00 6.2140E-011 8.921E-12 1.00E+00 8.921E-12
H2O3(g) 0.0000E+00 1.3133E-011 1.885E-12 1.00E+00 1.885E-12
KOH(g) 0.0000E+00 6.8727E-012 9.867E-13 1.00E+00 9.867E-13
NaOH(g) 0.0000E+00 2.6706E-012 3.834E-13 1.00E+00 3.834E-13
H2(g) 9.5000E-01 2.5933E-012 3.723E-13 1.00E+00 3.723E-13
PbO(g) 0.0000E+00 1.6424E-012 2.358E-13 1.00E+00 2.358E-13
CO(g) 0.0000E+00 1.0057E-012 1.444E-13 1.00E+00 1.444E-13
Ca(OH)2(g) 0.0000E+00 3.0512E-014 4.389E-15 1.00E+00 4.389E-15
K2O(g) 0.0000E+00 2.1604E-014 3.102E-15 1.00E+00 3.102E-15
K(g) 0.0000E+00 1.6307E-014 2.341E-15 1.00E+00 2.341E-15
Pb(g) 0.0000E+00 1.5346E-014 2.203E-15 1.00E+00 2.203E-15
Na(g) 0.0000E+00 1.1811E-014 1.696E-15 1.00E+00 1.696E-15
NH3(g) 0.0000E+00 9.5217E-015 1.367E-15 1.00E+00 1.367E-15
NH2(g) 0.0000E+00 2.7602E-016 3.963E-17 1.00E+00 3.963E-17
H(g) 0.0000E+00 1.4489E-017 2.080E-17 1.00E+00 2.080E-17
SiO2(g) 0.0000E+00 3.9578E-017 5.682E-18 1.00E+00 5.682E-18
NH(g) 0.0000E+00 3.8924E-017 5.588E-18 1.00E+00 5.588E-18
HgOH(g) 0.0000E+00 2.1054E-017 3.023E-18 1.00E+00 3.023E-18
FeO(g) 0.0000E+00 9.5610E-018 1.373E-18 1.00E+00 1.373E-18
HgO(g) 0.0000E+00 6.3592E-018 9.130E-19 1.00E+00 9.130E-19
AlO2(g) 0.0000E+00 3.8770E-018 5.566E-19 1.00E+00 5.566E-19
HCN(g) 0.0000E+00 6.7375E-020 9.673E-21 1.00E+00 9.673E-21
SiC(g) 0.0000E+00 3.6199E-020 5.197E-21 1.00E+00 5.197E-21
Hg(g) 0.0000E+00 2.8896E-020 4.148E-21 1.00E+00 4.148E-21
Fe(g) 0.0000E+00 2.7110E-020 3.892E-21 1.00E+00 3.892E-21
CH3OH(g) 0.0000E+00 2.1950E-020 3.151E-21 1.00E+00 3.151E-21
CaO(g) 0.0000E+00 5.9040E-021 8.476E-22 1.00E+00 8.476E-22
CH4(g) 0.0000E+00 2.0340E-022 2.920E-23 1.00E+00 2.920E-23
Ca(g) 0.0000E+00 1.1596E-022 1.665E-23 1.00E+00 1.665E-23
AlO(g) 0.0000E+00 1.0452E-022 1.500E-23 1.00E+00 1.500E-23
CH3(g) 0.0000E+00 1.0078E-023 1.447E-24 1.00E+00 1.447E-24
CH2(g) 0.0000E+00 1.8693E-026 2.684E-27 1.00E+00 2.684E-27
Al(g) 0.0000E+00 2.5212E-027 3.620E-28 1.00E+00 3.620E-28
C(g) 0.0000E+00 1.6671E-027 2.393E-28 1.00E+00 2.393E-28
Al2O2(g) 0.0000E+00 1.0748E-029 1.543E-30 1.00E+00 1.543E-30
Si(g) 0.0000E+00 1.0672E-031 1.532E-32 1.00E+00 1.532E-32
C2H2(g) 0.0000E+00 6.2242E-032 8.936E-33 1.00E+00 8.936E-33
C2H4(g) 0.0000E+00 1.0777E-034 1.547E-35 1.00E+00 1.547E-35
Al2O(g) 0.0000E+00 6.0589E-036 8.699E-37 1.00E+00 8.699E-37
C2H6(g) 0.0000E+00 4.7761E-039 6.857E-40 1.00E+00 6.857E-40
U(g) 0.0000E+00 6.8847E-043 9.949E-44 1.00E+00 9.949E-44
Total : 8.1050E+00 6.9655E+000 1.000E+00

PHASE 2 :
CaCO3 0.0000E+00 4.9400E-001 3.608E-01 1.00E+00 3.608E-01
SiO2 4.6900E-01 4.6900E-001 3.608E-01 1.00E+00 3.608E-01
Fe2O3 6.0000E-03 1.2950E-001 9.961E-02 1.00E+00 9.961E-02
Al2O3 7.8000E-02 9.9000E-002 7.615E-02 1.00E+00 7.615E-02
HgCO3 0.0000E+00 3.3000E-002 2.538E-02 1.00E+00 2.538E-02
K2CO3 0.0000E+00 3.1500E-002 2.423E-02 1.00E+00 2.423E-02
KH03 8.0000E-03 2.2000E-002 1.692E-02 1.00E+00 1.692E-02
Na2CO3 0.0000E+00 2.1000E-002 1.615E-02 1.00E+00 1.615E-02
U3O8 0.0000E+00 6.667E-004 5.128E-04 1.00E+00 5.128E-04
PbCO3 0.0000E+00 4.0000E-004 3.077E-04 1.00E+00 3.077E-04
H2O 9.8000E-02 3.0245E-009 2.328E-09 1.00E+00 2.328E-09
NaHCO3 0.0000E+00 2.3119E-009 1.778E-09 1.00E+00 1.778E-09
UO3 0.0000E+00 2.0557E-009 1.581E-09 1.00E+00 1.581E-09
Al(OH)3 6.0000E-03 1.8838E-009 1.449E-09 1.00E+00 1.449E-09
UO3(G) 0.0000E+00 1.6833E-009 1.295E-09 1.00E+00 1.295E-09
PbO2 0.0000E+00 1.6275E-009 1.253E-09 1.00E+00 1.253E-09
HNaO3 1.4000E-02 1.3855E-009 1.066E-09 1.00E+00 1.066E-09
Hg(OH)2 5.0000E-03 1.3022E-009 1.002E-09 1.00E+00 1.002E-09
Fe(OH)3 4.0000E-03 9.8131E-010 7.548E-10 1.00E+00 7.548E-10
PbO 0.0000E+00 9.6246E-010 7.403E-10 1.00E+00 7.403E-10
HgO2 0.0000E+00 9.1038E-010 7.003E-10 1.00E+00 7.003E-10
HgO 2.8000E-02 8.1370E-010 6.259E-10 1.00E+00 6.259E-10
NaFeO2 0.0000E+00 6.6768E-010 5.136E-10 1.00E+00 5.136E-10
Ca(OH)2 4.0000E-02 5.8216E-010 4.479E-10 1.00E+00 4.479E-10
NaOH 0.0000E+00 5.2957E-010 4.073E-10 1.00E+00 4.073E-10
KOH 5.0000E-03 3.8729E-010 2.979E-10 1.00E+00 2.979E-10
K02 0.0000E+00 1.8320E-010 1.409E-10 1.00E+00 1.409E-10

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Fe3O4 0.0000E+00 1.4104E-010 1.095E-10 1.00E+00 1.095E-10
CaO2 0.0000E+00 1.3583E-010 1.045E-10 1.00E+00 1.045E-10
CaO 4.9000E-01 1.3023E-010 1.002E-10 1.00E+00 1.002E-10
Pb3O4 0.0000E+00 1.2184E-010 9.372E-11 1.00E+00 9.372E-11
NaO2 0.0000E+00 1.1542E-010 8.878E-11 1.00E+00 8.878E-11
HNO3 0.0000E+00 9.8792E-011 7.599E-11 1.00E+00 7.599E-11
FeO 0.0000E+00 9.3970E-011 7.228E-11 1.00E+00 7.228E-11
FeCO3 0.0000E+00 7.5862E-011 5.835E-11 1.00E+00 5.835E-11
Ca(HO3)2 0.0000E+00 7.3159E-011 5.627E-11 1.00E+00 5.627E-11
Fe(OH)2 0.0000E+00 6.7247E-011 5.173E-11 1.00E+00 5.173E-11
Pb(HO3)2 0.0000E+00 5.5347E-011 4.257E-11 1.00E+00 4.257E-11
UO2 2.0000E-03 5.4801E-011 4.215E-11 1.00E+00 4.215E-11
U3O8 0.0000E+00 3.9883E-011 3.068E-11 1.00E+00 3.068E-11
K03 0.0000E+00 2.5819E-011 1.986E-11 1.00E+00 1.986E-11
Hg(HO3)2 0.0000E+00 8.7862E-012 6.758E-12 1.00E+00 6.758E-12
Na2O2 0.0000E+00 5.5037E-012 4.233E-12 1.00E+00 4.233E-12
K2O3 0.0000E+00 5.4151E-012 4.165E-12 1.00E+00 4.165E-12
Pb 4.0000E-04 2.6670E-012 2.051E-12 1.00E+00 2.051E-12
N2O4 0.0000E+00 1.7103E-012 1.316E-12 1.00E+00 1.316E-12
K2O2 0.0000E+00 1.5816E-012 1.217E-12 1.00E+00 1.217E-12
Na3UO4 0.0000E+00 7.4408E-013 5.723E-13 1.00E+00 5.723E-13
Na2O 1.4000E-02 6.5398E-013 5.030E-13 1.00E+00 5.030E-13
H2O5 0.0000E+00 5.9719E-013 4.594E-13 1.00E+00 4.594E-13
HCO2H 0.0000E+00 2.3695E-013 1.823E-13 1.00E+00 1.823E-13
HCOOH 0.0000E+00 2.2152E-013 1.704E-13 1.00E+00 1.704E-13
Na 0.0000E+00 1.3970E-013 8.438E-14 1.00E+00 8.438E-14
K 0.0000E+00 8.6196E-014 6.630E-14 1.00E+00 6.630E-14
K2O 3.6000E-02 2.4856E-014 1.912E-14 1.00E+00 1.912E-14
Fe 2.4300E-01 2.0529E-014 1.579E-14 1.00E+00 1.579E-14
U4O9 0.0000E+00 6.2483E-015 4.806E-15 1.00E+00 4.806E-15
C 1.0120E+00 4.4535E-015 3.426E-15 1.00E+00 3.426E-15
NaH 0.0000E+00 4.2986E-015 3.306E-15 1.00E+00 3.306E-15
NH4OH 0.0000E+00 4.0753E-015 3.135E-15 1.00E+00 3.135E-15
KH 0.0000E+00 3.3858E-015 2.604E-15 1.00E+00 2.604E-15
NH4NO3 0.0000E+00 1.2794E-015 9.841E-16 1.00E+00 9.841E-16
NaN3 0.0000E+00 3.0521E-018 2.348E-18 1.00E+00 2.348E-18
Hg 0.0000E+00 1.5327E-018 1.179E-18 1.00E+00 1.179E-18
UO 0.0000E+00 4.5922E-019 3.532E-19 1.00E+00 3.532E-19
KCN 0.0000E+00 9.0635E-020 6.972E-20 1.00E+00 6.972E-20
NaCN 0.0000E+00 4.9962E-020 3.843E-20 1.00E+00 3.843E-20
Ca 0.0000E+00 3.3337E-020 2.564E-20 1.00E+00 2.564E-20
CH3OH 0.0000E+00 1.3223E-020 1.017E-20 1.00E+00 1.017E-20
N2H4 0.0000E+00 5.5877E-021 4.298E-21 1.00E+00 4.298E-21
Al 3.6000E-02 1.0365E-021 7.973E-22 1.00E+00 7.973E-22
CaH2 0.0000E+00 4.9537E-022 3.810E-22 1.00E+00 3.810E-22
Si 0.0000E+00 6.7101E-023 5.161E-23 1.00E+00 5.161E-23
UN 0.0000E+00 6.8777E-025 5.290E-25 1.00E+00 5.290E-25
U 0.0000E+00 9.8979E-030 7.613E-30 1.00E+00 7.613E-30
C2H6O 0.0000E+00 2.5471E-035 1.959E-35 1.00E+00 1.959E-35
UH3 0.0000E+00 8.0490E-038 6.191E-38 1.00E+00 6.191E-38
UC 0.0000E+00 2.8675E-038 2.206E-38 1.00E+00 2.206E-38
Fe(CO)5 0.0000E+00 8.7645E-049 0.000E+00 1.00E+00 0.000E+00
UF6 0.0000E+00 5.1917E-052 0.000E+00 1.00E+00 0.000E+00
Ca3N2 0.0000E+00 1.9339E-052 0.000E+00 1.00E+00 0.000E+00
UC2 0.0000E+00 2.3336E-053 0.000E+00 1.00E+00 0.000E+00
Si3N4 0.0000E+00 1.6592E-060 0.000E+00 1.00E+00 0.000E+00
Si2H6 0.0000E+00 3.6561E-094 0.000E+00 1.00E+00 0.000E+00
UC3 0.0000E+00 4.0000E-178 0.000E+00 1.00E+00 0.000E+00
Total : 2.5584E+00 1.3001E+000 1.000E+00

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E

Temperature 498.15 K
 Pressure 1 bar
 Volume 1.561E-01 m³ (NPT)
 Reaction enthalpy -7.992E-02 kJ
 Reaction entropy 9.991E-00 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol		COEFFICIENT	
O ₂ (g)	7.1550E+00	5.4589E+00	7.837E-01	1.00E+00	7.837E-01
H ₂ O(g)	0.0000E+00	1.0745E+00	1.543E-01	1.00E+00	1.543E-01
CO ₂ (g)	0.0000E+00	4.3250E-001	6.209E-02	1.00E+00	6.209E-02
NO ₂ (g)	0.0000E+00	3.7286E-010	5.353E-11	1.00E+00	5.353E-11
NO(g)	0.0000E+00	1.8844E-010	2.705E-11	1.00E+00	2.705E-11
NO ₃ (g)	0.0000E+00	2.0420E-011	2.931E-12	1.00E+00	2.931E-12
KOH(g)	0.0000E+00	1.9012E-011	2.729E-12	1.00E+00	2.729E-12
NaOH(g)	0.0000E+00	6.9250E-012	9.941E-13	1.00E+00	9.941E-13
PbO(g)	0.0000E+00	6.6399E-012	9.532E-13	1.00E+00	9.532E-13
H ₂ (g)	9.5000E-01	4.3339E-012	6.222E-13	1.00E+00	6.222E-13
CO(g)	0.0000E+00	1.7929E-012	2.574E-13	1.00E+00	2.574E-13
Ca(OH) ₂ (g)	0.0000E+00	8.0296E-014	1.153E-14	1.00E+00	1.153E-14
Pb(g)	0.0000E+00	5.8420E-014	8.387E-15	1.00E+00	8.387E-15
K(g)	0.0000E+00	5.3384E-014	7.664E-15	1.00E+00	7.664E-15
Na(g)	0.0000E+00	3.1823E-014	4.291E-15	1.00E+00	4.291E-15
NH ₃ (g)	0.0000E+00	1.4354E-014	2.061E-15	1.00E+00	2.061E-15
NH ₂ (g)	0.0000E+00	4.2661E-016	6.124E-17	1.00E+00	6.124E-17
N(g)	0.0000E+00	2.7801E-016	3.991E-17	1.00E+00	3.991E-17
NH(g)	0.0000E+00	6.3539E-017	9.122E-18	1.00E+00	9.122E-18
SiO ₂ (g)	0.0000E+00	6.2914E-017	9.032E-18	1.00E+00	9.032E-18
MgO(g)	0.0000E+00	5.7257E-017	8.220E-18	1.00E+00	8.220E-18
FeO(g)	0.0000E+00	1.9714E-017	2.830E-18	1.00E+00	2.830E-18
Al ₂ O ₃ (g)	0.0000E+00	1.7963E-017	2.579E-18	1.00E+00	2.579E-18
Mg(g)	0.0000E+00	5.0362E-018	7.230E-19	1.00E+00	7.230E-19
HCl(g)	0.0000E+00	8.1149E-020	1.165E-20	1.00E+00	1.165E-20
SiO(g)	0.0000E+00	7.4795E-020	1.074E-20	1.00E+00	1.074E-20
Fe(g)	0.0000E+00	5.7972E-020	8.322E-21	1.00E+00	8.322E-21
CaO(g)	0.0000E+00	4.4940E-020	6.451E-21	1.00E+00	6.451E-21
CH ₃ OH(g)	0.0000E+00	1.3146E-020	1.867E-21	1.00E+00	1.867E-21
Ca(g)	0.0000E+00	6.4312E-021	9.21E-22	1.00E+00	9.21E-22
Al ₂ O ₃ (g)	0.0000E+00	2.5933E-022	3.723E-23	1.00E+00	3.723E-23
Al(g)	0.0000E+00	1.0721E-022	1.539E-23	1.00E+00	1.539E-23
CH ₄ (g)	0.0000E+00	5.5451E-023	7.960E-24	1.00E+00	7.960E-24
CH ₃ (g)	0.0000E+00	3.0111E-024	4.326E-25	1.00E+00	4.326E-25
CH ₂ (g)	0.0000E+00	4.4474E-027	6.384E-28	1.00E+00	6.384E-28
Al(g)	0.0000E+00	1.8952E-027	2.721E-28	1.00E+00	2.721E-28
C(g)	0.0000E+00	5.2623E-028	7.554E-29	1.00E+00	7.554E-29
Al ₂ O ₃ (g)	0.0000E+00	6.2704E-030	9.002E-31	1.00E+00	9.002E-31
Si(g)	0.0000E+00	5.9422E-032	8.530E-33	1.00E+00	8.530E-33
C ₂ H ₂ (g)	0.0000E+00	5.5481E-033	7.965E-34	1.00E+00	7.965E-34
Al ₂ O ₃ (g)	0.0000E+00	3.0683E-036	4.405E-37	1.00E+00	4.405E-37
C ₂ H ₄ (g)	0.0000E+00	3.0558E-036	4.387E-37	1.00E+00	4.387E-37
C ₂ H ₆ (g)	0.0000E+00	1.9610E-041	2.815E-42	1.00E+00	2.815E-42
U(g)	0.0000E+00	1.2823E-044	1.401E-45	1.00E+00	1.401E-45
Total :	8.1050E+00	6.9659E+000	1.060E+00		

PHASE 2 :	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol		COEFFICIENT	
CaCO ₃	0.0000E+00	4.9400E-001	3.800E-01	1.00E+00	3.800E-01
SiO ₂	4.6900E-01	4.6900E-001	3.608E-01	1.00E+00	3.608E-01
Fe ₂ O ₃	6.0000E-03	1.2950E-001	9.961E-02	1.00E+00	9.961E-02
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.615E-02	1.00E+00	7.615E-02
MgCO ₃	0.0000E+00	3.3000E-002	2.538E-02	1.00E+00	2.538E-02
K ₂ CO ₃	0.0000E+00	3.1500E-002	2.423E-02	1.00E+00	2.423E-02
KNO ₃	8.0000E-03	2.2000E-002	1.692E-02	1.00E+00	1.692E-02
Na ₂ CO ₃	0.0000E+00	2.1000E-002	1.615E-02	1.00E+00	1.615E-02
U ₃ O ₈	0.0000E+00	6.6667E-004	5.128E-04	1.00E+00	5.128E-04
PbO	0.0000E+00	4.0000E-004	3.077E-04	1.00E+00	3.077E-04
H ₂ O	9.8000E-02	4.2550E-009	3.273E-09	1.00E+00	3.273E-09
PbO ₂	0.0000E+00	3.5015E-009	2.693E-09	1.00E+00	2.693E-09
PbCO ₃	0.0000E+00	2.9165E-009	2.243E-09	1.00E+00	2.243E-09
MgO	2.8000E-02	2.7435E-009	2.110E-09	1.00E+00	2.110E-09
MgO ₂	0.0000E+00	2.6499E-009	2.038E-09	1.00E+00	2.038E-09
Mg(OH) ₂	5.0000E-03	2.5957E-009	1.997E-09	1.00E+00	1.997E-09
UO ₃	0.0000E+00	2.4584E-009	1.891E-09	1.00E+00	1.891E-09
NaHCO ₃	0.0000E+00	2.3800E-009	1.831E-09	1.00E+00	1.831E-09
NaNO ₃	1.4000E-02	2.2978E-009	1.767E-09	1.00E+00	1.767E-09
UO ₃ (g)	0.0000E+00	1.9897E-009	1.530E-09	1.00E+00	1.530E-09
NaF·CO ₂	0.0000E+00	1.5861E-009	1.220E-09	1.00E+00	1.220E-09
Al(OH) ₃	6.0000E-03	1.5589E-009	1.199E-09	1.00E+00	1.199E-09
Ca(OH) ₂	4.0000E-03	1.1946E-009	9.189E-10	1.00E+00	9.189E-10
NaOH	0.0000E+00	9.8978E-010	7.613E-10	1.00E+00	7.613E-10
Fe(OH) ₃	4.0000E-03	8.1496E-010	6.269E-10	1.00E+00	6.269E-10
KOH	5.0000E-03	7.3715E-010	5.670E-10	1.00E+00	5.670E-10
Pb ₃ O ₄	0.0000E+00	5.2773E-010	4.059E-10	1.00E+00	4.059E-10

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CaO	4.9000E-01	4.1900E-010	3.223E-10	1.00E+00	3.223E-10
CaO ₂	0.0000E+00	3.6807E-010	2.831E-10	1.00E+00	2.831E-10
K ₂ O	0.0000E+00	3.2578E-010	2.506E-10	1.00E+00	2.506E-10
Fe ₃ O ₄	0.0000E+00	2.8174E-010	2.167E-10	1.00E+00	2.167E-10
NaO ₂	0.0000E+00	1.9897E-010	1.530E-10	1.00E+00	1.530E-10
FeO	0.0000E+00	1.9845E-010	1.526E-10	1.00E+00	1.526E-10
HNO ₃	0.0000E+00	1.0458E-010	8.045E-11	1.00E+00	8.045E-11
Ca(HO ₃) ₂	0.0000E+00	9.3345E-011	7.180E-11	1.00E+00	7.180E-11
FeCO ₃	0.0000E+00	7.7562E-011	5.966E-11	1.00E+00	5.966E-11
Fe(OH) ₂	0.0000E+00	7.6953E-011	5.919E-11	1.00E+00	5.919E-11
UO ₂	2.0000E-03	6.9992E-011	5.376E-11	1.00E+00	5.376E-11
Pb(HO ₃) ₂	0.0000E+00	5.4642E-011	4.203E-11	1.00E+00	4.203E-11
KO ₃	0.0000E+00	2.9788E-011	2.291E-11	1.00E+00	2.291E-11
U ₃ O ₈	0.0000E+00	1.7005E-011	1.308E-11	1.00E+00	1.308E-11
Na ₂ O ₂	0.0000E+00	9.6385E-012	7.568E-12	1.00E+00	7.568E-12
Mg(HO ₃) ₂	0.0000E+00	8.9201E-012	6.961E-12	1.00E+00	6.961E-12
Pb	4.0000E-04	8.2093E-012	6.315E-12	1.00E+00	6.315E-12
K ₂ O ₃	0.0000E+00	7.4999E-012	5.769E-12	1.00E+00	5.769E-12
K ₂ O ₂	0.0000E+00	2.6705E-012	2.054E-12	1.00E+00	2.054E-12
N ₂ O ₄	0.0000E+00	1.7530E-012	1.348E-12	1.00E+00	1.348E-12
Na ₂ O	1.4000E-02	1.4037E-012	1.080E-12	1.00E+00	1.080E-12
Na ₃ UO ₄	0.0000E+00	1.3130E-012	1.010E-12	1.00E+00	1.010E-12
N ₂ O ₅	0.0000E+00	3.3457E-013	2.573E-13	1.00E+00	2.573E-13
Na	0.0000E+00	2.1823E-013	1.679E-13	1.00E+00	1.679E-13
K	0.0000E+00	1.7340E-013	1.334E-13	1.00E+00	1.334E-13
HCO ₂ H	0.0000E+00	1.4085E-013	1.083E-13	1.00E+00	1.083E-13
HCOOH	0.0000E+00	1.3113E-013	1.009E-13	1.00E+00	1.009E-13
K ₂ O	3.6000E-02	4.7348E-014	3.642E-14	1.00E+00	3.642E-14
Fe	2.4300E-01	3.5296E-014	2.715E-14	1.00E+00	2.715E-14
NaH	0.0000E+00	5.5207E-015	4.247E-15	1.00E+00	4.247E-15
KH	0.0000E+00	4.3706E-015	3.362E-15	1.00E+00	3.362E-15
C	1.0120E+00	3.9246E-015	3.019E-15	1.00E+00	3.019E-15
NH ₄ OH	0.0000E+00	2.5498E-015	1.961E-15	1.00E+00	1.961E-15
U ₄ O ₉	0.0000E+00	1.3928E-015	1.071E-15	1.00E+00	1.071E-15
NH ₄ NO ₃	0.0000E+00	4.6673E-016	3.590E-16	1.00E+00	3.590E-16
Na ₂ N ₃	0.0000E+00	6.8788E-018	5.291E-18	1.00E+00	5.291E-18
Mg	0.0000E+00	2.9566E-018	2.274E-18	1.00E+00	2.274E-18
UO	0.0000E+00	2.6405E-019	2.031E-19	1.00E+00	2.031E-19
KCN	0.0000E+00	1.2272E-019	9.439E-20	1.00E+00	9.439E-20
NaCN	0.0000E+00	6.5312E-020	5.024E-20	1.00E+00	5.024E-20
Ca	0.0000E+00	5.4516E-020	4.193E-20	1.00E+00	4.193E-20
N ₂ H ₄	0.0000E+00	2.6328E-021	2.025E-21	1.00E+00	2.025E-21
CH ₃ OH	0.0000E+00	2.2336E-021	1.718E-21	1.00E+00	1.718E-21
Al	3.6000E-02	7.6061E-022	5.851E-22	1.00E+00	5.851E-22
CaH ₂	0.0000E+00	4.0025E-022	3.079E-22	1.00E+00	3.079E-22
Si	0.0000E+00	4.7445E-023	3.649E-23	1.00E+00	3.649E-23
UH	0.0000E+00	3.4720E-025	2.671E-25	1.00E+00	2.671E-25
U	0.0000E+00	1.6605E-030	1.277E-30	1.00E+00	1.277E-30
C ₂ H ₆ O	0.0000E+00	8.4320E-038	6.486E-38	1.00E+00	6.486E-38
UH ₃	0.0000E+00	9.8426E-040	7.571E-40	1.00E+00	7.571E-40
UC	0.0000E+00	8.8049E-040	6.773E-40	1.00E+00	6.773E-40
Fe(CO) ₅	0.0000E+00	1.0535E-050	0.000E+00	1.00E+00	0.000E+00
Ca ₃ N ₂	0.0000E+00	1.2269E-052	0.000E+00	1.00E+00	0.000E+00
UF ₆	0.0000E+00	1.4142E-055	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	3.5268E-055	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	1.3127E-061	0.000E+00	1.00E+00	0.000E+00
Si ₂ N ₆	0.0000E+00	4.8561E-098	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	4.0000E-178	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.3001E+000	1.000E+00		

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B

Temperature 598.15 K
 Pressure 1 bar
 Volume 1.569E-01 m³ (NPT)
 Reaction enthalpy -7.593E-02 kJ
 Reaction entropy 8.163E-01 J/K
 Iterations 80 (Limit = 80)

	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRAC1	ACTIVITY	ACTIVITY
PHASE 1:					
O ₂ (g)	7.1550E+00	5.4589E+00	7.800E-01	1.00E+00	7.800E-01
H ₂ O(g)	0.0000E+00	1.0745E+00	1.535E-01	1.00E+00	1.535E-01
CO ₂ (g)	0.0000E+00	4.6550E+00	6.651E-02	1.00E+00	6.651E-02
NO ₂ (g)	0.0000E+00	1.0067E+00	1.438E-01	1.00E+00	1.438E-01
NO(g)	0.0000E+00	6.4725E+00	9.248E-01	1.00E+00	9.248E-01
KOH(g)	0.0000E+00	5.7307E+00	8.188E-02	1.00E+00	8.188E-02
NO ₃ (g)	0.0000E+00	3.2759E+00	4.681E-02	1.00E+00	4.681E-02
NaOH(g)	0.0000E+00	1.9384E+00	2.770E-02	1.00E+00	2.770E-02
H ₂ O(l)	0.0000E+00	1.5238E+00	2.177E-02	1.00E+00	2.177E-02
H ₂ (g)	9.5000E-01	7.5905E-02	1.085E-02	1.00E+00	1.085E-02
CO(g)	0.0000E+00	3.3801E-02	4.829E-03	1.00E+00	4.829E-03
Ca(OH) ₂ (g)	0.0000E+00	2.2017E-03	3.146E-04	1.00E+00	3.146E-04
K ₂ O(g)	0.0000E+00	1.3634E-03	1.948E-04	1.00E+00	1.948E-04
K(g)	0.0000E+00	1.2262E-03	1.754E-04	1.00E+00	1.754E-04
Pb(g)	0.0000E+00	1.1677E-03	1.668E-04	1.00E+00	1.668E-04
Na(g)	0.0000E+00	8.6329E-04	1.233E-04	1.00E+00	1.233E-04
NH ₃ (g)	0.0000E+00	2.1084E-04	3.012E-05	1.00E+00	3.012E-05
NH ₂ (g)	0.0000E+00	6.2892E-06	8.986E-07	1.00E+00	8.986E-07
H(g)	0.0000E+00	5.2270E-06	7.468E-07	1.00E+00	7.468E-07
HgO(l)	0.0000E+00	1.4912E-06	2.131E-07	1.00E+00	2.131E-07
NH(g)	0.0000E+00	9.8354E-07	1.405E-07	1.00E+00	1.405E-07
SiO ₂ (g)	0.0000E+00	9.3963E-07	1.343E-07	1.00E+00	1.343E-07
HgO(g)	0.0000E+00	5.8554E-07	8.364E-08	1.00E+00	8.364E-08
FeO(g)	0.0000E+00	3.1731E-07	4.534E-08	1.00E+00	4.534E-08
Al ₂ O ₃ (g)	0.0000E+00	5.9151E-08	8.452E-09	1.00E+00	8.452E-09
Hg(l)	0.0000E+00	2.0484E-09	2.927E-20	1.00E+00	2.927E-20
SiO(l)	0.0000E+00	8.1709E-020	1.167E-20	1.00E+00	1.167E-20
HCl(g)	0.0000E+00	7.1756E-020	1.025E-20	1.00E+00	1.025E-20
Fe(l)	0.0000E+00	6.5805E-020	9.402E-21	1.00E+00	9.402E-21
CaO(l)	0.0000E+00	2.5712E-020	3.671E-21	1.00E+00	3.671E-21
CH ₃ OH(g)	0.0000E+00	1.3059E-021	1.866E-22	1.00E+00	1.866E-22
Ca(l)	0.0000E+00	4.8897E-022	6.986E-23	1.00E+00	6.986E-23
Al ₂ O ₃ (l)	0.0000E+00	8.6459E-023	1.235E-23	1.00E+00	1.235E-23
CH ₄ (g)	0.0000E+00	9.9367E-024	1.424E-24	1.00E+00	1.424E-24
CH ₃ (g)	0.0000E+00	5.8907E-025	8.417E-26	1.00E+00	8.417E-26
Al(g)	0.0000E+00	9.5153E-028	1.367E-28	1.00E+00	1.367E-28
CH ₂ (g)	0.0000E+00	6.2420E-028	8.919E-29	1.00E+00	8.919E-29
C(g)	0.0000E+00	1.0060E-028	1.437E-29	1.00E+00	1.437E-29
Al ₂ O ₂ (g)	0.0000E+00	2.1595E-030	3.086E-31	1.00E+00	3.086E-31
Si(l)	0.0000E+00	1.8570E-032	2.653E-33	1.00E+00	2.653E-33
~?H ₂ (g)	0.0000E+00	2.2111E-034	3.159E-35	1.00E+00	3.159E-35
Al ₂ O(l)	0.0000E+00	7.6679E-037	1.096E-37	1.00E+00	1.096E-37
C ₂ H ₄ (g)	0.0000E+00	2.9488E-038	4.213E-39	1.00E+00	4.213E-39
C ₂ H ₆ (g)	0.0000E+00	2.5603E-044	4.204E-45	1.00E+00	4.204E-45
U(g)	0.0000E+00	7.0335E-046	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	6.9989E+00	1.000E+00		

	PHASE 2 :	MOLE FRAC2	ACTIVITY	ACTIVITY
CaCO ₃	0.0000E+00	4.9400E-001	3.800E-01	1.00E+00
SiO ₂	4.6900E-01	4.6900E-001	3.608E-01	1.00E+00
Fe ₂ O ₃	6.0000E-03	1.2950E-001	9.961E-02	1.00E+00
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.615E-02	1.00E+00
HgO	2.8000E-02	3.3000E-002	2.538E-02	1.00E+00
K ₂ CO ₃	0.0000E+00	3.1500E-002	2.423E-02	1.00E+00
KNO ₃	8.0000E-03	2.2000E-002	1.692E-02	1.00E+00
Na ₂ CO ₃	0.0000E+00	2.1000E-002	1.615E-02	1.00E+00
U ₃ O ₈	0.0000E+00	6.6667E-004	5.128E-04	1.00E+00
PbO	0.0000E+00	3.9999E-004	3.077E-04	1.00E+00
HgCO ₃	0.0000E+00	1.0245E-008	7.880E-09	1.00E+00
HgO ₂	0.0000E+00	8.5383E-009	6.568E-09	1.00E+00
H ₂ O	9.8000E-02	6.5692E-009	5.053E-09	1.00E+00
Hg(OH) ₂	5.0000E-03	5.5698E-009	4.284E-09	1.00E+00
PbO ₂	0.0000E+00	4.4053E-009	3.389E-09	1.00E+00
NaNO ₃	1.4000E-02	4.2309E-009	3.254E-09	1.00E+00
NaF·O ₂	0.0000E+00	4.1775E-009	3.213E-09	1.00E+00
UO ₃	0.0000E+00	3.0048E-009	2.311E-09	1.00E+00
PbCO ₃	0.0000E+00	2.8527E-009	2.194E-09	1.00E+00
Ca(OH) ₂	4.0000E-03	2.6885E-009	2.068E-09	1.00E+00
NaHCO ₃	0.0000E+00	2.5277E-009	1.944E-09	1.00E+00
UO ₃ (G)	0.0000E+00	2.3963E-009	1.843E-09	1.00E+00
NaOH	0.0000E+00	2.0488E-009	1.576E-09	1.00E+00
KOH	5.0000E-03	1.5897E-009	1.223E-09	1.00E+00
CaO	4.9000E-01	1.5256E-009	1.173E-09	1.00E+00
Al(OH) ₃	6.0000E-03	1.2915E-009	9.934E-10	1.00E+00
CaO ₂	0.0000E+00	1.1214E-009	8.626E-10	1.00E+00

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Fe(OH) ₃	4.0000E-03	6.6681E-010	5.129E-10	1.00E+00	5.129E-10
K ₂ O	0.0000E+00	6.2692E-010	4.822E-10	1.00E+00	4.822E-10
Fe ₃ O ₄	0.0000E+00	6.1505E-010	4.731E-10	1.00E+00	4.731E-10
FeO	0.0000E+00	4.5821E-010	3.525E-10	1.00E+00	3.525E-10
Pb ₃ O ₄	0.0000E+00	3.7564E-010	2.889E-10	1.00E+00	2.889E-10
Na ₂ O	0.0000E+00	3.6672E-010	2.821E-10	1.00E+00	2.821E-10
Ca(H ₂) ₂	0.0000E+00	1.2039E-010	9.260E-11	1.00E+00	9.260E-11
H ₂ N ₂	0.0000E+00	1.1231E-010	8.638E-11	1.00E+00	8.638E-11
UO ₂	2.0000E-03	8.9925E-011	6.917E-11	1.00E+00	6.917E-11
Fe(OH) ₂	0.0000E+00	8.9706E-011	6.900E-11	1.00E+00	6.900E-11
FeCO ₃	0.0000E+00	7.9877E-011	6.144E-11	1.00E+00	6.144E-11
K ₂ O	0.0000E+00	3.4781E-011	2.637E-11	1.00E+00	2.637E-11
Pb(NO ₃) ₂	0.0000E+00	2.6027E-011	2.002E-11	1.00E+00	2.002E-11
Na ₂ O	0.0000E+00	1.8146E-011	1.396E-11	1.00E+00	1.396E-11
Pb	4.0000E-04	1.4048E-011	1.081E-11	1.00E+00	1.081E-11
K ₂ O	0.0000E+00	1.0460E-011	8.046E-12	1.00E+00	8.046E-12
Mg(NO ₃) ₂	0.0000E+00	8.6109E-012	6.623E-12	1.00E+00	6.623E-12
U ₃ O ₈	0.0000E+00	6.0739E-012	4.672E-12	1.00E+00	4.672E-12
K ₂ O	0.0000E+00	4.6185E-012	3.553E-12	1.00E+00	3.553E-12
Na ₂ O	1.4000E-02	3.1217E-012	2.401E-12	1.00E+00	2.401E-12
Na ₃ UO ₄	0.0000E+00	2.2571E-012	1.736E-12	1.00E+00	1.736E-12
N ₂ O	0.0000E+00	1.8241E-012	1.403E-12	1.00E+00	1.403E-12
Na	0.0000E+00	4.4495E-013	3.423E-13	1.00E+00	3.423E-13
K	0.0000E+00	3.5773E-013	2.752E-13	1.00E+00	2.752E-13
N ₂ O ₅	0.0000E+00	1.6590E-013	1.276E-13	1.00E+00	1.276E-13
K ₂ O	3.6000E-02	9.0112E-014	6.931E-14	1.00E+00	6.931E-14
HCO ₂ H	0.0000E+00	7.6901E-014	5.915E-14	1.00E+00	5.915E-14
HCOOH	0.0000E+00	7.1221E-014	5.478E-14	1.00E+00	5.478E-14
Fe	2.4300E-01	6.0622E-014	4.663E-14	1.00E+00	4.663E-14
NaH	0.0000E+00	6.7271E-015	5.174E-15	1.00E+00	5.174E-15
KH	0.0000E+00	5.3619E-015	4.124E-15	1.00E+00	4.124E-15
C	1.0120E+00	3.1954E-015	2.458E-15	1.00E+00	2.458E-15
NH ₄ OH	0.0000E+00	1.4519E-015	1.117E-15	1.00E+00	1.117E-15
U ₄ O ₉	0.0000E+00	2.1542E-016	1.657E-16	1.00E+00	1.657E-16
NH ₄ NO ₃	0.0000E+00	1.3991E-016	1.076E-16	1.00E+00	1.076E-16
Na ₃ N	0.0000E+00	1.4399E-017	1.108E-17	1.00E+00	1.108E-17
Mg	0.0000E+00	5.1290E-018	3.945E-18	1.00E+00	3.945E-18
KCN	0.0000E+00	1.4596E-019	1.123E-19	1.00E+00	1.123E-19
UO	0.0000E+00	1.1632E-019	8.947E-20	1.00E+00	8.947E-20
Ca	0.0000E+00	7.7293E-020	5.945E-20	1.00E+00	5.945E-20
NaCN	0.0000E+00	7.4307E-020	5.716E-20	1.00E+00	5.716E-20
NH ₄	0.0000E+00	9.1898E-022	7.069E-22	1.00E+00	7.069E-22
Al	3.6000E-02	4.3180E-022	3.321E-22	1.00E+00	3.321E-22
CaH ₂	0.0000E+00	2.4233E-022	1.864E-22	1.00E+00	1.864E-22
CH ₃ OH	0.0000E+00	2.4055E-022	1.850E-22	1.00E+00	1.850E-22
Si	0.0000E+00	2.4879E-023	1.914E-23	1.00E+00	1.914E-23
UN	0.0000E+00	1.1416E-025	8.781E-26	1.00E+00	8.781E-26
U	0.0000E+00	1.3276E-031	1.021E-31	1.00E+00	1.021E-31
C ₂ H ₆ O	0.0000E+00	5.9269E-041	4.559E-41	1.00E+00	4.559E-41
UC	0.0000E+00	9.8811E-042	7.601E-42	1.00E+00	7.601E-42
UH ₃	0.0000E+00	3.4069E-042	2.620E-42	1.00E+00	2.620E-42
Ca ₃ N ₂	0.0000E+00	4.6696E-052	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	2.0747E-054	0.000E+00	1.00E+00	0.000E+00
UFe ₂	0.0000E+00	5.1614E-056	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	1.8252E-059	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	2.3084E-064	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	8.9022E-107	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	1.2064E-177	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.3001E+000	1.000E+00		

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Temperature 698.15 K
 Pressure 1 bar
 Volume 1.569E-01 m3 (NPT)
 Reaction enthalpy -7.223E+02 kJ
 Reaction entropy 1.388E+02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACT	ACTIVITY COEFFICIENT	ACTIVITY
O2(g)	7.1550E+00	5.4589E+00	7.800E-01	1.00E+00	7.800E-01
H2O(g)	0.0000E+00	1.0745E+00	1.535E-01	1.00E+00	1.535E-01
CO2(g)	0.0000E+00	4.6550E-01	6.651E-02	1.00E+00	6.651E-02
H2O2(g)	0.0000E+00	2.9916E-00	4.274E-10	1.00E+00	4.274E-10
NO(g)	0.0000E+00	2.5195E-00	3.600E-10	1.00E+00	3.600E-10
KOH(g)	0.0000E+00	1.9741E-010	2.821E-11	1.00E+00	2.821E-11
NaOH(g)	0.0000E+00	6.0368E-011	8.625E-12	1.00E+00	8.625E-12
NO3(g)	0.0000E+00	5.0919E-011	7.275E-12	1.00E+00	7.275E-12
PbO(g)	0.0000E+00	3.7652E-011	5.380E-12	1.00E+00	5.380E-12
H2(g)	9.5000E-01	1.1819E-011	1.974E-12	1.00E+00	1.974E-12
CO(g)	0.0000E+00	6.4872E-012	9.269E-13	1.00E+00	9.269E-13
Ca(OH)2(g)	0.0000E+00	6.1122E-013	9.019E-14	1.00E+00	9.019E-14
KO(g)	0.0000E+00	3.5266E-013	5.039E-14	1.00E+00	5.039E-14
K(g)	0.0000E+00	3.5115E-013	5.017E-14	1.00E+00	5.017E-14
Na(g)	0.0000E+00	2.3987E-013	3.427E-14	1.00E+00	3.427E-14
Pb(g)	0.0000E+00	2.2740E-013	3.249E-14	1.00E+00	3.249E-14
NH3(g)	0.0000E+00	2.5880E-014	3.698E-15	1.00E+00	3.698E-15
N(g)	0.0000E+00	7.9677E-016	1.138E-16	1.00E+00	1.138E-16
H2(g)	0.0000E+00	7.2377E-016	1.034E-16	1.00E+00	1.034E-16
HgOH(g)	0.0000E+00	1.4385E-016	2.055E-17	1.00E+00	2.055E-17
NH(g)	0.0000E+00	1.1538E-016	1.649E-17	1.00E+00	1.649E-17
SiO2(g)	0.0000E+00	1.1369E-016	1.624E-17	1.00E+00	1.624E-17
HgO(g)	0.0000E+00	6.3576E-017	9.084E-18	1.00E+00	9.084E-18
FeO(g)	0.0000E+00	4.5128E-017	6.448E-18	1.00E+00	6.448E-18
AlO2(g)	0.0000E+00	5.1129E-018	7.334E-19	1.00E+00	7.334E-19
Hg(g)	0.0000E+00	1.5215E-019	2.174E-20	1.00E+00	2.174E-20
SiO(g)	0.0000E+00	7.8170E-020	1.120E-20	1.00E+00	1.120E-20
Fe(g)	0.0000E+00	6.5602E-020	9.373E-21	1.00E+00	9.373E-21
HCN(g)	0.0000E+00	3.9824E-020	5.690E-21	1.00E+00	5.690E-21
CaO(g)	0.0000E+00	3.5111E-020	5.045E-21	1.00E+00	5.045E-21
Ca(g)	0.0000E+00	5.7864E-022	8.268E-23	1.00E+00	8.268E-23
CH3OH(g)	0.0000E+00	1.1075E-022	1.582E-23	1.00E+00	1.582E-23
AlO(g)	0.0000E+00	1.5941E-023	5.115E-24	1.00E+00	5.115E-24
CH4(g)	0.0000E+00	2.1009E-025	9.34E-26	1.00E+00	9.34E-26
CH3(g)	0.0000E+00	3.7803E-026	5.401E-27	1.00E+00	5.401E-27
Al(g)	0.0000E+00	1.5117E-028	2.160E-29	1.00E+00	2.160E-29
CH2(g)	0.0000E+00	2.0560E-029	2.938E-30	1.00E+00	2.938E-30
C(g)	0.0000E+00	4.4958E-030	6.424E-31	1.00E+00	6.424E-31
Al2O2(g)	0.0000E+00	1.6298E-031	2.329E-32	1.00E+00	2.329E-32
Si(g)	0.0000E+00	9.7945E-034	1.399E-34	1.00E+00	1.399E-34
C2H2(g)	0.0000E+00	6.6628E-037	9.520E-38	1.00E+00	9.520E-38
Al2O(g)	0.0000E+00	1.5138E-038	2.163E-39	1.00E+00	2.163E-39
C2H4(g)	0.0000E+00	6.7247E-042	9.613E-43	1.00E+00	9.613E-43
U(g)	0.0000E+00	3.0082E-050	0.000E+00	1.00E+00	0.000E+00
C2H6(g)	0.0000E+00	2.3213E-050	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	6.9989E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACT	ACTIVITY COEFFICIENT	ACTIVITY
CaCO3	0.0000E+00	4.9400E-001	3.800E-01	1.00E+00	3.800E-01
SiO2	4.6900E-01	4.6900E-001	3.608E-01	1.00E+00	3.608E-01
Fe2O3	6.0000E-03	1.2950E-001	9.961E-02	1.00E+00	9.961E-02
Al2O3	7.8000E-02	9.9000E-002	7.615E-02	1.00E+00	7.615E-02
HgO	2.8000E-02	3.1000E-002	2.538E-02	1.00E+00	2.538E-02
K2CO3	0.0000E+00	3.1500E-002	2.423E-02	1.00E+00	2.423E-02
KNO3	8.0000E-03	2.2000E-002	1.692E-02	1.00E+00	1.692E-02
Na2CO3	0.0000E+00	2.1000E-002	1.615E-02	1.00E+00	1.615E-02
U3O8	0.0000E+00	6.6667E-004	5.128E-04	1.00E+00	5.128E-04
PbO	0.0000E+00	3.9999E-004	3.077E-04	1.00E+00	3.077E-04
HgO2	0.0000E+00	1.6873E-008	1.298E-08	1.00E+00	1.298E-08
NaFeO2	0.0000E+00	1.3162E-008	1.012E-08	1.00E+00	1.012E-08
MgCO3	0.0000E+00	1.1817E-008	9.090E-09	1.00E+00	9.090E-09
H2O	9.8000E-02	1.1790E-008	9.068E-09	1.00E+00	9.068E-09
NaNO3	1.4000E-02	2.2617E-009	7.124E-09	1.00E+00	7.124E-09
Ca(OH)2	4.0000E-03	7.2045E-009	5.542E-09	1.00E+00	5.542E-09
Hg(OH)2	5.0000E-03	6.9625E-009	5.355E-09	1.00E+00	5.355E-09
CaO	4.9000E-01	6.9287E-009	5.330E-09	1.00E+00	5.330E-09
PbO2	0.0000E+00	5.9915E-009	4.609E-09	1.00E+00	4.609E-09
NaOH	0.0000E+00	5.2955E-009	4.073E-09	1.00E+00	4.073E-09
CaO2	0.0000E+00	4.1874E-009	3.221E-09	1.00E+00	3.221E-09
KOH	5.0000E-03	4.1090E-009	3.161E-09	1.00E+00	3.161E-09
UO3	0.0000E+00	1.6640E-009	2.972E-09	1.00E+00	2.972E-09
UO3(g)	0.0000E+00	3.0193E-009	2.322E-09	1.00E+00	2.322E-09
PHCO3	0.0000E+00	2.8735E-009	2.210E-09	1.00E+00	2.210E-09
NaHCO3	0.0000E+00	2.7715E-009	2.132E-09	1.00E+00	2.132E-09
Fe3O4	0.0000E+00	1.5408E-009	1.185E-09	1.00E+00	1.185E-09

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KO2	0.0000E+00	1.3718E-009	1.055E-09	1.00E+00	1.055E-09
FeO	0.0000E+00	1.2069E-009	9.283E-10	1.00E+00	9.283E-10
Al(OH)3	6.0000E-03	1.0860E-009	8.354E-10	1.00E+00	8.354E-10
NaO2	0.0000E+00	7.5215E-010	5.785E-10	1.00E+00	5.785E-10
Fe(OH)3	4.0000E-03	5.3644E-010	4.126E-10	1.00E+00	4.126E-10
PbO4	0.0000E+00	2.5523E-010	1.963E-10	1.00E+00	1.963E-10
Ca(NO3)2	0.0000E+00	1.4232E-010	1.095E-10	1.00E+00	1.095E-10
UO2	2.0000E-03	1.1670E-010	8.976E-11	1.00E+00	8.976E-11
HNO3	0.0000E+00	1.1339E-010	8.722E-11	1.00E+00	8.722E-11
Fe(OH)2	0.0000E+00	1.0602E-010	8.155E-11	1.00E+00	8.155E-11
FeCO3	0.0000E+00	8.0136E-011	6.164E-11	1.00E+00	6.164E-11
KO3	0.0000E+00	3.9270E-011	3.021E-11	1.00E+00	3.021E-11
Na2O2	0.0000E+00	3.5172E-011	2.705E-11	1.00E+00	2.705E-11
Pb	4.0000E-04	2.5706E-011	1.977E-11	1.00E+00	1.977E-11
K2O3	0.0000E+00	1.4826E-011	1.140E-11	1.00E+00	1.140E-11
Pb(NO3)2	0.0000E+00	8.8425E-012	6.802E-12	1.00E+00	6.802E-12
K2O2	0.0000E+00	8.2611E-012	6.354E-12	1.00E+00	6.354E-12
Na2O	1.4000E-02	7.2627E-012	5.586E-12	1.00E+00	5.586E-12
Na3UO4	0.0000E+00	3.7663E-012	2.897E-12	1.00E+00	2.897E-12
Mg(NO3)2	0.0000E+00	3.1918E-012	2.455E-12	1.00E+00	2.455E-12
U3O8	0.0000E+00	1.6351E-012	1.258E-12	1.00E+00	1.258E-12
N2O4	0.0000E+00	1.6127E-012	1.240E-12	1.00E+00	1.240E-12
Na	0.0000E+00	9.0829E-013	6.987E-13	1.00E+00	6.987E-13
K	0.0000E+00	7.4134E-013	5.702E-13	1.00E+00	5.702E-13
K2O	3.6000E-02	1.6657E-013	1.281E-13	1.00E+00	1.281E-13
Fe	2.4300E-01	9.7827E-014	7.525E-14	1.00E+00	7.525E-14
N2O5	0.0000E+00	5.5612E-014	4.278E-14	1.00E+00	4.278E-14
HCO2H	0.0000E+00	3.3170E-014	2.551E-14	1.00E+00	2.551E-14
HCOOH	0.0000E+00	3.0493E-014	2.346E-14	1.00E+00	2.346E-14
NaH	0.0000E+00	7.0717E-015	5.440E-15	1.00E+00	5.440E-15
KH	0.0000E+00	5.6909E-015	4.377E-15	1.00E+00	4.377E-15
Cl	1.0120E+00	2.0385E-015	1.568E-15	1.00E+00	1.568E-15
NH4OH	0.0000E+00	5.8796E-016	4.523E-16	1.00E+00	4.523E-16
NH4NO3	0.0000E+00	2.2259E-017	1.712E-17	1.00E+00	1.712E-17
NaN3	0.0000E+00	1.8959E-017	1.458E-17	1.00E+00	1.458E-17
U4O9	0.0000E+00	1.7108E-017	1.316E-17	1.00E+00	1.316E-17
Hg	0.0000E+00	2.7135E-018	2.133E-18	1.00E+00	2.133E-18
KCN	0.0000E+00	1.0608E-019	8.159E-20	1.00E+00	8.159E-20
Ca	0.0000E+00	7.5837E-020	5.833E-20	1.00E+00	5.833E-20
NaCN	0.0000E+00	5.0182E-020	3.860E-20	1.00E+00	3.860E-20
UO	0.0000E+00	2.8092E-020	2.161E-20	1.00E+00	2.161E-20
N2H4	0.0000E+00	1.2722E-022	9.786E-23	1.00E+00	9.786E-23
Al	3.6000E-02	1.2516E-022	9.627E-23	1.00E+00	9.627E-23
CaH2	0.0000E+00	7.4479E-023	5.729E-23	1.00E+00	5.729E-23
CH3OH	0.0000E+00	9.0138E-024	6.933E-24	1.00E+00	6.933E-24
Si	0.0000E+00	5.9753E-024	4.596E-24	1.00E+00	4.596E-24
UN	0.0000E+00	1.1473E-026	8.825E-27	1.00E+00	8.825E-27
U	0.0000E+00	1.4190E-033	1.091E-33	1.00E+00	1.091E-33
UC	0.0000E+00	1.0797E-045	1.401E-45	1.00E+00	1.401E-45
C2H6O	0.0000E+00	1.7365E-046	0.000E+00	1.00E+00	0.000E+00
UH3	0.0000E+00	6.3674E-047	0.000E+00	1.00E+00	0.000E+00
Ca3N2	0.0000E+00	1.4047E-052	0.000E+00	1.00E+00	0.000E+00
UF6	0.0000E+00	4.2353E-063	0.000E+00	1.00E+00	0.000E+00
Fe(CO)5	0.0000E+00	4.5268E-065	0.000E+00	1.00E+00	0.000E+00
UC2	0.0000E+00	5.4706E-071	0.000E+00	1.00E+00	0.000E+00
Si3N4	0.0000E+00	3.6106E-074	0.000E+00	1.00E+00	0.000E+00
Si2H6	0.0000E+00	4.5794E-115	0.000E+00	1.00E+00	0.000E+00
UC3	0.0000E+00	6.7382E-177	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.3001E+000	1.000E+00		

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R

Temperature 798.15 K
 Pressure 1 bar
 Volume 1.569E-01 m³ (NPT)
 Reaction enthalpy -6.844E-02 kJ
 Reaction entropy 1.896E-02 J/K
 Iterations 80 (Limit = 80)

	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol			
PHASE 1:					
O ₂ (g)	7.1550E+00	5.4589E+00	7.800E-01	1.00E+00	7.800E-01
H ₂ O(g)	0.0000E+00	1.0745E+00	1.235E-01	1.00E+00	1.235E-01
CO ₂ (g)	0.0000E+00	4.6550E+00	6.651E-02	1.00E+00	4.651E-02
NO ₂ (g)	0.0000E+00	1.3142E+00	1.879E-02	1.00E+00	1.878E-02
NO(g)	0.0000E+00	1.1355E+00	1.622E-02	1.00E+00	1.622E-02
KOH(g)	0.0000E+00	8.5322E-01	1.219E-01	1.00E+00	1.219E-01
NaOH(g)	0.0000E+00	2.2672E-01	3.239E-01	1.00E+00	3.239E-01
PbO(g)	0.0000E+00	1.0697E-01	1.528E-01	1.00E+00	1.528E-01
NO ₃ (g)	0.0000E+00	8.3471E-01	1.193E-01	1.00E+00	1.193E-01
H ₂ (g)	9.5000E-01	2.7248E-01	3.893E-02	1.00E+00	3.893E-02
CO(g)	0.0000E+00	1.3367E-01	1.910E-02	1.00E+00	1.910E-02
Ca(OH) ₂ (g)	0.0000E+00	1.9986E-02	2.856E-03	1.00E+00	2.856E-03
K(g)	0.0000E+00	1.0890E-02	1.556E-03	1.00E+00	1.556E-03
KO(g)	0.0000E+00	9.6846E-03	1.384E-03	1.00E+00	1.384E-03
Na(g)	0.0000E+00	7.0775E-03	1.011E-03	1.00E+00	1.011E-03
Pb(g)	0.0000E+00	4.4157E-03	6.309E-04	1.00E+00	6.309E-04
NH ₃ (g)	0.0000E+00	2.7326E-04	3.904E-05	1.00E+00	3.904E-05
N(g)	0.0000E+00	1.0140E-05	1.449E-06	1.00E+00	1.449E-06
NH ₂ (g)	0.0000E+00	6.4879E-06	9.270E-07	1.00E+00	9.270E-07
SiO ₂ (g)	0.0000E+00	1.0408E-06	1.487E-07	1.00E+00	1.487E-07
NH(g)	0.0000E+00	1.0113E-06	1.445E-07	1.00E+00	1.445E-07
HgOH(g)	0.0000E+00	1.0029E-06	1.433E-07	1.00E+00	1.433E-07
HgO(g)	0.0000E+00	5.0000E-07	7.144E-08	1.00E+00	7.144E-08
FeO(g)	0.0000E+00	4.8356E-07	6.909E-08	1.00E+00	6.909E-08
Al ₂ O ₃ (g)	0.0000E+00	2.8511E-08	4.074E-09	1.00E+00	4.074E-09
Hg(g)	0.0000E+00	6.1843E-09	8.836E-10	1.00E+00	8.836E-10
Si(g)	0.0000E+00	4.2800E-09	6.115E-10	1.00E+00	6.115E-10
Fe(g)	0.0000E+00	3.7091E-09	5.300E-10	1.00E+00	5.300E-10
CaO(g)	0.0000E+00	2.8940E-09	4.135E-10	1.00E+00	4.135E-10
HClN(g)	0.0000E+00	1.0612E-09	1.516E-10	1.00E+00	1.516E-10
Ca(g)	0.0000E+00	3.3604E-07	4.801E-03	1.00E+00	4.801E-03
AlO(g)	0.0000E+00	4.9087E-02	7.014E-05	1.00E+00	7.014E-05
CH ₃ OH(g)	0.0000E+00	1.9681E-02	2.812E-05	1.00E+00	2.812E-05
CH ₄ (g)	0.0000E+00	5.4945E-07	7.851E-08	1.00E+00	7.851E-08
CH ₃ (g)	0.0000E+00	2.8359E-08	4.054E-09	1.00E+00	4.052E-09
Al(g)	0.0000E+00	2.5264E-03	3.610E-03	1.00E+00	3.610E-03
CH ₂ (g)	0.0000E+00	3.0751E-03	4.394E-03	1.00E+00	4.394E-03
C(g)	0.0000E+00	8.9164E-03	1.274E-03	1.00E+00	1.274E-03
Al ₂ O ₃ (g)	0.0000E+00	4.4777E-03	6.398E-03	1.00E+00	6.398E-03
Si(g)	0.0000E+00	7.3905E-03	1.056E-03	1.00E+00	1.056E-03
C ₂ H ₂ (g)	0.0000E+00	4.4455E-03	6.306E-04	1.00E+00	6.306E-04
Al ₂ O ₃ (g)	0.0000E+00	7.1460E-04	9.809E-05	1.00E+00	9.809E-05
C ₂ H ₄ (g)	0.0000E+00	4.8178E-05	0.000E+00	1.00E+00	0.000E+00
U(g)	0.0000E+00	2.8301E-06	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ (g)	0.0000E+00	2.0476E-06	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	6.9989E+00	1.000E+00		

	MOLE FRACTION	ACTIVITY	ACTIVITY
PHASE 2 :			
CaCO ₃	0.0000E+00	4.9400E-001	3.800E-01
SiO ₂	4.6900E-01	4.6900E-001	3.608E-01
Fe ₂ O ₃	6.0000E-03	1.2950E-001	9.961E-02
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.615E-02
HgO	2.8000E-02	3.3000E-002	2.538E-02
K ₂ CO ₃	0.0000E+00	3.1500E-002	2.423E-02
KNO ₃	8.0000E-03	2.2000E-002	1.692E-02
Na ₂ CO ₃	0.0000E+00	2.1000E-002	1.615E-02
U ₂ O ₅	0.0000E+00	6.6667E-004	5.128E-04
PbO	0.0000E+00	3.9999E-004	3.077E-04
NaFeO ₂	0.0000E+00	5.4587E-008	4.199E-08
CaO	4.9000E-01	4.4162E-008	3.397E-08
HgO ₂	0.0000E+00	4.0619E-008	3.124E-08
H ₂ O	9.8000E-02	2.6430E-008	2.033E-08
NaNH ₃	1.4000E-02	2.5327E-008	1.948E-08
Ca(OH) ₂	4.0000E-03	2.4902E-008	1.915E-08
CaO ₂	0.0000E+00	2.1226E-008	1.633E-08
NaOH	0.0000E+00	1.7410E-008	1.339E-08
HgCO ₃	0.0000E+00	1.4969E-008	1.151E-08
KOH	5.0000E-03	1.4124E-008	1.086E-08
Hg(OH) ₂	5.0000E-03	9.7481E-009	7.498E-09
PbO ₂	0.0000E+00	9.1004E-009	7.000E-09
UO ₃	0.0000E+00	5.3751E-009	4.134E-09
Fe ₃ O ₄	0.0000E+00	4.8345E-009	3.719E-09
UO ₃ (g)	0.0000E+00	4.0824E-009	3.140E-09
FeO	0.0000E+00	3.9405E-009	3.031E-09
K ₂ O	0.0000E+00	3.6409E-009	2.801E-09

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NaHCO3	0.0000E+00	3.2738E-009	2.480E-09	1.00E+00	2.480E-09
PbCO3	0.0000E+00	3.0439E-009	2.341E-09	1.00E+00	2.341E-09
NaO2	0.0000E+00	1.8174E-009	1.398E-09	1.00E+00	1.398E-09
Al(OH)3	6.0000E-03	9.2808E-010	7.139E-10	1.00E+00	7.139E-10
Fe(OH)3	4.0000E-03	4.1691E-010	3.207E-10	1.00E+00	3.207E-10
Ca(NO3)2	0.0000E+00	1.7235E-010	1.326E-10	1.00E+00	1.326E-10
Pb3O4	0.0000E+00	1.5791E-010	1.214E-10	1.00E+00	1.214E-10
UO2	2.0000E-03	1.5540E-010	1.195E-10	1.00E+00	1.195E-10
Fe(OH)2	0.0000E+00	1.2823E-010	9.864E-11	1.00E+00	9.864E-11
HNO3	0.0000E+00	1.1251E-010	8.654E-11	1.00E+00	8.654E-11
FeCO3	0.0000E+00	7.8950E-011	6.073E-11	1.00E+00	6.073E-11
Na2O2	0.0000E+00	7.4346E-011	5.719E-11	1.00E+00	5.719E-11
Pb	4.0000E-04	5.0944E-011	3.919E-11	1.00E+00	3.919E-11
KO3	0.0000E+00	4.4653E-011	3.435E-11	1.00E+00	3.435E-11
K2O3	0.0000E+00	2.5268E-011	1.944E-11	1.00E+00	1.944E-11
Na2O	1.4000E-02	1.8414E-011	1.416E-11	1.00E+00	1.416E-11
K2O2	0.0000E+00	1.5652E-011	1.204E-11	1.00E+00	1.204E-11
Na3UO4	0.0000E+00	6.0655E-012	4.666E-12	1.00E+00	4.666E-12
Pb(NO3)2	0.0000E+00	2.0651E-012	1.588E-12	1.00E+00	1.588E-12
Na	0.0000E+00	1.9096E-012	1.469E-12	1.00E+00	1.469E-12
K	0.0000E+00	1.5914E-012	1.224E-12	1.00E+00	1.224E-12
N2O4	0.0000E+00	1.3195E-012	1.015E-12	1.00E+00	1.015E-12
Hg(NO3)2	0.0000E+00	8.8086E-013	6.775E-13	1.00E+00	6.775E-13
K2O	3.6000E-02	3.0068E-013	2.313E-13	1.00E+00	2.313E-13
U3O8	0.0000E+00	2.7945E-013	2.149E-13	1.00E+00	2.149E-13
Fe	2.4300E-01	1.4905E-013	1.147E-13	1.00E+00	1.147E-13
N2O5	0.0000E+00	1.1874E-014	9.133E-15	1.00E+00	9.133E-15
HCO2H	0.0000E+00	9.9356E-015	7.642E-15	1.00E+00	7.642E-15
HCOOH	0.0000E+00	9.0318E-015	6.947E-15	1.00E+00	6.947E-15
NaH	0.0000E+00	6.0298E-015	4.638E-15	1.00E+00	4.638E-15
KH	0.0000E+00	4.9155E-015	3.781E-15	1.00E+00	3.781E-15
C	1.0120E+00	9.1624E-016	7.048E-16	1.00E+00	7.048E-16
NH4OH	0.0000E+00	1.4969E-016	1.151E-16	1.00E+00	1.151E-16
NaN3	0.0000E+00	1.7249E-017	1.327E-17	1.00E+00	1.327E-17
NH4NO3	0.0000E+00	1.4859E-018	1.143E-18	1.00E+00	1.143E-18
Hg	0.0000E+00	8.3756E-019	6.442E-19	1.00E+00	6.442E-19
U4O9	0.0000E+00	4.3512E-019	3.347E-19	1.00E+00	3.347E-19
Ca	0.0000E+00	4.2673E-020	3.282E-20	1.00E+00	3.282E-20
KCN	0.0000E+00	4.0647E-020	3.127E-20	1.00E+00	3.127E-20
NaCN	0.0000E+00	1.6968E-020	1.305E-20	1.00E+00	1.305E-20
UO	0.0000E+00	2.4883E-021	1.914E-21	1.00E+00	1.914E-21
Al	3.6000E-02	1.1464E-023	8.818E-24	1.00E+00	8.818E-24
CaH2	0.0000E+00	7.0511E-024	5.424E-24	1.00E+00	5.424E-24
N2H4	0.0000E+00	4.3442E-024	3.342E-24	1.00E+00	3.342E-24
Si	0.0000E+00	3.6510E-025	2.808E-25	1.00E+00	2.808E-25
CH3OH	0.0000E+00	4.5721E-026	3.517E-26	1.00E+00	3.517E-26
UN	0.0000E+00	1.3896E-028	1.069E-28	1.00E+00	1.069E-28
U	0.0000E+00	8.7125E-038	6.702E-38	1.00E+00	6.702E-38
UC	0.0000E+00	6.2811E-057	0.000E+00	1.00E+00	0.000E+00
UH3	0.0000E+00	1.8774E-059	0.000E+00	1.00E+00	0.000E+00
C2H6O	0.0000E+00	2.0469E-060	0.000E+00	1.00E+00	0.000E+00
Ca3N2	0.0000E+00	4.6171E-061	0.000E+00	1.00E+00	0.000E+00
UFe2	0.0000E+00	1.3537E-075	0.000E+00	1.00E+00	0.000E+00
Fe(CO)5	0.0000E+00	1.1612E-080	0.000E+00	1.00E+00	0.000E+00
Si3N4	0.0000E+00	9.3353E-083	0.000E+00	1.00E+00	0.000E+00
UC2	0.0000E+00	1.2167E-083	0.000E+00	1.00E+00	0.000E+00
Si2H6	0.0000E+00	1.8831E-121	0.000E+00	1.00E+00	0.000E+00
UC3	0.0000E+00	5.7093E-177	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.3001E+000	1.000E+00		

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B

Temperature 898.15 K
 Pressure 1 bar
 Volume 1.573E-01 m3 (NPT)
 Reaction enthalpy -6.424E+02 kJ
 Reaction entropy 2.383E+02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACT	ACTIVITY	ACTIVITY
	mol	mol		COEFFIC1	
O2(g)	7.1550E+00	5.4589E+00	7.776E-01	1.00E+00	7.776E-01
H2O(g)	0.0000E+00	1.0745E+00	1.531E-01	1.00E+00	1.531E-01
CO2(g)	0.0000E+00	4.8650E+00	6.930E-02	1.00E+00	6.930E-02
NO(g)	0.0000E+00	1.2947E+00	1.844E-01	1.00E+00	1.844E-01
NO2(g)	0.0000E+00	7.4314E+00	1.059E-01	1.00E+00	1.059E-01
KOH(g)	0.0000E+00	5.7767E+00	8.229E-10	1.00E+00	8.229E-10
NaOH(g)	0.0000E+00	1.4132E+00	2.013E-10	1.00E+00	2.013E-10
PbO(g)	0.0000E+00	3.9049E+00	5.563E-11	1.00E+00	5.563E-11
NO3(g)	0.0000E+00	1.5128E+00	2.155E-11	1.00E+00	2.155E-11
H2(g)	9.5000E-01	5.9542E+00	8.482E-12	1.00E+00	8.482E-12
CO(g)	0.0000E+00	3.0266E+00	4.311E-12	1.00E+00	4.311E-12
Ca(OH)2(g)	0.0000E+00	6.895E+00	9.828E-13	1.00E+00	9.828E-13
K(g)	0.0000E+00	3.5486E+00	5.055E-13	1.00E+00	5.055E-13
KO(g)	0.0000E+00	2.6726E+00	3.807E-13	1.00E+00	3.807E-13
Na(g)	0.0000E+00	2.4797E+00	3.532E-13	1.00E+00	3.532E-13
Pb(g)	0.0000E+00	7.4579E+00	1.062E-13	1.00E+00	1.062E-13
NH3(g)	0.0000E+00	1.7664E+00	2.516E-15	1.00E+00	2.516E-15
N(g)	0.0000E+00	6.7661E+00	9.638E-17	1.00E+00	9.638E-17
NH2(g)	0.0000E+00	2.5655E+00	3.655E-17	1.00E+00	3.655E-17
SiO2(g)	0.0000E+00	1.5947E+00	5.122E-18	1.00E+00	5.122E-18
NH(g)	0.0000E+00	1.3402E+00	4.758E-18	1.00E+00	4.758E-18
MgOH(g)	0.0000E+00	2.3524E+00	3.351E-18	1.00E+00	3.351E-18
FeO(g)	0.0000E+00	1.8297E+00	2.606E-18	1.00E+00	2.606E-18
MgO(g)	0.0000E+00	1.3048E+00	1.859E-18	1.00E+00	1.859E-18
AlO2(g)	0.0000E+00	3.4334E+00	4.891E-20	1.00E+00	4.891E-20
SiO(g)	0.0000E+00	3.4731E+00	4.947E-22	1.00E+00	4.947E-22
CaO(g)	0.0000E+00	1.0617E+00	4.161E-22	1.00E+00	4.161E-22
Mg(g)	0.0000E+00	2.770E+00	2.41E-22	1.00E+00	2.41E-22
Fe(g)	0.0000E+00	2.5762E+00	3.670E-22	1.00E+00	3.670E-22
HCl(g)	0.0000E+00	2.1797E+00	3.10E-22	1.00E+00	3.10E-22
Ca(g)	0.0000E+00	1.2156E+00	1.732E-24	1.00E+00	1.732E-24
AlO(g)	0.0000E+00	6.1456E+00	8.75E-28	1.00E+00	8.75E-28
CH3OH(g)	0.0000E+00	1.1752E+00	4.52E-30	1.00E+00	4.52E-30
CH4(g)	0.0000E+00	1.1211E+00	1.6E-30	1.00E+00	1.6E-30
CH3(g)	0.0000E+00	1.1211E+00	1.6E-30	1.00E+00	1.6E-30
Al(g)	0.0000E+00	1.092E+00	2.0E-30	1.00E+00	2.0E-30
CH2(g)	0.0000E+00	5.1228E+00	7.301E-33	1.00E+00	7.301E-33
C(g)	0.0000E+00	3.4420E+00	4.90E-33	1.00E+00	4.90E-33
Al2O2(g)	0.0000E+00	2.0162E+00	2.80E-34	1.00E+00	2.80E-34
Si(g)	0.0000E+00	1.6567E+00	0.00E+00	1.00E+00	0.00E+00
Al2O(g)	0.0000E+00	3.2183E+00	0.00E+00	1.00E+00	0.00E+00
C2H2(g)	0.0000E+00	1.8846E+00	0.00E+00	1.00E+00	0.00E+00
C2H4(g)	0.0000E+00	1.2010E+00	0.00E+00	1.00E+00	0.00E+00
U(g)	0.0000E+00	2.7720E+00	0.00E+00	1.00E+00	0.00E+00
C2H6(g)	0.0000E+00	1.1590E+00	0.00E+00	1.00E+00	0.00E+00
Total :	8.1050E+00	7.0199E+00	1.00E+00		

PHASE 2 :	MOLE FRACT	ACTIVITY	ACTIVITY
CaCO3	0.0000E+00	4.9400E-001	3.800E-01
SiO2	4.690E-01	4.900E-001	3.608E-01
Fe2O3	6.000E-03	1.0850E-001	8.346E-02
Al2O3	7.800E-02	9.900E-002	7.615E-02
NaFeO2	0.0000E+00	4.1999E-002	3.231E-02
MgO	2.800E-02	3.3000E-002	2.538E-02
K2CO3	0.0000E+00	3.1500E-002	2.423E-02
KH2O	8.000E-03	2.2000E-002	1.692E-02
U3O8	0.0000E+00	6.666E-004	5.128E-04
PbO	0.0000E+00	3.9998E-004	3.077E-04
CaO	4.900E-01	5.6602E-007	4.354E-07
Na2CO3	0.0000E+00	4.6317E-007	3.563E-07
CaO2	0.0000E+00	2.0054E-007	1.543E-07
MgO2	0.0000E+00	1.5370E-007	1.182E-07
Ca(OH)2	4.000E-03	1.4608E-007	1.124E-07
NaNO3	1.400E-02	1.3879E-007	1.00E-07
NaOH	0.0000E+00	1.0959E-007	8.430E-08
H2O	9.800E-02	9.5456E-008	7.342E-08
KOH	5.000E-03	8.1206E-008	6.246E-08
MgCO3	0.0000E+00	2.4510E-008	1.885E-08
Fe3O4	0.0000E+00	2.1911E-008	1.686E-08
FeO	0.0000E+00	1.9511E-008	1.501E-08
PbO2	0.0000E+00	1.7916E-008	1.378E-08
Hg(OH)2	5.000E-03	1.7822E-008	1.371E-08
K2O	0.0000E+00	1.4681E-008	1.129E-08
UO3	0.0000E+00	9.1582E-009	7.044E-09
NaO2	0.0000E+00	7.1055E-009	5.465E-09

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UO3(g)	0.0000E+00	6.6263E-009	5.097E-09	1.00E+00	5.097E-09
NaHCO3	0.0000E+00	5.1171E-009	3.936E-09	1.00E+00	3.936E-09
PbCO3	0.0000E+00	3.7141E-009	2.857E-09	1.00E+00	2.857E-09
Al(OH)3	6.000E-03	8.2208E-010	6.323E-10	1.00E+00	6.323E-10
Fe(OH)3	4.000E-03	2.9054E-010	2.235E-10	1.00E+00	2.235E-10
Na2O	0.0000E+00	2.5114E-010	1.932E-10	1.00E+00	1.932E-10
Ca(NO3)2	0.0000E+00	2.2110E-010	1.701E-10	1.00E+00	1.701E-10
UO2	2.000E-03	2.1506E-010	1.654E-10	1.00E+00	1.654E-10
Fe(OH)2	0.0000E+00	1.5218E-010	1.171E-10	1.00E+00	1.171E-10
Pb	4.000E-04	1.1310E-010	8.700E-11	1.00E+00	8.700E-11
HNO3	0.0000E+00	1.0674E-010	8.210E-11	1.00E+00	8.210E-11
Pb3O4	0.0000E+00	7.7963E-011	5.997E-11	1.00E+00	5.997E-11
Na2O2	1.400E-02	7.1509E-011	5.500E-11	1.00E+00	5.500E-11
FeCO3	0.0000E+00	7.1294E-011	5.484E-11	1.00E+00	5.484E-11
KO3	0.0000E+00	4.7416E-011	3.647E-11	1.00E+00	3.647E-11
K2O3	0.0000E+00	4.4592E-011	3.430E-11	1.00E+00	3.430E-11
K2O2	0.0000E+00	3.0671E-011	2.359E-11	1.00E+00	2.359E-11
Na3UO4	0.0000E+00	1.3764E-011	1.059E-11	1.00E+00	1.059E-11
Na	0.0000E+00	4.5261E-012	3.481E-12	1.00E+00	3.481E-12
K	0.0000E+00	3.2775E-012	2.521E-12	1.00E+00	2.521E-12
N2O4	0.0000E+00	8.3712E-013	6.439E-13	1.00E+00	6.439E-13
K2O	3.600E-02	4.4156E-013	3.396E-13	1.00E+00	3.396E-13
Pb(NO3)2	0.0000E+00	2.0978E-013	1.614E-13	1.00E+00	1.614E-13
Fe	2.430E-01	1.6591E-013	1.276E-13	1.00E+00	1.276E-13
Hg(NO3)2	0.0000E+00	1.2026E-013	9.250E-14	1.00E+00	9.250E-14
U3O8	0.0000E+00	1.5719E-014	1.209E-14	1.00E+00	1.209E-14
NaH	0.0000E+00	3.0643E-015	2.357E-15	1.00E+00	2.357E-15
KH	0.0000E+00	2.0966E-015	1.613E-15	1.00E+00	1.613E-15
HCO2H	0.0000E+00	1.0587E-015	8.143E-16	1.00E+00	8.143E-16
HCOOH	0.0000E+00	9.4042E-016	7.234E-16	1.00E+00	7.234E-16
N2O5	0.0000E+00	7.8118E-016	6.009E-16	1.00E+00	6.009E-16
C	1.0120E+00	1.4257E-016	1.097E-16	1.00E+00	1.097E-16
NH4OH	0.0000E+00	9.0966E-018	6.997E-18	1.00E+00	6.997E-18
NaH3	0.0000E+00	6.1518E-018	4.732E-18	1.00E+00	4.732E-18
Mg	0.0000E+00	3.5848E-020	2.757E-20	1.00E+00	2.757E-20
NH4NO3	0.0000E+00	6.9110E-021	5.316E-21	1.00E+00	5.316E-21
Ca	0.0000E+00	3.1077E-021	2.390E-21	1.00E+00	2.390E-21
KCN	0.0000E+00	1.7241E-021	1.326E-21	1.00E+00	1.326E-21
NaCN	0.0000E+00	6.9630E-022	5.356E-22	1.00E+00	5.356E-22
U4O9	0.0000E+00	3.1633E-022	2.433E-22	1.00E+00	2.433E-22
UO	0.0000E+00	6.1340E-024	4.718E-24	1.00E+00	4.718E-24
Al	3.600E-02	8.9312E-027	6.870E-27	1.00E+00	6.870E-27
CaH2	0.0000E+00	4.7685E-027	3.668E-27	1.00E+00	3.668E-27
NH4	0.0000E+00	3.9184E-028	3.014E-28	1.00E+00	3.014E-28
Si	0.0000E+00	3.7605E-029	2.893E-29	1.00E+00	2.893E-29
CH3OH	0.0000E+00	8.5838E-034	6.603E-34	1.00E+00	6.603E-34
UN	0.0000E+00	1.2940E-035	9.953E-36	1.00E+00	9.953E-36
U	0.0000E+00	1.4920E-049	0.00E+00	1.00E+00	0.00E+00
Ca3N2	0.0000E+00	1.5555E-066	0.00E+00	1.00E+00	0.00E+00
UC	0.0000E+00	1.3944E-067	0.00E+00	1.00E+00	0.00E+00
UH3	0.0000E+00	1.0549E-070	0.00E+00	1.00E+00	0.00E+00
C2H6O	0.0000E+00	9.3821E-073	0.00E+00	1.00E+00	0.00E+00
UF6	0.0000E+00	7.1260E-083	0.00E+00	1.00E+00	0.00E+00
Si3N4	0.0000E+00	1.3913E-087	0.00E+00	1.00E+00	0.00E+00
Fe(CO)5	0.0000E+00	1.5549E-089	0.00E+00	1.00E+00	0.00E+00
UC2	0.0000E+00	5.9403E-091	0.00E+00	1.00E+00	0.00E+00
Si2H6	0.0000E+00	1.8033E-123	0.00E+00	1.00E+00	0.00E+00
UC3	0.0000E+00	3.4728E-174	0.00E+00	1.00E+00	0.00E+00
Total :	2.5594E+00	1.3001E+000	1.00E+00		

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R

Temperature 998.15 K
 Pressure 1 bar
 Volume 1.684E-01 m³ (NPT)
 Reaction enthalpy -5.189E-02 kJ
 Reaction entropy 3.549E-02 J/K
 Iterations 80 (Limit = 80)

	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACT	ACTIVITY	ACTIVITY
	mol	mol			
PHASE 1:					
O ₂ (g)	7.1550E+00	5.4589E+00	7.265E-01	1.00E+00	7.265E-01
H ₂ O(g)	0.0000E+00	1.0745E+00	1.430E-01	1.00E+00	1.430E-01
CO ₂ (g)	0.0000E+00	9.8039E-01	1.305E-01	1.00E+00	1.305E-01
NO(g)	0.0000E+00	1.5417E-005	2.054E-07	1.00E+00	2.054E-06
NO ₂ (g)	0.0000E+00	4.4211E-006	5.884E-07	1.00E+00	5.884E-07
KOH(g)	0.0000E+00	1.7726E-007	2.359E-08	1.00E+00	2.359E-08
NaOH(g)	0.0000E+00	1.7635E-008	2.347E-09	1.00E+00	2.347E-09
PbO(g)	0.0000E+00	3.6192E-009	4.817E-10	1.00E+00	4.817E-10
NO ₃ (g)	0.0000E+00	4.4541E-010	5.928E-11	1.00E+00	5.928E-11
H ₂ (g)	9.5000E-01	1.6322E-010	2.172E-11	1.00E+00	2.172E-11
CO(g)	0.0000E+00	1.1936E-010	1.589E-11	1.00E+00	1.589E-11
Ca(OH) ₂ (g)	0.0000E+00	1.9252E-011	2.562E-12	1.00E+00	2.562E-12
K(g)	0.0000E+00	8.3837E-012	1.116E-12	1.00E+00	1.116E-12
Ka(g)	0.0000E+00	4.2374E-012	5.640E-13	1.00E+00	5.640E-13
Na(g)	0.0000E+00	3.0436E-012	4.051E-13	1.00E+00	4.051E-13
Pb(g)	0.0000E+00	4.2993E-013	5.722E-14	1.00E+00	5.722E-14
NH ₃ (g)	0.0000E+00	3.4624E-016	4.608E-17	1.00E+00	4.608E-17
N(g)	0.0000E+00	7.5771E-019	1.008E-19	1.00E+00	1.008E-19
NH ₂ (g)	0.0000E+00	1.0214E-020	1.359E-21	1.00E+00	1.359E-21
NH(g)	0.0000E+00	7.8831E-021	1.049E-21	1.00E+00	1.049E-21
SiO ₂ (g)	0.0000E+00	6.9492E-021	9.249E-22	1.00E+00	9.249E-22
FeO(g)	0.0000E+00	4.1215E-021	5.485E-22	1.00E+00	5.485E-22
HgOH(g)	0.0000E+00	1.8666E-021	2.484E-22	1.00E+00	2.484E-22
HgO(g)	0.0000E+00	9.6627E-022	1.286E-22	1.00E+00	1.286E-22
AlO ₂ (g)	0.0000E+00	3.9097E-025	5.203E-26	1.00E+00	5.203E-26
Fe(g)	0.0000E+00	1.8412E-027	2.450E-28	1.00E+00	2.450E-28
Hg(g)	0.0000E+00	1.8248E-027	2.429E-28	1.00E+00	2.429E-28
SiO(g)	0.0000E+00	1.0469E-027	1.386E-28	1.00E+00	1.386E-28
CaO(g)	0.0000E+00	2.3894E-028	3.180E-29	1.00E+00	3.180E-29
HCH(g)	0.0000E+00	6.6147E-030	8.801E-31	1.00E+00	8.801E-31
Ca(g)	0.0000E+00	1.0526E-030	1.401E-31	1.00E+00	1.401E-31
AlO(g)	0.0000E+00	2.1970E-036	2.924E-37	1.00E+00	2.924E-37
CH ₃ OH(g)	0.0000E+00	2.9821E-039	3.969E-40	1.00E+00	3.969E-40
CH ₄ (g)	0.0000E+00	6.5361E-043	8.688E-44	1.00E+00	8.688E-44
CH ₃ (g)	0.0000E+00	5.8989E-044	8.408E-45	1.00E+00	8.408E-45
Al(g)	0.0000E+00	2.3436E-045	1.401E-45	1.00E+00	1.401E-45
C(g)	0.0000E+00	2.4661E-049	0.000E+00	1.00E+00	0.000E+00
CH ₂ (g)	0.0000E+00	1.1907E-049	0.000E+00	1.00E+00	0.000E+00
Al ₂ O ₂ (g)	0.0000E+00	9.8978E-050	0.000E+00	1.00E+00	0.000E+00
Si(g)	0.0000E+00	4.4933E-054	0.000E+00	1.00E+00	0.000E+00
Al ₂ O(g)	0.0000E+00	5.8438E-059	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₂ (g)	0.0000E+00	5.6571E-061	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₄ (g)	0.0000E+00	2.3436E-069	0.000E+00	1.00E+00	0.000E+00
U(g)	0.0000E+00	5.5849E-075	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ (g)	0.0000E+00	1.5551E-079	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.5138E+00	1.000E+00		

		MOLE FRACT			
PHASE 2 :					
CaO	4.9000E-01	4.9389E-001	3.799E-01	1.00E+00	3.799E-01
SiO ₂	4.6900E-01	4.6900E-001	3.608E-01	1.00E+00	3.608E-01
Fe ₂ O ₃	6.0000E-03	1.0851E-002	8.347E-02	1.00E+00	8.347E-02
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.615E-02	1.00E+00	7.615E-02
NaFeO ₂	0.0000E+00	4.1974E-002	3.229E-02	1.00E+00	3.229E-02
HgO	2.8000E-02	3.2966E-002	2.538E-02	1.00E+00	2.538E-02
K ₂ CO ₃	0.0000E+00	3.1510E-002	2.424E-02	1.00E+00	2.424E-02
KNO ₃	8.0000E-03	2.1977E-002	1.690E-02	1.00E+00	1.690E-02
U ₃ O ₈	0.0000E+00	6.6665E-004	5.128E-04	1.00E+00	5.128E-04
PbO	0.0000E+00	3.9988E-004	3.076E-04	1.00E+00	3.076E-04
CaCO ₃	0.0000E+00	6.5119E-005	6.547E-05	1.00E+00	6.547E-05
CaO ₂	0.0000E+00	1.5128E-005	1.164E-05	1.00E+00	1.164E-05
Na ₂ CO ₃	0.0000E+00	1.0417E-005	8.013E-06	1.00E+00	8.013E-06
Ca(OH) ₂	4.0000E-03	5.0941E-006	3.918E-06	1.00E+00	3.918E-06
HgO ₂	0.0000E+00	3.3997E-006	2.615E-06	1.00E+00	2.615E-06
NaNO ₃	1.4000E-02	2.8691E-006	2.207E-06	1.00E+00	2.207E-06
KOH	5.0000E-03	2.7054E-006	2.081E-06	1.00E+00	2.081E-06
NaOH	0.0000E+00	2.5961E-006	1.997E-06	1.00E+00	1.997E-06
H ₂ O	9.8000E-02	1.9846E-006	1.527E-06	1.00E+00	1.527E-06
Fe ₃ O ₄	0.0000E+00	5.7477E-007	4.421E-07	1.00E+00	4.421E-07
FeO	0.0000E+00	5.3780E-007	4.137E-07	1.00E+00	4.137E-07
K ₂ O	0.0000E+00	2.3976E-007	1.844E-07	1.00E+00	1.844E-07
MgCO ₃	0.0000E+00	1.6577E-007	1.275E-07	1.00E+00	1.275E-07
PbO ₂	0.0000E+00	1.0611E-007	8.162E-08	1.00E+00	8.162E-08
Hg(OH) ₂	5.0000E-03	9.5172E-008	7.321E-08	1.00E+00	7.321E-08
Na ₂ O	0.0000E+00	5.1301E-008	4.092E-08	1.00E+00	4.092E-08
UO ₃	0.0000E+00	3.7758E-008	2.904E-08	1.00E+00	2.904E-08

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UO ₄ (g)	0.0000E+00	2.3932E-008	1.841E-08	1.00E+00	1.841E-08
NaHCO ₃	0.0000E+00	1.2219E-008	9.399E-09	1.00E+00	9.399E-09
PbCO ₃	0.0000E+00	1.1891E-008	9.146E-09	1.00E+00	9.146E-09
Al(OH) ₃	6.0000E-03	7.8241E-010	6.018E-10	1.00E+00	6.018E-10
Ca(NO ₃) ₂	0.0000E+00	3.7397E-010	2.877E-10	1.00E+00	2.877E-10
Pb	4.0000E-04	3.5642E-010	2.742E-10	1.00E+00	2.742E-10
H ₂ O ₂	0.0000E+00	3.5273E-010	2.713E-10	1.00E+00	2.713E-10
UO ₂	2.0000E-03	3.2759E-010	2.520E-10	1.00E+00	2.520E-10
Fe(OH) ₂	0.0000E+00	1.7220E-010	1.325E-10	1.00E+00	1.325E-10
Fe(OH) ₃	4.0000E-03	1.4220E-010	1.094E-10	1.00E+00	1.094E-10
Na ₂ O	1.4000E-02	9.7781E-011	7.521E-11	1.00E+00	7.521E-11
HNO ₃	0.0000E+00	8.9065E-011	6.851E-11	1.00E+00	6.851E-11
FeCO ₃	0.0000E+00	6.7175E-011	5.167E-11	1.00E+00	5.167E-11
K ₂ O ₃	0.0000E+00	4.7932E-011	3.687E-11	1.00E+00	3.687E-11
K ₂ O ₂	0.0000E+00	3.7330E-011	2.871E-11	1.00E+00	2.871E-11
K ₂ O	0.0000E+00	2.5451E-011	1.958E-11	1.00E+00	1.958E-11
Pb ₃ O ₄	0.0000E+00	1.4678E-011	1.129E-11	1.00E+00	1.129E-11
K	0.0000E+00	3.1491E-012	2.422E-12	1.00E+00	2.422E-12
Na	0.0000E+00	3.0611E-012	2.355E-12	1.00E+00	2.355E-12
Na ₃ UO ₄	0.0000E+00	1.6834E-012	1.295E-12	1.00E+00	1.295E-12
H ₂ O ₄	0.0000E+00	1.3012E-013	1.001E-13	1.00E+00	1.001E-13
K ₂ O	3.6000E-02	9.0595E-014	6.969E-14	1.00E+00	6.969E-14
C	2.4300E-01	2.5040E-014	1.926E-14	1.00E+00	1.926E-14
Hg(NO ₃) ₂	0.0000E+00	2.1377E-016	1.644E-16	1.00E+00	1.644E-16
Pb(NO ₃) ₂	0.0000E+00	1.8982E-016	1.460E-16	1.00E+00	1.460E-16
NaH	0.0000E+00	6.1707E-019	4.747E-19	1.00E+00	4.747E-19
KH	0.0000E+00	5.9907E-019	4.608E-19	1.00E+00	4.608E-19
HCCO ₂ H	0.0000E+00	1.6844E-020	1.296E-20	1.00E+00	1.296E-20
HCCO ₂ H	0.0000E+00	1.6443E-020	1.265E-20	1.00E+00	1.265E-20
U ₃ O ₈	0.0000E+00	1.3711E-020	1.055E-20	1.00E+00	1.055E-20
H ₂ O ₅	0.0000E+00	1.2324E-020	9.480E-21	1.00E+00	9.480E-21
C	1.0120E+00	1.0714E-020	8.241E-21	1.00E+00	8.241E-21
H ₂ N ₃	0.0000E+00	4.5527E-022	3.502E-22	1.00E+00	3.502E-22
NH ₄ OH	0.0000E+00	3.1657E-023	2.435E-23	1.00E+00	2.435E-23
Mg	0.0000E+00	1.0956E-026	8.427E-27	1.00E+00	8.427E-27
Ca	0.0000E+00	2.0360E-027	1.566E-27	1.00E+00	1.566E-27
KCN	0.0000E+00	1.8670E-027	1.436E-27	1.00E+00	1.436E-27
NaCH ₃	0.0000E+00	2.3184E-028	1.783E-28	1.00E+00	1.783E-28
NH ₄ NO ₃	0.0000E+00	1.0610E-030	8.161E-31	1.00E+00	8.161E-31
UO ₄	0.0000E+00	3.4050E-032	2.619E-32	1.00E+00	2.619E-32
UO	0.0000E+00	7.2603E-033	5.585E-33	1.00E+00	5.585E-33
Al	3.6000E-02	3.1767E-035	2.444E-35	1.00E+00	2.444E-35
CaH ₂	0.0000E+00	4.1813E-037	3.216E-37	1.00E+00	3.216E-37
N ₂ H ₄	0.0000E+00	3.9383E-037	3.029E-37	1.00E+00	3.029E-37
Si	0.0000E+00	5.2766E-038	4.059E-38	1.00E+00	4.059E-38
CH ₃ OH	0.0000E+00	1.1364E-042	8.744E-43	1.00E+00	8.744E-43
UH	0.0000E+00	1.2187E-043	9.389E-44	1.00E+00	9.389E-44
U	0.0000E+00	1.3266E-056	0.000E+00	1.00E+00	0.000E+00
Ca ₃ N ₂	0.0000E+00	1.3771E-068	0.000E+00	1.00E+00	0.000E+00
UC	0.0000E+00	2.5102E-072	0.000E+00	1.00E+00	0.000E+00
UH ₃	0.0000E+00	3.9939E-076	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	3.3609E-079	0.000E+00	1.00E+00	0.000E+00
UF ₆	0.0000E+00	1.4292E-085	0.000E+00	1.00E+00	0.000E+00
Si ₃ H ₄	0.0000E+00	2.1107E-086	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	3.0433E-092	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	2.6865E-093	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	6.2405E-122	0.000E+00	1.00E+00	0.000E+00
UC ₃	0.0000E+00	3.9970E-167	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.3001E+000	1.000E+00		

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Temperature 1098.15 K
 Pressure 1 bar
 Volume 1.671E-01 m³ (NPT)
 Reaction enthalpy 4.883E-02 kJ
 Reaction entropy 3.839E-02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACT	ACTIVITY	ACTIVITY
	mol	mol		COEFFICIENT	
O ₂ (g)	7.1550E+00	5.4642E+00	7.330E-01	1.00E+00	7.330E-01
H ₂ O(g)	0.0000E+00	1.0709E+00	1.437E-01	1.00E+00	1.437E-01
CO ₂ (g)	0.0000E+00	8.9956E-01	1.207E-01	1.00E+00	1.207E-01
NO(g)	0.0000E+00	1.8343E-02	2.461E-03	1.00E+00	2.461E-03
NO ₂ (g)	0.0000E+00	9.5743E-04	1.284E-04	1.00E+00	1.284E-04
KOH(g)	0.0000E+00	1.3653E-04	1.832E-05	1.00E+00	1.832E-05
NaOH(g)	0.0000E+00	1.3662E-06	1.833E-07	1.00E+00	1.833E-07
PbO(g)	0.0000E+00	1.9515E-07	2.618E-08	1.00E+00	2.618E-08
H ₂ (g)	9.5000E-01	1.5716E-09	2.108E-10	1.00E+00	2.108E-10
CO(g)	0.0000E+00	1.3309E-09	1.786E-10	1.00E+00	1.786E-10
NO ₃ (g)	0.0000E+00	3.0082E-10	4.036E-11	1.00E+00	4.036E-11
K(g)	0.0000E+00	2.3252E-10	3.119E-11	1.00E+00	3.119E-11
KO(g)	0.0000E+00	7.5617E-11	1.014E-11	1.00E+00	1.014E-11
Ca(OH) ₂ (g)	0.0000E+00	7.0253E-11	9.425E-12	1.00E+00	9.425E-12
Na(g)	0.0000E+00	2.2823E-11	3.062E-12	1.00E+00	3.062E-12
Pb(g)	0.0000E+00	2.3077E-12	3.095E-13	1.00E+00	3.095E-13
NH ₃ (g)	0.0000E+00	9.0274E-17	1.211E-17	1.00E+00	1.211E-17
N(g)	0.0000E+00	4.6308E-18	6.212E-19	1.00E+00	6.212E-19
NH ₂ (g)	0.0000E+00	2.1257E-19	2.852E-20	1.00E+00	2.852E-20
SiO ₂ (g)	0.0000E+00	1.5436E-19	2.071E-20	1.00E+00	2.071E-20
FeO(g)	0.0000E+00	1.3571E-19	1.821E-20	1.00E+00	1.821E-20
MgO(g)	0.0000E+00	2.2075E-20	2.961E-21	1.00E+00	2.961E-21
Mg(g)	0.0000E+00	2.1251E-20	2.851E-21	1.00E+00	2.851E-21
NH(g)	0.0000E+00	1.8491E-20	2.481E-21	1.00E+00	2.481E-21
Al ₂ O ₃ (g)	0.0000E+00	7.7516E-23	1.040E-23	1.00E+00	1.040E-23
SiO(g)	0.0000E+00	7.4577E-25	1.000E-25	1.00E+00	1.000E-25
Fe(g)	0.0000E+00	6.8147E-25	9.142E-26	1.00E+00	9.142E-26
CaO(g)	0.0000E+00	4.3571E-25	5.845E-26	1.00E+00	5.845E-26
Mg(g)	0.0000E+00	1.6878E-25	2.264E-26	1.00E+00	2.264E-26
HCl(g)	0.0000E+00	6.8291E-28	9.162E-29	1.00E+00	9.162E-29
Ca(g)	0.0000E+00	6.2123E-28	8.361E-29	1.00E+00	8.361E-29
AlO(g)	0.0000E+00	4.6762E-32	6.273E-33	1.00E+00	6.273E-33
CH ₃ OH(g)	0.0000E+00	3.8652E-37	5.185E-38	1.00E+00	5.185E-38
CH ₄ (g)	0.0000E+00	2.8932E-40	3.881E-41	1.00E+00	3.881E-41
Al(g)	0.0000E+00	1.4095E-40	1.891E-41	1.00E+00	1.891E-41
CH ₃ (g)	0.0000E+00	3.3390E-41	4.460E-42	1.00E+00	4.460E-42
Al ₂ O ₂ (g)	0.0000E+00	2.5398E-45	0.000E+00	1.00E+00	0.000E+00
C(g)	0.0000E+00	2.0678E-45	0.000E+00	1.00E+00	0.000E+00
CH ₂ (g)	0.0000E+00	6.4291E-46	0.000E+00	1.00E+00	0.000E+00
Si(g)	0.0000E+00	8.9190E-48	0.000E+00	1.00E+00	0.000E+00
Al ₂ O(g)	0.0000E+00	3.0314E-53	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₂ (g)	0.0000E+00	1.3692E-56	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₄ (g)	0.0000E+00	1.8789E-64	0.000E+00	1.00E+00	0.000E+00
U(g)	0.0000E+00	1.6141E-68	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ (g)	0.0000E+00	2.4336E-74	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.4541E+00	1.000E+00		

PHASE 2 :	MOLE FRACT			
SiO ₂	4.6900E-01	4.6900E-01	3.627E-01	1.00E+00
CaO	4.9000E-01	4.0551E-01	3.136E-01	1.00E+00
Fe ₂ O ₃	6.0000E-03	1.1031E-01	8.531E-02	1.00E+00
Al ₂ O ₃	7.8000E-02	9.9000E-02	7.656E-02	1.00E+00
CaCO ₃	0.0000E+00	7.1143E-02	5.502E-02	1.00E+00
K ₂ CO ₃	0.0000E+00	3.9499E-02	3.055E-02	1.00E+00
NaFeO ₂	0.0000E+00	3.7459E-02	2.897E-02	1.00E+00
MgO	2.8000E-02	3.1924E-02	2.469E-02	1.00E+00
CaO ₂	0.0000E+00	1.6452E-02	1.272E-02	1.00E+00
KOH	5.0000E-03	3.1784E-03	2.458E-03	1.00E+00
KNO ₃	8.0000E-03	2.6322E-03	2.036E-03	1.00E+00
Na ₂ CO ₃	0.0000E+00	1.7954E-03	1.389E-03	1.00E+00
MgO ₂	0.0000E+00	1.0725E-03	8.294E-04	1.00E+00
Ca(OH) ₂	4.0000E-03	8.9379E-04	6.912E-04	1.00E+00
NaOH	0.0000E+00	8.7980E-04	6.804E-04	1.00E+00
U ₃ O ₈	0.0000E+00	6.6651E-04	5.155E-04	1.00E+00
H ₂ O	9.8000E-02	6.4152E-04	4.961E-04	1.00E+00
PbO	0.0000E+00	3.9796E-04	3.078E-04	1.00E+00
FeO	0.0000E+00	2.3799E-04	1.841E-04	1.00E+00
Fe ₃ O ₄	0.0000E+00	2.3047E-04	1.782E-04	1.00E+00
NaNO ₃	1.4000E-02	6.7129E-05	5.192E-05	1.00E+00
K ₂ O	0.0000E+00	5.4526E-05	4.217E-05	1.00E+00
HgCO ₃	0.0000E+00	1.9795E-06	1.531E-06	1.00E+00
PbO ₂	0.0000E+00	1.8071E-06	1.398E-06	1.00E+00
Na ₂ O	0.0000E+00	1.4613E-06	1.130E-06	1.00E+00
Mg(OH) ₂	5.0000E-03	1.3878E-06	1.073E-06	1.00E+00
UO ₃	0.0000E+00	3.1464E-07	2.433E-07	1.00E+00

UO ₃ (G)	0.0000E+00	1.5702E-007	1.214E-07	1.00E+00	1.214E-07
PbCO ₃	0.0000E+00	3.8103E-008	2.947E-08	1.00E+00	2.947E-08
NaHCO ₃	0.0000E+00	1.9633E-008	1.518E-08	1.00E+00	1.518E-08
Pb	4.0000E-04	1.5770E-009	1.765E-09	1.00E+00	1.765E-09
UO ₂	2.0000E-03	8.0474E-010	6.224E-10	1.00E+00	6.224E-10
Al(OH) ₃	6.0000E-03	7.2867E-010	5.635E-10	1.00E+00	5.635E-10
Na ₂ O ₂	0.0000E+00	6.0663E-010	4.691E-10	1.00E+00	4.691E-10
Fe(OH) ₂	0.0000E+00	3.0320E-010	2.345E-10	1.00E+00	2.345E-10
K ₂ O ₂	0.0000E+00	2.7626E-010	2.137E-10	1.00E+00	2.137E-10
K ₂ O ₃	0.0000E+00	2.5960E-010	2.008E-10	1.00E+00	2.008E-10
Na ₂ O	1.4000E-02	2.3075E-010	1.785E-10	1.00E+00	1.785E-10
FeCO ₃	0.0000E+00	9.7628E-011	4.622E-11	1.00E+00	4.622E-11
Fe(OH) ₃	4.0000E-03	5.1729E-011	4.001E-11	1.00E+00	4.001E-11
KO ₃	0.0000E+00	3.0502E-011	2.359E-11	1.00E+00	2.359E-11
K	0.0000E+00	2.5611E-011	1.981E-11	1.00E+00	1.981E-11
HNO ₃	0.0000E+00	8.2521E-012	6.382E-12	1.00E+00	6.382E-12
Na	0.0000E+00	7.8205E-012	6.048E-12	1.00E+00	6.048E-12
Pb ₃ O ₄	0.0000E+00	1.7545E-012	1.357E-12	1.00E+00	1.357E-12
Ca(NO ₃) ₂	0.0000E+00	1.4219E-012	1.100E-12	1.00E+00	1.100E-12
K ₂ O	3.6000E-02	4.4971E-013	3.478E-13	1.00E+00	3.478E-13
Na ₃ UO ₄	0.0000E+00	1.7322E-013	1.340E-13	1.00E+00	1.340E-13
Fe	2.4300E-01	7.7353E-014	5.982E-14	1.00E+00	5.982E-14
N ₂ O ₄	0.0000E+00	1.0427E-015	8.064E-16	1.00E+00	8.064E-16
KH	0.0000E+00	1.0841E-017	8.384E-18	1.00E+00	8.384E-18
NaH	0.0000E+00	3.6255E-018	2.804E-18	1.00E+00	2.804E-18
Mg(NO ₃) ₂	0.0000E+00	1.3060E-019	1.010E-19	1.00E+00	1.010E-19
HCO ₂ H	0.0000E+00	3.2890E-020	2.544E-20	1.00E+00	2.544E-20
Pb(NO ₃) ₂	0.0000E+00	1.1849E-020	2.463E-20	1.00E+00	2.463E-20
C	1.0120E+00	3.1166E-020	2.410E-20	1.00E+00	2.410E-20
HCOOH	0.0000E+00	2.6995E-020	2.088E-20	1.00E+00	2.088E-20
U ₃ O ₈	0.0000E+00	9.6204E-021	7.440E-21	1.00E+00	7.440E-21
N ₂ O ₅	0.0000E+00	3.9262E-023	3.036E-23	1.00E+00	3.036E-23
NaH ₃	0.0000E+00	1.2052E-023	9.321E-24	1.00E+00	9.321E-24
NH ₄ OH	0.0000E+00	7.8163E-024	6.045E-24	1.00E+00	6.045E-24
Mg	0.0000E+00	4.5674E-025	3.532E-25	1.00E+00	3.532E-25
Ca	0.0000E+00	6.8669E-026	5.311E-26	1.00E+00	5.311E-26
KCN	0.0000E+00	2.4542E-026	1.898E-26	1.00E+00	1.898E-26
NaCN	0.0000E+00	1.2576E-027	9.726E-28	1.00E+00	9.726E-28
NH ₄ NO ₃	0.0000E+00	7.9205E-031	6.125E-31	1.00E+00	6.125E-31
UO	0.0000E+00	4.6470E-031	3.594E-31	1.00E+00	3.594E-31
Al	3.6000E-02	1.1760E-032	9.095E-33	1.00E+00	9.095E-33
U ₄ O ₉	0.0000E+00	9.9694E-033	7.710E-33	1.00E+00	7.710E-33
CaH ₂	0.0000E+00	5.3438E-034	4.133E-34	1.00E+00	4.133E-34
Si	0.0000E+00	7.6828E-035	5.942E-35	1.00E+00	5.942E-35
N ₂ H ₄	0.0000E+00	3.9447E-037	3.051E-37	1.00E+00	3.051E-37
CH ₃ OH	0.0000E+00	3.4507E-041	2.669E-41	1.00E+00	2.669E-41
UN	0.0000E+00	1.9409E-041	1.501E-41	1.00E+00	1.501E-41
U	0.0000E+00	2.5430E-052	0.000E+00	1.00E+00	0.000E+00
Ca ₃ N ₂	0.0000E+00	1.0056E-063	0.000E+00	1.00E+00	0.000E+00
UC	0.0000E+00	6.5126E-067	0.000E+00	1.00E+00	0.000E+00
UH ₃	0.0000E+00	5.1121E-071	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	2.1844E-074	0.000E+00	1.00E+00	0.000E+00
UF ₆	0.0000E+00	1.5214E-077	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	8.6779E-081	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	2.0573E-085	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	3.8486E-086	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	7.0130E-111	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	9.2694E-153	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.2930E+000	1.000E+00		

Temperature 1198 15 K
 Pressure 1 bar
 Volume 1.684E-01 m³ (HPT)
 Reaction enthalpy -4.377E+02 kJ
 Reaction entropy 4.282E+02 J/K
 Iterations 80 (Limit = 80)

PHASE 1.	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
O ₂ (g)	0.0000E+00	5.4661E-000	7.277E-01	1.00E+00	7.277E-01
H ₂ O(g)	0.0000E+00	1.0686E-000	1.423E-01	1.00E+00	1.423E-01
CO ₂ (g)	0.0000E+00	9.5421E-001	1.270E-01	1.00E+00	1.270E-01
NO(g)	0.0000E+00	2.0840E-002	2.774E-03	1.00E+00	2.774E-03
KOH(g)	0.0000E+00	1.1682E-003	1.555E-04	1.00E+00	1.555E-04
NO ₂ (g)	0.0000E+00	6.3603E-004	8.467E-05	1.00E+00	8.467E-05
NaOH(g)	0.0000E+00	9.5134E-006	1.266E-06	1.00E+00	1.266E-06
PbO(g)	0.0000E+00	1.7501E-006	2.330E-07	1.00E+00	2.330E-07
CO(g)	0.0000E+00	1.8749E-008	2.496E-09	1.00E+00	2.496E-09
H ₂ (g)	9.5000E-01	1.5295E-008	2.036E-09	1.00E+00	2.036E-09
K(g)	0.0000E+00	1.2637E-008	1.682E-09	1.00E+00	1.682E-09
KO(g)	0.0000E+00	3.4832E-009	4.637E-10	1.00E+00	4.637E-10
Ca(OH) ₂ (g)	0.0000E+00	8.8341E-010	1.176E-10	1.00E+00	1.176E-10
Na(g)	0.0000E+00	8.3184E-010	1.07E-10	1.00E+00	1.07E-10
NO ₃ (g)	0.0000E+00	2.9290E-010	3.899E-11	1.00E+00	3.899E-11
Pb(g)	0.0000E+00	8.0818E-011	1.076E-11	1.00E+00	1.076E-11
NH ₃ (g)	0.0000E+00	8.1173E-016	1.081E-16	1.00E+00	1.081E-16
N(g)	0.0000E+00	1.8101E-016	2.410E-17	1.00E+00	2.410E-17
FeO(g)	0.0000E+00	4.7079E-017	6.268E-18	1.00E+00	6.268E-18
SiO ₂ (g)	0.0000E+00	3.5461E-017	4.721E-18	1.00E+00	4.721E-18
NH ₂ (g)	0.0000E+00	5.5474E-018	7.385E-19	1.00E+00	7.385E-19
MgO(g)	0.0000E+00	4.9710E-018	6.619E-19	1.00E+00	6.619E-19
MgOH(g)	0.0000E+00	3.4360E-018	4.574E-19	1.00E+00	4.574E-19
NH(g)	0.0000E+00	9.9499E-019	1.300E-19	1.00E+00	1.300E-19
Al ₂ O ₃ (g)	0.0000E+00	2.8889E-020	3.846E-21	1.00E+00	3.846E-21
SiO(g)	0.0000E+00	1.0861E-021	1.446E-22	1.00E+00	1.446E-22
Fe(g)	0.0000E+00	1.0500E-021	1.398E-22	1.00E+00	1.398E-22
CaO(g)	0.0000E+00	2.8970E-022	3.857E-23	1.00E+00	3.857E-23
Mg(g)	0.0000E+00	1.4700E-022	1.957E-23	1.00E+00	1.957E-23
Ca(g)	0.0000E+00	1.0753E-024	1.432E-25	1.00E+00	1.432E-25
HCl(g)	0.0000E+00	1.4063E-025	1.872E-26	1.00E+00	1.872E-26
Al(g)	0.0000E+00	2.0536E-028	2.734E-29	1.00E+00	2.734E-29
CH ₃ OH(g)	0.0000E+00	1.9277E-034	2.560E-35	1.00E+00	2.560E-35
Al(g)	0.0000E+00	5.4712E-036	7.284E-37	1.00E+00	7.284E-37
CH ₄ (g)	0.0000E+00	4.6601E-037	6.204E-38	1.00E+00	6.204E-38
CH ₃ (g)	0.0000E+00	1.2448E-037	1.657E-38	1.00E+00	1.657E-38
Al ₂ O ₃ (g)	0.0000E+00	2.2962E-040	3.057E-41	1.00E+00	3.057E-41
C(g)	0.0000E+00	5.8835E-041	7.833E-42	1.00E+00	7.833E-42
CH ₂ (g)	0.0000E+00	8.8916E-042	1.184E-42	1.00E+00	1.184E-42
Si(g)	0.0000E+00	2.0666E-042	2.747E-43	1.00E+00	2.747E-43
Al ₂ O ₃ (g)	0.0000E+00	3.1382E-047	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₂ (g)	0.0000E+00	1.5895E-051	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₄ (g)	0.0000E+00	3.8301E-059	0.000E+00	1.00E+00	0.000E+00
U(g)	0.0000E+00	6.1007E-062	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ (g)	0.0000E+00	1.2899E-068	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.5116E+000	1.000E+00		

PHASE 2 :	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
SiO ₂	4.6900E-01	4.6900E-001	3.625E-01	1.00E+00	3.625E-01
CaO	4.9000E-01	4.5774E-001	3.538E-01	1.00E+00	3.538E-01
Fe ₂ O ₃	6.0000E-03	1.0837E-001	8.377E-02	1.00E+00	8.377E-02
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.652E-02	1.00E+00	7.652E-02
NaFeO ₂	0.0000E+00	3.9449E-002	3.049E-02	1.00E+00	3.049E-02
K ₂ CO ₃	0.0000E+00	3.8080E-002	2.943E-02	1.00E+00	2.943E-02
MgO	2.8000E-02	3.2153E-002	2.485E-02	1.00E+00	2.485E-02
CaCO ₃	0.0000E+00	1.8957E-002	1.465E-02	1.00E+00	1.465E-02
CaO ₂	0.0000E+00	1.6874E-002	1.304E-02	1.00E+00	1.304E-02
KOH	5.0000E-03	7.0150E-003	5.422E-03	1.00E+00	5.422E-03
NaOH	0.0000E+00	1.0263E-003	7.933E-04	1.00E+00	7.933E-04
MgO ₂	0.0000E+00	8.4522E-004	6.533E-04	1.00E+00	6.533E-04
H ₂ O	9.8000E-02	8.2973E-004	6.413E-04	1.00E+00	6.413E-04
FeO	0.0000E+00	8.0818E-004	6.247E-04	1.00E+00	6.247E-04
Na ₂ CO ₃	0.0000E+00	7.5080E-004	5.803E-04	1.00E+00	5.803E-04
U ₃ O ₈	0.0000E+00	6.6657E-004	5.152E-04	1.00E+00	5.152E-04
Fe ₃ O ₄	0.0000E+00	6.6557E-004	5.145E-04	1.00E+00	5.145E-04
KNO ₃	8.0000E-03	5.1258E-004	3.962E-04	1.00E+00	3.962E-04
Ca(OH) ₂	4.0000E-03	4.2487E-004	3.284E-04	1.00E+00	3.284E-04
PbO	0.0000E+00	3.9720E-004	3.070E-04	1.00E+00	3.070E-04
K ₂ O	0.0000E+00	1.4418E-004	1.114E-04	1.00E+00	1.114E-04
NaNO ₃	1.4000E-02	1.1344E-005	8.768E-06	1.00E+00	8.768E-06
Na ₂ O	0.0000E+00	2.3893E-006	1.847E-06	1.00E+00	1.847E-06
PbO ₂	0.0000E+00	1.0609E-006	7.736E-07	1.00E+00	7.736E-07
Mg(OH) ₂	5.0000E-03	8.6467E-007	6.684E-07	1.00E+00	6.684E-07
HgCO ₃	0.0000E+00	8.3159E-007	6.428E-07	1.00E+00	6.428E-07
UO ₃	0.0000E+00	1.8767E-007	1.451E-07	1.00E+00	1.451E-07

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UO ₃ (g)	0.0000E+00	9.8204E-008	7.591E-08	1.00E+00	7.591E-08
Pb	4.0000E-04	2.3202E-008	1.791E-08	1.00E+00	1.791E-08
PbCO ₃	0.0000E+00	2.1447E-008	1.658E-08	1.00E+00	1.658E-08
NaHCO ₃	0.0000E+00	7.9898E-009	6.176E-09	1.00E+00	6.176E-09
K ₂ O ₂	0.0000E+00	2.4610E-009	1.902E-09	1.00E+00	1.902E-09
UO ₂	2.0000E-03	1.8212E-009	1.408E-09	1.00E+00	1.408E-09
K ₂ O ₃	0.0000E+00	1.5966E-009	1.234E-09	1.00E+00	1.234E-09
Na ₂ O ₂	0.0000E+00	1.3840E-009	1.070E-09	1.00E+00	1.070E-09
Na ₂ O	1.4000E-02	1.1730E-009	9.067E-10	1.00E+00	9.067E-10
Fe(OH) ₂	0.0000E+00	6.8840E-010	5.321E-10	1.00E+00	5.321E-10
K	0.0000E+00	6.7301E-010	5.204E-10	1.00E+00	5.202E-10
Al(OH) ₃	6.0000E-03	5.6696E-010	4.382E-10	1.00E+00	4.382E-10
FeCO ₃	0.0000E+00	1.3097E-010	1.012E-10	1.00E+00	1.012E-10
Na	0.0000E+00	1.1587E-010	8.956E-11	1.00E+00	8.956E-11
KOH	0.0000E+00	8.4737E-011	6.511E-11	1.00E+00	6.511E-11
Fe(OH) ₃	4.0000E-03	3.4187E-011	2.642E-11	1.00E+00	2.642E-11
K ₂ O	3.6000E-02	1.4255E-011	1.102E-11	1.00E+00	1.102E-11
Fe	2.4300E-01	3.1376E-012	2.425E-12	1.00E+00	2.425E-12
HNO ₃	0.0000E+00	2.9305E-012	2.265E-12	1.00E+00	2.265E-12
Pb ₃ O ₄	0.0000E+00	7.9132E-013	6.117E-13	1.00E+00	6.117E-13
Na ₃ UO ₄	0.0000E+00	2.7522E-013	2.127E-13	1.00E+00	2.127E-13
Ca(NO ₃) ₂	0.0000E+00	4.0286E-014	3.114E-14	1.00E+00	3.114E-14
KH	0.0000E+00	5.5174E-016	4.265E-16	1.00E+00	4.265E-16
N ₂ O ₄	0.0000E+00	5.2146E-016	4.031E-16	1.00E+00	4.031E-16
NaH	0.0000E+00	1.0703E-016	8.273E-17	1.00E+00	8.273E-17
C	0.0000E+00	1.2792E-018	9.502E-19	1.00E+00	9.502E-19
HCO ₂ H	0.0000E+00	2.9643E-019	2.291E-19	1.00E+00	2.291E-19
HCOOH	0.0000E+00	2.4785E-019	1.916E-19	1.00E+00	1.916E-19
Mg(NO ₃) ₂	0.0000E+00	1.2349E-020	9.545E-21	1.00E+00	9.545E-21
U ₃ O ₈	0.0000E+00	6.9509E-021	5.373E-21	1.00E+00	5.373E-21
Pb(NO ₃) ₂	0.0000E+00	7.2479E-022	5.602E-22	1.00E+00	5.602E-22
Mg	0.0000E+00	1.2040E-022	9.306E-23	1.00E+00	9.306E-23
HNH ₄ OH	0.0000E+00	6.0069E-023	4.643E-23	1.00E+00	4.643E-23
Ca	0.0000E+00	2.7226E-023	2.104E-23	1.00E+00	2.104E-23
NaH ₂	0.0000E+00	2.6421E-023	2.042E-23	1.00E+00	2.042E-23
N ₂ O ₅	0.0000E+00	8.0334E-024	6.210E-24	1.00E+00	6.210E-24
KCN	0.0000E+00	5.2051E-024	4.023E-24	1.00E+00	4.023E-24
NaCN	0.0000E+00	1.8130E-025	1.401E-25	1.00E+00	1.401E-25
UO	0.0000E+00	1.3093E-028	1.012E-28	1.00E+00	1.012E-28
Al	3.6000E-02	2.7010E-029	2.088E-29	1.00E+00	2.088E-29
HNH ₄ NO ₃	0.0000E+00	8.2765E-031	6.397E-31	1.00E+00	6.397E-31
CaH ₂	0.0000E+00	3.0878E-031	2.387E-31	1.00E+00	2.387E-31
Si	0.0000E+00	2.9514E-031	2.281E-31	1.00E+00	2.281E-31
U ₄ O ₉	0.0000E+00	6.5815E-032	5.087E-32	1.00E+00	5.087E-32
NH ₄	0.0000E+00	1.5478E-035	1.196E-35	1.00E+00	1.196E-35
CH	0.0000E+00	2.8626E-038	2.213E-38	1.00E+00	2.213E-38
CH ₃ OH	0.0000E+00	1.3012E-038	1.006E-38	1.00E+00	1.006E-38
U	0.0000E+00	1.1634E-047	0.000E+00	1.00E+00	0.000E+00
Ca ₃ H ₂	0.0000E+00	2.4638E-058	0.000E+00	1.00E+00	0.000E+00
UC	0.0000E+00	4.6549E-061	0.000E+00	1.00E+00	0.000E+00
UH ₃	0.0000E+00	1.7656E-065	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	1.9178E-069	0.000E+00	1.00E+00	0.000E+00
UFe ₂	0.0000E+00	6.6458E-070	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	3.2984E-074	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	9.8929E-078	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	1.7281E-079	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	1.7257E-100	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	2.0007E-139	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.2237E+000	1.000E+00		

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Temperature 1298.15 K
 Pressure 1 bar
 Volume 1.688E-01 m³ (NPT)
 Reaction enthalpy -3.927E-02 kJ
 Reaction entropy 4.637E-02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACT	ACTIVITY	ACTIVITY (COEFFICIENT)
O2(g)	7.1550E-00	5.4675E-00	7.259E-01	1.00E+00	7.259E-01
H2O(g)	0.0000E+00	1.0635E-00	1.412E-01	1.00E+00	1.412E-01
CO2(g)	0.0000E+00	9.7279E-01	1.292E-01	1.00E+00	1.292E-01
NO(g)	0.0000E+00	2.1476E-02	2.851E-03	1.00E+00	2.851E-03
KOH(g)	0.0000E+00	6.1051E-03	8.106E-04	1.00E+00	8.106E-04
NO2(g)	0.0000E+00	4.1717E-04	5.539E-05	1.00E+00	5.539E-05
NaOH(g)	0.0000E+00	4.7025E-05	6.244E-06	1.00E+00	6.244E-06
PbO(g)	0.0000E+00	9.4138E-06	1.250E-06	1.00E+00	1.250E-06
K(g)	0.0000E+00	3.1568E-07	4.191E-08	1.00E+00	4.191E-08
CO(g)	0.0000E+00	1.6967E-07	2.253E-08	1.00E+00	2.253E-08
H2(g)	9.5000E-01	1.0472E-07	1.390E-08	1.00E+00	1.390E-08
KO(g)	0.0000E+00	7.5778E-08	1.006E-08	1.00E+00	1.006E-08
Na(g)	0.0000E+00	1.6603E-08	2.204E-09	1.00E+00	2.204E-09
Ca(OH)2(g)	0.0000E+00	6.9592E-09	9.240E-10	1.00E+00	9.240E-10
Pb(g)	0.0000E+00	1.3755E-09	1.826E-10	1.00E+00	1.826E-10
NO3(g)	0.0000E+00	2.6759E-10	3.551E-11	1.00E+00	3.551E-11
FeO(g)	0.0000E+00	6.4499E-15	8.564E-16	1.00E+00	8.564E-16
NH3(g)	0.0000E+00	4.8159E-15	6.394E-16	1.00E+00	6.394E-16
N(g)	0.0000E+00	3.7254E-15	4.946E-16	1.00E+00	4.946E-16
SiO2(g)	0.0000E+00	3.4803E-15	4.621E-16	1.00E+00	4.621E-16
HgO(g)	0.0000E+00	4.9360E-16	6.554E-17	1.00E+00	6.554E-17
HgOH(g)	0.0000E+00	2.4258E-16	3.221E-17	1.00E+00	3.221E-17
NH2(g)	0.0000E+00	8.0937E-17	1.075E-17	1.00E+00	1.075E-17
NH(g)	0.0000E+00	2.1994E-17	2.920E-18	1.00E+00	2.920E-18
AlO2(g)	0.0000E+00	4.2703E-18	5.670E-19	1.00E+00	5.670E-19
Fe(g)	0.0000E+00	5.0990E-19	6.770E-20	1.00E+00	6.770E-20
SiO(g)	0.0000E+00	5.0540E-19	6.710E-20	1.00E+00	6.710E-20
CaO(g)	0.0000E+00	6.4751E-20	8.597E-21	1.00E+00	8.597E-21
Hg(g)	0.0000E+00	4.4358E-20	5.889E-21	1.00E+00	5.889E-21
Ca(g)	0.0000E+00	5.3816E-22	7.145E-23	1.00E+00	7.145E-23
HCH(g)	0.0000E+00	1.1442E-23	1.519E-24	1.00E+00	1.519E-24
AlO(g)	0.0000E+00	2.4305E-25	3.227E-26	1.00E+00	3.227E-26
Al(g)	0.0000E+00	4.0895E-32	5.43E-33	1.00E+00	5.43E-33
CH3OH(g)	0.0000E+00	3.5683E-32	4.738E-33	1.00E+00	4.738E-33
CH4(g)	0.0000E+00	2.3339E-34	3.099E-35	1.00E+00	3.099E-35
CH3(g)	0.0000E+00	1.2683E-34	1.684E-35	1.00E+00	1.684E-35
Al2O2(g)	0.0000E+00	3.4716E-36	4.612E-37	1.00E+00	4.612E-37
C(g)	0.0000E+00	3.336E-37	4.430E-38	1.00E+00	4.430E-38
Si(g)	0.0000E+00	7.0071E-38	9.301E-39	1.00E+00	9.301E-39
CH2(g)	0.0000E+00	2.7415E-38	3.640E-39	1.00E+00	3.640E-39
Al2O(g)	0.0000E+00	3.7124E-42	4.933E-43	1.00E+00	4.933E-43
C2H2(g)	0.0000E+00	2.8829E-47	0.000E+00	1.00E+00	0.000E+00
C2H4(g)	0.0000E+00	1.1227E-54	0.000E+00	1.00E+00	0.000E+00
U(g)	0.0000E+00	2.1726E-56	0.000E+00	1.00E+00	0.000E+00
C2H6(g)	0.0000E+00	8.5022E-64	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.5318E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACT	ACTIVITY	ACTIVITY (COEFFICIENT)
CaO	4.9000E-01	4.7220E-01	3.649E-01	1.00E+00	3.649E-01
SiO2	4.6900E-01	4.6900E-01	3.624E-01	1.00E+00	3.624E-01
Fe2O3	6.0000E-03	1.0592E-01	8.184E-02	1.00E+00	8.184E-02
Al2O3	7.8000E-02	9.9000E-02	7.649E-02	1.00E+00	7.649E-02
NaFeO2	0.0000E+00	4.0079E-02	3.097E-02	1.00E+00	3.097E-02
K2CO3	0.0000E+00	3.3298E-02	2.571E-02	1.00E+00	2.571E-02
HgO	2.8000E-02	3.2313E-02	2.497E-02	1.00E+00	2.497E-02
CaO2	0.0000E+00	1.6039E-02	1.239E-02	1.00E+00	1.239E-02
KOH	5.0000E-03	1.1903E-02	9.197E-03	1.00E+00	9.197E-03
CaCO3	0.0000E+00	5.5502E-03	4.288E-03	1.00E+00	4.288E-03
FeO	0.0000E+00	2.2586E-03	1.745E-03	1.00E+00	1.745E-03
Fe3O4	0.0000E+00	1.6071E-03	1.242E-03	1.00E+00	1.242E-03
H2O	9.8000E-02	1.1831E-03	9.141E-04	1.00E+00	9.141E-04
NaOH	0.0000E+00	1.1462E-03	8.856E-04	1.00E+00	8.856E-04
HgO2	0.0000E+00	6.8575E-04	5.299E-04	1.00E+00	5.299E-04
U3O8	0.0000E+00	6.6660E-04	5.151E-04	1.00E+00	5.151E-04
PbO	0.0000E+00	3.8995E-04	3.013E-04	1.00E+00	3.013E-04
Na2CO3	0.0000E+00	3.6103E-04	2.790E-04	1.00E+00	2.790E-04
KO2	0.0000E+00	2.9064E-04	2.246E-04	1.00E+00	2.246E-04
Ca(OH)2	4.0000E-03	2.1446E-04	1.657E-04	1.00E+00	1.657E-04
KNO3	8.0000E-03	1.0443E-04	8.069E-05	1.00E+00	8.069E-05
NaO2	0.0000E+00	3.6214E-06	2.798E-06	1.00E+00	2.798E-06
NaHCO3	1.4000E-02	2.3631E-06	1.826E-06	1.00E+00	1.826E-06
Hg(OH)2	5.0000E-03	6.1363E-07	4.741E-07	1.00E+00	4.741E-07
PbO2	0.0000E+00	5.2342E-07	4.044E-07	1.00E+00	4.044E-07
HgCO3	0.0000E+00	4.0036E-07	3.093E-07	1.00E+00	3.093E-07
UO3	0.0000E+00	1.1950E-07	9.234E-08	1.00E+00	9.234E-08

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Pb	4.0000E-04	9.5770E-008	7.400E-08	1.00E+00	7.400E-08
UO3 (G)	0.0000E+00	6.4554E-008	4.988E-08	1.00E+00	4.988E-08
K2O2	0.0000E+00	1.2103E-008	9.352E-09	1.00E+00	9.352E-09
PbCO3	0.0000E+00	1.1444E-008	9.075E-09	1.00E+00	9.075E-09
K	0.0000E+00	9.1909E-009	7.101E-09	1.00E+00	7.101E-09
K2O3	0.0000E+00	5.6712E-009	4.382E-09	1.00E+00	4.382E-09
Na2O	1.4000E-02	4.6043E-009	3.558E-09	1.00E+00	3.558E-09
NaHCO3	0.0000E+00	3.7954E-009	2.933E-09	1.00E+00	2.933E-09
UO2	2.0000E-03	3.5782E-009	2.765E-09	1.00E+00	2.765E-09
Na2O2	0.0000E+00	2.6270E-009	2.030E-09	1.00E+00	2.030E-09
Fe(OH)2	0.0000E+00	1.3930E-009	1.076E-09	1.00E+00	1.076E-09
Na	0.0000E+00	1.0916E-009	8.434E-10	1.00E+00	8.434E-10
Al(OH)3	6.0000E-03	5.1636E-010	3.990E-10	1.00E+00	3.990E-10
FeCO3	0.0000E+00	2.5943E-010	2.005E-10	1.00E+00	2.005E-10
K2O	3.6000E-02	1.9932E-010	1.540E-10	1.00E+00	1.540E-10
KO3	0.0000E+00	1.7735E-010	1.370E-10	1.00E+00	1.370E-10
Fe	2.4300E-01	7.1513E-011	5.526E-11	1.00E+00	5.526E-11
Fe(OH)3	4.0000E-03	2.4673E-011	1.906E-11	1.00E+00	1.906E-11
HNO3	0.0000E+00	1.1371E-012	8.786E-13	1.00E+00	8.786E-13
Na3UO4	0.0000E+00	3.6120E-013	2.791E-13	1.00E+00	2.791E-13
Pb3O4	0.0000E+00	2.6002E-013	2.009E-13	1.00E+00	2.009E-13
KH	0.0000E+00	1.3443E-014	1.039E-14	1.00E+00	1.039E-14
NaNH	0.0000E+00	1.8568E-015	1.435E-15	1.00E+00	1.435E-15
Ca(NO3)2	0.0000E+00	1.7627E-015	1.362E-15	1.00E+00	1.362E-15
N2O4	0.0000E+00	2.9036E-016	2.243E-16	1.00E+00	2.243E-16
C	1.0120E+00	2.6776E-017	2.069E-17	1.00E+00	2.069E-17
HCOOH	0.0000E+00	1.8786E-018	1.452E-18	1.00E+00	1.452E-18
HC2OH	0.0000E+00	1.5957E-018	1.233E-18	1.00E+00	1.233E-18
Mg	0.0000E+00	1.3391E-020	1.035E-20	1.00E+00	1.035E-20
U3O8	0.0000E+00	5.1614E-021	3.988E-21	1.00E+00	3.988E-21
Ca	0.0000E+00	4.0077E-021	3.097E-21	1.00E+00	3.097E-21
Hg(NO3)2	0.0000E+00	1.7346E-021	1.340E-21	1.00E+00	1.340E-21
KCN	0.0000E+00	3.7667E-022	2.910E-22	1.00E+00	2.910E-22
NH4OH	0.0000E+00	3.2593E-022	2.518E-22	1.00E+00	2.518E-22
NaN3	0.0000E+00	3.9351E-023	3.041E-23	1.00E+00	3.041E-23
Pb(NO3)2	0.0000E+00	2.1503E-023	1.662E-23	1.00E+00	1.662E-23
NaCN	0.0000E+00	1.0636E-023	8.218E-24	1.00E+00	8.218E-24
N2O5	0.0000E+00	1.8492E-024	1.429E-24	1.00E+00	1.429E-24
Al	3.6000E-02	1.8694E-026	1.444E-26	1.00E+00	1.444E-26
UO	0.0000E+00	1.4995E-026	1.159E-26	1.00E+00	1.159E-26
Si	0.0000E+00	3.1467E-028	2.431E-28	1.00E+00	2.431E-28
CaH2	0.0000E+00	6.2002E-029	4.791E-29	1.00E+00	4.791E-29
NH4NO3	0.0000E+00	7.5334E-031	5.821E-31	1.00E+00	5.821E-31
U4O9	0.0000E+00	3.1245E-031	2.414E-31	1.00E+00	2.414E-31
N2H4	0.0000E+00	2.9920E-034	2.312E-34	1.00E+00	2.312E-34
UN	0.0000E+00	1.2402E-035	9.583E-36	1.00E+00	9.583E-36
CH3OH	0.0000E+00	1.8971E-036	1.466E-36	1.00E+00	1.466E-36
U	0.0000E+00	9.8903E-044	7.707E-44	1.00E+00	7.707E-44
Ca3N2	0.0000E+00	6.1957E-054	0.000E+00	1.00E+00	0.000E+00
UC	0.0000E+00	3.9479E-056	0.000E+00	1.00E+00	0.000E+00
UH3	0.0000E+00	8.3133E-061	0.000E+00	1.00E+00	0.000E+00
UF6	0.0000E+00	1.8189E-063	0.000E+00	1.00E+00	0.000E+00
C2H6O	0.0000E+00	2.6923E-065	0.000E+00	1.00E+00	0.000E+00
Si3N4	0.0000E+00	8.8205E-069	0.000E+00	1.00E+00	0.000E+00
UC2	0.0000E+00	2.9899E-071	0.000E+00	1.00E+00	0.000E+00
Fe(CO)5	0.0000E+00	6.3628E-074	0.000E+00	1.00E+00	0.000E+00
Si2H6	0.0000E+00	1.0558E-091	0.000E+00	1.00E+00	0.000E+00
U2C3	0.0000E+00	3.2911E-128	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.2942E+000	1.000E+00		

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Temperature: 1399.15 K
Pressure: 1 bar
Volume: 1.693E-01 m3 (NPT)
Reaction enthalpy: -3.470E+02 kJ
Reaction entropy: 4.969E+02 J/K
Iterations: 80 (Limit = 80)

INPUT AMOUNT EQUIL AMOUNT MOLE FRACTION ACTIVITY ACTIVITY
mol mol EFFICIENCY
PHASE 1:
O2(g) 7.1550E+00 5.4692E+00 7.242E-01 1.00E+00 7.242E-01
H2O(g) 0.0000E+00 1.0529E+00 1.394E-01 1.00E+00 1.394E-01
CO2(g) 0.0000E+00 9.8660E-01 1.306E-01 1.00E+00 1.306E-01
NO(g) 0.0000E+00 2.1690E-02 2.872E-03 1.00E+00 2.872E-03
KOH(g) 0.0000E+00 2.1600E-02 2.860E-03 1.00E+00 2.860E-03
H2(g) 0.0000E+00 2.8632E-04 3.791E-05 1.00E+00 3.791E-05
NaOH(g) 0.0000E+00 1.8077E-04 2.394E-05 1.00E+00 2.394E-05
PbO(g) 0.0000E+00 3.7054E-05 4.906E-06 1.00E+00 4.906E-06
K(g) 0.0000E+00 4.2877E-06 5.677E-07 1.00E+00 5.677E-07
CO(g) 0.0000E+00 1.1151E-06 1.477E-07 1.00E+00 1.477E-07
XO(g) 0.0000E+00 9.1391E-07 1.210E-07 1.00E+00 1.210E-07
H2(g) 9.5000E-01 5.4298E-07 7.189E-08 1.00E+00 7.189E-08
Na(g) 0.0000E+00 2.1122E-07 2.797E-08 1.00E+00 2.797E-08
Ca(OH)2(g) 0.0000E+00 9.989E-08 5.283E-09 1.00E+00 5.283E-09
Pb(g) 0.0000E+00 1.4549E-08 1.926E-09 1.00E+00 1.926E-09
NO3(g) 0.0000E+00 2.4499E-10 3.244E-11 1.00E+00 3.244E-11
FeO(g) 0.0000E+00 4.2654E-13 5.648E-14 1.00E+00 5.648E-14
SiO2(g) 0.0000E+00 1.7654E-13 2.338E-14 1.00E+00 2.338E-14
N(g) 0.0000E+00 4.9098E-14 6.501E-15 1.00E+00 6.501E-15
MgO(g) 0.0000E+00 2.5216E-14 3.339E-15 1.00E+00 3.339E-15
H3(g) 0.0000E+00 2.1676E-14 2.870E-15 1.00E+00 2.870E-15
H2O(g) 0.0000E+00 9.2549E-15 1.225E-15 1.00E+00 1.225E-15
NH2(g) 0.0000E+00 7.8868E-16 1.044E-16 1.00E+00 1.044E-16
NH(g) 0.0000E+00 3.3639E-16 4.454E-17 1.00E+00 4.454E-17
AlO2(g) 0.0000E+00 3.0689E-16 4.063E-17 1.00E+00 4.063E-17
Fe(g) 0.0000E+00 1.0028E-16 1.328E-17 1.00E+00 1.328E-17
SiO(g) 0.0000E+00 9.6964E-17 1.284E-17 1.00E+00 1.284E-17
CaO(g) 0.0000E+00 6.5108E-18 8.621E-19 1.00E+00 8.621E-19
Hg(g) 0.0000E+00 5.8819E-18 7.789E-19 1.00E+00 7.789E-19
Ca(g) 0.0000E+00 1.0811E-19 1.431E-20 1.00E+00 1.431E-20
HCl(g) 0.0000E+00 4.8689E-22 6.447E-23 1.00E+00 6.447E-23
AlO(g) 0.0000E+00 1.0347E-22 1.370E-23 1.00E+00 1.370E-23
Al(g) 0.0000E+00 8.4590E-29 1.120E-29 1.00E+00 1.120E-29
CH3OH(g) 0.0000E+00 3.1039E-30 4.110E-31 1.00E+00 4.110E-31
CH3(g) 0.0000E+00 4.7663E-32 6.311E-33 1.00E+00 6.311E-33
CH4(g) 0.0000E+00 4.7614E-32 6.304E-33 1.00E+00 6.304E-33
Al2O2(g) 0.0000E+00 1.3042E-32 1.727E-33 1.00E+00 1.727E-33
C(g) 0.0000E+00 5.4888E-34 7.268E-35 1.00E+00 7.268E-35
Si(g) 0.0000E+00 5.3145E-34 7.037E-35 1.00E+00 7.037E-35
CH2(g) 0.0000E+00 2.6641E-35 3.527E-36 1.00E+00 3.527E-36
Al2O(g) 0.0000E+00 8.0955E-38 1.072E-38 1.00E+00 1.072E-38
C2H2(g) 0.0000E+00 1.2788E-43 1.682E-44 1.00E+00 1.682E-44
C2H4(g) 0.0000E+00 7.5168E-51 0.000E+00 1.00E+00 0.000E+00
U(g) 0.0000E+00 1.2215E-51 0.000E+00 1.00E+00 0.000E+00
C2H6(g) 0.0000E+00 1.1333E-59 0.000E+00 1.00E+00 0.000E+00
Total: 8.1050E+00 7.5524E+00 1.000E+00

PHASE 2:
CaO 4.9000E-01 4.7676E-01 3.696E-01 1.00E+00 3.696E-01
SiO2 4.6900E-01 4.6900E-01 3.636E-01 1.00E+00 3.636E-01
Fe2O3 6.0000E-01 1.0175E-01 7.887E-02 1.00E+00 7.887E-02
Al2O3 7.8000E-02 9.9000E-02 7.674E-02 1.00E+00 7.674E-02
NaFeO2 0.0000E+00 4.0179E-02 3.115E-02 1.00E+00 3.115E-02
MgO 2.8000E-02 3.2429E-02 2.514E-02 1.00E+00 2.514E-02
K2CO3 0.0000E+00 2.3278E-02 1.804E-02 1.00E+00 1.804E-02
KOH 5.0000E-03 1.6348E-02 1.267E-02 1.00E+00 1.267E-02
CaO2 0.0000E+00 1.5193E-02 1.178E-02 1.00E+00 1.178E-02
FeO 0.0000E+00 5.3829E-03 4.173E-03 1.00E+00 4.173E-03
Fe3O4 0.0000E+00 3.3153E-03 2.570E-03 1.00E+00 2.570E-03
CaCO3 0.0000E+00 1.9257E-03 1.493E-03 1.00E+00 1.493E-03
H2O 9.8000E-02 1.8208E-03 1.411E-03 1.00E+00 1.411E-03
NaOH 0.0000E+00 1.2493E-03 9.684E-04 1.00E+00 9.684E-04
U3O8 0.0000E+00 6.6662E-04 5.167E-04 1.00E+00 5.167E-04
MgO2 0.0000E+00 5.7024E-04 4.420E-04 1.00E+00 4.420E-04
K2O 0.0000E+00 4.6800E-04 3.628E-04 1.00E+00 3.628E-04
PbO 0.0000E+00 3.214E-04 2.809E-04 1.00E+00 2.809E-04
Na2CO3 0.0000E+00 1.9234E-04 1.491E-04 1.00E+00 1.491E-04
Ca(OH)2 4.0000E-03 1.1815E-04 9.159E-05 1.00E+00 9.159E-05
KH2PO4 8.0000E-03 2.3026E-05 1.785E-05 1.00E+00 1.785E-05
Na2O 0.0000E+00 5.2280E-06 4.053E-06 1.00E+00 4.053E-06
NaNO3 1.4000E-02 6.1591E-07 4.774E-07 1.00E+00 4.774E-07
Mg(OH)2 5.0000E-03 4.7990E-07 3.720E-07 1.00E+00 3.720E-07
Pb 4.0000E-04 3.0115E-07 2.334E-07 1.00E+00 2.334E-07
PbO2 0.0000E+00 2.8289E-07 2.193E-07 1.00E+00 2.193E-07
HgCO3 0.0000E+00 2.1956E-07 1.702E-07 1.00E+00 1.702E-07

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UO3 0.0000E+00 7.9776E-08 6.186E-08 1.00E+00 6.186E-08
K 0.0000E+00 7.4560E-08 5.780E-08 1.00E+00 5.780E-08
UO3(G) 0.0000E+00 4.3837E-08 3.398E-08 1.00E+00 3.398E-08
K2O2 0.0000E+00 3.6826E-08 2.855E-08 1.00E+00 2.855E-08
Na2O 1.4000E-02 1.5075E-08 1.169E-08 1.00E+00 1.169E-08
K2O3 0.0000E+00 1.2855E-08 9.965E-09 1.00E+00 9.965E-09
Na 0.0000E+00 7.3157E-09 5.671E-09 1.00E+00 5.671E-09
PbCO3 0.0000E+00 6.9916E-09 5.420E-09 1.00E+00 5.420E-09
UO2 2.0000E-03 6.2788E-09 4.867E-09 1.00E+00 4.867E-09
Na2O2 0.0000E+00 4.4367E-09 3.439E-09 1.00E+00 3.439E-09
Fe(OH)2 0.0000E+00 2.5333E-09 1.964E-09 1.00E+00 1.964E-09
NaHCO3 0.0000E+00 2.1082E-09 1.634E-09 1.00E+00 1.634E-09
K2O 3.6000E-02 1.4482E-09 1.123E-09 1.00E+00 1.123E-09
Fe 2.4300E-01 1.0236E-09 7.935E-10 1.00E+00 7.935E-10
Al(OH)3 6.0000E-03 5.2769E-10 4.090E-10 1.00E+00 4.090E-10
FeCO3 0.0000E+00 4.8108E-10 3.745E-10 1.00E+00 3.745E-10
K3 0.0000E+00 2.9824E-10 2.312E-10 1.00E+00 2.312E-10
Fe(OH)3 4.0000E-03 1.8685E-11 1.448E-11 1.00E+00 1.448E-11
HNO3 0.0000E+00 4.9218E-13 3.815E-13 1.00E+00 3.815E-13
Na3UO4 0.0000E+00 4.2850E-13 3.322E-13 1.00E+00 3.322E-13
KH 0.0000E+00 1.8197E-13 1.411E-13 1.00E+00 1.411E-13
Pb3O4 0.0000E+00 8.5347E-14 6.616E-14 1.00E+00 6.616E-14
NaH 0.0000E+00 2.1489E-14 1.666E-14 1.00E+00 1.666E-14
C 0.0120E+00 3.7401E-16 2.899E-16 1.00E+00 2.899E-16
N2O4 0.0000E+00 1.9406E-16 1.504E-16 1.00E+00 1.504E-16
Ca(NO3)2 0.0000E+00 1.2618E-16 9.781E-17 1.00E+00 9.781E-17
HCO2H 0.0000E+00 9.1284E-18 7.076E-18 1.00E+00 7.076E-18
HCOOH 0.0000E+00 7.8601E-18 6.093E-18 1.00E+00 6.093E-18
Mg 0.0000E+00 7.5781E-19 5.874E-19 1.00E+00 5.874E-19
Ca 0.0000E+00 2.8257E-19 2.190E-19 1.00E+00 2.190E-19
U 0.0000E+00 1.2594E-20 9.763E-21 1.00E+00 9.763E-21
U3O8 0.0000E+00 3.9016E-21 3.024E-21 1.00E+00 3.024E-21
NH4OH 0.0000E+00 1.3880E-21 1.076E-21 1.00E+00 1.076E-21
Hg(NO3)2 0.0000E+00 3.6949E-22 2.864E-22 1.00E+00 2.864E-22
NaCl 0.0000E+00 3.3826E-22 2.622E-22 1.00E+00 2.622E-22
NaN3 0.0000E+00 5.1673E-23 4.006E-23 1.00E+00 4.006E-23
Al 3.6000E-02 5.0487E-24 3.914E-24 1.00E+00 3.914E-24
Pb(NO3)2 0.0000E+00 9.4107E-25 7.295E-25 1.00E+00 7.295E-25
UO 0.0000E+00 8.4773E-25 6.571E-25 1.00E+00 6.571E-25
N2O5 0.0000E+00 5.1284E-25 3.975E-25 1.00E+00 3.975E-25
Si 0.0000E+00 1.2312E-25 9.544E-26 1.00E+00 9.544E-26
CaH2 0.0000E+00 5.6888E-27 4.410E-27 1.00E+00 4.410E-27
U4O9 0.0000E+00 1.1440E-30 8.868E-31 1.00E+00 8.868E-31
NH4NO3 0.0000E+00 6.7060E-31 5.198E-31 1.00E+00 5.198E-31
N2H4 0.0000E+00 3.6389E-33 2.821E-33 1.00E+00 2.821E-33
UN 0.0000E+00 2.1723E-33 1.684E-33 1.00E+00 1.684E-33
CH3OH 0.0000E+00 1.3228E-34 1.025E-34 1.00E+00 1.025E-34
U 0.0000E+00 2.2470E-40 1.742E-40 1.00E+00 1.742E-40
Ca3N2 0.0000E+00 3.4178E-50 0.000E+00 1.00E+00 0.000E+00
UC 0.0000E+00 6.4544E-52 0.000E+00 1.00E+00 0.000E+00
UH3 0.0000E+00 8.1505E-57 0.000E+00 1.00E+00 0.000E+00
UFe2 0.0000E+00 5.6581E-58 0.000E+00 1.00E+00 0.000E+00
C2H6O 0.0000E+00 9.2215E-62 0.000E+00 1.00E+00 0.000E+00
Si3H4 0.0000E+00 3.7232E-64 0.000E+00 1.00E+00 0.000E+00
UC2 0.0000E+00 1.0818E-06 0.000E+00 1.00E+00 0.000E+00
Fe(CO)5 0.0000E+00 3.6754E-06 0.000E+00 1.00E+00 0.000E+00
Si2H6 0.0000E+00 3.5299E-08 0.000E+00 1.00E+00 0.000E+00
U2C3 0.0000E+00 1.2795E-118 0.000E+00 1.00E+00 0.000E+00
Total: 2.5584E+00 1.2900E+00 1.000E+00

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Temperature 1498.15 K
 Pressure 1 bar
 Volume 1.699E-01 m³ (NPT)
 Reaction enthalpy -2.988E+02 kJ
 Reaction entropy 5.292E+02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol		COEFFICIENT	
O ₂ (g)	7.1550E+00	5.4717E+00	7.217E 01	1.00E+00	7.217E 01
H ₂ O(g)	1.0383E+00	1.369E 01	1.369E 01	1.00E+00	1.369E 01
CO ₂ (g)	1.0011E+00	1.320E 01	1.320E 01	1.00E+00	1.320E 01
KOH(g)	0.0000E+00	4.8138E+02	6.349E 03	1.00E+00	6.349E 03
NO(g)	0.0000E+00	2.1789E+02	2.874E 03	1.00E+00	2.874E 03
NaOH(g)	0.0000E+00	5.7906E+04	7.637E 05	1.00E+00	7.637E 05
NO ₂ (g)	0.0000E+00	2.0587E+04	2.715E 05	1.00E+00	2.715E 05
PbO(g)	0.0000E+00	1.0439E+04	1.377E 05	1.00E+00	1.377E 05
K(g)	0.0000E+00	3.0804E+05	4.063E 06	1.00E+00	4.063E 06
KO(g)	0.0000E+00	5.9180E+06	7.805E 07	1.00E+00	7.805E 07
CO(g)	0.0000E+00	5.7041E+06	7.523E 07	1.00E+00	7.523E 07
H ₂ (g)	9.5000E-01	2.2547E+06	2.974E 07	1.00E+00	2.974E 07
Na(g)	0.0000E+00	1.9115E+06	2.521E 07	1.00E+00	2.521E 07
Ca(OH) ₂ (g)	0.0000E+00	1.7988E+07	2.372E 08	1.00E+00	2.372E 08
Pb(g)	0.0000E+00	9.6705E+08	1.275E 08	1.00E+00	1.275E 08
NO ₃ (g)	0.0000E+00	2.2677E+10	2.991E 11	1.00E+00	2.991E 11
FeO(g)	0.0000E+00	1.5704E+11	2.071E 12	1.00E+00	2.071E 12
SiO ₂ (g)	0.0000E+00	5.3027E+12	6.994E 13	1.00E+00	6.994E 13
HgO(g)	0.0000E+00	7.6016E+13	1.003E 13	1.00E+00	1.003E 13
N(g)	0.0000E+00	4.5804E+13	6.041E 14	1.00E+00	6.041E 14
HgOH(g)	0.0000E+00	2.1663E+13	2.857E 14	1.00E+00	2.857E 14
NH ₃ (g)	0.0000E+00	7.9048E+14	1.043E 14	1.00E+00	1.043E 14
Al ₂ O ₃ (g)	0.0000E+00	1.2417E+14	1.638E 15	1.00E+00	1.638E 15
Fe(g)	0.0000E+00	9.5416E+15	1.258E 15	1.00E+00	1.258E 15
SiO(g)	0.0000E+00	9.2012E+15	5.214E 15	1.00E+00	5.214E 15
NH ₂ (g)	0.0000E+00	5.6249E+15	7.419E 16	1.00E+00	7.419E 16
NH(g)	0.0000E+00	3.5568E+15	4.691E 16	1.00E+00	4.691E 16
Hg(g)	0.0000E+00	4.0589E+16	5.353E 17	1.00E+00	5.353E 17
CnO(g)	0.0000E+00	3.5099E+16	4.629E 17	1.00E+00	4.629E 17
Ca(g)	0.0000E+00	1.0634E+17	1.403E 18	1.00E+00	1.403E 18
AlO(g)	0.0000E+00	1.9504E+17	2.572E 21	1.00E+00	2.572E 21
HCl(g)	0.0000E+00	1.2552E+17	1.652E 21	1.00E+00	1.652E 21
Al(g)	0.0000E+00	6.2847E+17	8.289E 27	1.00E+00	8.289E 27
CH ₃ OH(g)	0.0000E+00	1.4774E+18	1.949E 29	1.00E+00	1.949E 29
Al ₂ O ₃ (g)	0.0000E+00	1.6146E+19	2.130E 30	1.00E+00	2.130E 30
CH ₃ (g)	0.0000E+00	8.1052E+19	1.069E 30	1.00E+00	1.069E 30
CH ₄ (g)	0.0000E+00	4.7588E+19	6.276E 31	1.00E+00	6.276E 31
Si(g)	0.0000E+00	1.2230E+19	1.613E 31	1.00E+00	1.613E 31
C(g)	0.0000E+00	3.3717E+19	4.450E 32	1.00E+00	4.450E 32
KOH(g)	0.0000E+00	1.0331E+19	1.363E 33	1.00E+00	1.363E 33
Al ₂ O ₃ (g)	0.0000E+00	4.5912E+19	6.055E 35	1.00E+00	6.055E 35
C ₂ H ₂ (g)	0.0000E+00	1.8559E+19	2.448E 41	1.00E+00	2.448E 41
U(g)	0.0000E+00	1.5745E+19	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₄ (g)	0.0000E+00	1.5608E+19	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ (g)	0.0000E+00	4.2399E+19	0.000E+00	1.00E+00	0.000E+00
Total 1:	8.1050E+00	7.5819E+00	1.000E+00		

PHASE 2:	MOLE FRACTION	ACTIVITY	ACTIVITY
CaO	4.9000E-01	4.7865E-001	3.742E-01
SiO ₂	4.6900E-01	3.666E-01	1.00E+00
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.739E-02
Fe ₂ O ₃	6.0000E-03	9.5107E-002	7.434E-02
NaFeO ₂	0.0000E+00	3.9827E-002	3.113E-02
HgO	2.8000E-02	3.2516E-002	2.542E-02
KOH	5.0000E-03	1.6232E-002	1.269E-02
CaO ₂	0.0000E+00	1.4499E-002	1.133E-02
FeO	0.0000E+00	1.1214E-002	8.766E-03
K ₂ CO ₃	0.0000E+00	1.0024E-002	7.836E-03
Fe ₃ O ₄	0.0000E+00	5.9151E-003	4.624E-03
H ₂ O	9.8000E-02	2.9922E-003	2.339E-03
NaOH	0.0000E+00	1.3541E-003	1.058E-03
CaCO ₃	0.0000E+00	7.7651E-004	6.070E-04
U ₃ O ₈	0.0000E+00	6.6661E-004	5.211E-04
K ₂ O	0.0000E+00	5.3916E-004	4.215E-04
HgO ₂	0.0000E+00	4.8374E-004	3.781E-04
PbO	0.0000E+00	2.9467E-004	2.303E-04
Na ₂ CO ₃	0.0000E+00	1.1505E-004	8.993E-05
Ca(OH) ₂	4.0000E-03	7.0487E-005	5.510E-05
Na ₂ O	0.0000E+00	5.766E-006	5.766E-06
K ₂ O	0.0000E+00	4.6724E-006	3.653E-06
Pb	4.0000E-04	6.9766E-007	5.454E-07
Hg(OH) ₂	5.0000E-03	4.0593E-007	3.173E-07
K	0.0000E+00	3.4212E-007	2.674E-07
NaHCO ₃	1.4000E-02	1.9624E-007	1.531E-07
PbO ₂	0.0000E+00	1.4344E-007	1.121E-07

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MgCO ₃	0.0000E+00	1.3420E-007	1.049E-07	1.00E+00	1.049E-07
K ₂ O ₂	0.0000E+00	5.6243E-008	4.396E-08	1.00E+00	4.396E-08
UO ₃	0.0000E+00	5.5273E-008	4.321E-08	1.00E+00	4.321E-08
Na ₂ O	1.4000E-02	5.5000E-008	4.299E-08	1.00E+00	4.299E-08
Na	0.0000E+00	3.7958E-008	2.967E-08	1.00E+00	2.967E-08
UO ₃ (G)	0.0000E+00	3.0428E-008	2.378E-08	1.00E+00	2.378E-08
K ₂ O ₃	0.0000E+00	1.4956E-008	1.169E-08	1.00E+00	1.169E-08
UO ₂	2.0000E-03	1.0055E-008	7.860E-09	1.00E+00	7.860E-09
Fe	2.4300E-01	1.0036E-008	7.845E-09	1.00E+00	7.845E-09
Na ₂ O ₂	0.0000E+00	7.0468E-009	5.508E-09	1.00E+00	5.508E-09
K ₂ O	3.6000E-02	4.5953E-009	3.592E-09	1.00E+00	3.592E-09
Fe(OH) ₂	0.0000E+00	4.1864E-009	3.272E-09	1.00E+00	3.272E-09
PbCO ₃	0.0000E+00	4.0938E-009	3.200E-09	1.00E+00	3.200E-09
NaHCO ₃	0.0000E+00	1.3552E-009	1.059E-09	1.00E+00	1.059E-09
FeCO ₃	0.0000E+00	8.5463E-010	6.680E-10	1.00E+00	6.680E-10
Al(OH) ₃	6.0000E-03	5.9177E-010	4.626E-10	1.00E+00	4.626E-10
K ₂ O	0.0000E+00	3.5912E-010	2.807E-10	1.00E+00	2.807E-10
Fe(OH) ₃	4.0000E-03	1.4542E-011	1.137E-11	1.00E+00	1.137E-11
KH	0.0000E+00	1.3203E-012	1.032E-12	1.00E+00	1.032E-12
Na ₃ UO ₄	0.0000E+00	4.9443E-013	3.865E-13	1.00E+00	3.865E-13
NH ₃	0.0000E+00	2.3345E-013	1.825E-13	1.00E+00	1.825E-13
NaH	0.0000E+00	1.8288E-013	1.430E-13	1.00E+00	1.430E-13
Pb ₃ O ₄	0.0000E+00	2.1540E-014	1.684E-14	1.00E+00	1.684E-14
C	1.0120E+00	3.6685E-015	2.868E-15	1.00E+00	2.868E-15
N ₂ O ₄	0.0000E+00	1.5251E-016	1.192E-16	1.00E+00	1.192E-16
HCO ₂ H	0.0000E+00	3.5834E-017	2.801E-17	1.00E+00	2.801E-17
HCCOH	0.0000E+00	3.1223E-017	2.441E-17	1.00E+00	2.441E-17
Hg	0.0000E+00	2.4999E-017	1.954E-17	1.00E+00	1.954E-17
Ca(NO ₃) ₂	0.0000E+00	1.3809E-017	1.079E-17	1.00E+00	1.079E-17
Ca	0.0000E+00	1.1194E-017	8.750E-18	1.00E+00	8.750E-18
KCN	0.0000E+00	1.9751E-019	1.544E-19	1.00E+00	1.544E-19
NaCN	0.0000E+00	6.7884E-021	5.306E-21	1.00E+00	5.306E-21
NH ₄ OH	0.0000E+00	4.8825E-021	3.817E-21	1.00E+00	3.817E-21
U ₃ O ₈	0.0000E+00	2.9923E-021	2.339E-21	1.00E+00	2.339E-21
Al	3.6000E-02	6.4219E-022	5.020E-22	1.00E+00	5.020E-22
Mg(NO ₃) ₂	0.0000E+00	1.1235E-022	8.782E-23	1.00E+00	8.782E-23
Na ₃ N	0.0000E+00	6.4240E-023	5.022E-23	1.00E+00	5.022E-23
UO	0.0000E+00	2.7259E-023	2.131E-23	1.00E+00	2.131E-23
Si	0.0000E+00	2.1643E-023	1.692E-23	1.00E+00	1.692E-23
CaH ₂	0.0000E+00	2.8249E-025	2.208E-25	1.00E+00	2.208E-25
N ₂ O ₅	0.0000E+00	1.6741E-025	1.309E-25	1.00E+00	1.309E-25
Pb(NO ₃) ₂	0.0000E+00	5.2369E-026	4.094E-26	1.00E+00	4.094E-26
U ₄ O ₉	0.0000E+00	3.4081E-030	2.664E-30	1.00E+00	2.664E-30
NH ₄ NO ₃	0.0000E+00	5.9430E-031	4.646E-31	1.00E+00	4.646E-31
UN	0.0000E+00	1.6634E-031	1.457E-31	1.00E+00	1.457E-31
N ₂ H ₄	0.0000E+00	3.1027E-032	2.425E-32	1.00E+00	2.425E-32
CH ₃ OH	0.0000E+00	5.1123E-033	3.996E-33	1.00E+00	3.996E-33
U	0.0000E+00	1.8642E-037	1.457E-37	1.00E+00	1.457E-37
Ca ₃ N ₂	0.0000E+00	5.9530E-047	0.000E+00	1.00E+00	0.000E+00
UC	0.0000E+00	2.8422E-048	0.000E+00	1.00E+00	0.000E+00
UFe ₂	0.0000E+00	3.3705E-053	0.000E+00	1.00E+00	0.000E+00
UH ₃	0.0000E+00	2.2807E-053	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	1.0261E-058	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	3.7723E-060	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	7.2155E-061	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	4.8750E-065	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	1.1569E-077	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	2.5285E-110	0.000E+00	1.00E+00	0.000E+00
Total 1:	2.5584E+00	1.2793E+000	1.000E+00		

A-28

Temperature 1598.15 K
 Pressure 1 bar
 Volume 1.704E-01 m³ (NPT)
 Reaction enthalpy 2.513E-02 kJ
 Reaction entropy 5.592E-02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol			
O ₂ (g)	7.1550E+00	5.4755E+00	1.200E-01	1.00E+00	1.200E-01
H ₂ O(g)	0.0000E+00	1.0279E+00	1.352E-01	1.00E+00	1.352E-01
CO ₂ (g)	0.0000E+00	1.0091E+00	1.327E-01	1.00E+00	1.327E-01
KOH(g)	0.0000E+00	6.7993E-02	8.941E-03	1.00E+00	8.941E-03
NO(g)	0.0000E+00	2.1845E-02	2.871E-03	1.00E+00	2.871E-03
NaOH(g)	0.0000E+00	1.5945E-03	2.097E-04	1.00E+00	2.097E-04
PbO(g)	0.0000E+00	2.0257E-04	2.664E-05	1.00E+00	2.664E-05
NO ₂ (g)	0.0000E+00	1.5423E-04	2.028E-05	1.00E+00	2.028E-05
K(g)	0.0000E+00	1.2109E-04	1.592E-05	1.00E+00	1.592E-05
CO(g)	0.0000E+00	2.3611E-05	3.105E-06	1.00E+00	3.105E-06
KO(g)	0.0000E+00	2.1246E-05	2.794E-06	1.00E+00	2.794E-06
Na(g)	0.0000E+00	1.3015E-05	1.712E-06	1.00E+00	1.712E-06
H ₂ (g)	9.5000E-01	7.8622E-06	1.034E-06	1.00E+00	1.034E-06
Ca(OH) ₂ (g)	0.0000E+00	6.6909E-07	8.799E-08	1.00E+00	8.799E-08
FeO(g)	0.0000E+00	3.9799E-07	5.234E-08	1.00E+00	5.234E-08
Fe ₂ O ₃ (g)	0.0000E+00	3.5540E-10	4.674E-11	1.00E+00	4.674E-11
NO ₃ (g)	0.0000E+00	2.1263E-10	2.796E-11	1.00E+00	2.796E-11
SiO ₂ (g)	0.0000E+00	1.0321E-10	1.357E-11	1.00E+00	1.357E-11
MgO(g)	0.0000E+00	1.4810E-11	1.948E-12	1.00E+00	1.948E-12
MgOH(g)	0.0000E+00	3.3949E-12	4.465E-13	1.00E+00	4.465E-13
N(g)	0.0000E+00	3.2101E-12	4.249E-13	1.00E+00	4.249E-13
Fe(g)	0.0000E+00	4.9733E-13	6.540E-14	1.00E+00	6.540E-14
Si(g)	0.0000E+00	4.8844E-13	6.421E-14	1.00E+00	6.421E-14
Al ₂ O ₃ (g)	0.0000E+00	3.1362E-13	4.124E-14	1.00E+00	4.124E-14
NH ₃ (g)	0.0000E+00	2.4617E-13	3.237E-14	1.00E+00	3.237E-14
NH ₂ (g)	0.0000E+00	3.1420E-14	4.137E-15	1.00E+00	4.137E-15
NH(g)	0.0000E+00	2.8007E-14	3.683E-15	1.00E+00	3.683E-15
Mg(g)	0.0000E+00	1.6129E-14	2.147E-15	1.00E+00	2.147E-15
Ca(g)	0.0000E+00	1.1342E-14	1.492E-15	1.00E+00	1.492E-15
Al(g)	0.0000E+00	5.8185E-16	7.652E-17	1.00E+00	7.652E-17
NCH(g)	0.0000E+00	1.8871E-18	2.482E-19	1.00E+00	2.482E-19
Al(g)	0.0000E+00	2.1368E-19	2.810E-20	1.00E+00	2.810E-20
Al ₂ O ₃ (g)	0.0000E+00	2.0197E-23	2.656E-24	1.00E+00	2.656E-24
Al ₂ O ₃ (g)	0.0000E+00	8.0462E-27	1.058E-27	1.00E+00	1.058E-27
CH ₃ OH(g)	0.0000E+00	4.3371E-27	5.704E-28	1.00E+00	5.704E-28
Si(g)	0.0000E+00	1.0574E-27	1.391E-28	1.00E+00	1.391E-28
CH ₃ (g)	0.0000E+00	7.2554E-28	9.541E-29	1.00E+00	9.541E-29
CH ₄ (g)	0.0000E+00	2.6817E-28	3.527E-29	1.00E+00	3.527E-29
C(g)	0.0000E+00	9.2341E-29	1.214E-29	1.00E+00	1.214E-29
CH ₂ (g)	0.0000E+00	1.8969E-30	2.494E-31	1.00E+00	2.494E-31
Al ₂ O ₃ (g)	0.0000E+00	8.6361E-31	1.136E-31	1.00E+00	1.136E-31
C ₂ H ₂ (g)	0.0000E+00	1.0773E-37	1.417E-38	1.00E+00	1.417E-38
U(g)	0.0000E+00	6.1033E-44	8.408E-45	1.00E+00	8.408E-45
C ₂ H ₄ (g)	0.0000E+00	1.2528E-44	1.601E-45	1.00E+00	1.601E-45
C ₂ H ₆ (g)	0.0000E+00	5.6859E-53	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.6043E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol			
CaO	4.9000E-01	4.7964E-01	3.771E-01	1.00E+00	3.771E-01
SiO ₂	4.6900E-01	4.6900E-01	3.688E-01	1.00E+00	3.688E-01
Al ₂ O ₃	7.8000E-02	9.9000E-02	7.784E-02	1.00E+00	7.784E-02
Fe ₂ O ₃	6.0000E-03	8.5915E-02	6.755E-02	1.00E+00	6.755E-02
NaFeO ₂	0.0000E+00	3.8765E-02	3.048E-02	1.00E+00	3.048E-02
MgO	2.8000E-02	3.2582E-02	2.562E-02	1.00E+00	2.562E-02
FeO	0.0000E+00	2.0892E-02	1.642E-02	1.00E+00	1.642E-02
CaO ₂	0.0000E+00	1.3963E-02	1.098E-02	1.00E+00	1.098E-02
KOH	5.0000E-03	1.1504E-02	9.045E-03	1.00E+00	9.045E-03
Fe ₂ O ₄	0.0000E+00	9.1741E-03	7.213E-03	1.00E+00	7.213E-03
H ₂ O	9.0000E-02	5.3059E-03	4.172E-03	1.00E+00	4.172E-03
K ₂ CO ₃	0.0000E+00	2.4598E-03	1.934E-03	1.00E+00	1.934E-03
NaOH	0.0000E+00	1.4672E-03	1.154E-03	1.00E+00	1.154E-03
U ₃ O ₈	0.0000E+00	6.6664E-04	5.241E-04	1.00E+00	5.241E-04
K ₂ O	0.0000E+00	4.3854E-04	3.448E-04	1.00E+00	3.448E-04
MgO ₂	0.0000E+00	4.1770E-04	3.284E-04	1.00E+00	3.284E-04
CaCO ₃	0.0000E+00	3.5283E-04	2.774E-04	1.00E+00	2.774E-04
PbO	0.0000E+00	1.9582E-04	1.540E-04	1.00E+00	1.540E-04
Na ₂ CO ₃	0.0000E+00	7.4666E-05	5.871E-05	1.00E+00	5.871E-05
Ca(OH) ₂	4.0000E-03	4.5347E-05	3.565E-05	1.00E+00	3.565E-05
Na ₂ O	0.0000E+00	1.0210E-05	8.028E-06	1.00E+00	8.028E-06
Pb	4.0000E-04	1.141E-06	9.027E-07	1.00E+00	9.027E-07
K	0.0000E+00	9.1456E-07	7.191E-07	1.00E+00	7.191E-07
KNO ₃	8.0000E-03	8.2459E-07	6.483E-07	1.00E+00	6.483E-07
Mg(OH) ₂	5.0000E-03	3.6968E-07	2.907E-07	1.00E+00	2.907E-07
Na ₂ O	1.4000E-02	1.7500E-07	1.376E-07	1.00E+00	1.376E-07
Na	0.0000E+00	1.6013E-07	1.259E-07	1.00E+00	1.259E-07

MgCO ₃	0.0000E+00	8.9193E-08	7.011E-08	1.00E+00	7.011E-08
Na ₂ SiO ₃	1.4000E-02	7.1931E-08	5.813E-08	1.00E+00	5.813E-08
Fe	2.4100E-01	7.2113E-08	5.670E-08	1.00E+00	5.670E-08
PbO ₂	0.0000E+00	6.2927E-08	4.948E-08	1.00E+00	4.948E-08
K ₂ O ₇	0.0000E+00	4.1841E-08	3.290E-08	1.00E+00	3.290E-08
UO ₃	0.0000E+00	3.9700E-08	3.121E-08	1.00E+00	3.121E-08
UO ₃ (g)	0.0000E+00	2.1579E-08	1.697E-08	1.00E+00	1.697E-08
UO ₂	2.0000E-03	1.5031E-08	1.182E-08	1.00E+00	1.182E-08
Na ₂ O	0.0000E+00	1.0598E-08	8.333E-09	1.00E+00	8.333E-09
K ₂ O ₃	0.0000E+00	8.6248E-09	6.781E-09	1.00E+00	6.781E-09
Fe(OH) ₂	0.0000E+00	6.1259E-09	5.052E-09	1.00E+00	5.052E-09
K ₂ O	3.0000E-02	6.3357E-09	4.981E-09	1.00E+00	4.981E-09
PbCO ₃	0.0000E+00	2.1471E-09	1.688E-09	1.00E+00	1.688E-09
FeCO ₃	0.0000E+00	1.4412E-09	1.133E-09	1.00E+00	1.133E-09
NaHCO ₃	0.0000E+00	9.8295E-10	7.728E-10	1.00E+00	7.728E-10
Al(OH) ₃	6.0000E-03	7.2965E-10	5.737E-10	1.00E+00	5.737E-10
K ₂ O	0.0000E+00	3.0621E-10	2.408E-10	1.00E+00	2.408E-10
Fe(OH) ₃	4.0000E-03	1.1672E-11	9.177E-12	1.00E+00	9.177E-12
KH	0.0000E+00	5.3638E-12	4.217E-12	1.00E+00	4.217E-12
NaH	0.0000E+00	1.2184E-12	9.580E-13	1.00E+00	9.580E-13
Na ₃ UO ₄	0.0000E+00	5.164E-13	4.337E-13	1.00E+00	4.337E-13
HNO ₃	0.0000E+00	1.2109E-13	9.520E-14	1.00E+00	9.520E-14
C	1.0120E+00	2.6984E-14	2.122E-14	1.00E+00	2.122E-14
Pb ₃ O ₄	0.0000E+00	3.2805E-15	2.579E-15	1.00E+00	2.579E-15
Mg	0.0000E+00	5.3146E-16	4.179E-16	1.00E+00	4.179E-16
Ca	0.0000E+00	2.7811E-16	2.187E-16	1.00E+00	2.187E-16
H ₂ O ₄	0.0000E+00	1.3909E-16	1.094E-16	1.00E+00	1.094E-16
HCO ₂ H	0.0000E+00	1.1924E-16	9.375E-17	1.00E+00	9.375E-17
HCOOH	0.0000E+00	1.0499E-16	8.255E-17	1.00E+00	8.255E-17
Ca(NO ₃) ₂	0.0000E+00	2.1671E-18	1.704E-18	1.00E+00	1.704E-18
KCN	0.0000E+00	1.5427E-18	1.213E-18	1.00E+00	1.213E-18
NaCN	0.0000E+00	9.3329E-20	7.338E-20	1.00E+00	7.338E-20
NH ₄ OH	3.6000E-02	4.4397E-20	3.491E-20	1.00E+00	3.491E-20
U ₃ O ₈	0.0000E+00	1.5118E-20	1.189E-20	1.00E+00	1.189E-20
Si	0.0000E+00	2.3322E-21	1.834E-21	1.00E+00	1.834E-21
UO	0.0000E+00	1.9831E-21	1.559E-21	1.00E+00	1.559E-21
NaH ₃	0.0000E+00	5.5708E-22	4.380E-22	1.00E+00	4.380E-22
Mg(NO ₃) ₂	0.0000E+00	7.7147E-23	6.066E-23	1.00E+00	6.066E-23
CaH ₂	0.0000E+00	6.323E-23	3.642E-23	1.00E+00	3.642E-23
Na ₂ O ₅	0.0000E+00	8.6075E-24	6.768E-24	1.00E+00	6.768E-24
Pb(NO ₃) ₂	0.0000E+00	6.3451E-24	4.989E-24	1.00E+00	4.989E-24
UN	0.0000E+00	3.2653E-27	2.567E-27	1.00E+00	2.567E-27
U ₄ O ₉	0.0000E+00	9.0122E-30	7.086E-30	1.00E+00	7.086E-30
U ₄ O ₉	0.0000E+00	8.6016E-30	6.763E-30	1.00E+00	6.763E-30
NH ₄ NO ₃	0.0000E+00	5.4081E-31	4.252E-31	1.00E+00	4.252E-31
N ₂ H ₄	0.0000E+00	2.0380E-31	1.602E-31	1.00E+00	1.602E-31
CH ₃ OH	0.0000E+00	1.2427E-31	9.771E-32	1.00E+00	9.771E-32
U	0.0000E+00	6.6021E-35	5.191E-35	1.00E+00	5.191E-35
Ca ₃ N ₂	0.0000E+00	4.0561E-44	3.223E-44	1.00E+00	3.223E-44
UC	0.0000E+00	4.2973E-45	2.803E-45	1.00E+00	2.803E-45
UF ₆	0.0000E+00	6.1773E-49	0.000E+00	1.00E+00	0.000E+00
U ₃	0.0000E+00	2.3437E-50	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	4.6564E-56	0.000E+00	1.00E+00	0.000E+00
UC ₂	0.0000E+00	1.2031E-56	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	1.1927E-56	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	1.8862E-61	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	5.8175E-72	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	4.3503E-103	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.2719E+00	1.000E+00		

R

Temperature 1698.15 K
 Pressure 1 bar
 Volume 1.707E-01 m3 (NPT)
 Reaction enthalpy -2.015E+02 kJ
 Reaction entropy 5.888E+02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACTION	ACTIVITY COEFFICIENT	ACTIVITY
O2(g)	7.1550E+00	5.4806E+00	7.198E-01	1.00E+00	7.198E-01
H2O(g)	0.0000E+00	1.0203E+00	1.340E-01	1.00E+00	1.340E-01
CO2(g)	0.0000E+00	1.0112E+00	1.328E-01	1.00E+00	1.328E-01
KOH(g)	0.0000E+00	7.6109E-02	9.996E-03	1.00E+00	9.996E-03
NO(g)	0.0000E+00	2.1880E-02	2.874E-03	1.00E+00	2.874E-03
NaOH(g)	0.0000E+00	3.2859E-03	4.315E-04	1.00E+00	4.315E-04
K(g)	0.0000E+00	3.3407E-04	4.387E-05	1.00E+00	4.387E-05
PbO(g)	0.0000E+00	2.8724E-04	3.772E-05	1.00E+00	3.772E-05
NO2(g)	0.0000E+00	1.1964E-04	1.571E-05	1.00E+00	1.571E-05
CO(g)	0.0000E+00	8.2024E-05	1.077E-05	1.00E+00	1.077E-05
Na(g)	0.0000E+00	5.9414E-05	7.803E-06	1.00E+00	7.803E-06
KO(g)	0.0000E+00	5.4139E-05	7.110E-06	1.00E+00	7.110E-06
H2(g)	9.5000E-01	2.3714E-05	3.114E-06	1.00E+00	3.114E-06
Ca(OH)2(g)	0.0000E+00	2.1104E-06	2.772E-07	1.00E+00	2.772E-07
Pb(g)	0.0000E+00	1.0960E-06	1.439E-07	1.00E+00	1.439E-07
FeO(g)	0.0000E+00	5.3145E-09	6.980E-10	1.00E+00	6.980E-10
SiO2(g)	0.0000E+00	1.3949E-09	1.832E-10	1.00E+00	1.832E-10
NO3(g)	0.0000E+00	2.0176E-10	2.650E-11	1.00E+00	2.650E-11
MgO(g)	0.0000E+00	1.9998E-10	2.626E-11	1.00E+00	2.626E-11
MgOH(g)	0.0000E+00	1.8107E-11	2.378E-12	1.00E+00	2.378E-12
N(g)	0.0000E+00	1.5949E-11	2.095E-12	1.00E+00	2.095E-12
Fe(g)	0.0000E+00	1.5567E-11	2.044E-12	1.00E+00	2.044E-12
AlO2(g)	0.0000E+00	5.3542E-12	7.032E-13	1.00E+00	7.032E-13
NH3(g)	0.0000E+00	6.7312E-13	8.840E-14	1.00E+00	8.840E-14
Mg(g)	0.0000E+00	4.1799E-13	5.489E-14	1.00E+00	5.489E-14
CaO(g)	0.0000E+00	2.3890E-13	3.137E-14	1.00E+00	3.137E-14
HI(g)	0.0000E+00	1.7302E-13	2.277E-14	1.00E+00	2.277E-14
NH2(g)	0.0000E+00	1.4353E-13	1.885E-14	1.00E+00	1.885E-14
Ca(g)	0.0000E+00	1.9504E-14	2.567E-15	1.00E+00	2.567E-15
AlO(g)	0.0000E+00	1.0501E-16	1.379E-17	1.00E+00	1.379E-17
HCN(g)	0.0000E+00	2.5970E-18	3.411E-19	1.00E+00	3.411E-19
Al(g)	0.0000E+00	3.2407E-21	4.256E-22	1.00E+00	4.256E-22
Al2O3(g)	0.0000E+00	1.8813E-24	2.471E-25	1.00E+00	2.471E-25
Si(g)	0.0000E+00	4.0502E-25	5.319E-26	1.00E+00	5.319E-26
CH3OH(g)	0.0000E+00	8.5304E-26	1.120E-26	1.00E+00	1.120E-26
CH3(g)	0.0000E+00	3.8215E-26	5.019E-27	1.00E+00	5.019E-27
C(g)	0.0000E+00	1.2962E-26	1.702E-27	1.00E+00	1.702E-27
CH4(g)	0.0000E+00	9.4096E-27	1.236E-27	1.00E+00	1.236E-27
Al2O(g)	0.0000E+00	6.4965E-28	8.537E-29	1.00E+00	8.537E-29
CH2(g)	0.0000E+00	1.8784E-28	2.467E-29	1.00E+00	2.467E-29
C2H2(g)	0.0000E+00	2.9333E-35	3.852E-36	1.00E+00	3.852E-36
U(g)	0.0000E+00	8.7676E-41	1.151E-41	1.00E+00	1.151E-41
C2H4(g)	0.0000E+00	4.5912E-42	6.026E-43	1.00E+00	6.026E-43
C2H6(g)	0.0000E+00	3.2638E-050	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.6143E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACTION	ACTIVITY COEFFICIENT	ACTIVITY
CaO	4.9000E-01	4.8023E-001	3.764E-01	1.00E+00	3.764E-01
SiO2	4.6900E-01	4.6900E-001	3.676E-01	1.00E+00	3.676E-01
Al2O3	7.8000E-02	9.9000E-002	7.760E-02	1.00E+00	7.760E-02
Pb2O3	6.0000E-03	7.3988E-002	5.799E-02	1.00E+00	5.799E-02
NaFeO2	0.0000E+00	3.7210E-002	2.917E-02	1.00E+00	2.917E-02
FeO	0.0000E+00	3.7030E-002	2.902E-02	1.00E+00	2.902E-02
MgO	2.8000E-02	3.2633E-002	2.558E-02	1.00E+00	2.558E-02
CaO2	0.0000E+00	1.3557E-002	1.063E-02	1.00E+00	1.063E-02
Fe3O4	0.0000E+00	1.2261E-002	9.610E-03	1.00E+00	9.610E-03
H2O	9.0000E-02	1.0158E-002	7.962E-03	1.00E+00	7.962E-03
KOH	5.0000E-03	7.1730E-003	5.622E-03	1.00E+00	5.622E-03
NaOH	0.0000E+00	1.3563E-003	1.063E-03	1.00E+00	1.063E-03
U3O8	0.0000E+00	6.6664E-004	5.225E-04	1.00E+00	5.225E-04
K2CO3	0.0000E+00	5.0816E-004	3.983E-04	1.00E+00	3.983E-04
MgO2	0.0000E+00	3.6634E-004	2.871E-04	1.00E+00	2.871E-04
KO2	0.0000E+00	3.1121E-004	2.439E-04	1.00E+00	2.439E-04
CaCO3	0.0000E+00	1.7704E-004	1.388E-04	1.00E+00	1.388E-04
PbO	0.0000E+00	1.1022E-004	8.639E-05	1.00E+00	8.639E-05
Na2CO3	0.0000E+00	3.7462E-005	2.936E-05	1.00E+00	2.936E-05
Ca(OH)2	4.0000E-03	3.1059E-005	2.434E-05	1.00E+00	2.434E-05
NaO2	0.0000E+00	1.1922E-005	9.345E-06	1.00E+00	9.345E-06
K	0.0000E+00	1.8203E-006	1.427E-06	1.00E+00	1.427E-06
Pb	4.0000E-04	1.4260E-006	1.114E-06	1.00E+00	1.114E-06
Na	0.0000E+00	4.8659E-007	3.814E-07	1.00E+00	3.814E-07
Fe	2.4300E-01	3.9904E-007	3.128E-07	1.00E+00	3.128E-07
Mg(OH)2	5.0000E-03	1.5829E-007	2.808E-07	1.00E+00	2.808E-07
Na2O	1.4000E-02	3.5408E-007	2.775E-07	1.00E+00	2.775E-07

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KNO3	8.0000E-03	1.5092E-007	1.183E-07	1.00E+00	1.183E-07
MgCO3	0.0000E+00	6.3563E-008	4.982E-08	1.00E+00	4.982E-08
UO3	0.0000E+00	2.9550E-008	2.316E-08	1.00E+00	2.316E-08
NaNO3	1.4000E-02	2.7312E-008	2.141E-08	1.00E+00	2.141E-08
PbO2	0.0000E+00	2.4507E-008	1.921E-08	1.00E+00	1.921E-08
K2O2	0.0000E+00	2.3098E-008	1.810E-08	1.00E+00	1.810E-08
UO2	2.0000E-03	2.1342E-008	1.673E-08	1.00E+00	1.673E-08
UO3(G)	0.0000E+00	1.5624E-008	1.225E-08	1.00E+00	1.225E-08
Na2O2	0.0000E+00	1.1034E-008	8.648E-09	1.00E+00	8.648E-09
Fe(OH)2	0.0000E+00	9.2077E-009	7.217E-09	1.00E+00	7.217E-09
K2O	3.6000E-02	5.8968E-009	4.622E-09	1.00E+00	4.622E-09
K2O3	0.0000E+00	3.7410E-009	2.932E-09	1.00E+00	2.932E-09
FeCO3	0.0000E+00	2.3251E-009	1.822E-09	1.00E+00	1.822E-09
PbCO3	0.0000E+00	1.0307E-009	8.078E-10	1.00E+00	8.078E-10
Al(OH)3	6.0000E-03	9.7883E-010	7.672E-10	1.00E+00	7.672E-10
NaHCO3	0.0000E+00	6.7389E-010	5.282E-10	1.00E+00	5.282E-10
KO3	0.0000E+00	2.2870E-010	1.793E-10	1.00E+00	1.793E-10
KH	0.0000E+00	1.5702E-011	1.231E-11	1.00E+00	1.231E-11
Fe(OH)3	4.0000E-03	9.5338E-012	7.473E-12	1.00E+00	7.473E-12
NaH	0.0000E+00	5.6669E-012	4.442E-12	1.00E+00	4.442E-12
Na3UO4	0.0000E+00	3.6731E-013	2.879E-13	1.00E+00	2.879E-13
C	1.0120E+01	1.5754E-013	1.235E-13	1.00E+00	1.235E-13
HNH3	0.0000E+00	6.8144E-014	5.341E-14	1.00E+00	5.341E-14
Mg	0.0000E+00	7.8657E-015	6.165E-15	1.00E+00	6.165E-15
Ca	0.0000E+00	4.7079E-015	3.690E-15	1.00E+00	3.690E-15
HCO2H	0.0000E+00	3.4840E-016	2.731E-16	1.00E+00	2.731E-16
Pb3O4	0.0000E+00	3.2590E-016	2.554E-16	1.00E+00	2.554E-16
HCOOH	0.0000E+00	3.0961E-016	2.427E-16	1.00E+00	2.427E-16
H2O4	0.0000E+00	1.4496E-016	1.136E-16	1.00E+00	1.136E-16
KCH	0.0000E+00	7.8854E-018	6.181E-18	1.00E+00	6.181E-18
Al	3.6000E-02	1.8631E-018	1.460E-18	1.00E+00	1.460E-18
NaCN	0.0000E+00	8.0210E-019	6.287E-19	1.00E+00	6.287E-19
Ca(NO3)2	0.0000E+00	4.6051E-019	3.609E-19	1.00E+00	3.609E-19
Si	0.0000E+00	1.0919E-019	8.558E-20	1.00E+00	8.558E-20
HNH4OH	0.0000E+00	4.2384E-020	3.322E-20	1.00E+00	3.322E-20
UO	0.0000E+00	7.8810E-021	6.177E-21	1.00E+00	6.177E-21
U3O8	0.0000E+00	1.8467E-021	1.447E-21	1.00E+00	1.447E-21
CaH2	0.0000E+00	1.7557E-022	1.376E-22	1.00E+00	1.376E-22
NaH3	0.0000E+00	7.7109E-023	6.044E-23	1.00E+00	6.044E-23
Mg(NO3)2	0.0000E+00	2.4741E-023	1.939E-23	1.00E+00	1.939E-23
N2O5	0.0000E+00	2.7481E-026	2.154E-26	1.00E+00	2.154E-26
UN	0.0000E+00	2.7342E-028	2.143E-28	1.00E+00	2.143E-28
Pb(NO3)2	0.0000E+00	2.2478E-028	1.762E-28	1.00E+00	1.762E-28
U4O9	0.0000E+00	1.8942E-029	1.485E-29	1.00E+00	1.485E-29
CH3OH	0.0000E+00	2.0746E-030	1.626E-30	1.00E+00	1.626E-30
N2H4	0.0000E+00	1.0883E-030	8.530E-31	1.00E+00	8.530E-31
HNH4NO3	0.0000E+00	5.0744E-031	3.977E-31	1.00E+00	3.977E-31
U	0.0000E+00	1.1614E-032	9.103E-33	1.00E+00	9.103E-33
Ca3N2	0.0000E+00	1.2622E-041	9.893E-42	1.00E+00	9.893E-42
UC	0.0000E+00	2.7052E-042	2.120E-42	1.00E+00	2.120E-42
UF62	0.0000E+00	3.2941E-045	2.803E-45	1.00E+00	2.803E-45
UH3	0.0000E+00	1.0612E-047	0.000E+00	1.00E+00	0.000E+00
UC2	0.0000E+00	6.4160E-053	0.000E+00	1.00E+00	0.000E+00
Si3N4	0.0000E+00	1.4291E-053	0.000E+00	1.00E+00	0.000E+00
C2H6O	0.0000E+00	1.0150E-053	0.000E+00	1.00E+00	0.000E+00
Fe(CO)5	0.0000E+00	2.6216E-058	0.000E+00	1.00E+00	0.000E+00
Si2H6	0.0000E+00	6.1861E-067	0.000E+00	1.00E+00	0.000E+00
U2C3	0.0000E+00	1.0029E-096	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.2758E+000	1.000E+00		

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B

Temperature 1798.15 K
 Pressure 1 bar
 Volume 1.707E-01 m³ (NPT)
 Reaction enthalpy -1.516E-02 kJ
 Reaction entropy 6.167E-02 J/K
 Iterations 80 (Limit = 80)

	INPUT AMOUNT	EQUIL AMOUNT	MOL FRACT	ACTIVITY	ACTIVITY
	mol	mol			
PHASE 1:					
O ₂ (g)	7.1550E+00	5.4879E+00	7.205E-01	1.00E+00	7.205E-01
CO ₂ (g)	0.0000E+00	1.0115E+00	1.328E-01	1.00E+00	1.328E-01
H ₂ O(g)	0.0000E+00	1.0083E+00	1.324E-01	1.00E+00	1.324E-01
KOH(g)	0.0000E+00	7.9106E-02	1.039E-02	1.00E+00	1.039E-02
NO(g)	0.0000E+00	2.1904E-02	2.876E-03	1.00E+00	2.876E-03
NaOH(g)	0.0000E+00	5.8413E-03	7.672E-04	1.00E+00	7.672E-04
K(g)	0.0000E+00	7.7615E-04	1.019E-04	1.00E+00	1.019E-04
PbO(g)	0.0000E+00	3.3782E-04	4.435E-05	1.00E+00	4.435E-05
CO(g)	0.0000E+00	2.4702E-04	3.243E-05	1.00E+00	3.243E-05
Na(g)	0.0000E+00	2.1436E-04	2.814E-05	1.00E+00	2.814E-05
KO(g)	0.0000E+00	1.1726E-04	1.540E-05	1.00E+00	1.540E-05
NO ₂ (g)	0.0000E+00	9.5548E-05	1.254E-05	1.00E+00	1.254E-05
H ₂ (g)	9.5000E-01	6.2948E-05	8.265E-06	1.00E+00	8.265E-06
Ca(OH) ₂ (g)	0.0000E+00	5.7430E-06	7.540E-07	1.00E+00	7.540E-07
Pb(g)	0.0000E+00	2.3270E-06	3.055E-07	1.00E+00	3.055E-07
FeO(g)	0.0000E+00	5.5588E-08	7.298E-09	1.00E+00	7.298E-09
SiO ₂ (g)	0.0000E+00	1.3873E-08	1.821E-09	1.00E+00	1.821E-09
MgO(g)	0.0000E+00	1.9838E-09	2.605E-10	1.00E+00	2.605E-10
SiO(g)	0.0000E+00	3.4644E-10	4.549E-11	1.00E+00	4.549E-11
MgOH(g)	0.0000E+00	3.1810E-10	4.176E-11	1.00E+00	4.176E-11
Fe(g)	0.0000E+00	3.1468E-10	4.132E-11	1.00E+00	4.132E-11
NO ₃ (g)	0.0000E+00	1.9334E-10	2.538E-11	1.00E+00	2.538E-11
N(g)	0.0000E+00	8.3791E-11	1.100E-11	1.00E+00	1.100E-11
AlO ₂ (g)	0.0000E+00	6.5868E-11	8.648E-12	1.00E+00	8.648E-12
Mg(g)	0.0000E+00	7.3213E-12	9.613E-13	1.00E+00	9.613E-13
CaO(g)	0.0000E+00	3.5117E-12	4.611E-13	1.00E+00	4.611E-13
NH ₃ (g)	0.0000E+00	1.6346E-12	2.146E-13	1.00E+00	2.146E-13
NH ₄ (g)	0.0000E+00	7.7016E-13	1.011E-13	1.00E+00	1.011E-13
HI ₂ (g)	0.0000E+00	5.5075E-13	7.231E-14	1.00E+00	7.231E-14
Ca(g)	0.0000E+00	4.3357E-13	5.691E-14	1.00E+00	5.691E-14
AlO(g)	0.0000E+00	3.6815E-15	4.831E-16	1.00E+00	4.831E-16
HCl(g)	0.0000E+00	2.3787E-17	3.121E-18	1.00E+00	3.121E-18
Al(g)	0.0000E+00	2.9122E-19	3.824E-20	1.00E+00	3.824E-20
Al ₂ O ₃ (g)	0.0000E+00	2.355E-22	3.066E-23	1.00E+00	3.066E-23
Si(g)	0.0000E+00	1.851E-23	2.413E-24	1.00E+00	2.413E-24
CH ₃ (g)	0.0000E+00	1.2840E-24	1.666E-25	1.00E+00	1.666E-25
CH ₃ OH(g)	0.0000E+00	1.869E-24	2.459E-25	1.00E+00	2.459E-25
C(g)	0.0000E+00	1.0463E-24	1.374E-25	1.00E+00	1.374E-25
Al ₂ O(g)	0.0000E+00	2.2720E-25	2.983E-26	1.00E+00	2.983E-26
CH ₄ (g)	0.0000E+00	2.2003E-25	2.889E-26	1.00E+00	2.889E-26
CH ₂ (g)	0.0000E+00	1.1076E-26	1.454E-27	1.00E+00	1.454E-27
C ₂ H ₂ (g)	0.0000E+00	4.2449E-33	5.571E-34	1.00E+00	5.571E-34
U(g)	0.0000E+00	5.5066E-38	7.230E-39	1.00E+00	7.230E-39
C ₂ H ₄ (g)	0.0000E+00	8.6925E-40	1.141E-40	1.00E+00	1.141E-40
C ₂ H ₆ (g)	0.0000E+00	9.0880E-48	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.6164E+00	1.000E+00		

			MOL FRACT		
PHASE 2 :					
CaO	4.9000E-01	4.8063E-01	3.715E-01	1.00E+00	3.715E-01
SiO ₂	4.6900E-01	4.6900E-01	3.625E-01	1.00E+00	3.625E-01
Al ₂ O ₃	7.8000E-02	9.9000E-02	7.652E-02	1.00E+00	7.652E-02
FeO	0.0000E+00	6.2730E-02	4.848E-02	1.00E+00	4.848E-02
Fe ₂ O ₃	6.0000E-03	5.9851E-02	4.626E-02	1.00E+00	4.626E-02
NaFeO ₂	0.0000E+00	3.4680E-02	2.680E-02	1.00E+00	2.680E-02
MgO	2.8000E-02	3.2674E-02	2.525E-02	1.00E+00	2.525E-02
H ₂ O	9.8000E-02	2.0785E-02	1.606E-02	1.00E+00	1.606E-02
Fe ₃ O ₄	0.0000E+00	1.3362E-02	1.079E-02	1.00E+00	1.079E-02
CaO ₂	0.0000E+00	1.3250E-02	1.024E-02	1.00E+00	1.024E-02
KOH	5.0000E-03	4.5402E-03	3.509E-03	1.00E+00	3.509E-03
NaOH	0.0000E+00	1.2096E-03	9.348E-04	1.00E+00	9.348E-04
U ₃ O ₈	0.0000E+00	6.6665E-04	5.152E-04	1.00E+00	5.152E-04
MgO ₂	0.0000E+00	3.2558E-04	2.516E-04	1.00E+00	2.516E-04
K ₂ O	0.0000E+00	2.2349E-04	1.727E-04	1.00E+00	1.727E-04
K ₂ CO ₃	0.0000E+00	1.1671E-04	9.020E-05	1.00E+00	9.020E-05
CaCO ₃	0.0000E+00	9.4787E-05	7.478E-05	1.00E+00	7.478E-05
PbO	0.0000E+00	5.8331E-05	4.508E-05	1.00E+00	4.508E-05
Ca(OH) ₂	4.0000E-03	2.2248E-05	1.720E-05	1.00E+00	1.720E-05
Na ₂ CO ₃	0.0000E+00	1.8511E-05	1.431E-05	1.00E+00	1.431E-05
Na ₂ O	0.0000E+00	1.3349E-05	1.032E-05	1.00E+00	1.032E-05
K	0.0000E+00	3.2145E-06	2.484E-06	1.00E+00	2.484E-06
Fe	2.4300E-01	1.7638E-06	1.363E-06	1.00E+00	1.363E-06
Pb	4.0000E-04	1.5138E-06	1.170E-06	1.00E+00	1.170E-06
Na	0.0000E+00	1.2450E-06	9.622E-07	1.00E+00	9.622E-07
Na ₂ O	1.400E-02	5.9845E-07	4.625E-07	1.00E+00	4.625E-07
Mg(OH) ₂	5.000E-03	3.6347E-07	2.809E-07	1.00E+00	2.809E-07

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MgCO ₃	0.0000E+00	4.8167E-08	3.723E-08	1.00E+00	3.723E-08
K ₂ SO ₄	8.0000E-03	3.2269E-08	2.494E-08	1.00E+00	2.494E-08
UO ₂	2.0000E-03	2.9107E-08	2.250E-08	1.00E+00	2.250E-08
UO ₃	0.0000E+00	2.2719E-08	1.756E-08	1.00E+00	1.756E-08
K ₂ SO ₄	0.0000E+00	1.2753E-08	9.857E-09	1.00E+00	9.857E-09
Fe(OH) ₂	0.0000E+00	1.2232E-08	9.454E-09	1.00E+00	9.454E-09
UO ₃ (g)	0.0000E+00	1.1509E-08	8.895E-09	1.00E+00	8.895E-09
NaNO ₃	1.4000E-02	1.0960E-08	8.471E-09	1.00E+00	8.471E-09
Na ₂ O ₂	0.0000E+00	1.0300E-08	7.961E-09	1.00E+00	7.961E-09
PbO ₂	0.0000E+00	9.3280E-09	7.209E-09	1.00E+00	7.209E-09
K ₂ O	3.6000E-02	5.0728E-09	3.921E-09	1.00E+00	3.921E-09
FeCO ₃	0.0000E+00	3.5961E-09	2.779E-09	1.00E+00	2.779E-09
K ₂ CO ₃	0.0000E+00	1.6393E-09	1.267E-09	1.00E+00	1.267E-09
Al(OH) ₃	6.0000E-03	1.3988E-09	1.081E-09	1.00E+00	1.081E-09
PbCO ₃	0.0000E+00	4.9836E-10	3.852E-10	1.00E+00	3.852E-10
NaHCO ₃	0.0000E+00	4.8781E-10	3.770E-10	1.00E+00	3.770E-10
KO ₃	0.0000E+00	1.7355E-10	1.341E-10	1.00E+00	1.341E-10
KH	0.0000E+00	3.9549E-11	3.057E-11	1.00E+00	3.057E-11
NaH	0.0000E+00	2.1542E-11	1.665E-11	1.00E+00	1.665E-11
Fe(OH) ₃	4.0000E-03	7.7271E-12	5.972E-12	1.00E+00	5.972E-12
C	1.0120E+00	7.6347E-13	5.901E-13	1.00E+00	5.901E-13
Na ₃ UO ₄	0.0000E+00	2.1363E-13	1.651E-13	1.00E+00	1.651E-13
Mg	0.0000E+00	8.6099E-14	6.654E-14	1.00E+00	6.654E-14
Ca	0.0000E+00	5.7914E-14	4.476E-14	1.00E+00	4.476E-14
HNH ₃	0.0000E+00	4.0990E-14	3.168E-14	1.00E+00	3.168E-14
HCO ₂ H	0.0000E+00	9.1189E-16	7.048E-16	1.00E+00	7.048E-16
HCOOH	0.0000E+00	8.1711E-16	6.315E-16	1.00E+00	6.315E-16
H ₂ O ₄	0.0000E+00	1.6941E-16	1.309E-16	1.00E+00	1.309E-16
Al	3.6000E-02	5.1675E-17	3.994E-17	1.00E+00	3.994E-17
KCN	0.0000E+00	3.2195E-17	2.488E-17	1.00E+00	2.488E-17
Pb ₃ CO ₄	0.0000E+00	2.8395E-17	2.195E-17	1.00E+00	2.195E-17
NaCN	0.0000E+00	5.1676E-18	3.994E-18	1.00E+00	3.994E-18
Si	0.0000E+00	4.5553E-18	3.521E-18	1.00E+00	3.521E-18
Ca(NO ₃) ₂	0.0000E+00	1.2610E-19	9.746E-20	1.00E+00	9.746E-20
HNH ₄ OH	0.0000E+00	1.0764E-19	8.320E-20	1.00E+00	8.320E-20
UO	0.0000E+00	8.2331E-20	6.363E-20	1.00E+00	6.363E-20
CaH ₂	0.0000E+00	2.5473E-21	1.969E-21	1.00E+00	1.969E-21
U ₃ O ₈	0.0000E+00	1.4828E-21	1.146E-21	1.00E+00	1.146E-21
NaH ₃	0.0000E+00	7.3157E-23	5.654E-23	1.00E+00	5.654E-23
Mg(NO ₃) ₂	0.0000E+00	1.6435E-23	1.270E-23	1.00E+00	1.270E-23
Na ₂ O ₅	0.0000E+00	1.3333E-26	1.031E-26	1.00E+00	1.031E-26
UN	0.0000E+00	5.6421E-27	4.361E-27	1.00E+00	4.361E-27
U ₄ O ₉	0.0000E+00	3.7227E-29	2.877E-29	1.00E+00	2.877E-29
CH ₃ OH	0.0000E+00	2.5115E-29	1.941E-29	1.00E+00	1.941E-29
Pb(NO ₃) ₂	0.0000E+00	1.8152E-29	1.403E-29	1.00E+00	1.403E-29
NH ₄ H	0.0000E+00	4.8351E-30	3.737E-30	1.00E+00	3.737E-30
U	0.0000E+00	1.1438E-30	8.840E-31	1.00E+00	8.840E-31
HNH ₄ NO ₃	0.0000E+00	4.8265E-31	3.730E-31	1.00E+00	3.730E-31
Ca ₃ N ₂	0.0000E+00	2.0322E-39	1.571E-39	1.00E+00	1.571E-39
UC	0.0000E+00	8.2565E-40	6.381E-40	1.00E+00	6.381E-40
UFe ₂	0.0000E+00	6.1351E-42	4.742E-42	1.00E+00	4.742E-42
UH ₃	0.0000E+00	2.4113E-45	1.891E-45	1.00E+00	1.891E-45
UC ₂	0.0000E+00	1.3334E-49	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	7.5839E-51	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	1.1864E-51	0.000E+00	1.00E+00	0.000E+00
Fe(CO) ₅	0.0000E+00	1.5581E-55	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	1.7572E-56	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	4.3817E-59	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.2939E+00	1.000E+00		

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B

Temperature 1898.15 K
 Pressure 1 bar
 Volume 1.705E-01 m³ (NPT)
 Reaction enthalpy -9.188E+01 kJ
 Reaction entropy 6.470E+02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol			
O ₂ (g)	7.1550E+00	5.4971E+00	7.227E-01	1.00E+00	7.227E-01
CO ₂ (g)	0.0000E+00	1.0112E+00	1.330E-01	1.00E+00	1.330E-01
H ₂ O(g)	0.0000E+00	9.8255E-001	1.292E-01	1.00E+00	1.292E-01
KOH(g)	0.0000E+00	7.9887E-002	1.050E-02	1.00E+00	1.050E-02
NaOH(g)	0.0000E+00	2.1922E-002	2.882E-03	1.00E+00	2.882E-03
K(g)	0.0000E+00	9.4684E-003	1.245E-03	1.00E+00	1.245E-03
CO(g)	0.0000E+00	1.6209E-003	2.131E-04	1.00E+00	2.131E-04
Na(g)	0.0000E+00	6.5994E-004	8.677E-05	1.00E+00	8.677E-05
PbO(g)	0.0000E+00	6.5747E-004	8.644E-05	1.00E+00	8.644E-05
KO(g)	0.0000E+00	3.6277E-004	4.770E-05	1.00E+00	4.770E-05
H ₂ (g)	0.0000E+00	2.3019E-004	3.026E-05	1.00E+00	3.026E-05
NO ₂ (g)	0.0000E+00	1.4845E-004	1.952E-05	1.00E+00	1.952E-05
Ca(OH) ₂ (g)	0.0000E+00	7.8231E-005	1.029E-05	1.00E+00	1.029E-05
Pb(g)	0.0000E+00	1.3601E-005	1.788E-06	1.00E+00	1.788E-06
FeO(g)	0.0000E+00	4.2405E-006	5.575E-07	1.00E+00	5.575E-07
SiO ₂ (g)	0.0000E+00	4.2020E-007	5.525E-08	1.00E+00	5.525E-08
MgO(g)	0.0000E+00	1.0602E-007	1.394E-08	1.00E+00	1.394E-08
Fe(g)	0.0000E+00	1.5104E-008	1.986E-09	1.00E+00	1.986E-09
HgO(g)	0.0000E+00	5.3103E-009	6.982E-10	1.00E+00	6.982E-10
Al ₂ O ₃ (g)	0.0000E+00	4.2964E-009	5.649E-10	1.00E+00	5.649E-10
NaCl(g)	0.0000E+00	2.0711E-009	2.723E-10	1.00E+00	2.723E-10
Al ₂ O ₃ (g)	0.0000E+00	6.1331E-010	8.064E-11	1.00E+00	8.064E-11
N(g)	0.0000E+00	3.2989E-010	4.337E-11	1.00E+00	4.337E-11
NO(g)	0.0000E+00	1.8692E-010	2.458E-11	1.00E+00	2.458E-11
Mg(g)	0.0000E+00	9.2661E-011	1.218E-11	1.00E+00	1.218E-11
CaO(g)	0.0000E+00	3.8004E-011	4.997E-12	1.00E+00	4.997E-12
Ca(g)	0.0000E+00	6.7833E-012	8.918E-13	1.00E+00	8.918E-13
NH(g)	0.0000E+00	3.6615E-012	4.817E-13	1.00E+00	4.817E-13
NH ₃ (g)	0.0000E+00	3.5386E-012	4.652E-13	1.00E+00	4.652E-13
NH ₂ (g)	0.0000E+00	1.8064E-012	2.375E-13	1.00E+00	2.375E-13
AlO(g)	0.0000E+00	8.7224E-014	1.147E-14	1.00E+00	1.147E-14
HCl(g)	0.0000E+00	1.7093E-016	2.247E-17	1.00E+00	2.247E-17
Al(g)	0.0000E+00	1.6009E-017	2.105E-18	1.00E+00	2.105E-18
Al ₂ O ₃ (g)	0.0000E+00	1.6923E-017	2.225E-18	1.00E+00	2.225E-18
Si(g)	0.0000E+00	8.5291E-021	1.121E-21	1.00E+00	1.121E-21
C(g)	0.0000E+00	5.3001E-023	6.964E-24	1.00E+00	6.964E-24
Al ₂ O ₃ (g)	0.0000E+00	4.1458E-023	5.451E-24	1.00E+00	5.451E-24
CH ₃ (g)	0.0000E+00	2.9109E-023	3.827E-24	1.00E+00	3.827E-24
CH ₃ OH(g)	0.0000E+00	1.2098E-023	1.589E-24	1.00E+00	1.589E-24
CH ₄ (g)	0.0000E+00	3.5837E-024	4.712E-25	1.00E+00	4.712E-25
CH ₂ (g)	0.0000E+00	4.1788E-025	5.494E-26	1.00E+00	5.494E-26
C ₂ H ₂ (g)	0.0000E+00	3.5746E-031	4.700E-32	1.00E+00	4.700E-32
U(g)	0.0000E+00	1.7189E-035	2.260E-36	1.00E+00	2.260E-36
C ₂ H ₄ (g)	0.0000E+00	9.2685E-038	1.219E-38	1.00E+00	1.219E-38
C ₂ H ₆ (g)	0.0000E+00	1.3354E-045	0.000E+00	1.00E+00	0.000E+00
Total :	8.1050E+00	7.6059E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol			
CaO	4.9000E-01	4.8089E-001	3.615E-01	1.00E+00	3.615E-01
SiO ₂	4.6900E-01	4.6900E-001	3.525E-01	1.00E+00	3.525E-01
Al ₂ O ₃	7.8000E-02	9.9000E-002	7.442E-02	1.00E+00	7.442E-02
FeO	0.0000E+00	9.5637E-002	7.189E-02	1.00E+00	7.189E-02
H ₂ O	9.8000E-02	4.5038E-002	3.385E-02	1.00E+00	3.385E-02
Fe ₂ O ₃	6.0000E-03	4.4037E-002	3.310E-02	1.00E+00	3.310E-02
MgO	2.8000E-02	3.2707E-002	2.459E-02	1.00E+00	2.459E-02
NaFeO ₂	0.0000E+00	3.0750E-002	2.311E-02	1.00E+00	2.311E-02
Fe ₃ O ₄	0.0000E+00	1.4844E-002	1.116E-02	1.00E+00	1.116E-02
CaO ₂	0.0000E+00	1.3023E-002	9.789E-03	1.00E+00	9.789E-03
KOH	5.0000E-03	3.0236E-003	2.273E-03	1.00E+00	2.273E-03
NaOH	0.0000E+00	1.0848E-003	8.154E-04	1.00E+00	8.154E-04
U ₃ O ₈	0.0000E+00	6.6664E-004	5.011E-04	1.00E+00	5.011E-04
HgO ₂	0.0000E+00	2.9280E-004	2.201E-04	1.00E+00	2.201E-04
K ₂ O	0.0000E+00	1.6933E-004	1.271E-04	1.00E+00	1.271E-04
CaCO ₃	0.0000E+00	5.6915E-005	4.278E-05	1.00E+00	4.278E-05
K ₂ CO ₃	0.0000E+00	3.1808E-005	2.391E-05	1.00E+00	2.391E-05
PbO	0.0000E+00	3.1477E-005	2.366E-05	1.00E+00	2.366E-05
Ca(OH) ₂	4.0000E-03	1.6389E-005	1.232E-05	1.00E+00	1.232E-05
Na ₂ O	0.0000E+00	1.5044E-005	1.131E-05	1.00E+00	1.131E-05
Na ₂ CO ₃	0.0000E+00	9.7602E-006	7.337E-06	1.00E+00	7.337E-06
Fe	2.4300E-01	6.6008E-006	4.962E-06	1.00E+00	4.962E-06
K	0.0000E+00	5.3594E-006	4.029E-06	1.00E+00	4.029E-06
Na	0.0000E+00	2.8721E-006	2.159E-06	1.00E+00	2.159E-06
Pb	4.0000E-04	1.5122E-006	1.137E-06	1.00E+00	1.137E-06
Na ₂ O	1.4000E-02	9.3891E-007	7.058E-07	1.00E+00	7.058E-07
Hg(OH) ₂	5.0000E-03	3.7988E-007	2.856E-07	1.00E+00	2.856E-07

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MgCO ₃	0.0000E+00	3.6513E-008	2.895E-08	1.00E+00	2.895E-08
UO ₂	2.0000E-03	3.8510E-008	2.895E-08	1.00E+00	2.895E-08
UO ₃	0.0000E+00	1.8022E-008	1.355E-08	1.00E+00	1.355E-08
Fe(OH) ₂	0.0000E+00	1.4795E-008	1.112E-08	1.00E+00	1.112E-08
Na ₂ O ₂	0.0000E+00	9.4794E-009	7.126E-09	1.00E+00	7.126E-09
U ₃ (O) ₈	0.0000E+00	8.6132E-009	6.474E-09	1.00E+00	6.474E-09
K ₂ O	8.0000E-03	8.2215E-009	6.180E-09	1.00E+00	6.180E-09
K ₂ O ₂	0.0000E+00	7.6499E-009	5.750E-09	1.00E+00	5.750E-09
FeCO ₃	0.0000E+00	5.2810E-009	3.970E-09	1.00E+00	3.970E-09
NaNO ₃	1.4000E-02	4.9146E-009	3.694E-09	1.00E+00	3.694E-09
K ₂ O	3.6000E-02	4.4343E-009	3.333E-09	1.00E+00	3.333E-09
PbO ₂	0.0000E+00	3.7393E-009	2.811E-09	1.00E+00	2.811E-09
Al(OH) ₃	6.0000E-03	2.0871E-009	1.569E-09	1.00E+00	1.569E-09
K ₂ O ₃	0.0000E+00	7.8667E-010	5.913E-10	1.00E+00	5.913E-10
NaHCO ₃	0.0000E+00	3.8442E-010	2.890E-10	1.00E+00	2.890E-10
PbCO ₃	0.0000E+00	2.6110E-010	1.963E-10	1.00E+00	1.963E-10
K ₂ O	0.0000E+00	1.3957E-010	1.049E-10	1.00E+00	1.049E-10
KH	0.0000E+00	9.1195E-011	6.855E-11	1.00E+00	6.855E-11
NaNH	0.0000E+00	7.1655E-011	5.386E-11	1.00E+00	5.386E-11
Fe(OH) ₃	4.0000E-03	6.0091E-012	4.517E-12	1.00E+00	4.517E-12
C	1.0120E+00	3.1796E-012	2.390E-12	1.00E+00	2.390E-12
Mg	0.0000E+00	7.3079E-013	5.493E-13	1.00E+00	5.493E-13
Ca	0.0000E+00	5.4436E-013	4.092E-13	1.00E+00	4.092E-13
Na ₃ UO ₄	0.0000E+00	1.2420E-013	9.336E-14	1.00E+00	9.336E-14
HNO ₃	0.0000E+00	2.6089E-014	1.961E-14	1.00E+00	1.961E-14
HCO ₂ H	0.0000E+00	2.1661E-015	1.628E-15	1.00E+00	1.628E-15
HCOOH	0.0000E+00	1.9555E-015	1.470E-15	1.00E+00	1.470E-15
Al	3.6000E-02	1.0131E-015	7.616E-16	1.00E+00	7.616E-16
H ₂ O ₄	0.0000E+00	2.1961E-016	1.651E-16	1.00E+00	1.651E-16
Si	0.0000E+00	1.2758E-016	9.590E-17	1.00E+00	9.590E-17
KCN	0.0000E+00	1.1371E-016	8.547E-17	1.00E+00	8.547E-17
NaCN	0.0000E+00	2.7234E-017	2.047E-17	1.00E+00	2.047E-17
Pb ₃ O ₄	0.0000E+00	2.7222E-018	2.046E-18	1.00E+00	2.046E-18
UO	0.0000E+00	6.6868E-019	5.026E-19	1.00E+00	5.026E-19
NH ₄ OH	0.0000E+00	2.4641E-019	1.852E-19	1.00E+00	1.852E-19
Ca(NO ₃) ₂	0.0000E+00	4.2910E-020	3.225E-20	1.00E+00	3.225E-20
CaH ₂	0.0000E+00	2.7478E-020	2.065E-20	1.00E+00	2.065E-20
U ₃ O ₈	0.0000E+00	1.2071E-021	9.074E-22	1.00E+00	9.074E-22
Na ₃	0.0000E+00	6.9299E-023	5.209E-23	1.00E+00	5.209E-23
Mg(NO ₃) ₂	0.0000E+00	1.3189E-023	9.914E-24	1.00E+00	9.914E-24
UN	0.0000E+00	8.4444E-026	6.348E-26	1.00E+00	6.348E-26
N ₂ O ₅	0.0000E+00	7.1674E-027	5.388E-27	1.00E+00	5.388E-27
CH ₃ OH	0.0000E+00	2.2874E-028	1.719E-28	1.00E+00	1.719E-28
U	0.0000E+00	6.9300E-029	5.209E-29	1.00E+00	5.209E-29
U ₄ O ₉	0.0000E+00	6.6495E-029	4.998E-29	1.00E+00	4.998E-29
N ₂ H ₄	0.0000E+00	1.8132E-029	1.363E-29	1.00E+00	1.363E-29
Pb(NO ₃) ₂	0.0000E+00	1.8067E-030	1.358E-30	1.00E+00	1.358E-30
NH ₄ NO ₃	0.0000E+00	4.5800E-031	3.443E-31	1.00E+00	3.443E-31
Ca ₃ N ₂	0.0000E+00	1.8614E-037	1.399E-37	1.00E+00	1.399E-37
UC	0.0000E+00	1.3751E-037	1.034E-37	1.00E+00	1.034E-37
UF ₆	0.0000E+00	4.5039E-039	3.386E-39	1.00E+00	3.386E-39
U ₃	0.0000E+00	3.0323E-043	2.284E-43	1.00E+00	2.284E-43
UC ₂	0.0000E+00	1.2576E-046	0.000E+00	1.00E+00	0.000E+00
Si ₃ N ₄	0.0000E+00	2.0066E-048	0.000E+00	1.00E+00	0.000E+00
C ₂ H ₆ O	0.0000E+00	8.0188E-050	0.000E+00	1.00E+00	0.000E+00
Fe(OH) ₅	0.0000E+00	4.4642E-053	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	1.5832E-058	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	4.7348E-086	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.3303E+00	1.000E+00		

2.5584E+00	1.9977E+00	1.000E+00	1.000E+00	2.5584E+00	1.9977E+00	1.000E+00	1.000E+00
1.5415E+00	1.9510E+00	1.000E+00	1.000E+00	1.5415E+00	1.9510E+00	1.000E+00	1.000E+00
4.9726E+00	4.9555E+00	1.000E+00	1.000E+00	4.9726E+00	4.9555E+00	1.000E+00	1.000E+00
6.1945E+00	6.1945E+00	1.000E+00	1.000E+00	6.1945E+00	6.1945E+00	1.000E+00	1.000E+00
2.7272E+00	2.7272E+00	1.000E+00	1.000E+00	2.7272E+00	2.7272E+00	1.000E+00	1.000E+00
6.0850E+00	6.0850E+00	1.000E+00	1.000E+00	6.0850E+00	6.0850E+00	1.000E+00	1.000E+00
2.2449E+00	2.2449E+00	1.000E+00	1.000E+00	2.2449E+00	2.2449E+00	1.000E+00	1.000E+00
2.3836E+00	2.3836E+00	1.000E+00	1.000E+00	2.3836E+00	2.3836E+00	1.000E+00	1.000E+00
1.0309E+00	1.0309E+00	1.000E+00	1.000E+00	1.0309E+00	1.0309E+00	1.000E+00	1.000E+00
1.1769E+00	1.1769E+00	1.000E+00	1.000E+00	1.1769E+00	1.1769E+00	1.000E+00	1.000E+00
2.7870E+00	2.7870E+00	1.000E+00	1.000E+00	2.7870E+00	2.7870E+00	1.000E+00	1.000E+00
5.1913E+00	5.1913E+00	1.000E+00	1.000E+00	5.1913E+00	5.1913E+00	1.000E+00	1.000E+00
7.8242E+00	7.8242E+00	1.000E+00	1.000E+00	7.8242E+00	7.8242E+00	1.000E+00	1.000E+00
9.0952E+00	9.0952E+00	1.000E+00	1.000E+00	9.0952E+00	9.0952E+00	1.000E+00	1.000E+00
1.5848E+00	1.5848E+00	1.000E+00	1.000E+00	1.5848E+00	1.5848E+00	1.000E+00	1.000E+00
2.7943E+00	2.7943E+00	1.000E+00	1.000E+00	2.7943E+00	2.7943E+00	1.000E+00	1.000E+00
2.9648E+00	2.9648E+00	1.000E+00	1.000E+00	2.9648E+00	2.9648E+00	1.000E+00	1.000E+00
9.7967E+00	9.7967E+00	1.000E+00	1.000E+00	9.7967E+00	9.7967E+00	1.000E+00	1.000E+00
1.6573E+00	1.6573E+00	1.000E+00	1.000E+00	1.6573E+00	1.6573E+00	1.000E+00	1.000E+00
7.1515E+00	7.1515E+00	1.000E+00	1.000E+00	7.1515E+00	7.1515E+00	1.000E+00	1.000E+00
9.8797E+00	9.8797E+00	1.000E+00	1.000E+00	9.8797E+00	9.8797E+00	1.000E+00	1.000E+00
1.7744E+00	1.7744E+00	1.000E+00	1.000E+00	1.7744E+00	1.7744E+00	1.000E+00	1.000E+00
2.5117E+00	2.5117E+00	1.000E+00	1.000E+00	2.5117E+00	2.5117E+00	1.000E+00	1.000E+00
3.9069E+00	3.9069E+00	1.000E+00	1.000E+00	3.9069E+00	3.9069E+00	1.000E+00	1.000E+00
4.9469E+00	4.9469E+00	1.000E+00	1.000E+00	4.9469E+00	4.9469E+00	1.000E+00	1.000E+00
4.4172E+00	4.4172E+00	1.000E+00	1.000E+00	4.4172E+00	4.4172E+00	1.000E+00	1.000E+00
1.2272E+00	1.2272E+00	1.000E+00	1.000E+00	1.2272E+00	1.2272E+00	1.000E+00	1.000E+00
1.6584E+00	1.6584E+00	1.000E+00	1.000E+00	1.6584E+00	1.6584E+00	1.000E+00	1.000E+00
1.8188E+00	1.8188E+00	1.000E+00	1.000E+00	1.8188E+00	1.8188E+00	1.000E+00	1.000E+00
4.2868E+00	4.2868E+00	1.000E+00	1.000E+00	4.2868E+00	4.2868E+00	1.000E+00	1.000E+00
4.6969E+00	4.6969E+00	1.000E+00	1.000E+00	4.6969E+00	4.6969E+00	1.000E+00	1.000E+00
1.4848E+00	1.4848E+00	1.000E+00	1.000E+00	1.4848E+00	1.4848E+00	1.000E+00	1.000E+00
1.5047E+00	1.5047E+00	1.000E+00	1.000E+00	1.5047E+00	1.5047E+00	1.000E+00	1.000E+00
1.4514E+00	1.4514E+00	1.000E+00	1.000E+00	1.4514E+00	1.4514E+00	1.000E+00	1.000E+00
4.6058E+00	4.6058E+00	1.000E+00	1.000E+00	4.6058E+00	4.6058E+00	1.000E+00	1.000E+00
3.7676E+00	3.7676E+00	1.000E+00	1.000E+00	3.7676E+00	3.7676E+00	1.000E+00	1.000E+00
4.9940E+00	4.9940E+00	1.000E+00	1.000E+00	4.9940E+00	4.9940E+00	1.000E+00	1.000E+00
1.2189E+00	1.2189E+00	1.000E+00	1.000E+00	1.2189E+00	1.2189E+00	1.000E+00	1.000E+00
1.4526E+00	1.4526E+00	1.000E+00	1.000E+00	1.4526E+00	1.4526E+00	1.000E+00	1.000E+00
1.9877E+00	1.9877E+00	1.000E+00	1.000E+00	1.9877E+00	1.9877E+00	1.000E+00	1.000E+00
1.5262E+00	1.5262E+00	1.000E+00	1.000E+00	1.5262E+00	1.5262E+00	1.000E+00	1.000E+00
1.9867E+00	1.9867E+00	1.000E+00	1.000E+00	1.9867E+00	1.9867E+00	1.000E+00	1.000E+00
2.1010E+00	2.1010E+00	1.000E+00	1.000E+00	2.1010E+00	2.1010E+00	1.000E+00	1.000E+00
1.7525E+00	1.7525E+00	1.000E+00	1.000E+00	1.7525E+00	1.7525E+00	1.000E+00	1.000E+00
1.9151E+00	1.9151E+00	1.000E+00	1.000E+00	1.9151E+00	1.9151E+00	1.000E+00	1.000E+00
1.9567E+00	1.9567E+00	1.000E+00	1.000E+00	1.9567E+00	1.9567E+00	1.000E+00	1.000E+00
1.9	1.9	1.000E+00	1.000E+00	1.9	1.9	1.000E+00	1.000E+00

[illegible]

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Temperature 2098.15 K
 Pressure 1 bar
 Volume 1.669E-01 m3 (NPT)
 Reaction enthalpy 7.861E+01 kJ
 Reaction entropy 7.314E-02 J/K
 Iterations 80 (Limit = 80)

PHASE 1:	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACTION	ACTIVITY COEFFICIENT	ACTIVITY
O2(g)	7.1550E+00	5.5176E+00	7.408E-01	1.00E+00	7.408E-01
CO2(g)	0.0000E+00	1.0088E+00	1.354E-01	1.00E+00	1.354E-01
H2O(g)	0.0000E+00	7.9058E-01	1.061E-01	1.00E+00	1.061E-01
KOH(g)	0.0000E+00	7.6634E-02	1.029E-02	1.00E+00	1.029E-02
NO(g)	0.0000E+00	2.1944E-02	2.946E-03	1.00E+00	2.946E-03
NaOH(g)	0.0000E+00	1.7640E-02	2.368E-03	1.00E+00	2.368E-03
K(g)	0.0000E+00	5.8159E-03	7.809E-04	1.00E+00	7.809E-04
Na(g)	0.0000E+00	3.9208E-03	5.264E-04	1.00E+00	5.264E-04
CO(g)	0.0000E+00	3.4944E-03	4.692E-04	1.00E+00	4.692E-04
KO(g)	0.0000E+00	7.4973E-04	1.007E-04	1.00E+00	1.007E-04
H2(g)	9.5000E-01	5.3897E-04	7.237E-05	1.00E+00	7.237E-05
PbO(g)	0.0000E+00	3.7601E-04	5.049E-05	1.00E+00	5.049E-05
NO2(g)	0.0000E+00	5.6090E-05	7.531E-06	1.00E+00	7.531E-06
Ca(OH)2(g)	0.0000E+00	4.4831E-05	6.019E-06	1.00E+00	6.019E-06
Pb(g)	0.0000E+00	1.0824E-05	1.453E-06	1.00E+00	1.453E-06
FeO(g)	0.0000E+00	9.6611E-06	1.297E-06	1.00E+00	1.297E-06
SiO2(g)	0.0000E+00	2.9392E-06	3.946E-07	1.00E+00	3.946E-07
SiO(g)	0.0000E+00	4.7843E-07	6.423E-08	1.00E+00	6.423E-08
HgO(g)	0.0000E+00	2.693E-08	3.62E-09	1.00E+00	3.62E-09
Fe(g)	0.0000E+00	2.7138E-07	3.644E-08	1.00E+00	3.644E-08
MgOH(g)	0.0000E+00	4.1412E-08	5.560E-09	1.00E+00	5.560E-09
AlO2(g)	0.0000E+00	2.5941E-08	3.483E-09	1.00E+00	3.483E-09
Mg(g)	0.0000E+00	6.2086E-09	8.336E-10	1.00E+00	8.336E-10
N(g)	0.0000E+00	3.4295E-09	4.605E-10	1.00E+00	4.605E-10
CaO(g)	0.0000E+00	1.9543E-09	2.624E-10	1.00E+00	2.624E-10
Ca(g)	0.0000E+00	6.5156E-10	8.748E-11	1.00E+00	8.748E-11
NO3(g)	0.0000E+00	1.8093E-10	2.429E-11	1.00E+00	2.429E-11
NH(g)	0.0000E+00	3.9291E-11	5.275E-12	1.00E+00	5.275E-12
AlO(g)	0.0000E+00	1.8025E-11	2.426E-12	1.00E+00	2.426E-12
NH2(g)	0.0000E+00	1.1643E-11	1.563E-12	1.00E+00	1.563E-12
NH3(g)	0.0000E+00	1.0337E-11	1.388E-12	1.00E+00	1.388E-12
Al(g)	0.0000E+00	1.3884E-11	1.864E-12	1.00E+00	1.864E-12
HCl(g)	0.0000E+00	4.5656E-15	6.13E-16	1.00E+00	6.13E-16
Al2O3(g)	0.0000E+00	2.1412E-17	2.93E-18	1.00E+00	2.93E-18
Si(g)	0.0000E+00	2.1897E-17	2.940E-18	1.00E+00	2.940E-18
Al2O(g)	0.0000E+00	2.6040E-19	3.496E-20	1.00E+00	3.496E-20
C(g)	0.0000E+00	4.3212E-20	5.802E-21	1.00E+00	5.802E-21
CH3(g)	0.0000E+00	4.6974E-21	6.307E-22	1.00E+00	6.307E-22
CH3OH(g)	0.0000E+00	4.5196E-22	6.068E-23	1.00E+00	6.068E-23
CH4(g)	0.0000E+00	3.0366E-22	4.069E-23	1.00E+00	4.069E-23
CH2(g)	0.0000E+00	1.7485E-22	2.348E-23	1.00E+00	2.348E-23
C2H2(g)	0.0000E+00	5.9129E-28	7.939E-29	1.00E+00	7.939E-29
U(g)	0.0000E+00	2.9312E-31	3.936E-32	1.00E+00	3.936E-32
C2H4(g)	0.0000E+00	2.0115E-34	2.701E-35	1.00E+00	2.701E-35
C2H6(g)	0.0000E+00	4.1151E-42	5.521E-43	1.00E+00	5.521E-43
Total :	8.1050E+00	7.4479E+00	1.000E+00		

PHASE 2 :	INPUT AMOUNT mol	EQUIL AMOUNT mol	MOLE FRACTION	ACTIVITY COEFFICIENT	ACTIVITY
CaO	4.9000E-01	4.8110E-01	3.109E-01	1.00E+00	3.109E-01
SiO2	4.6900E-01	4.6900E-01	3.031E-01	1.00E+00	3.031E-01
H2O	9.8000E-02	2.3496E-01	1.518E-01	1.00E+00	1.518E-01
FeO	0.0000E+00	1.6412E-01	1.061E-01	1.00E+00	1.061E-01
Al2O3	7.8000E-02	9.9000E-02	6.397E-02	1.00E+00	6.397E-02
MgO	2.8000E-02	3.2753E-02	2.117E-02	1.00E+00	2.117E-02
NaFeO2	0.0000E+00	1.9550E-02	1.263E-02	1.00E+00	1.263E-02
Fe2O3	6.0000E-02	1.6318E-02	1.054E-02	1.00E+00	1.054E-02
Fe3O4	0.0000E+00	1.4211E-02	9.183E-03	1.00E+00	9.183E-03
CaO2	0.0000E+00	1.2827E-02	8.288E-03	1.00E+00	8.288E-03
KOH	5.0000E-03	1.6474E-03	1.065E-03	1.00E+00	1.065E-03
NaOH	0.0000E+00	8.4719E-04	5.475E-04	1.00E+00	5.475E-04
U3O8	0.0000E+00	6.6644E-04	4.308E-04	1.00E+00	4.308E-04
MgO2	0.0000E+00	2.4566E-04	1.587E-04	1.00E+00	1.587E-04
K2O	0.0000E+00	8.329E-04	5.329E-05	1.00E+00	5.329E-05
Fe	2.4300E-01	5.2623E-05	3.400E-05	1.00E+00	3.400E-05
CaCO3	0.0000E+00	2.3846E-05	1.541E-05	1.00E+00	1.541E-05
NnO2	0.0000E+00	1.9961E-05	1.290E-05	1.00E+00	1.290E-05
K	0.0000E+00	1.4898E-05	9.627E-06	1.00E+00	9.627E-06
Na	0.0000E+00	1.2087E-05	7.811E-06	1.00E+00	7.811E-06
PbO	0.0000E+00	1.1604E-05	7.499E-06	1.00E+00	7.499E-06
Ca(OH)2	4.0000E-03	8.4532E-06	5.462E-06	1.00E+00	5.462E-06
K2CO3	0.0000E+00	4.5132E-06	2.916E-06	1.00E+00	2.916E-06
Na2CO3	0.0000E+00	3.1203E-06	2.016E-06	1.00E+00	2.016E-06
Na2O	1.4000E-02	1.8742E-06	1.211E-06	1.00E+00	1.211E-06
Pb	4.0000E-04	1.5638E-06	1.011E-06	1.00E+00	1.011E-06
Mg(OH)2	5.0000E-03	3.9759E-07	2.569E-07	1.00E+00	2.569E-07

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UO2	2.0000E-03	6.5491E-008	4.232E-08	1.00E+00	4.232E-08
MgCO3	0.0000E+00	2.8462E-008	1.839E-08	1.00E+00	1.839E-08
Fe(OH)2	0.0000E+00	1.4538E-008	9.395E-09	1.00E+00	9.395E-09
UO3	0.0000E+00	1.2887E-008	8.327E-09	1.00E+00	8.327E-09
FeCO3	0.0000E+00	9.7475E-009	6.299E-09	1.00E+00	6.299E-09
Na2O2	0.0000E+00	7.5917E-009	4.906E-09	1.00E+00	4.906E-09
UO3(g)	0.0000E+00	5.2294E-009	3.379E-09	1.00E+00	3.379E-09
Al(OH)3	6.0000E-03	4.4847E-009	2.898E-09	1.00E+00	2.898E-09
K2O	3.6000E-02	4.4064E-009	2.847E-09	1.00E+00	2.847E-09
K2O2	0.0000E+00	4.2412E-009	2.741E-09	1.00E+00	2.741E-09
NaHCO3	1.4000E-02	1.3445E-009	8.688E-10	1.00E+00	8.688E-10
KNO3	8.0000E-03	9.6415E-010	6.230E-10	1.00E+00	6.230E-10
PbO2	0.0000E+00	8.2711E-010	5.345E-10	1.00E+00	5.345E-10
NaH	0.0000E+00	5.4696E-010	3.534E-10	1.00E+00	3.534E-10
KH	0.0000E+00	4.2289E-010	2.733E-10	1.00E+00	2.733E-10
NaHCO3	0.0000E+00	2.8644E-010	1.851E-10	1.00E+00	1.851E-10
K2O3	0.0000E+00	2.8569E-010	1.846E-10	1.00E+00	1.846E-10
KO3	0.0000E+00	1.2216E-010	7.894E-11	1.00E+00	7.894E-11
PbCO3	0.0000E+00	1.0699E-010	6.913E-11	1.00E+00	6.913E-11
C	1.0120E+00	4.0572E-011	2.622E-11	1.00E+00	2.622E-11
Mg	0.0000E+00	2.8193E-011	1.822E-11	1.00E+00	1.822E-11
Ca	0.0000E+00	2.4858E-011	1.606E-11	1.00E+00	1.606E-11
Fe(OH)3	4.0000E-03	2.6192E-012	1.693E-12	1.00E+00	1.693E-12
Al	3.6000E-02	1.7129E-013	1.107E-13	1.00E+00	1.107E-13
Na3UO4	0.0000E+00	3.8552E-014	2.491E-14	1.00E+00	2.491E-14
Si	0.0000E+00	3.6424E-014	2.354E-14	1.00E+00	2.354E-14
HNO3	0.0000E+00	1.2432E-014	8.034E-15	1.00E+00	8.034E-15
HCO2H	0.0000E+00	9.1762E-015	5.930E-15	1.00E+00	5.930E-15
HCOOH	0.0000E+00	8.3912E-015	5.422E-15	1.00E+00	5.422E-15
KCN	0.0000E+00	1.1537E-015	7.455E-16	1.00E+00	7.455E-16
N2O4	0.0000E+00	5.2731E-016	3.407E-16	1.00E+00	3.407E-16
NaCN	0.0000E+00	4.7378E-016	3.062E-16	1.00E+00	3.062E-16
UO	0.0000E+00	2.4895E-017	1.609E-17	1.00E+00	1.609E-17
CaH2	0.0000E+00	1.3670E-018	8.834E-19	1.00E+00	8.834E-19
NH4OH	0.0000E+00	7.8975E-019	5.103E-19	1.00E+00	5.103E-19
Pb3O4	0.0000E+00	4.9628E-020	3.207E-20	1.00E+00	3.207E-20
Ca(NO3)2	0.0000E+00	8.8748E-021	5.735E-21	1.00E+00	5.735E-21
U3O8	0.0000E+00	8.4646E-022	5.470E-22	1.00E+00	5.470E-22
NaN3	0.0000E+00	6.4255E-023	4.152E-23	1.00E+00	4.152E-23
Mg(NO3)2	0.0000E+00	1.4234E-023	9.198E-24	1.00E+00	9.198E-24
UN	0.0000E+00	9.0171E-024	5.827E-24	1.00E+00	5.827E-24
U	0.0000E+00	8.0660E-026	5.212E-26	1.00E+00	5.212E-26
CH3OH	0.0000E+00	7.9303E-027	5.124E-27	1.00E+00	5.124E-27
N2O5	0.0000E+00	2.9649E-027	1.916E-27	1.00E+00	1.916E-27
U4O9	0.0000E+00	1.6796E-028	1.085E-28	1.00E+00	1.085E-28
N2H4	0.0000E+00	1.4201E-028	9.176E-29	1.00E+00	9.176E-29
NH4NO3	0.0000E+00	3.5168E-031	2.273E-31	1.00E+00	2.273E-31
Pb(NO3)2	0.0000E+00	3.7810E-032	2.443E-32	1.00E+00	2.443E-32
UC	0.0000E+00	9.0450E-034	5.845E-34	1.00E+00	5.845E-34
Ca3N2	0.0000E+00	3.4842E-034	2.251E-34	1.00E+00	2.251E-34
UF6	0.0000E+00	2.0697E-034	1.337E-34	1.00E+00	1.337E-34
UH3	0.0000E+00	9.7853E-040	6.323E-40	1.00E+00	6.323E-40
UC2	0.0000E+00	1.6871E-041	1.090E-41	1.00E+00	1.090E-41
Si3H4	0.0000E+00	2.0813E-044	1.401E-44	1.00E+00	1.401E-44
C2H6O	0.0000E+00	7.1344E-047	0.000E+00	1.00E+00	0.000E+00
Fe(CO)5	0.0000E+00	6.0787E-049	0.000E+00	1.00E+00	0.000E+00
Si2H6	0.0000E+00	4.6644E-052	0.000E+00	1.00E+00	0.000E+00
U2C3	0.0000E+00	1.8578E-077	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.5475E+000	1.000E+00		

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B

Temperature 2198.15 K
 Pressure 1 bar
 Volume 1.617E-01 m³ (NPT)
 Reaction enthalpy 2.191E+02 kJ
 Reaction entropy 8.072E+02 J/K
 Iterations 80 (Limit = 80)

	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol			
PHASE 1:					
O ₂ (g)	7.1550E+00	5.5286E+00	7.665E-01	1.00E+00	7.665E-01
CO ₂ (g)	0.0000E+00	1.0049E+00	1.393E-01	1.00E+00	1.393E-01
H ₂ O(g)	0.0000E+00	5.3886E-01	7.471E-02	1.00E+00	7.471E-02
KOH(g)	0.0000E+00	7.1238E-02	9.81E-03	1.00E+00	9.877E-03
NO(g)	0.0000E+00	2.1951E-02	3.043E-03	1.00E+00	3.043E-03
NaOH(g)	0.0000E+00	1.8674E-02	2.589E-03	1.00E+00	2.589E-03
K(g)	0.0000E+00	1.0860E-02	1.506E-03	1.00E+00	1.506E-03
Na(g)	0.0000E+00	7.7818E-03	1.079E-03	1.00E+00	1.079E-03
CO(g)	0.0000E+00	7.0573E-03	9.785E-04	1.00E+00	9.785E-04
KO(g)	0.0000E+00	1.3581E-03	1.883E-04	1.00E+00	1.883E-04
H ₂ (g)	9.5000E-01	6.9641E-04	9.655E-05	1.00E+00	9.655E-05
PbO(g)	0.0000E+00	3.7411E-04	5.187E-05	1.00E+00	5.187E-05
Ca(OH) ₂ (g)	0.0000E+00	5.0856E-05	7.051E-06	1.00E+00	7.051E-06
H ₂ O ₂ (g)	0.0000E+00	4.9161E-05	6.816E-06	1.00E+00	6.816E-06
FeO(g)	0.0000E+00	3.1166E-05	4.321E-06	1.00E+00	4.321E-06
Pb(g)	0.0000E+00	1.5745E-05	2.183E-06	1.00E+00	2.183E-06
SiO ₂ (g)	0.0000E+00	1.0723E-05	1.487E-06	1.00E+00	1.487E-06
SiO(g)	0.0000E+00	2.8634E-06	3.970E-07	1.00E+00	3.970E-07
HgO(g)	0.0000E+00	1.5939E-06	2.210E-07	1.00E+00	2.210E-07
Fe(g)	0.0000E+00	1.3428E-06	1.862E-07	1.00E+00	1.862E-07
Al ₂ O ₃ (g)	0.0000E+00	1.2167E-07	1.687E-08	1.00E+00	1.687E-08
Hg ₁₉ (g)	0.0000E+00	1.1607E-07	1.609E-08	1.00E+00	1.609E-08
Hg(g)	0.0000E+00	3.3282E-08	4.614E-09	1.00E+00	4.614E-09
CaO(g)	0.0000E+00	9.4322E-09	1.308E-09	1.00E+00	1.308E-09
N(g)	0.0000E+00	9.3243E-09	1.293E-09	1.00E+00	1.293E-09
Ca(g)	0.0000E+00	4.0739E-09	5.648E-10	1.00E+00	5.648E-10
NO ₃ (g)	0.0000E+00	1.8308E-10	2.538E-11	1.00E+00	2.538E-11
AlO(g)	0.0000E+00	1.6540E-10	2.293E-11	1.00E+00	2.293E-11
NH(g)	0.0000E+00	1.1607E-11	1.609E-12	1.00E+00	1.609E-12
NH ₂ (g)	0.0000E+00	1.9494E-11	2.703E-12	1.00E+00	2.703E-12
NH ₃ (g)	0.0000E+00	1.0717E-11	1.486E-12	1.00E+00	1.486E-12
Al(g)	0.0000E+00	2.3406E-13	3.245E-14	1.00E+00	3.245E-14
HCN(g)	0.0000E+00	1.6170E-14	2.242E-15	1.00E+00	2.242E-15
Si(g)	0.0000E+00	5.5102E-16	7.640E-17	1.00E+00	7.640E-17
Al ₂ O ₃ (g)	0.0000E+00	4.2444E-16	5.884E-17	1.00E+00	5.884E-17
Al ₂ O(g)	0.0000E+00	9.6932E-18	1.344E-18	1.00E+00	1.344E-18
C(g)	0.0000E+00	7.5999E-19	1.054E-19	1.00E+00	1.054E-19
CH ₃ (g)	0.0000E+00	2.7097E-20	3.757E-21	1.00E+00	3.757E-21
CH ₂ (g)	0.0000E+00	1.7474E-21	2.423E-22	1.00E+00	2.423E-22
CH ₃ OH(g)	0.0000E+00	1.2073E-21	1.674E-22	1.00E+00	1.674E-22
CH ₄ (g)	0.0000E+00	1.1522E-21	1.597E-22	1.00E+00	1.597E-22
C ₂ H ₂ (g)	0.0000E+00	1.0672E-26	1.480E-27	1.00E+00	1.480E-27
U(g)	0.0000E+00	1.8016E-29	2.498E-30	1.00E+00	2.498E-30
C ₂ H ₄ (g)	0.0000E+00	3.1425E-33	4.357E-34	1.00E+00	4.357E-34
C ₂ H ₆ (g)	0.0000E+00	5.5480E-41	7.692E-42	1.00E+00	7.692E-42
Total :	8.1050E+00	7.2126E+00	1.000E+00		

PHASE 2 :		MOLE FRACT			
H2O	9.8000E-02	4.8899E-01	2.691E-01	1.00E+00	2.691E-01
CaO	4.9000E-01	4.8101E-01	2.647E-01	1.00E+00	2.647E-01
SiO2	4.6900E-01	4.6899E-01	2.581E-01	1.00E+00	2.581E-01
FeO	0.0000E+00	1.9669E-01	1.082E-01	1.00E+00	1.082E-01
Al2O3	7.8000E-02	9.9000E-02	5.448E-02	1.00E+00	5.448E-02
Hg	2.8000E-02	3.2768E-02	1.803E-02	1.00E+00	1.803E-02
NaFeO2	0.0000E+00	1.4787E-02	8.137E-03	1.00E+00	8.137E-03
CaO2	0.0000E+00	1.2915E-02	7.107E-03	1.00E+00	7.107E-03
Fe3O4	0.0000E+00	9.9332E-03	5.466E-03	1.00E+00	5.466E-03
Fe2O3	6.0000E-03	8.7832E-03	4.834E-03	1.00E+00	4.834E-03
KOH	5.0000E-03	1.3655E-03	7.515E-04	1.00E+00	7.515E-04
NaOH	0.0000E+00	7.0044E-04	3.855E-04	1.00E+00	3.855E-04
U3O8	0.0000E+00	6.6663E-04	3.669E-04	1.00E+00	3.669E-04
HgO2	0.0000E+00	2.3012E-04	1.266E-04	1.00E+00	1.266E-04
KO2	0.0000E+00	1.4502E-04	7.981E-05	1.00E+00	7.981E-05
Fe	2.4300E-01	1.2083E-04	6.649E-05	1.00E+00	6.649E-05
K	0.0000E+00	2.8154E-05	1.549E-05	1.00E+00	1.549E-05
Na2O	0.0000E+00	2.4658E-05	1.358E-05	1.00E+00	1.358E-05
Na	0.0000E+00	2.3419E-05	1.290E-05	1.00E+00	1.290E-05
CaCO3	0.0000E+00	1.6901E-05	9.301E-06	1.00E+00	9.301E-06
PbO	0.0000E+00	8.4052E-06	4.626E-06	1.00E+00	4.626E-06
Ca(OH)2	4.0000E-03	4.9013E-06	2.697E-06	1.00E+00	2.697E-06
K2CO3	0.0000E+00	2.7660E-06	1.522E-06	1.00E+00	1.522E-06
Na2O	1.4000E-02	2.5251E-06	1.390E-06	1.00E+00	1.390E-06
Na2CO3	0.0000E+00	1.9636E-06	1.081E-06	1.00E+00	1.081E-06
Pb	4.0000E-04	1.7365E-06	9.56E-07	1.00E+00	9.56E-07
Hg(OH)2	5.0000E-03	3.3001E-07	1.816E-07	1.00E+00	1.816E-07

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UO ₂	2.00E+00	8.7266E-06	4.862E-08	1.00E+00	4.802E-08
MgCO ₃	0.0000E+00	2.6108E-08	1.448E-08	1.00E+00	1.448E-08
FeCO ₃	0.0000E+00	1.3060E-08	7.187E-09	1.00E+00	7.187E-09
UO ₃	0.0000E+00	1.1957E-08	6.560E-09	1.00E+00	6.580E-09
Fe(OH) ₂	0.0000E+00	1.0435E-08	5.743E-09	1.00E+00	5.743E-09
Na ₂ O ₂	0.0000E+00	6.9490E-09	3.824E-09	1.00E+00	3.824E-09
K ₂ O	3.6000E-02	6.0437E-09	3.326E-09	1.00E+00	3.326E-09
Al(OH) ₃	6.0000E-03	4.9777E-09	2.739E-09	1.00E+00	2.739E-09
K ₂ O ₂	0.0000E+00	4.6908E-09	2.581E-09	1.00E+00	2.581E-09
UO ₃ (G)	0.0000E+00	4.3644E-09	2.402E-09	1.00E+00	2.402E-09
NaH	0.0000E+00	1.2221E-09	6.726E-10	1.00E+00	6.726E-10
KH	0.0000E+00	8.8332E-10	4.861E-10	1.00E+00	4.861E-10
NaNH ₂	1.4000E-02	8.5162E-10	4.687E-10	1.00E+00	4.687E-10
KNO ₃	8.0000E-03	4.8996E-10	2.696E-10	1.00E+00	2.696E-10
PbO ₂	0.0000E+00	4.8108E-10	2.659E-10	1.00E+00	2.659E-10
K ₂ O	0.0000E+00	2.5969E-10	1.429E-10	1.00E+00	1.429E-10
NaNHCO ₃	0.0000E+00	2.5606E-10	1.409E-10	1.00E+00	1.409E-10
K ₂ O	0.0000E+00	1.4981E-10	8.244E-11	1.00E+00	8.244E-11
Hg	0.0000E+00	1.3467E-10	7.411E-11	1.00E+00	7.411E-11
C	1.0120E+00	1.3363E-10	7.354E-11	1.00E+00	7.354E-11
Ca	0.0000E+00	1.2733E-10	7.007E-11	1.00E+00	7.007E-11
PbCO ₃	0.0000E+00	8.8659E-11	4.879E-11	1.00E+00	4.879E-11
Al	1.6115E-02	1.6115E-12	8.868E-13	1.00E+00	8.868E-13
Fe(OH) ₃	4.0000E-03	1.1737E-12	6.459E-13	1.00E+00	6.459E-13
Si	0.0000E+00	4.0053E-13	2.204E-13	1.00E+00	2.204E-13
Na ₃ UO ₄	0.0000E+00	2.1309E-14	1.173E-14	1.00E+00	1.173E-14
HCO ₂ H	0.0000E+00	1.4575E-14	8.021E-15	1.00E+00	8.021E-15
HCOOH	0.0000E+00	1.3403E-14	7.376E-15	1.00E+00	7.376E-15
HNO ₃	0.0000E+00	8.9289E-15	4.914E-15	1.00E+00	4.914E-15
KCH	0.0000E+00	3.8487E-15	2.118E-15	1.00E+00	2.118E-15
NH ₂ CH	0.0000E+00	1.7057E-15	9.387E-16	1.00E+00	9.387E-16
N ₂ O ₄	0.0000E+00	1.0331E-15	5.685E-16	1.00E+00	5.685E-16
UO	0.0000E+00	1.2349E-16	6.796E-17	1.00E+00	6.796E-17
CaH ₂	0.0000E+00	5.5422E-18	3.050E-18	1.00E+00	3.050E-18
NH ₄ OH	0.0000E+00	7.4393E-19	4.094E-19	1.00E+00	4.094E-19
Pb ₃ O ₄	0.0000E+00	1.0371E-20	5.708E-21	1.00E+00	5.708E-21
Ca(NO ₃) ₂	0.0000E+00	5.3825E-21	2.962E-21	1.00E+00	2.962E-21
U ₃ O ₈	0.0000E+00	7.4178E-22	4.082E-22	1.00E+00	4.082E-22
NaH ₃	0.0000E+00	7.0675E-23	3.889E-23	1.00E+00	3.889E-23
Mg(NO ₃) ₂	0.0000E+00	6.6606E-23	3.665E-23	1.00E+00	3.665E-23
U	0.0000E+00	1.9254E-23	1.060E-23	1.00E+00	1.060E-23
CH ₃ OH	0.0000E+00	1.7536E-24	9.650E-25	1.00E+00	9.650E-25
N ₂ O ₅	0.0000E+00	2.3076E-26	1.270E-26	1.00E+00	1.270E-26
U ₄ O ₉	0.0000E+00	2.4276E-27	1.336E-27	1.00E+00	1.336E-27
N ₂ H ₄	0.0000E+00	2.4322E-28	1.338E-28	1.00E+00	1.338E-28
NH ₄ NO ₃	0.0000E+00	2.2266E-28	1.225E-28	1.00E+00	1.225E-28
UC	0.0000E+00	2.0986E-31	1.155E-31	1.00E+00	1.155E-31
UF ₆	0.0000E+00	4.1476E-32	2.282E-32	1.00E+00	2.282E-32
Pb(NO ₃) ₂	0.0000E+00	1.5951E-32	8.777E-33	1.00E+00	8.777E-33
Ca ₃ N ₂	0.0000E+00	8.4596E-33	4.655E-33	1.00E+00	4.655E-33
U ₃	0.0000E+00	7.3911E-33	4.067E-33	1.00E+00	4.067E-33
UC ₂	0.0000E+00	2.1953E-38	1.208E-38	1.00E+00	1.208E-38
Si ₃ N ₄	0.0000E+00	2.8939E-39	1.593E-39	1.00E+00	1.593E-39
C ₂ H ₆ O	0.0000E+00	8.6558E-43	4.764E-43	1.00E+00	4.764E-43
Fe(CO) ₅	0.0000E+00	6.2947E-46	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	3.5966E-47	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	1.0443E-49	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	1.8171E+00	1.000E+00		

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B

Temperature 2298.15 K
 Pressure 1 bar
 Volume 1.559E-01 m³ (HPT)
 Reaction enthalpy 4.413E-02 kJ
 Reaction entropy 9.005E-02 J/K
 Iterations 80 (Limit = 80)

	INPUT AMOUNT	EQUIL AMOUNT	MOLE FRACTION	ACTIVITY	ACTIVITY
	mol	mol		COEFFICIENT	
PHASE 1:					
O ₂ (g)	7.1550E+00	5.5405E+00	7.965E-01	1.00E+00	7.965E-01
CO ₂ (g)	0.0000E+00	9.989E-01	1.436E-01	1.00E+00	1.436E-01
H ₂ O(g)	0.0000E+00	6.657E-01	8.832E-02	1.00E+00	8.832E-02
KOH(g)	0.0000E+00	6.0476E-02	8.693E-03	1.00E+00	8.693E-03
NO(g)	0.0000E+00	2.1956E-02	3.156E-03	1.00E+00	3.156E-03
K(g)	0.0000E+00	2.0700E-02	2.976E-03	1.00E+00	2.976E-03
NaOH(g)	0.0000E+00	1.6253E-02	2.336E-03	1.00E+00	2.336E-03
Na(g)	0.0000E+00	1.4266E-02	2.051E-03	1.00E+00	2.051E-03
CO(g)	0.0000E+00	1.3296E-02	1.911E-03	1.00E+00	1.911E-03
KO(g)	0.0000E+00	2.5264E-03	3.632E-04	1.00E+00	3.632E-04
H ₂ (g)	9.5000E-01	1.1572E-04	8.851E-05	1.00E+00	8.851E-05
PbO(g)	0.0000E+00	1.6980E-04	5.316E-05	1.00E+00	5.316E-05
FeO(g)	0.0000E+00	8.4893E-05	1.220E-05	1.00E+00	1.220E-05
NO ₂ (g)	0.0000E+00	4.3743E-05	6.288E-06	1.00E+00	6.288E-06
Ca(OH) ₂ (g)	0.0000E+00	3.9883E-05	5.733E-06	1.00E+00	5.733E-06
SiO ₂ (g)	0.0000E+00	3.4452E-05	4.953E-06	1.00E+00	4.953E-06
Pb(g)	0.0000E+00	2.1972E-05	3.159E-06	1.00E+00	3.159E-06
SiO(g)	0.0000E+00	2.3169E-05	2.068E-06	1.00E+00	2.068E-06
Fe(g)	0.0000E+00	5.3958E-06	7.757E-07	1.00E+00	7.757E-07
MgO(g)	0.0000E+00	5.2383E-06	7.530E-07	1.00E+00	7.530E-07
Al ₂ O ₃ (g)	0.0000E+00	4.9388E-07	7.100E-08	1.00E+00	7.100E-08
MgOH(g)	0.0000E+00	2.4663E-07	3.545E-08	1.00E+00	3.545E-08
Mg(g)	0.0000E+00	1.5170E-07	2.181E-08	1.00E+00	2.181E-08
CaO(g)	0.0000E+00	3.9151E-08	5.628E-09	1.00E+00	5.628E-09
N(g)	0.0000E+00	2.3169E-08	3.331E-09	1.00E+00	3.331E-09
Ca(g)	0.0000E+00	2.1353E-08	3.069E-09	1.00E+00	3.069E-09
AlO(g)	0.0000E+00	1.2332E-09	1.773E-10	1.00E+00	1.773E-10
NO ₃ (g)	0.0000E+00	1.8667E-10	2.683E-11	1.00E+00	2.683E-11
NH(g)	0.0000E+00	1.7493E-10	2.515E-11	1.00E+00	2.515E-11
NH ₂ (g)	0.0000E+00	2.1911E-11	3.150E-12	1.00E+00	3.150E-12
NH ₃ (g)	0.0000E+00	6.5321E-12	9.390E-13	1.00E+00	9.390E-13
Al	0.0000E+00	3.0110E-12	4.357E-13	1.00E+00	4.357E-13
HCl(g)	0.0000E+00	2.1445E-14	6.09E-15	1.00E+00	6.09E-15
Si	0.0000E+00	1.0246E-14	1.471E-15	1.00E+00	1.471E-15
Al ₂ O ₃ (g)	0.0000E+00	6.1557E-15	8.849E-16	1.00E+00	8.849E-16
Al ₂ O(g)	0.0000E+00	2.5653E-16	3.686E-17	1.00E+00	3.686E-17
C(g)	0.0000E+00	1.0299E-17	1.480E-18	1.00E+00	1.480E-18
CH ₃ (g)	0.0000E+00	7.8493E-20	1.128E-20	1.00E+00	1.128E-20
CH ₂ (g)	0.0000E+00	9.9579E-21	1.431E-21	1.00E+00	1.431E-21
CH ₃ OH(g)	0.0000E+00	1.9154E-21	2.753E-22	1.00E+00	2.753E-22
C ₂ H ₂ (g)	0.0000E+00	1.4459E-21	2.078E-22	1.00E+00	2.078E-22
U(g)	0.0000E+00	1.0400E-25	1.495E-26	1.00E+00	1.495E-26
C ₂ H ₄ (g)	0.0000E+00	7.5675E-28	1.088E-28	1.00E+00	1.088E-28
C ₂ H ₆ (g)	0.0000E+00	1.9121E-32	2.749E-33	1.00E+00	2.749E-33
Total :	8.1050E+00	6.9565E+00	1.000E+00		

	MOLE FRACTION	ACTIVITY	ACTIVITY
		COEFFICIENT	
PHASE 2 :			
H ₂ O	9.8000E-02	7.6813E-001	3.644E-01
CaO	4.9000E-01	4.8089E-001	2.282E-01
SiO ₂	4.6900E-01	4.6895E-001	2.225E-01
FeO	0.0000E+00	2.2039E-001	1.046E-01
Al ₂ O ₃	7.8000E-02	9.9000E-002	4.697E-02
MgO	2.8000E-02	3.2777E-002	1.555E-02
CaO ₂	0.0000E+00	1.3054E-002	6.193E-03
NaFeO ₂	0.0000E+00	1.0906E-002	5.174E-03
Fe ₃ O ₄	0.0000E+00	6.1223E-003	2.905E-03
Fe ₂ O ₃	6.0000E-03	4.5018E-003	2.136E-03
KOH	5.0000E-03	1.0598E-003	5.028E-04
U ₃ O ₈	0.0000E+00	6.6662E-004	3.163E-04
NaOH	0.0000E+00	4.9352E-004	2.341E-04
Fe	2.4300E-01	2.4405E-004	1.158E-04
HgO ₂	0.0000E+00	2.1742E-004	1.032E-04
K ₂ O	0.0000E+00	1.7912E-004	8.498E-05
K	0.0000E+00	5.4847E-005	2.602E-05
Na	0.0000E+00	4.2692E-005	2.025E-05
Na ₂ O	0.0000E+00	3.0499E-005	1.447E-05
CaCO ₃	0.0000E+00	1.2475E-005	5.919E-06
PbO	0.0000E+00	6.3106E-006	2.994E-06
Na ₂ O	1.4000E-02	3.2817E-006	1.557E-06
K ₂ CO ₃	0.0000E+00	2.1448E-006	1.018E-06
Ca(OH) ₂	4.0000E-03	2.1156E-006	1.004E-06
Pb	4.0000E-04	1.9120E-006	9.071E-07
Na ₂ CO ₃	0.0000E+00	1.2850E-006	6.097E-07
Mg(OH) ₂	5.0000E-03	2.0461E-007	9.707E-08

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UO ₂	2.0000E-03	1.1301E-007	5.362E-08	1.00E+00	5.362E-08
MgCO ₃	0.0000E+00	2.5077E-008	1.190E-08	1.00E+00	1.190E-08
FeCO ₃	0.0000E+00	1.6907E-008	8.021E-09	1.00E+00	8.021E-09
UO ₃	0.0000E+00	1.1172E-008	5.300E-09	1.00E+00	5.300E-09
K ₂ O	3.6000E-02	9.6667E-009	4.586E-09	1.00E+00	4.586E-09
Na ₂ O ₂	0.0000E+00	6.3529E-009	3.014E-09	1.00E+00	3.014E-09
K ₂ O ₂	0.0000E+00	6.2864E-009	2.983E-09	1.00E+00	2.983E-09
Fe(OH) ₃	0.0000E+00	5.1477E-009	2.442E-09	1.00E+00	2.442E-09
UO ₃ (G)	0.0000E+00	3.6079E-009	1.712E-09	1.00E+00	1.712E-09
Al(OH) ₃	6.0000E-03	3.5332E-009	1.676E-09	1.00E+00	1.676E-09
NaH	0.0000E+00	2.1576E-009	1.024E-09	1.00E+00	1.024E-09
KH	0.0000E+00	1.6009E-009	7.595E-10	1.00E+00	7.595E-10
NaNO ₃	1.4000E-02	5.7090E-010	2.709E-10	1.00E+00	2.709E-10
Ca	0.0000E+00	5.6226E-010	2.668E-10	1.00E+00	2.668E-10
Mg	0.0000E+00	5.5885E-010	2.651E-10	1.00E+00	2.651E-10
C	1.0120E+00	3.9602E-010	1.879E-10	1.00E+00	1.879E-10
PbO ₂	0.0000E+00	2.9766E-010	1.412E-10	1.00E+00	1.412E-10
KNO ₃	8.0000E-03	2.9300E-010	1.390E-10	1.00E+00	1.390E-10
NaHCO ₃	0.0000E+00	2.8715E-010	1.362E-10	1.00E+00	1.362E-10
K ₂ O ₃	0.0000E+00	2.0466E-010	9.710E-11	1.00E+00	9.710E-11
NaNO ₂	0.0000E+00	2.0282E-010	9.623E-11	1.00E+00	9.623E-11
PbCO ₃	0.0000E+00	7.8995E-011	3.748E-11	1.00E+00	3.748E-11
Al	3.6000E-02	1.2390E-011	5.878E-12	1.00E+00	5.878E-12
Si	0.0000E+00	3.5320E-012	1.676E-12	1.00E+00	1.676E-12
Fe(OH) ₂	4.0000E-03	3.1849E-013	1.511E-13	1.00E+00	1.511E-13
HCO ₂ H	0.0000E+00	1.5754E-014	7.475E-15	1.00E+00	7.475E-15
HCO ₂ H	0.0000E+00	1.4563E-014	6.909E-15	1.00E+00	6.909E-15
KCN	0.0000E+00	1.2598E-014	5.977E-15	1.00E+00	5.977E-15
Na ₃ UO ₄	0.0000E+00	1.2112E-014	5.746E-15	1.00E+00	5.746E-15
HNO ₃	0.0000E+00	5.5747E-015	2.645E-15	1.00E+00	2.645E-15
NaCN	0.0000E+00	5.4508E-015	2.586E-15	1.00E+00	2.586E-15
N ₂ O ₄	0.0000E+00	2.1210E-015	1.006E-15	1.00E+00	1.006E-15
Co	0.0000E+00	5.2712E-016	2.501E-16	1.00E+00	2.501E-16
UO ₂	0.0000E+00	1.3990E-017	6.638E-18	1.00E+00	6.638E-18
NH ₄ OH	0.0000E+00	2.9813E-019	1.414E-19	1.00E+00	1.414E-19
Ca(NO ₃) ₂	0.0000E+00	3.7253E-021	1.767E-21	1.00E+00	1.767E-21
Pb ₃ O ₄	0.0000E+00	2.5745E-021	1.221E-21	1.00E+00	1.221E-21
U ₃ O ₈	0.0000E+00	6.5914E-022	3.127E-22	1.00E+00	3.127E-22
UN	0.0000E+00	4.5872E-022	2.176E-22	1.00E+00	2.176E-22
NaH ₃	0.0000E+00	6.8805E-023	3.264E-23	1.00E+00	3.264E-23
Hg(NO ₃) ₂	0.0000E+00	2.9363E-023	1.393E-23	1.00E+00	1.393E-23
U	0.0000E+00	2.8792E-023	1.366E-23	1.00E+00	1.366E-23
CH ₃ OH	0.0000E+00	3.0192E-026	1.432E-26	1.00E+00	1.432E-26
N ₂ O ₅	0.0000E+00	2.0818E-027	9.877E-28	1.00E+00	9.877E-28
U ₄ O ₉	0.0000E+00	3.3839E-028	1.605E-28	1.00E+00	1.605E-28
N ₂ H ₄	0.0000E+00	1.6778E-028	7.960E-29	1.00E+00	7.960E-29
UF ₆	0.0000E+00	1.3430E-030	6.372E-31	1.00E+00	6.372E-31
Fe ₂	0.0000E+00	7.4077E-031	3.515E-31	1.00E+00	3.515E-31
CaH ₂	0.0000E+00	1.9666E-031	5.677E-32	1.00E+00	5.677E-32
NH ₄ NO ₃	0.0000E+00	6.6220E-032	3.142E-32	1.00E+00	3.142E-32
Pb(NO ₃) ₂	0.0000E+00	2.2037E-033	1.046E-33	1.00E+00	1.046E-33
UC ₂	0.0000E+00	3.1514E-037	1.495E-37	1.00E+00	1.495E-37
UN ₃	0.0000E+00	2.2056E-037	1.046E-37	1.00E+00	1.046E-37
Si ₃ N ₄	0.0000E+00	2.5527E-041	1.211E-41	1.00E+00	1.211E-41
C ₂ H ₆ O	0.0000E+00	1.5805E-045	1.401E-45	1.00E+00	1.401E-45
Fe(CO) ₅	0.0000E+00	1.4030E-045	0.000E+00	1.00E+00	0.000E+00
Si ₂ H ₆	0.0000E+00	4.9486E-048	0.000E+00	1.00E+00	0.000E+00
U ₂ C ₃	0.0000E+00	2.0337E-070	0.000E+00	1.00E+00	0.000E+00
Total :	2.5584E+00	2.1077E+000	1.000E+00		

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APPENDIX B

FIDAP INPUT FILE

APPENDIX B

FIDAP INPUT FILE

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Problem(steady,nonlinear,2-d,buoyancy=0,species=1)
Scale(value=0.01)
Clip(minimum)
0 0 0 0 300.0
Icnod(velo,read)
Icnod(temp,read)
Icnod(spec=1,read)
Execution(newjob)
Solution(s.s.=10,velconv=0.001,resconv=0.01)
Options(upwind)
Relax
0.9 0.9 0.9 0.9 0.9 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
Dataprint(normal)
Printout(none)
Post
Entity(fluid,name="soil",      property="slag",      snoconv=1)
Entity(fluid,name="soil2",    property="slag",      snoconv=1)
Entity(fluid,name="soil3",    property="slag",      snoconv=1)
Entity(fluid,name="soil4",    property="slag",      snoconv=1)
Entity(fluid,name="soil5",    property="slag",      snoconv=1)
Entity(fluid,name="soil6",    property="slag",      snoconv=1)
Entity(fluid,name="metal",    property="slag",      snoconv=1)
Entity(conv ,name="bottom",   property="convbot")
Entity(conv ,name="convexit", property="convexit")
Entity(conv ,name="airsides", property="convair")
Entity(plot ,name="top")
Entity(plot ,name="electrode+")
Entity(plot ,name="electrode-")
Entity(plot ,name="soilenter")
Entity(plot ,name="outside")
Entity(plot ,name="exit")
Entity(plot ,name="interface")
Entity(plot ,name="airleft")
Entity(plot ,name="airmiddle")
Entity(plot ,name="airright")
Conductivity(set="slag",curv=10)
-1e10 0 673 1073 1428 1773 2173 2573 5000 1e10
0.2 0.2 0.23 0.45 8.5 18.0 50.0 80.0 80.0 80.0
Conductivity(set="metal",const=30.0)
Diffusivity(set="slag",curv=10)
-1e10      0.0      673.      1073.      1428.
1773.      2173.      2573.      5000.      1e10
0.50e-6 0.50e-6 0.50e-6 0.80e-5 0.49e-3
0.28e-2 0.10e-1 0.22e-1 0.44e-1 0.44e-1
Diffusivity(set="metal",const=1282)
Htransfer(set="convbot",const=50,reftemp=300)
Htransfer(set="convexit",const=50,reftemp=300)
Htransfer(set="convair",const=100,reftemp=1500)
Density(set="slag",const=2180)
Density(set="metal",const=7800)
Volume(set="slag",gravity=9.8,reftemp=0.0,curv=22,temp)
-1.00E+10 300 600 700 800 900
1000 1100 1200 1300 1400
1500 1600 1700 1800 1900

```



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2000 2100 2200 2300 3000 1.00E+10
0.00E-00 8.87E-04 4.05E-04 3.08E-04 2.01E-04 1.07E-04
5.96E-05 2.92E-05 1.15E-05 3.53E-06 0.00E+00
3.06E-06 1.43E-05 1.89E-05 2.04E-05 2.41E-05
2.75E-05 3.06E-05 3.34E-05 3.59E-05 4.28E-05 3.12E-11
Volume(set="metal",grav=9.8,reftemp=1673,curv=5)
-1e10 1670 1673 5000 1e10
0.0 0.0 1e-7 1e-8 1e-14
Viscosity(set="slag",curv=8,temp)
-1.e20 1428 1473 1673 1873 2073 2273 1.e20
1e6 1e6 100 30 7.5 2.7 1.0 1.0
Viscosity(set="metal",curv=4)
-1e10 1673 1700 1e10
1e9 1e9 2.25e-1 2.25e-1
Specificheat(set="slag",const=1300)
Specificheat(set="metal",const=460)
Source(joule=1,entity="soil",constant=1.0)
Source(joule=1,entity="soil2",constant=1.0)
Source(joule=1,entity="soil3",constant=1.0)
Source(joule=1,entity="soil4",constant=1.0)
Source(joule=1,entity="soil5",constant=1.0)
Source(joule=1,entity="soil6",constant=1.0)
Source(joule=1,entity="metal",constant=1.0)
Bcnod(velo,entity="outside",zero)
Bcnod(ux,entity="soilenter",zero)
Bcnod(uy,entity="soilenter",const=-1.72e-4)
Bcnod(temp,entity="soilenter",const=500)
Bcnod(spec=1,entity="electrode+",const=250)
Bcnod(spec=1,entity="electrode-",const=100)
Bcnod(ux,const=0.00363,entity="exit")
Bcnod(uy,zero,entity="exit")
Bcflux(heat,entity="airleft",poly=1)
-16875e2 562.5e2 1
Bcflux(heat,entity="electrode+",const=5625e2)
Bcflux(heat,entity="airmiddle",poly=2)
455625e2 -16500e2 1 0 0 150e2 2 0 0
Bcflux(heat,entity="electrode-",const=5625e2)
Bcflux(heat,entity="airright",poly=1)
45000e2 -562.5e2 1
Renummer(profile)
End
Create(fisolv)

```